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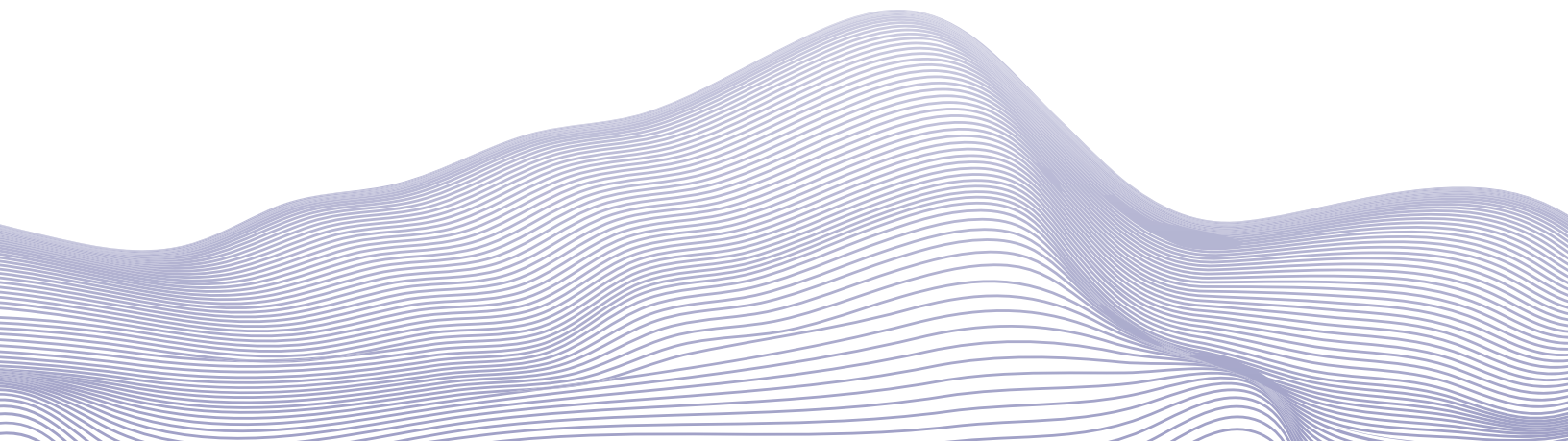
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The Usefulness of Seismic Attribute Mapping in the Interpretation of Submarine Channel Seismic Geomorphology: A Comparative Review

Muchamad Ocky Bayu Nugroho^{1,a} 

Abstract

Submarine channels are major components that transport and store sediments across the continental margins that act as confined pathways for turbidity currents, facilitating sediment transfer from the shallow to the deep ocean and forming important sand-rich deposits with high hydrocarbon reservoir potential. Sedimentary processes are crucial for sculpting submarine channel morphologies and the building blocks of their architectural elements. This could be understood by seismic geomorphology analysis, which reveals the geological and geomorphological features through seismic data. Understanding the submarine channels through their morphology and architecture will help to build detailed geometry and evolution for further application, such as reservoir prediction, hydrocarbon migration and geological carbon storage. This review evaluates the effectiveness of seismic attributes in characterizing submarine channel geomorphology. This study examines 20 peer-reviewed articles published between 2016 and 2023 that applied seismic attribute analyses for geological interpretation of submarine channels. Seismic attributes such as RMS (root-mean square), variance, instantaneous frequency, sweetness, dip, curvature, coherence, and envelope were commonly applied in the reviewed case studies. Physical attributes highlight amplitude-related variations that may reflect lithological contrasts, depending on data calibration and depositional context, while geometrical attributes delineate channel margins and planform geometries and are strongly dependent on seismic data quality. In cases where single attributes are insufficient to clearly reveal channel geomorphology, additional analyses such as co-rendering and spectral decomposition were employed to enhance interpretation. This study confirms that seismic attributes provide reliable insights into submarine channel deposits, including possible lithological contrasts, channel boundaries, channel-belt morphology, and the distribution of sediment accumulations within channel systems. However, the accuracy of interpretation depends on seismic data quality and the geological understanding of the study area. Inadequate knowledge or poor-quality seismic data can lead to misapplication of attribute parameters and potential misinterpretation.

Key words: Seismic Interpretation, Seismic Attributes, Seismic Geomorphology, Submarine channels.

Resumen

Los canales submarinos son componentes principales que transportan y almacenan sedimentos a lo largo de los márgenes continentales, actuando como vías confinadas para las corrientes de turbidez, facilitando la transferencia de sedimentos desde aguas someras hacia el océano profundo y formando depósitos importantes ricos en arena con alto potencial como reservorios de hidrocarburos. Los procesos sedimentarios son fundamentales para modelar la morfología de los canales submarinos y los elementos arquitectónicos que los componen. Esto puede comprenderse mediante el análisis de geomorfología sísmica, el cual revela características geológicas y geomorfológicas a partir de datos sísmicos. El entendimiento de los canales submarinos a través de su morfología y arquitectura permite construir geometrías detalladas y su evolución, con aplicaciones en la predicción de reservorios, la migración de hidrocarburos y el almacenamiento geológico de carbono. Esta revisión evalúa la eficacia de los atributos sísmicos en la caracterización de la geomorfología de canales submarinos. El estudio analiza 20 artículos revisados por pares publicados entre 2016 y 2023 que aplican análisis de atributos sísmicos para la interpretación geológica de canales submarinos. Los atributos sísmicos como RMS (raíz cuadrática media), varianza, frecuencia instantánea, "sweetness", inclinación (dip), curvatura, coherencia y envolvente fueron comúnmente utilizados en los casos de estudio revisados. Los atributos físicos destacan variaciones relacionadas con la amplitud que pueden reflejar contrastes litológicos, dependiendo de la calibración de los datos y del contexto deposicional, mientras que los atributos geométricos delimitan los márgenes de los canales y sus geometrías en planta, y dependen fuertemente de la calidad de los datos sísmicos. En los casos donde los atributos individuales no son suficientes para revelar claramente la geomorfología de los canales, se emplearon análisis adicionales como la co-visualización (co-rendering) y la descomposición espectral para mejorar la interpretación. Este estudio confirma que los atributos sísmicos proporcionan información confiable sobre los depósitos de canales submarinos, incluyendo posibles contrastes litológicos, límites de canal, morfología de los sistemas de canal y la distribución de las acumulaciones sedimentarias dentro de estos sistemas. Sin embargo, la precisión de la interpretación depende de la calidad de los datos sísmicos y del conocimiento geológico del área de estudio. Un conocimiento insuficiente o datos sísmicos de baja calidad pueden conducir a una aplicación inadecuada de los parámetros de atributos y a posibles interpretaciones erróneas.

Palabras clave: Interpretación sísmica, atributos sísmicos, geomorfología sísmica, canales submarinos.

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1. Introduction

Submarine channels are important morphological and sedimentary systems observed across the continental slope to the deep. They facilitate sediment transport to the deep ocean by acting as confined pathways for turbidity currents and serving as significant sand reservoirs with high hydrocarbon potential (Pickering *et al.*, 1989; Deptuck *et al.*, 2007; Mulder *et al.*, 2012; Bouchakour *et al.*, 2024 and 2025). These channels exhibit a dynamic response to variations in seafloor topography (Posamentier and Kolla, 2003; Deb *et al.*, 2012; Gamboa *et al.*, 2012; Gamboa & Alves, 2015; Bouchakour *et al.*, 2022 and 2023). Over the past decade, submarine channels have been widely studied due to the expansion of hydrocarbon exploration and the technological evolution of data quality (Mayall *et al.*, 2006, 2010; Weimer *et al.*, 2007; Di Celma *et al.*, 2010) and their relevance in assessing geohazards (Bruschi *et al.*, 2006; Thomas *et al.*, 2010; Carter *et al.*, 2014). In addition, submarine channels can archive valuable sedimentological signatures and paleoclimatic information that provide insights into the processes governing their formation (Bouma, 2001; Brenchley *et al.*, 2006; Zühlendorf *et al.*, 2007).

In many case studies, channel features are difficult to interpret properly due to poor seismic data quality, limited seismic resolution, and pitfalls of time slice interpretation (Clark and Pickering, 1996). The use of three-dimensional seismic data for interpretation of channel geomorphology is referred to as seismic geomorphology (Posamentier *et al.*, 2023). Seismic geomorphology plays a key role in identifying and mapping the distribution of seismic facies (Posamentier and Kolla, 2003; Posamentier, 2005). Seismic characteristics are obtained from seismic data parameters and measurements such as amplitude, frequency, and attenuation, as well as combinations of seismic attributes (Sheriff, 1994; Coren *et al.*, 2001; Chopra and Marfurt, 2007a). Various reflection properties, including amplitude, dip magnitude, dip azimuth, time/depth structure, and curvature, can be analyzed to generate direct images of features relevant to deposition and structural frameworks (Posamentier, 2004). Seismic attributes are useful both quantitatively and qualitatively. Quantitative applications involve predicting physical properties such as porosity or lithology (Leiphart & Hart, 2001; Sagan & Hart, 2006), while qualitative uses focus on identifying stratigraphic and structural elements (Hart, 2008). Over the past decades, advances in seismic data visualization techniques and increased calibration through well ties have enabled seismic attributes to provide valuable insights into geological structures, lithology, and stratigraphic channels (Taner, 2001; Chopra & Marfurt, 2007a; Azevedo & Pereira, 2009). Among their applications, the most critical is the extraction of information from raw seismic data that may not be immediately apparent (Anees, 2013). Although seismic attributes

are widely used by both academic and industrial communities for geological and depositional interpretations, a number of uncertainties remain when applying different attributes across varying geological settings and datasets. Therefore, improving our understanding of seismic attribute behavior and systematically testing their usefulness is essential.

This review aims to comprehensively evaluate the application of various seismic attributes in interpreting channel system deposits within a seismic geomorphology framework. By synthesizing case studies from the Taranaki Basin, Gulf of Mexico, Gulf of Thailand, Levant Basin, Offshore Nile Delta, and Kribi-Campo Basin, this review highlights the specific roles, advantages, and limitations of each attribute type in resolving channel morphology and associated depositional features. The analysis also seeks to identify the most effective attributes for enhancing the detection, visualization, and characterization of submarine channels, thereby providing guidance for future exploration and geomorphological studies.

2. Material and Methods

This review was conducted using literature sourced from the Scopus database and reputable open-access journals. The literature search applied targeted keywords, including “seismic attribute” and “submarine channel” or “seismic geomorphology”, to prioritize studies explicitly addressing seismic-based attribute analysis within a seismic geomorphology framework, while maintaining a focused and reproducible review scope. This approach does not aim to provide an exhaustive compilation of all related studies, and additional relevant literature may exist beyond the selected keyword combinations. The keyword selection was designed to prioritize specificity over completeness; consequently, studies addressing geological processes without explicit seismic attribute analysis may not be fully represented. The inclusion criteria were as follows: (1) the article was written in English, (2) it was published between 2016 and 2023, and (3) it explicitly focused on seismic attributes and their application to submarine channel interpretation. The initial search retrieved 28 articles from the Scopus database and one additional article from an open-access journal. The selection of articles have been further optimized based on filtering works focusing on submarine channel interpretation and their sedimentological context using 3D seismic data. Following this process, a total of 20 articles were selected for this review. The scope of this review focuses on the utilization of seismic attributes for interpreting submarine channel deposits within a seismic geomorphology framework. The analysis addresses three main objectives: (1) identifying the types of seismic attributes used, (2) classifying the attributes according to their purposes in submarine channel characterization,

and (3) evaluating their relative usefulness and applicability for specific geomorphological and depositional objectives.

In this review, “usefulness” is defined in relation to the interpretation objectives established in this study, rather than the original objectives of the individual case studies. It refers to the capability of a seismic attribute to identify geological features based on a set of predefined interpretation purposes established in this study, as evidenced by their application in the published literature. The usefulness of each seismic attribute was evaluated using a qualitative binary scoring approach based on six predefined interpretation purposes including lithological variation and distribution, channel boundary identification, channel orientation, channel planform geometry, channel thalweg distribution, and channel-associated deposits. Channel-associated deposits include channel-fill sediments, levee–overbank deposits, and adjacent lobe or crevasse-splay deposits, which may be expressed in seismic attribute maps through variations in amplitude, continuity, and geometric patterns. For each attribute–purpose combination, a binary score of 1 was assigned

when the applicability of the attribute to a given purpose was explicitly demonstrated or could be reasonably inferred from the interpretation results and discussion presented in the literature; otherwise, a score of 0 was assigned. The usefulness score was calculated as the sum of achieved purposes divided by the total number of purposes (six) and expressed as a percentage (%). The workflow of the review process is illustrated in Figure 1.

3. Results

The selected studies in this review employed a range of seismic attributes to characterize submarine channels. These include amplitude- and frequency-related attributes (e.g., RMS, envelope, sweetness, instantaneous frequency) as well as attributes that emphasize reflector continuity and geometry (e.g., coherence, variance, dip, and curvature) (Taner, 2001; Posamentier, 2004; Chopra and Marfurt, 2006; Chopra and Marfurt, 2007a; Subrahmanyam and Rao, 2008; Posamentier *et al.*, 2022). In most studies,

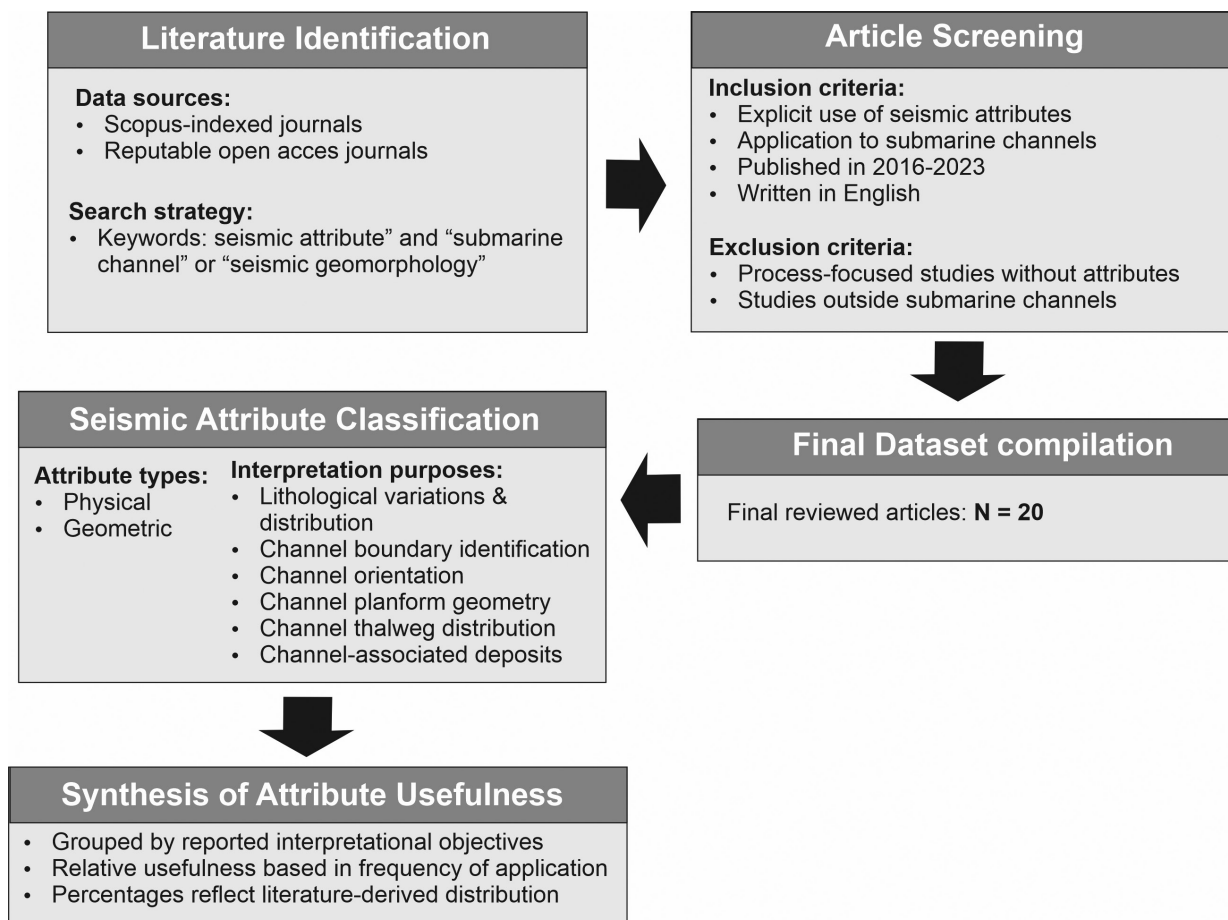


Figure 1. Integrated workflow illustrating literature identification, screening, chronological selection, classification, and synthesis of seismic attribute applications in submarine channel studies.

these attributes are not interpreted individually but are integrated to provide complementary insights into channel geomorphology, stratigraphic architecture, and associated lithological variability.

3.1. RMS Amplitude

RMS is calculated using the standard deviation, $\sigma(t)$, of the seismic amplitude values, $d(t)$, within a moving analysis window, where $\sigma(t)$ quantifies the dispersion of amplitude values around their mean and thus provides a measure of reflectivity within that window (Taner, 2001; Chopra and Marfurt, 2007a; Brown, 2004; Posamentier *et al.*, 2022). The root-mean square (RMS) attribute enhances high-amplitude reflections within specific intervals or horizons, thereby aiding the delineation of channel-related depositional bodies and their planform geometries by highlighting the lateral distribution and continuity of amplitude features (Brown,

2004; Omosanya & Alves, 2013; Posamentier *et al.*, 2022). It is calculated in specific time windows around horizons where it reflects the signatures of reflection amplitudes and contrasts with background components (Posamentier *et al.*, 2022).

Figure 2a illustrates strong RMS attribute contrast within channel deposits. The channel is expressed by relatively higher RMS amplitudes, suggesting a lithological contrast with the surrounding lower-amplitude deposits, such as overbank or levee deposits. These are commonly associated with coarser- and finer-grained lithologies, which should be confirmed by well data calibration. The asymmetric distribution of high RMS amplitudes outside the channel margin further suggests preferential sediment accumulation related to channel-adjacent depositional processes, which may include overbank sedimentation and/or flow-stripping-related splay-like deposits. The sinuous channel system is highlighted by elevated RMS amplitudes along the channel thalweg and inner

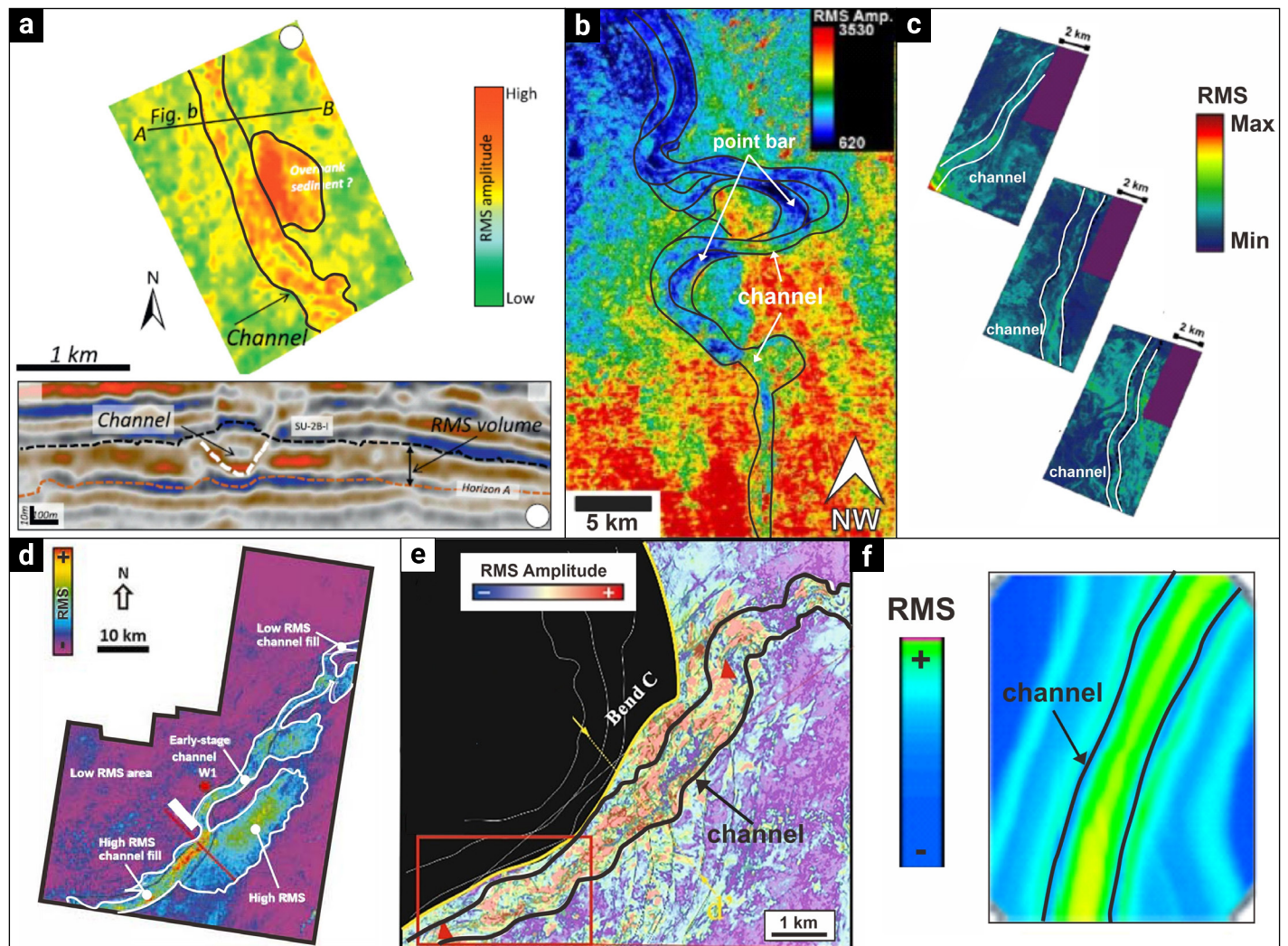


Figure 2. Submarine channel geometries highlighted by the RMS amplitude attribute, modified and compiled from previous studies: (a) Levant Basin (Niyazi *et al.*, 2018); (b) Taranaki Basin (Naewboonien, 2019); (c) Canterbury Basin (Harishidayat and Raja, 2022); (d) Kribi-Campo Basin (Gouott *et al.*, 2023); (e) Niger Delta (Bouchakour *et al.*, 2023); (f) Offshore New Zealand (La Marca *et al.*, 2023).

bends (Figure 2b). The high amplitude contrast suggests a different lithological composition between the channel body and overbank deposits, potentially reflecting sand-rich channel fills surrounded by fine-grained slope or overbank sediments. Localized amplitude enhancement at channel bends is interpreted to reflect variations in seismic response associated with changes in flow behavior along the curved channel pathway. Figure 2c illustrates relatively high RMS amplitudes confined within the channel margins, indicating a contrast in seismic response with the surrounding lower-amplitude channel-edge and overbank areas. The integration with dip-angle attributes further assists in delineating channel edges and internal stratigraphic boundaries associated with erosional surfaces. Figure 2d highlights along-channel variations in RMS amplitude that reflect temporal changes in channel infill. The channels are characterized by relatively high RMS amplitudes interpreted as sand-rich channel fills or possible sediment splays. Figure 2e shows a pattern of relatively high RMS amplitude values that can be interpreted as zones of preferential sand accumulation within the channel body. In contrast, Figure 2f shows a pronounced RMS amplitude contrast that clearly delineates channel boundaries, reflecting a sensitivity analysis performed at a smaller scale on individual channel elements within a channel complex (La Marca *et al.*, 2023), where channel geometry and attribute responses can be resolved more distinctly. Overall, these examples demonstrate that RMS amplitude is effective for lithological variation, channel boundary identification, channel trend delineation, and the interpretation of depositional elements within submarine channel deposits.

3.2. Envelope Amplitude

Envelope, also referred to as instantaneous amplitude, represents reflection strength independent of phase and highlights contrasts in acoustic impedance (Posamentier *et al.*, 2022). Essentially, this attribute primarily captures variations in acoustic impedance, that may reflect subsurface reflectivity associated with lithological contrasts, internal stratigraphic heterogeneity, and variations in bed thickness (Subrahmanyam and Rao, 2008). The envelope is effective for emphasizing discontinuities, seismic facies variations, faults, depositional changes, tuning effects, sequence boundaries, and areas of hydrocarbon accumulation such as bright spots. As an amplitude-based attribute, envelope extractions reflect differences in density and velocity, facilitating high contrast in values corresponding to lithological changes and clearer delineation of the channel bodies. Figure 3a shows the envelope attribute extracted along the mapped horizon, exhibiting relatively low envelope values within portions of the channel body. It may reflect reduced reflection strength and locally disrupted seismic continuity within a defined amplitude

range. Such areas are interpreted to represent segments of the channel characterized by lower-amplitude seismic facies expression, associated with channel-related features such as channel margins and slump scars. In contrast, Figures 3b and 3c display envelope attributes extracted within a defined time window relative to the mapped horizon. These maps exhibit relatively high envelope values within the channel body, which are interpreted as sand-prone channel fills characterized by strong reflectivity. This interpretation is supported by calibration with well-log data, and the enhanced reflectivity facilitates the delineation of channel boundaries. The envelope also provides the amplitude context for other instantaneous attributes, particularly instantaneous frequency, which may become unstable in low-amplitude or noisy zones.

3.3. Instantaneous Frequency

Instantaneous frequency is computed as the time derivative of the instantaneous phase (Taner *et al.* 1979; Barnes 1991). The analytic signal also yields instantaneous amplitude (envelope), which is used to provide amplitude context for frequency interpretation. Subrahmanyam and Rao (2008) suggested that the instantaneous frequency attribute might reflect seismic-scale layer thickness and provide lithological insights. In some cases, it could be used to identify the thin-bed tuning effects and zones of abnormal seismic attenuation, where high-frequency energy is preferentially lost due to intrinsic absorption or scattering effects (Chopra and Marfurt, 2007a). Intrinsic absorption refers to energy loss caused by inelastic attenuation related to lithology, pore fluids, and rock properties, whereas scattering effects are triggered by small-scale heterogeneities such as thin interbedded sand–mud layers, erosional surfaces, or internal channel-fill complexity that redistribute seismic energy. Frequency-based seismic attributes are sensitive to seismic noise, and their application in stratigraphic and reservoir analysis remains limited in the industry. However, some studies have demonstrated their potential utility as part of an integrated attribute approach for identifying hydrocarbon-related indicators (Brown, 2011). As a physical attribute, the instantaneous frequency attribute has been shown to enhance the submarine channel features, including lithology prediction, depositional elements, and vertical layer thickness.

Figure 4a displays a channel pathway that is expressed by systematic variations in instantaneous frequency values relative to the surrounding background. The channel body is associated with contrasting frequency magnitudes, forming a continuous, sinuous pattern, while adjacent areas exhibit more uniform and laterally continuous frequency values. Figure 4b highlights that relatively lower instantaneous frequency values occur within

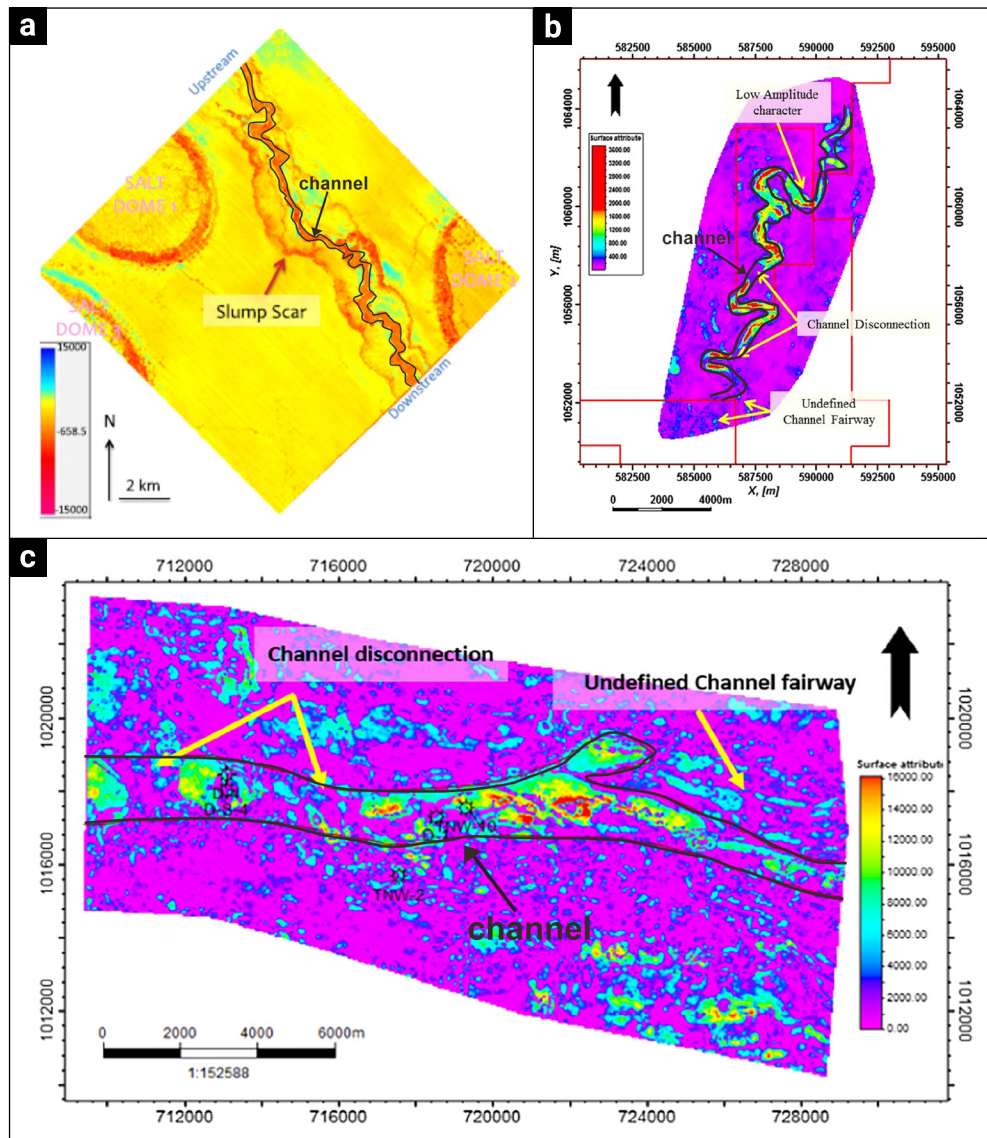


Figure 3. Submarine channel geometries highlighted by the envelope amplitude attribute modified and compiled from previous studies: (a) Gulf of Mexico (Carter *et al.*, 2016); (b) Nile Delta (Othman *et al.*, 2016); (c) Nile Delta (Othman *et al.*, 2018).

the channel body and display pronounced spatial variability. The instantaneous frequency attribute enhances internal variability within the channel body, which may be associated with thin-bedded successions and internal heterogeneities linked to lateral channel migration and stacking patterns, rather than primary channel boundaries. The channel margins are more clearly delineated by sharp contrasts between higher and lower instantaneous frequency values, indicating that frequency magnitude variations enhance the visibility of channel geometry (Figure 4c). In vertical section, the channel interval is characterized by higher and laterally variable frequency values compared to the surrounding background strata which display lower and more uniform responses, with localized low-frequency anomalies

potentially indicating attenuation or stratigraphic complexity within the channel fill (Figure 4d).

3.4. Sweetness

Sweetness is a composite seismic attribute designed to emphasize high-amplitude, low-frequency responses commonly associated with thick, clean reservoir-prone intervals. It is computed by dividing the instantaneous amplitude (or amplitude envelope) by the square root of the instantaneous frequency (Radovich and Oliveros, 1998). This attribute could be used for sand-shale ratio prediction. However, it is not particularly useful when the contrast in acoustic impedance between these lithologies is low

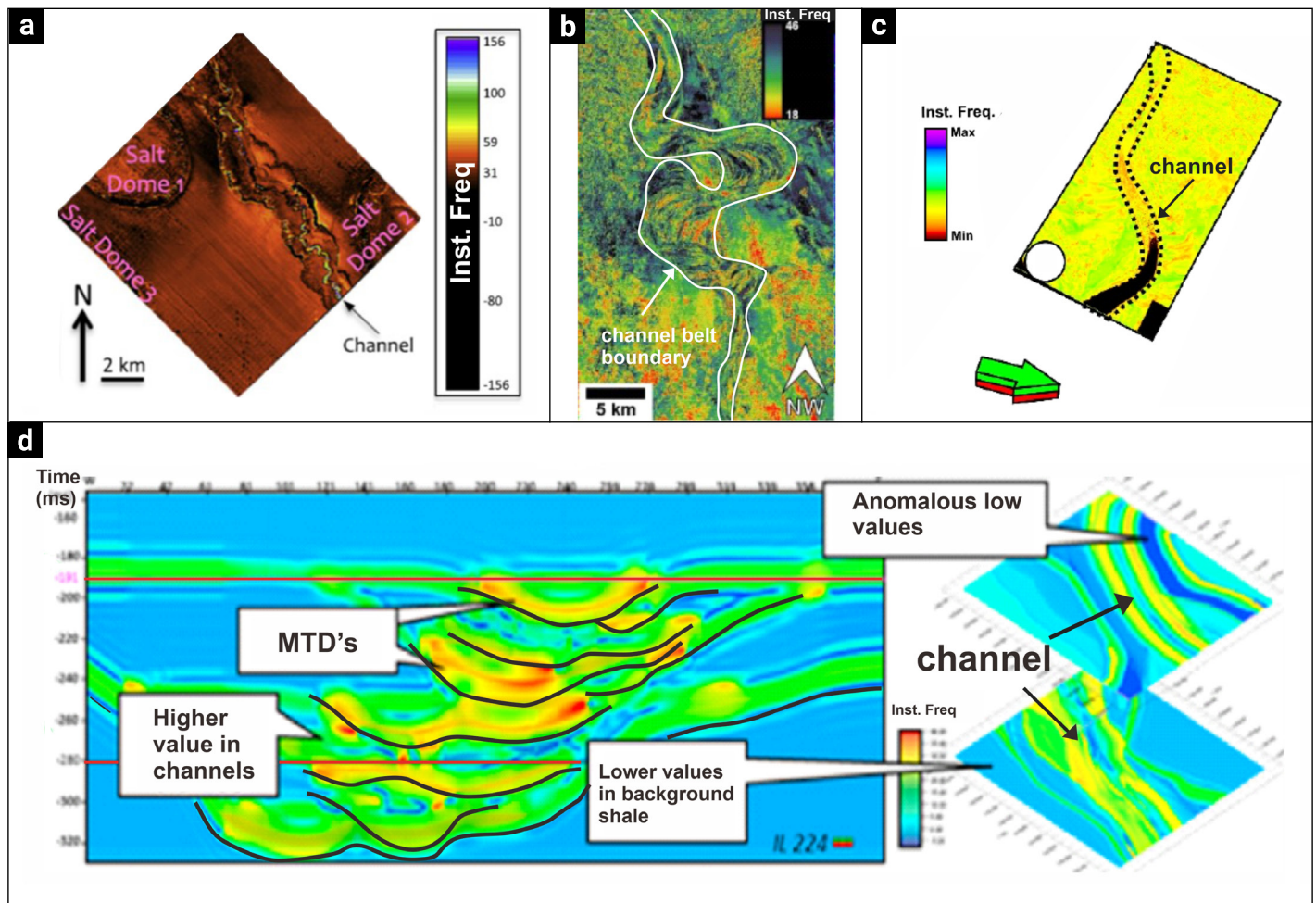


Figure 4. Submarine channel geometries highlighted by the instantaneous frequency attribute modified and compiled from previous studies: (a) Gulf of Mexico (Carter *et al.*, 2016); (b) Taranaki Basin (Naewboonien, 2019); (c) Canterbury Basin (Harishidayat and Raja, 2022); (d) Offshore New Zealand (La Marca *et al.*, 2023).

(Hart, 2008). Theoretically, identifying the sand and shale composition that forms some trend or channel features is a means to illustrate the channel features more easily. On the other hand, several authors combine the sweetness attribute with geometrical attributes (coherence) to identify submarine channels in more detail (Li *et al.*, 2017). The sweetness attribute becomes more effective for indicating potential pay zones when integrated with other seismic attributes, such as RMS amplitude, frequency, and phase, as demonstrated by Azeem *et al.* (2016) in the Sawan gas field, Pakistan. Figure 5a shows a plan-view sweetness attribute map in which the submarine channel body is characterized by relatively low to moderate sweetness values, consistent with a heterogeneous seismic response commonly associated with internally complex channel fills. In contrast, relatively higher sweetness values outside the channel zone correspond to a more uniform seismic character which may be associated with a more homogeneous lithological composition.

In Figure 5b, the alignment between the interpreted channel margins (dashed lines) and the sweetness contrast demonstrates that sweetness is a robust attribute for channel boundary delineation, particularly in areas where amplitude alone may be ambiguous due to noise or tuning effects. Figure 5c highlights internal variations in sweetness within the channel belt, suggesting heterogeneity within the channel fill, potentially related to changes in grain size, layer thickness, or stacking patterns of channel elements. Figure 5d illustrates a sweetness attribute extracted along a time-slice horizon intersecting the submarine channel and integrated with well data, seismic inversion, and AVO analysis. Relatively high-sweetness anomalies along the channel axis are interpreted as sand-prone channel fills, supported by the association of strong amplitudes and reduced frequencies. In contrast, low-sweetness regions away from the channel axis are interpreted as shale-dominated background deposits.

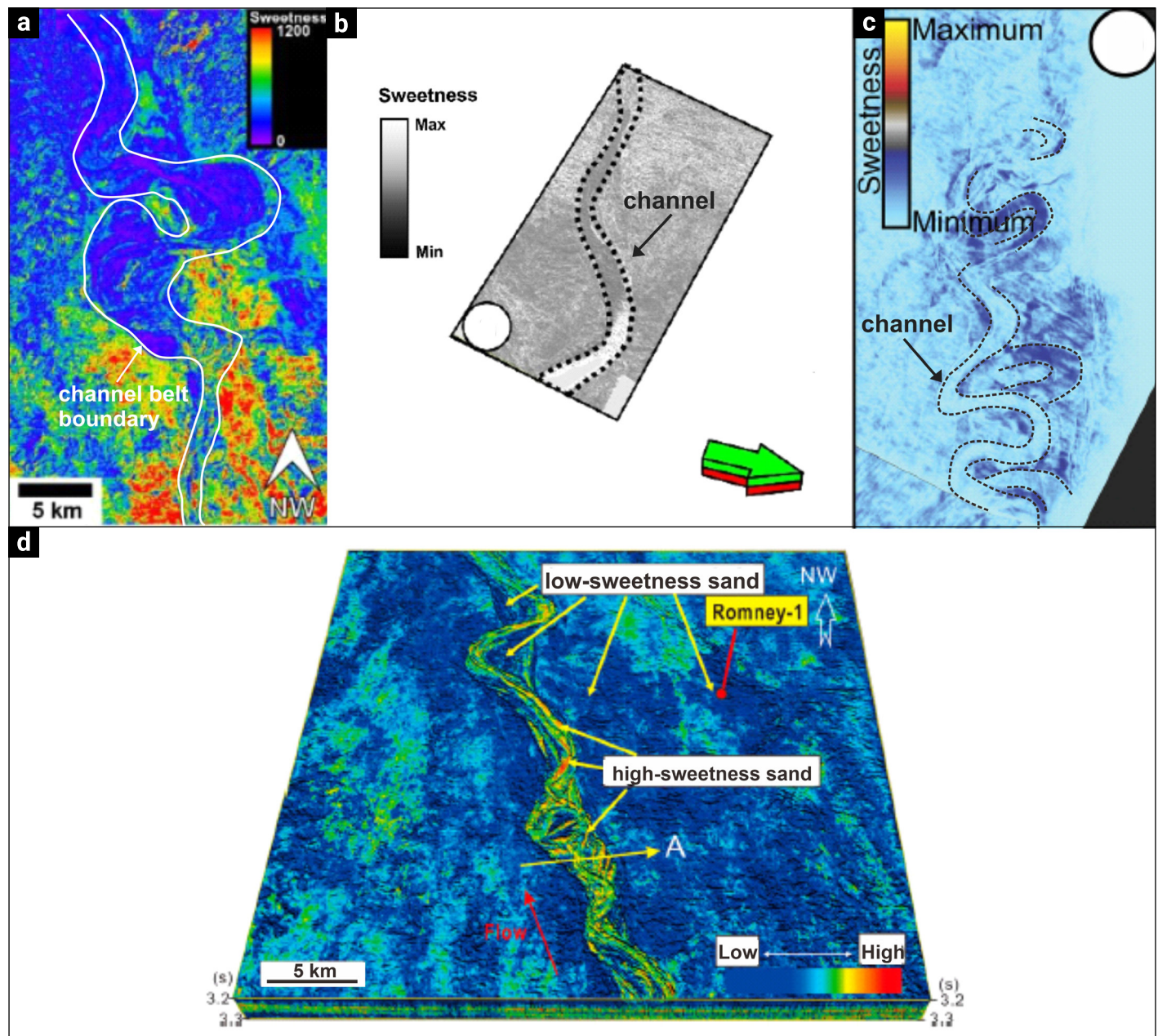


Figure 5. Submarine channel geometries highlighted by the sweetness attribute modified and compiled from previous studies: (a) Taranaki Basin (Naewboonien, 2019); (b) Canterbury Basin (Harishidayat and Raja, 2022); (c) Taranaki Basin (Larsen *et al.*, 2023); (d) Taranaki Basin (Li *et al.*, 2017).

3.5. Variance and Coherence

Variance and coherence are closely related seismic attributes that image lateral variations in seismic signals over horizons or intervals and are widely used to enhance structural and stratigraphic discontinuities (Posamentier *et al.*, 2022). They are fundamental to seismic interpretation and are commonly integrated with other attributes, such as RMS or RGB spectral decomposition, to improve the visualization of channel architectures and associated features, including mass-transport deposits

(Almasgari *et al.*, 2020; Howlett *et al.*, 2022; Larsen *et al.*, 2023). They are computed from trace-to-trace waveform similarity and statistical variability, whereby seismic traces across faults or stratigraphic discontinuities exhibit reduced similarity relative to surrounding, laterally continuous reflections (Bahorich and Farmer, 1995; Gersztenkorn and Marfurt, 1999). The primary distinction between the two attributes lies in their computational approach, where coherence relies on trace-to-trace similarity measures, whereas variance quantifies statistical dispersion within a defined analysis window. Variance quantifies local

dissimilarities in seismic signals, while coherence evaluates the degree of similarity between neighboring seismic traces (Posamentier *et al.*, 2022). Together, coherence and variance enhance the detection and visualization of seismic reflector discontinuities associated with faults and stratigraphic changes, delineating fault planes and channel margins across both horizon slices and vertical seismic sections.

These attributes are processed within a three-dimensional analysis window, this attribute quantifies trace-to-trace variability across a sample interval, enhancing lateral acoustic impedance contrasts associated with stratigraphic discontinuities such as channel belts and mass transport complex as demonstrated by Bouchakour *et al.* (2022). Higher variance values correspond to zones of increased discontinuity, for example where strong contrasts occur between the submarine channel belt axis and its bounding levees (Naewbonieen, 2019). In contrast, coherence typically exhibits low values along faults and stratigraphic boundaries, indicating geological discontinuities associated with lateral changes in seismic character (Li *et al.*, 2017). In terms of submarine channel identification, coherence provides better constraints in distinguishing the channel axis from the surrounding levee background compared to variance, as it is based on the similarity of seismic traces. Similarity-based coherence evaluates a short “mini-trace” in multiple directions, allowing systematic comparison with neighboring traces, which enhances sensitivity to subtle lateral changes in seismic character and typically results in more precise delineation of channel-related discontinuities (Posamentier *et al.*, 2022).

Previous studies demonstrate that variance and coherence attributes enhance the imaging of submarine channel architecture and are commonly used in combination with other seismic attributes to improve channel delineation (Deptuck *et al.*, 2007; Hansen *et al.*, 2017; Li *et al.*, 2017; Naewboonien, 2019; Gouott *et al.*, 2023; Larsen *et al.*, 2023; La Marca *et al.*, 2023; Silver and Bedle, 2021; Bouchakour *et al.*, 2025). Figure 6a shows that the variance attribute highlights high trace-to-trace variability along sinuous channel margins, delineating erosional boundaries and stepwise lateral channel shifting relative to the surrounding overbank deposits. Elevated variance values delineate channel edges and zones of internal architectural complexity, reflecting abrupt lateral changes in seismic character associated with channel incision and fill (Figure 6b). Figure 6c exhibits low variance values outlining the channel axis, with additional associated channel-related elements, whereas higher variance values may indicate internal variability within the channel fill. The coherence attribute exhibits pronounced low-coherence lineaments along channel margins, clearly defining channel boundaries and zones of lateral discontinuity within the submarine channel system as shown in Figure 6d and 6e. Figure

6f further demonstrates that coherence contrasts effectively image channel margins and erosional features, enabling detailed mapping of channel geometry.

3.6. Dip Attribute

The strike and dip of sedimentary layers are analogous to the magnitude and azimuth of the dip. Marfurt (2006) emphasizes that accurate estimation of reflector dip magnitude and azimuth (i.e., vector dip) constitutes the fundamental building block for geometric seismic attributes and structurally oriented filtering. Such estimates can be obtained using several approaches, including complex trace analysis, discrete vector dip scanning, and gradient structure tensor methods; reliable vector dip estimation further enables the calculation of coherent amplitude gradients along structural dip, thereby enhancing the delineation of subtle stratigraphic features such as channels expressed through lateral variations in thin-bed tuning. Compared to variance and RMS attributes, which primarily emphasize discontinuities and amplitude contrasts, dip attributes capture changes in reflector orientation, providing improved imaging of subtle structural features surrounding or crosscutting submarine channels, such as internal channel terraces. Dip magnitude represents the magnitude of the reflector’s local slope, quantifying the steepness of the seismic reflector relative to the horizontal plane, with values ranging from 0 to 90. Dip azimuth defines the horizontal direction of the maximum reflector slope and corresponds to the azimuthal direction of the vector dip, typically measured clockwise from north or relative to the survey coordinate system. In terms of submarine channel characterization, dip attributes reveal increased reflector tilting along channel flanks, as well as a broad downstream gradient following the channel flow.

In recent quantitative workflows for submarine channel analysis, spatial variations in dip magnitude have been used to highlight structural gradients and localized deformation, aiding the identification of channel-bounding structural markers such as channel margins and bank failure-related features (Bouchakour *et al.*, 2025). Figure 7a exhibits systematic variations between low and high dip azimuth values that define the sinuous channel pathway, including meandering segments and shifts in channel orientation. These azimuthal contrasts emphasize channel curvature and inferred flow direction, while also revealing the influence of adjacent salt domes that locally deflect channel trajectories. The dip magnitude attribute shows higher dip angle values concentrated along the channel flanks, reflecting increased reflector tilting associated with channel incision and lateral relief, whereas lower dip magnitudes characterize the channel axis and produce a clear and continuous expression of the channel thalweg (Figure 7b).

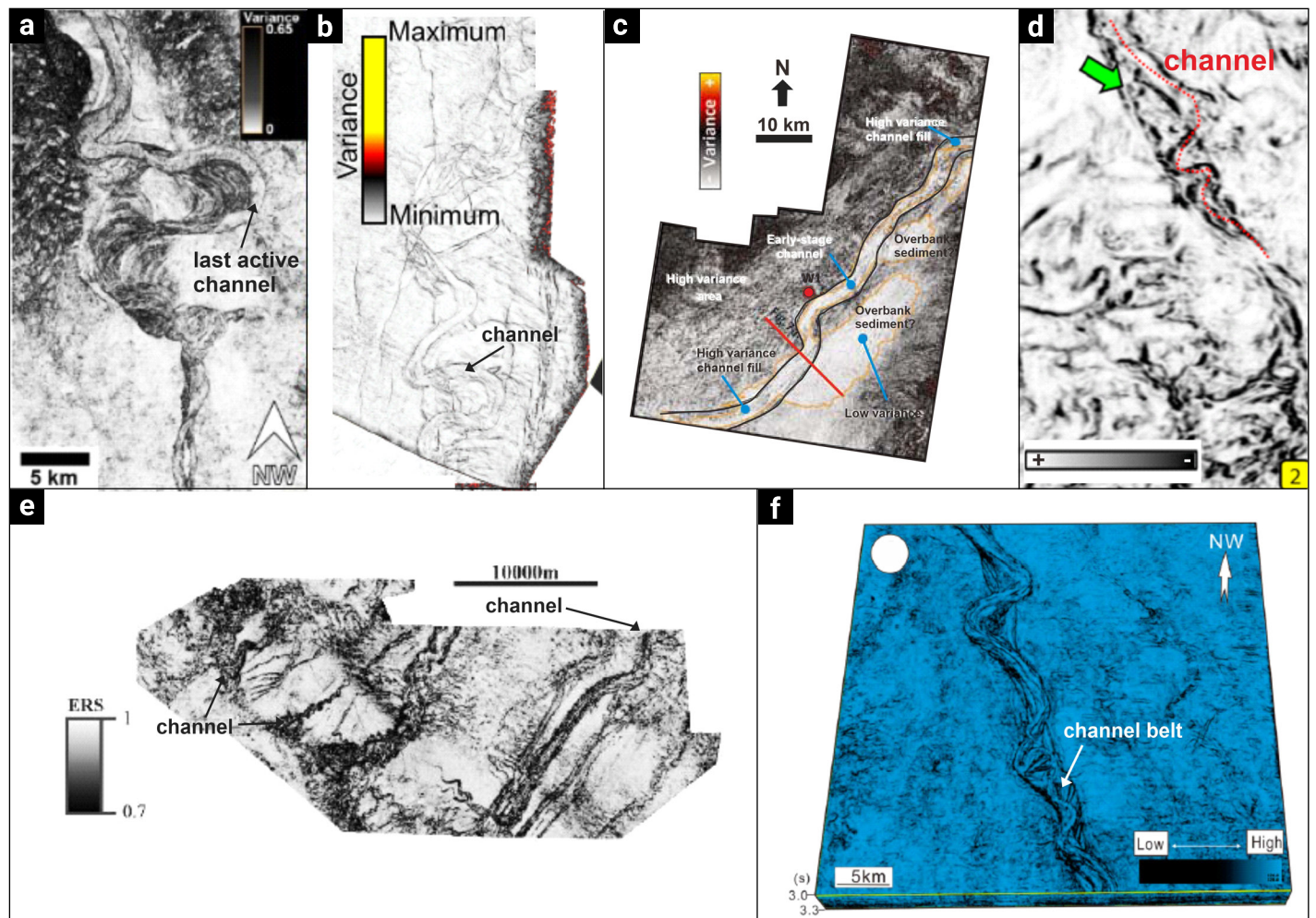


Figure 6. Examples of submarine channel identification using discontinuity-based seismic attributes, modified and compiled from previous studies: (a) variance attribute, Taranaki Basin (Naewboonien, 2019); (b) variance attribute, Taranaki Basin (Larsen *et al.*, 2023); (c) variance attribute, Karibi/Campo Basin (Gouott *et al.*, 2023); (d) coherence attribute, Offshore New Zealand (La Marca *et al.*, 2023); (e) coherence attribute (ERS is energy ratio similarity), Taranaki Basin (Silver and Bedle, 2021); (f) coherence attribute, Taranaki Basin (Li *et al.*, 2017).

3.7. Curvature

Curvature is a three-dimensional seismic attribute that represents the local second-order geometric variation of a surface, quantifying the degree to which a horizon deviates from planarity (Chopra and Marfurt, 2006; Chopra and Marfurt, 2007b). By minimizing the influence of regional dip, curvature analysis enhances subtle, small-scale surface irregularities that are commonly associated with primary depositional elements or minor structural features such as small-scale faults. However, curvature attributes are sensitive to disrupted seismic images or limited depositional continuity, where noise, reflector truncation, or poor imaging may generate spurious curvature anomalies and lead to misleading geological interpretations. This attribute enhances subtle geometric irregularities and abrupt changes in surface curvature, making it particularly effective for identifying minor structural flexures and fault-related deformation.

Curvature can be applied to surfaces or time slices and is also helpful for the stratigraphic analysis of features such as channel margins, reefs, compaction structures, and debris flows (Chopra & Marfurt, 2007b). Two main types of curvature exist: (1) maximum curvature (k_{max}), defined as the curvature of a circle with the smallest radius and representing the direction of the most pronounced surface bending, and (2) minimum curvature (k_{min}), which characterizes the curvature of a second circle oriented perpendicular to the k_{max} direction and corresponds to the least pronounced bending of the surface at that point (Al-Dossary and Marfurt, 2006; Chopra and Marfurt, 2007b). In seismic geomorphology, maximum curvature commonly accentuates sharp ridges and levee crests, whereas minimum curvature emphasizes channel axes and erosional troughs, making the combined analysis particularly effective for delineating channel geometry and subtle structural deformation (Chopra and Marfurt, 2006; Chopra and Marfurt, 2007b). Positive values in the

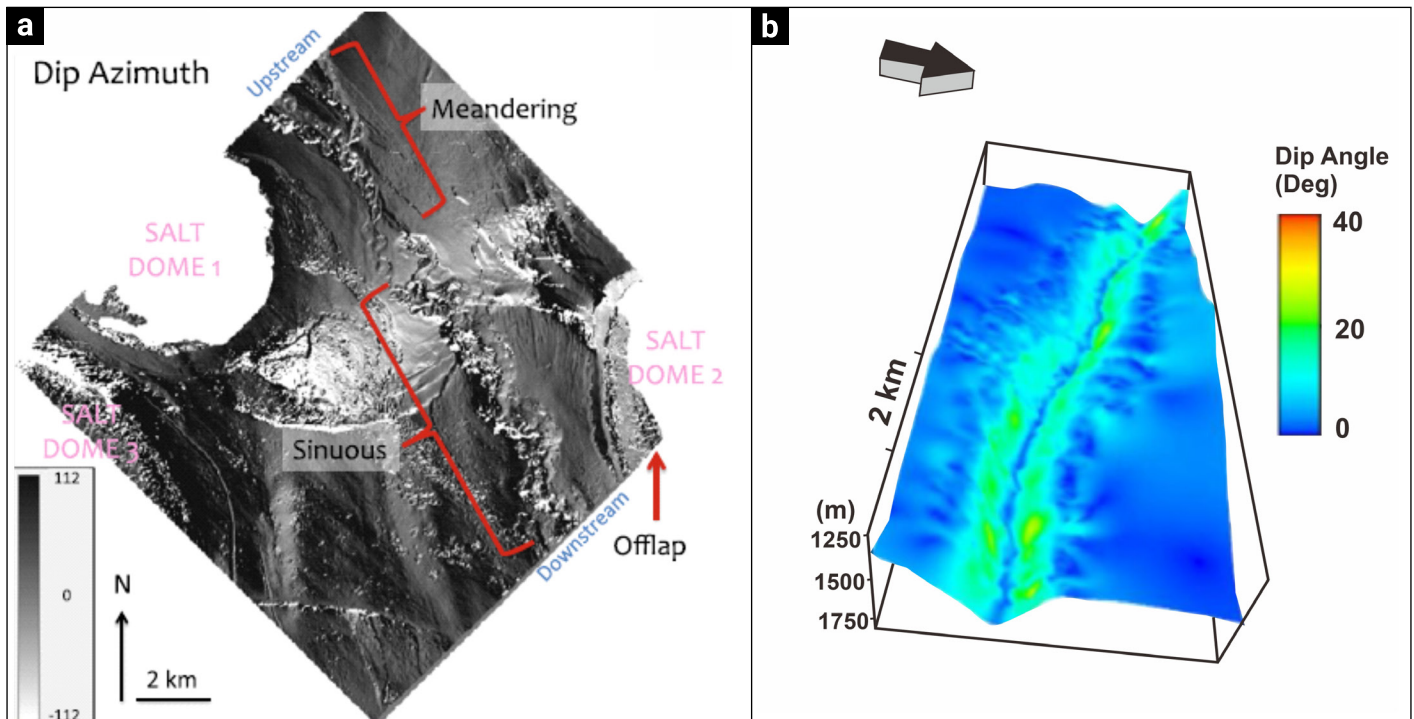


Figure 7. Dip attribute extraction for identifying submarine channels, modified and compiled from previous studies: (a) Gulf of Mexico (Carter *et al.*, 2016) and (b) Canterbury Basin (Harishidayat and Raja, 2022).

most-positive curvature (k_1) highlight concave-down structures, including channel banks and levees, while negative anomalies in the most-negative curvature (k_2) indicate concave-up features, such as the base of a channel (Figure 8a; Silver and Bedle, 2021). Figure 8b highlights the contrast between minimum and maximum curvature which enhances the geometric definition of the channel outline, allowing the channel pathway and boundaries to be accurately delineated.

4. Discussion

Since the 1990s, seismic attribute analysis has been increasingly applied to visualize and interpret submarine channel deposits within deep-water systems, with continued methodological development driven by advances in computerized seismic processing and interpretation technologies (Posamentier and Kolla, 2003; Chopra and Marfurt, 2007a; Mayall *et al.*, 2010; Mayall and Kneller, 2021; Bouchakour *et al.*, 2022; Bouchakour *et al.*, 2025). Many researchers have used specific attributes and have made combinations between them or have applied additional methods to enhance the visualization of channel features. For instance, spectral decomposition and RGB color blending (Partyka *et al.*, 1999; Chopra and Marfurt, 2007a; Carter *et al.*, 2016; Othman *et al.*, 2018; Almasgari *et al.*, 2020; Silver and Bedle, 2021; Bouchakour *et al.*, 2023; Kamaruzaman *et al.*, 2023). Spectral

decomposition has been widely integrated with other seismic attributes to enhance the visualization of channel features by exploiting frequency-dependent seismic responses, particularly in areas with limited seismic imaging quality or subtle channel expression. This integration improves the identification of channel morphology and planform characteristics, as well as associated depositional elements in submarine channel systems. Other studies have applied co-rendering of two seismic attributes, typically integrating amplitude-based and discontinuity-based attributes, to enhance the visualization of channel features (Li *et al.*, 2017; Niyazi *et al.*, 2018; Naewboonien, 2019). Such integration provides effective visualization of channel features but generally relies on good seismic image quality and clear channel expression.

Table 1 highlights a synthesis of the reviewed literature, illustrating how different seismic attributes contribute to the identification of submarine channel deposits across various interpretation purposes, as reflected by their respective usefulness scores. The review qualitatively compares the effectiveness of seismic attributes in identifying channel features based on the usefulness score.

The usefulness scores highlight clear contrasts between amplitude-based, frequency-related, and geometric attributes in terms of their versatility and functional scope. Amplitude-related attributes, particularly RMS amplitude, exhibit the highest usefulness score (100%), indicating that they have been reported to support all predefined interpretation purposes. This reflects

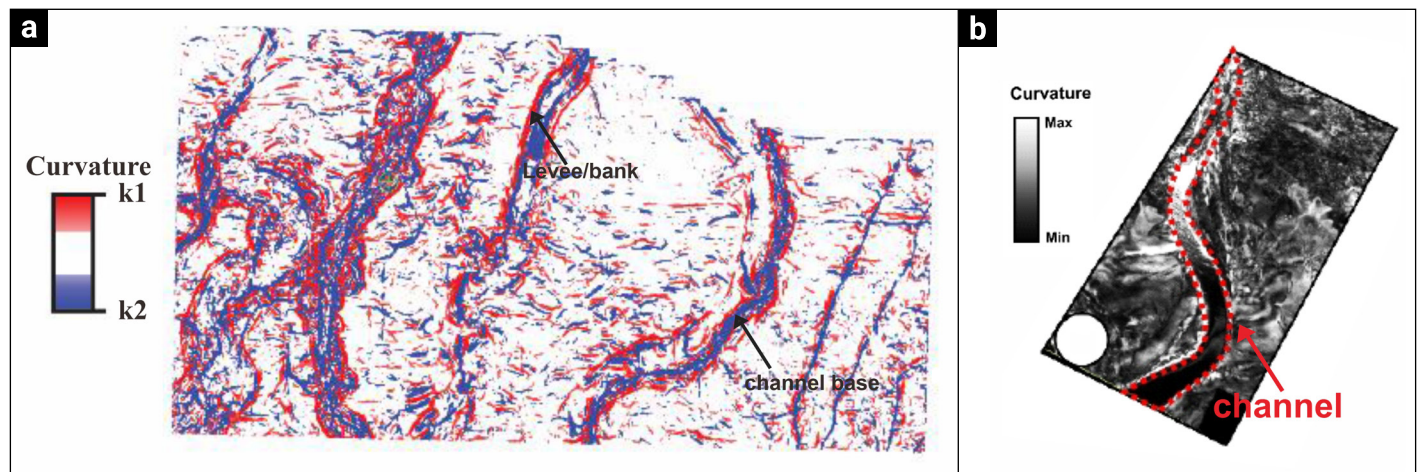


Figure 8. Curvature attribute extraction for identifying submarine channels, modified and compiled from previous studies: (a) Taranaki Basin (Silver and Bedle, 2021) and (b) Canterbury Basin (Harishidayat and Raja, 2022).

the well-established sensitivity of RMS amplitude to changes in lithology and impedance contrasts, which are fundamental to identifying channel boundaries, internal geometries, and associated depositional elements (Posamentier and Kolla, 2003; Chopra and Marfurt, 2007a; Bernhardt *et al.*, 2012; Posamentier *et al.*, 2022). The high applicability of RMS amplitude across studies underscores its role as a first-order attribute in submarine channel analysis, particularly in settings where sand–mud contrasts and stratigraphic variability are pronounced. Envelope amplitude and sweetness attributes also show high usefulness scores (83.3%), suggesting broad applicability, though dependent on geological and data quality context. This pattern indicates that amplitude-derived attributes are highly effective for outlining channel architecture and depositional elements but may be less consistently applied to more detailed geomorphological elements, depending on data resolution and depositional complexity. Although instantaneous frequency can assist in identifying lithological variations and channel-associated deposits, its application to channel trend delineation and thalweg interpretation remains inconsistent, indicating strong context dependence. This variability likely reflects the sensitivity of frequency attributes to tuning effects, attenuation, and noise, which can complicate their application in laterally heterogeneous channel systems. The high usefulness score of variance, coherence, and curvatures (83.3%) highlights their robustness in capturing lateral discontinuities and channel margins, whereas the lower score of dip attributes (66.7%) reflects their limited application in lithological prediction and channel-associated deposit identification.

These results highlight that geometrical attributes are most effective when integrated with physical attributes, underscoring the value of multi-attribute approaches in submarine channel interpretation (Chopra and Marfurt, 2006; Chopra and Marfurt,

2007a; Chopra and Marfurt, 2007b). Overall, physical attributes provide lithological context, whereas geometrical attributes define structural and morphological characteristics. Combining both types enhances overall interpretation, and the usefulness score provides guidance on selecting the most suitable attributes for specific geomorphological tasks. Attributes with lower usefulness scores should therefore not be interpreted as having inferior performance; rather, they reflect a relative scarcity of documented applications linking these attributes to specific interpretation purposes in the existing literature, highlighting opportunities for further methodological exploration.

5. Conclusion

This study investigated the usefulness of seismic attributes to visualize the morphologies of submarine channel systems and associated deposits within several areas, including Taranaki Basin, Gulf of Mexico, Gulf of Thailand, Levant Basin, Offshore Nile Delta, offshore Niger Delta, and Kribi-Campo Basin. The method used a qualitative review of 20 articles, which applied different techniques and attributes to their analysis. Generally, two types of seismic attributes were used according to Taner's (2001) classification: physical attributes and geometrical attributes. Physical attributes include RMS amplitude, sweetness, envelope, and instantaneous frequency, whereas, geometrical attributes are variance, coherence, dip attribute, and curvature.

Physical attributes, particularly amplitude-based measures such as RMS amplitude, exhibit the broadest reported applicability across lithological, architectural, and depositional elements, highlighting their strong depositional usefulness in characterizing submarine channels and associated deposits. In contrast, geo-

Table 1. The summary of seismic attribute application by interpretation purposes and their usefulness score.

No	Name of Attribute	Type of Attribute (Taner, 2001)	Interpretation purposes	Binary score	Usefulness score (%)
1	RMS Amplitude	Physical	Lithological variations and distribution	1	100
			Channel boundary identification	1	
			Channel orientation	1	
			Channel planform geometry	1	
			Channel thalweg distribution	1	
			Channel-associated deposits	1	
2	Envelope Amplitude	Physical	Lithological variations and distribution	1	83.3
			Channel boundary identification	1	
			Channel orientation	1	
			Channel planform geometry	1	
			Channel thalweg distribution	0	
			Channel-associated deposits	1	
3	Instantaneous Frequency	Physical	Lithological variations and distribution	1	66.7
			Channel boundary identification	1	
			Channel orientation	0	
			Channel planform geometry	1	
			Channel thalweg distribution	0	
			Channel-associated deposits	1	
4	Sweetness	Physical	Lithological variations and distribution	1	83.3
			Channel boundary identification	1	
			Channel orientation	1	
			Channel planform geometry	1	
			Channel thalweg distribution	0	
			Channel-associated deposits	1	
5	Variance & Coherence	Geometrical	Lithological variations and distribution	0	83.3
			Channel boundary identification	1	
			Channel orientation	1	
			Channel planform geometry	1	
			Channel thalweg distribution	1	
			Channel-associated deposits	1	
6	Dip attribute	Geometrical	Lithological variations and distribution	0	66.7
			Channel boundary identification	1	
			Channel orientation	1	
			Channel planform geometry	1	
			Channel thalweg distribution	1	
			Channel-associated deposits	0	
7	Curvature	Geometrical	Lithological variations and distribution	0	83.3
			Channel boundary identification	1	
			Channel orientation	1	
			Channel planform geometry	1	
			Channel thalweg distribution	1	
			Channel-associated deposits	1	

metrical attributes primarily enhance the delineation of channel boundaries, trends, and planform geometries, demonstrating pronounced morphological usefulness by capturing lateral discontinuities and channel-scale geometry rather than detailed lithological variations.

These results underscore that robust interpretation of submarine channel systems requires a purpose-driven integration of physical and geometrical attributes rather than reliance on any single attribute type. The direct application of individual seismic attributes may not always be sufficient and often requires complementary analyses such as attribute co-rendering, parameter tuning, and spectral decomposition. Overall, any interpretation method depends on seismic data quality and geological conditions. Therefore, strong geological understanding is essential in seismic interpretation and the use of the seismic attributes.

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Nota sobre la definición de demandas sísmicas para el diseño de edificaciones en Colombia

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Abstract

The definition of seismic design parameters for all types of infrastructure is crucial to ensuring good performance in countries located in areas with significant seismic risk. The main objective of the codes or standards governing earthquake-resistant design is to protect life; however, the definition of the design coefficient (cs), which determines the lateral load resistance of a structure under seismic actions, also has an economic and social impact related to the construction cost, and the expected future losses. Seismic hazard focuses on the study of expected seismic intensity (PGA, PGV, among others) and its recurrence, while seismic risk is related to the study of the impacts generated due to seismic actions on a single element or a portfolio of exposed elements, usually expressed with different metrics, such as probability of collapse, number of fatalities, and economic losses. In this context, the definition of cs , often represented in parametric design spectra, should include both threat and risk analysis that allows for the integration of different approaches, always prioritizing safety aspects. This paper explores the most widely accepted methodologies worldwide for defining cs in earthquake-resistant standards and proposes the use of its envelope, justifying that the benefit in terms of collapse safety is much greater than the impact on the total expected cost over the useful life. To this end, Colombia was taken as a case study, a country that has various seismic hazard and risk studies, design codes, and openly and freely available information.

Key words: Seismic design, PSHA, Probability of collapse, Optimal design, RTGM.

Resumen

La definición de los parámetros de diseño sismorresistente de todo tipo de infraestructura resulta crucial para asegurar un buen desempeño en países ubicados en zonas con amenaza sísmica significativa. El objetivo principal de los códigos o normas que rigen el diseño sismorresistente es la protección de la vida; sin embargo, la definición del coeficiente de diseño (cs), que determina la resistencia a carga lateral de una estructura ante acciones sísmicas, tiene además un impacto económico y social, debido al costo de construcción y a las pérdidas futuras esperadas. La amenaza sísmica se centra en el estudio de la intensidad sísmica esperada (PGA, PGV, entre otros), y su recurrencia, mientras que el riesgo sísmico se relaciona con el estudio de los impactos generados debido a las acciones sísmicas sobre un único elemento o un portafolio de elementos expuestos, usualmente expresado con diferentes métricas, como probabilidad de colapso, número de fatalidades y pérdidas económicas. En este contexto, la definición de cs , a menudo representada en espectros de diseño paramétrico, debería incluir un análisis tanto de amenaza como riesgo que permita integrar diferentes métricas como la probabilidad de excedencia, la probabilidad de colapso o las pérdidas futuras esperadas. En este trabajo se exploran las metodologías más aceptadas a nivel mundial para la definición de cs en normas sismorresistentes y se propone el uso de su envolvente, justificando que el beneficio en términos de seguridad de colapso es mucho mayor que el impacto en el costo total esperado a lo largo de la vida útil. Para ello, se tomó como caso de estudio a Colombia, un país que cuenta con diversos estudios de amenaza y riesgo sísmico, códigos de diseño e información disponible de manera abierta y libre.

Palabras clave: Diseño sismorresistente, PSHA, Probabilidad de colapso, Diseño Óptimo, RTGM.

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1. Introducción

Colombia es un país localizado en el noroeste del continente suramericano, en una zona geológicamente compleja debido a la interacción de las placas tectónicas de Nazca, Sudamérica y Caribe, las cuales generan sismos con diversas características (Sarria Molina, 2003; Vargas *et al.*, 2004). En el territorio nacional, es posible encontrar sismos corticales, sismos de subducción interplaca e intraplaca (Zona de Benioff), y eventos de sismicidad intermedia concentrados en el nido de Bucaramanga (Taboada *et al.*, 2000; Pulido, 2003).

Debido a estas condiciones, en el país se han registrado al menos 15 sismos con intensidad estimada IX o mayor en la escala EMS-98, clasificados como muy destructivos o catastróficos. La Tabla 1 presenta la magnitud y la máxima intensidad macrosísmica registrada para cada uno de los sismos (Sarabia Gómez *et al.*, 2022), siendo el más antiguo el evento ocurrido en 1644 en la zona de Pamplona, Norte de Santander.

La reconocida sismicidad en Colombia ha impulsado el desarrollo de diversos estudios y mapas de amenaza sísmica a escala nacional (Ramírez & Estrada, 1977; Sarria, 1978; AIS, 1984, AIS, 1996, AIS, 2010; Gallego, 2000; Salgado *et al.*, 2010; Salgado-Gálvez *et al.*, 2016; Arcila *et al.*, 2020), así como la estimación de riesgo tanto a nivel nacional (UNGRD *et al.*, 2018), como en áreas de gran interés (Yamin & Bernal, 2013; Salgado-Gálvez *et al.*, 2014; Acevedo *et al.*, 2020). Estos estudios buscan comprender cuantitativamente la sismicidad del territorio

en términos de las intensidades sísmicas esperadas -amenaza-, o de sus afectaciones -riesgo-, y su probabilidad de ser excedidas.

La mayoría de estos estudios se enfocan en la evaluación probabilística de la amenaza sísmica (PSHA por sus siglas en inglés), cuya principal aplicación es en la formulación de normas de diseño sismorresistente. A nivel global, existe una estrecha relación entre los modelos PSHA y las normas sismorresistente (Esteva, 1970; Algermissen & Perkins, 1976, ATC3, 1978; Leyendecker *et al.*, 1995; García-Mayordomo *et al.*, 2004; Stucchi *et al.*, 2011; Khose *et al.*, 2012; Crowley *et al.*, 2021; Pavel *et al.*, 2024), y Colombia no es la excepción. Los modelos de amenaza sísmica formulados en el país han servido como base para el desarrollo de los distintos códigos de diseño sismorresistente, tales como el código colombiano de construcciones sismo-resistentes (AIS, 1983; MOPT, 1984), la Norma Colombiana de Diseño y Construcción Sismo Resistente NSR-98 (MDE, 1998; AIS, 1998), y su actualización de 2010 (MAVDT, 2010), la Norma Colombiana de Diseño de Puentes CCP-14 (AIS, 2014), y la próxima actualización de la NSR-10, en desarrollo desde la década anterior.

Como parte de las discusiones en torno a la actualización de la NSR-10, y en particular sobre la demanda sísmica de diseño, en esta nota se discuten diferentes metodologías para la definición de *cs*, y se justifica el uso de su envolvente.

Es importante aclarar que este trabajo no pretende recomendar el uso de un modelo de amenaza sísmica en particular, sino analizar las metodologías utilizadas para definir parámetros de

Tabla 1. Resumen de sismos registrados en Colombia con intensidad EMS-98 IX o mayor.

Fecha	Hora local	Mw	Autor Magnitud	Intensidad máxima (EMS-98)	Autor Intensidad
1644/01/16	05:00	6.5	(Sarabia, 2016)	9	(Cifuentes & Sarabia, 2007b)
1805/06/16	03:15	6.1	(Sarabia, 2016)	9	(Cifuentes & Sarabia, 2007c)
1827/11/16	18:00	7.1	(Gómez-Capera <i>et al.</i> , 2020)	10	(Sarabia <i>et al.</i> , 2006b)
1834/01/20	07:00	6.7	(Sarabia, 2016)	9	(Sarabia <i>et al.</i> , 2006a)
1875/05/18	11:15	6.8	(Sarabia, 2016)	10	(Cifuentes & Sarabia, 2006b)
1882/09/07	03:20	6.5	(Sarabia, 2016)	9	(Sarabia & Cifuentes, 2007a)
1906/01/31	10:36	8.4	ISC-GEM*	10	(Sarabia & Cifuentes, 2007d)
1917/08/31	06:36	7	ISC-GEM*	9	(Cifuentes & Sarabia, 2006a)
1923/12/14	05:31	6.2	(Beauval <i>et al.</i> , 2010)	9	(Sarabia & Cifuentes, 2007c)
1950/07/08	21:35	6.2	(Gómez-Capera <i>et al.</i> , 2020)	9	(Cifuentes & Sarabia, 2007a)
1967/02/09	10:24	7	ISC-GEM*	10	(Cifuentes & Sarabia, 2009c)
1979/12/12	02:59	8.1	ISC-GEM*	10	(Sarabia & Cifuentes, 2007b)
1983/03/31	08:12	5.6	ISC-GEM*	9	(Cifuentes & Sarabia, 2009b)
1992/10/18	11:12	7.1	ISC-GEM*	10	(Cifuentes & Sarabia, 2009a)
1999/01/25	13:19	6.1	ISC-GEM*	9	(Sarabia & Cifuentes, 2010)

*Hace referencia al catálogo ISC-GEM soportado por el International Seismological Centre (ISC, 2025)

diseño. Los hallazgos aquí expuestos muestran consistencia con estudios realizados en otras regiones del mundo, utilizando distintos modelos de amenaza y en diferentes ambientes tectónicos. Por lo tanto, las conclusiones presentadas en este documento pueden considerarse independientes del modelo de amenaza empleado.

2. Metodologías

En la práctica, los parámetros de diseño suelen definirse directamente de la amenaza sísmica; sin embargo, en los últimos años ha crecido la tendencia a incluir métricas de riesgo en este proceso. Esto se debe a que el parámetro de diseño de una estructura debe ser definido en función de su comportamiento y desempeño esperado. A continuación, se resumen brevemente los métodos más utilizados para la definición del coeficiente de diseño o de carga lateral (cs), orientados a la amenaza y el riesgo sísmico. No se detalla cada método en su totalidad, pues existen estudios específicos que los analizan y profundizan (Gkimprxis *et al.*, 2019; Ordaz *et al.*, 2023), o el lector puede remitirse directamente a la literatura en donde se desarrolla cada uno. Las metodologías seleccionadas son además presentadas en términos de aceleraciones espectrales (SA), la medida de intensidad sísmica más empleada para definir cs a nivel global.

2.1. Metodología orientada a la amenaza

Una curva de amenaza sísmica se puede entender como la probabilidad de excedencia en un periodo de tiempo T , o la tasa anual de excedencia de un valor determinado de SA en un sitio determinado. Asumiendo que la ocurrencia de sismos sigue una distribución de Poisson, la probabilidad de excedencia de un valor de SA igual a cs en T años se expresa como:

$$Pr(SA \geq cs, T) = 1 - e^{-\lambda(cs)T} \quad (1)$$

El periodo de retorno (T_R) se define como:

$$T_R = \frac{1}{\lambda(cs)} \quad (2)$$

donde $\lambda(cs)$ representa la tasa anual de excedencia promedio dado un valor de SA igual a cs .

Las normas sismorresistentes que definen valores de cs basados en amenaza suelen emplear como input el concepto espectro de amenaza uniforme (UHS por sus siglas en inglés). En un UHS, para cada sitio se calcula el valor de aceleración como

$Sa_{UHS}T_R$, que corresponde a la aceleración espectral esperada para un periodo de retorno T_R según el UHS.

En el caso de Colombia, la norma NSR-10 define un espectro de diseño paramétrico a partir del coeficiente A_a , que representa la aceleración pico del terreno y afecta los periodos cortos, y el coeficiente A_v , que representa la velocidad pico efectiva y controla el diseño para periodos intermedios a largos (AIS, 2010). Estos coeficientes son estimados a partir de los resultados de un análisis probabilista de amenaza sísmica para PGA y $Sa(1.0)$ asumiendo un periodo de retorno de 475 años, que corresponde a intensidades sísmicas con una probabilidad de 10% de ser excedidas en 50 años.

En consecuencia, en este trabajo se definió un valor de T_R de 475 años, para ser consistentes con el periodo de retorno de diseño definido en la NSR-10 para A_a y A_v . Así, la demanda sísmica para una determinada ordenada espectral puede ser definida como:

$$cs = Sa_{UHS475} \quad (3)$$

2.2. Metodologías orientadas al riesgo

Entre las metodologías basadas en riesgo, se seleccionaron los enfoques de "tasa de colapso uniforme" y "diseño óptimo". La primera se basa en la probabilidad de alcanzar un estado de colapso, mientras que la segunda optimiza el diseño en función del costo total esperado a lo largo de la vida útil de la estructura.

2.2.1. Tasa de Colapso Uniforme

Conocida como *Risk Targeted Design* o *RTGM*, esta metodología fue propuesta por primera vez por Luco (2006), y luego extendida por Luco *et al.* (2007), y busca definir valores de SA de manera que la probabilidad de colapso esperada sea uniforme para todos los sitios. Este enfoque reconoce que diferentes edificaciones diseñadas con similares valores de Sa_{UHS475} pueden tener riesgo de colapso muy diferente, debido a que el cálculo de riesgo probabilístico depende de la curva de amenaza en su totalidad, y no solo de un único punto en esta.

Para esta metodología, la probabilidad de colapso f_{Col} de una edificación sigue una distribución lognormal indexada a un valor de intensidad que, en este caso se identifica como c . De esta manera:

$$f_{Col}(c) = \phi \left[\frac{\ln(c) - (\ln(c_{10\%}) + 1.28\beta)}{\beta} \right] \frac{1}{c\beta} \quad (4)$$

A su vez, la probabilidad de colapso puede ser estimada a partir de f_{Col} y la curva de amenaza de tal manera que:

$$PCol[c, T] = \int_0^{\infty} [1 - e^{-\lambda(c)T}] f_{Col}(c) dc \quad (5)$$

β representa la incertidumbre en la probabilidad de colapso, y en su formulación original asume un valor de $\beta=0.8$, argumentando que luego de un análisis de sensibilidad con valores entre 0.6 y 1.0, es un parámetro que no afecta los resultados considerablemente. Además, se define el sismo máximo considerado como aquel que genera un valor de $SA_{c10\%}$ para el cual la probabilidad de colapso en 50 años es del 1%. Para motivos de esta nota, este valor está definido como SA_{RTGM} .

Los parámetros descritos previamente fueron definidos para Estados Unidos, con base en la probabilidad de colapso promedio estimada para edificaciones diseñadas en California. Con lo anterior, si SA_{RTGM} es compatible con el sismo máximo considerado orientado a riesgo (MCE_R por sus siglas en inglés), la aceleración de diseño debe incluir un factor de reducción de 1.5 (NEHRP, 2003). De esta manera, se obtiene que:

$$cs = Sa_{2/3RTGM} = \frac{2}{3} Sa_{RTGM} \quad (6)$$

El factor de 1.5 (2/3) representa el límite inferior de margen con respecto a la probabilidad de colapso definida para el MCE_R , pero a su vez se ha encontrado que representa de manera aproximada la relación entre los valores de $Sa(0.2s)$ con una probabilidad de 2 y 10% de ser excedidos en 50 años en algunos sitios en California (Leyendecker *et al.*, 2000). Si bien, la introducción de un factor de 2/3 hace que la probabilidad de colapso varíe espacialmente, se ha demostrado que $PCol[2/3 Sa_{RTGM}, 50]$ es mucho más uniforme que $PCol[Sa_{UHS475}, 50]$ (Luco, 2006).

Esta metodología ha sido ampliamente replicada en diferentes regiones debido a que el estado de daño de colapso está directamente relacionado con la seguridad esperada en términos de fatalidades. Algunos ejemplos de mapas de coeficientes utilizando esta metodología se encuentran para Europa (Silva *et al.*, 2016), México (Sandoval & Ordaz, 2025), Irán (Taherian & Kalantari, 2019) y Nueva Zelanda (Horspool *et al.*, 2021). Dentro de los países que han adoptado esta metodología oficialmente para el diseño de edificaciones se encuentra Indonesia (National Standardization Agency, 2019) y Estados Unidos (BSSC, 2020), mientras que países como El Salvador la han incluido en borradores de actualización (López Menjivar *et al.*, 2021).

2.2.2. Diseño Óptimo

Según esta metodología, el riesgo esperado durante el ciclo

de vida de una estructura debería incluirse en la definición de la demanda de fuerza lateral por sismo, aceptando un cierto umbral considerado como admisible (Wiggins, 1972; Wiggins & Moran, 1970). El diseño óptimo se basa principalmente en los trabajos de Rosenblueth (1976a, 1976b), con el objetivo de definir cs a partir de un proceso de optimización del costo de una edificación, incluyendo su construcción y sus pérdidas asociadas en su vida útil.

El diseño óptimo ha sido la metodología propuesta para la actualización de la norma NSR-10 (Bernal & Cardona, 2021, 2024), con base en trabajos previos realizados para Colombia y México (Ordaz *et al.*, 2017). La metodología se basa en la optimización del costo total (CT) de una edificación a lo largo de su vida útil, incluyendo su costo inicial de construcción (CI) y pérdidas futuras por sismo (CFL). Las funciones de costo normalizadas en términos del costo esperado de una edificación diseñada para soportar únicamente cargas gravitacionales, C_0 , y su resistencia lateral, c_0 , se presentan a continuación en términos de cs :

$$C_I(c_s) = \frac{C_I(c_s)}{C_0} = \begin{cases} 1 & , \text{ si } c_s < c_0 \\ 1 + \varepsilon \left[\frac{c_s - c_0}{c_0} \right]^\alpha & , \text{ si } c_s \geq c_0 \end{cases} \quad (7)$$

$$C_{FL}(cs) = \frac{C_{FL}(cs)}{C_0} = \frac{C_I(cs)}{C_0} (1 + S_L) \frac{\lambda(cs)}{\gamma} \quad (8)$$

$$CT(cs) = CI(cs) + CFL(cs) \quad (9)$$

Este método, también conocido como diseño de mínimo costo, requiere la calibración de diversos parámetros. En este trabajo se utilizaron los mismos parámetros que Ordaz *et al.* (2017) propusieron para Colombia. En los parámetros requeridos destaca S_L , que representa las pérdidas secundarias o indirectas por sismo, y puede variar dependiendo de las condiciones socioeconómicas. Para el presente estudio, S_L se fijó en un valor de 12, utilizado previamente para Colombia (Ordaz *et al.*, 2017), con base en análisis realizados previamente para el terremoto de 1985 que afectó Ciudad de México (Ordaz *et al.*, 1989). En este trabajo no se consideraron las variaciones locales de S_L propuestas para Colombia (Bernal & Cardona, 2021) en zonas específicas del país.

La definición de cs en esta metodología se obtiene mediante la optimización de $CT(cs)$, buscando el valor óptimo sa_{OPT} que minimiza los costos.

3. Resultados y comparaciones

Para comparar las metodologías presentadas, se utilizó el modelo de amenaza probabilista de Arcila et al (2020) para calcular curvas de amenaza en roca ($V_{s30} = 760$ m/s) para $S_a(0.2s)$ y $S_a(1.0s)$ utilizando OpenQuake (Pagani et al., 2014) en 1,103 sitios correspondientes a las cabeceras municipales definidas por el Departamento Nacional de Estadística de Colombia (DANE, n.d.). Es importante aclarar que la propuesta de actualización de la norma NSR-10 utiliza un modelo de amenaza diferente.

Debido a que todas las diferentes metodologías expresan el coeficiente de diseño en términos de aceleración espectral, podría compararse directamente el cambio relativo o absoluto de estos valores, sin embargo, no es una métrica que permita conclusiones profundas. Una segunda opción sería comparar los resultados en términos de su probabilidad de ser excedidos (asociada a un periodo de retorno) haciendo uso de las curvas de amenaza. De manera similar al trabajo realizado por Ordaz et al. (2023), en su sección 3 (figura 2 del artículo original), decidimos estimar y comparar la de colapso asociadas a los coeficientes de diseño definidos por cada metodología, y además añadimos los costos totales normalizados a la comparación.

Si bien la función de costo total utilizada para la definición de S_{aOPT} , y los parámetros asociados para el cálculo de S_{aRTGM} deberían ajustarse para diferentes tipologías estructurales, las dos metodologías comparten algunas suposiciones como la no inclusión de acumulación de daño o el continuo deterioro de las estructuras. Además, si bien el diseño óptimo podría incluir pérdidas económicas asociadas a la pérdida de vidas, con el debate ético y moral que esto conlleva (Keller et al., 2021), no incluir estas pérdidas permite consistencia entre las dos metodologías (Ordaz et al., 2023).

Bajo este enfoque, con el objetivo de comparar las diferentes metodologías, se realizó el siguiente procedimiento:

1. Estimación de coeficientes siguiendo las diferentes metodologías.
2. Estimación de la probabilidad de colapso, $PCol[cs, 50 \text{ años}]$. Con la ecuación (5) se estimó la probabilidad esperada de colapso para cada valor de cs . Esto permite comparar el impacto de los diferentes valores de cs en cada sitio, bajo el supuesto —coherente con el método RTGM— de que la fragilidad depende únicamente de cs y β .
3. Estimación del costo total normalizado esperado, $CT(cs)$. Mediante la ecuación (9) se calculó el costo total esperado en cada sitio. En un escenario en el que un nuevo reglamento colombiano se derive de esta función de costo

generalizada para todo el territorio y todas las tipologías, esta comparación permite evaluar el impacto de diseñar con un valor de cs distinto bajo las mismas condiciones de amenaza. Con ello es posible comparar, de manera simplificada, las implicaciones económicas de distintos valores de cs para cada sitio de interés.

La comparación de pérdidas económicas y probabilidad de colapso esperadas utilizando diferentes valores de aceleración y bajo las mismas suposiciones permiten comparar la implicación de diferentes valores de cs utilizando métricas asociadas al riesgo esperado.

3.1. Ejemplos de resultados

A modo de ilustración, se seleccionaron 4 diferentes ciudades en condiciones de amenaza sísmica diferentes. La Figura 1 presenta los valores de cs y $CT(cs)$ y la Figura 2 presenta los valores de cs y $PCol[cs, 50 \text{ años}]$ obtenidos para las diferentes ciudades.

En términos de costo total (Figura 1), es posible observar cómo el costo total estimado para las demandas sísmicas en las diferentes metodologías toma valores estables en la vecindad de S_{aOPT} , a pesar de que el valor de cs presenta variaciones considerables. En términos de la probabilidad de colapso (Figura 2), el efecto fue diferente, en donde cambios en cs afectan considerablemente el riesgo de colapso esperado.

El [anexo A](#) incluye la distribución de las diferentes métricas por metodología, en donde se evidencia la misma tendencia al comparar los 1,103 sitios de cálculo.

3.2. Comparación entre metodologías basadas en riesgo

La tendencia actual en las normas de diseño ha evolucionado hacia metodologías con base en riesgo sísmico; en este contexto, un mayor énfasis debe realizarse en la comparación entre S_{aOPT} y $S_{a2/3 RTGM}$. Para esto, se calculó la diferencia relativa porcentual de $S_{a2/3 RTGM}$ con respecto a S_{aOPT} en términos de costo total $CT(cs)$ y la probabilidad de colapso en 50 años. La Figura 3 presenta la comparación de S_{aOPT} y $S_{a2/3 RTGM}$ para $S_a(0.2s)$ y $S_a(1.0s)$ en términos de $CT(cs)$ y la probabilidad de colapso en 50 años.

Para $S_a(0.2s)$, el aumento porcentual de $CT(cs)$ de $S_{a2/3 RTGM}$ con respecto a S_{aOPT} , está concentrado en valores menores al 5%, con una mediana de 2.9%. Al comparar las probabilidades de colapso, los valores $S_{a2/3 RTGM}$ conducen a valores mucho menores con una mediana de -35.8%, implicando una disminución considerable.

En términos de $S_a(1.0s)$, debido a que los valores de S_a tienden a ser numéricamente menores, los valores de $CT(cs)$ y probabilidad de colapso estimados a partir de $S_{a2/3 RTGM}$, tienden

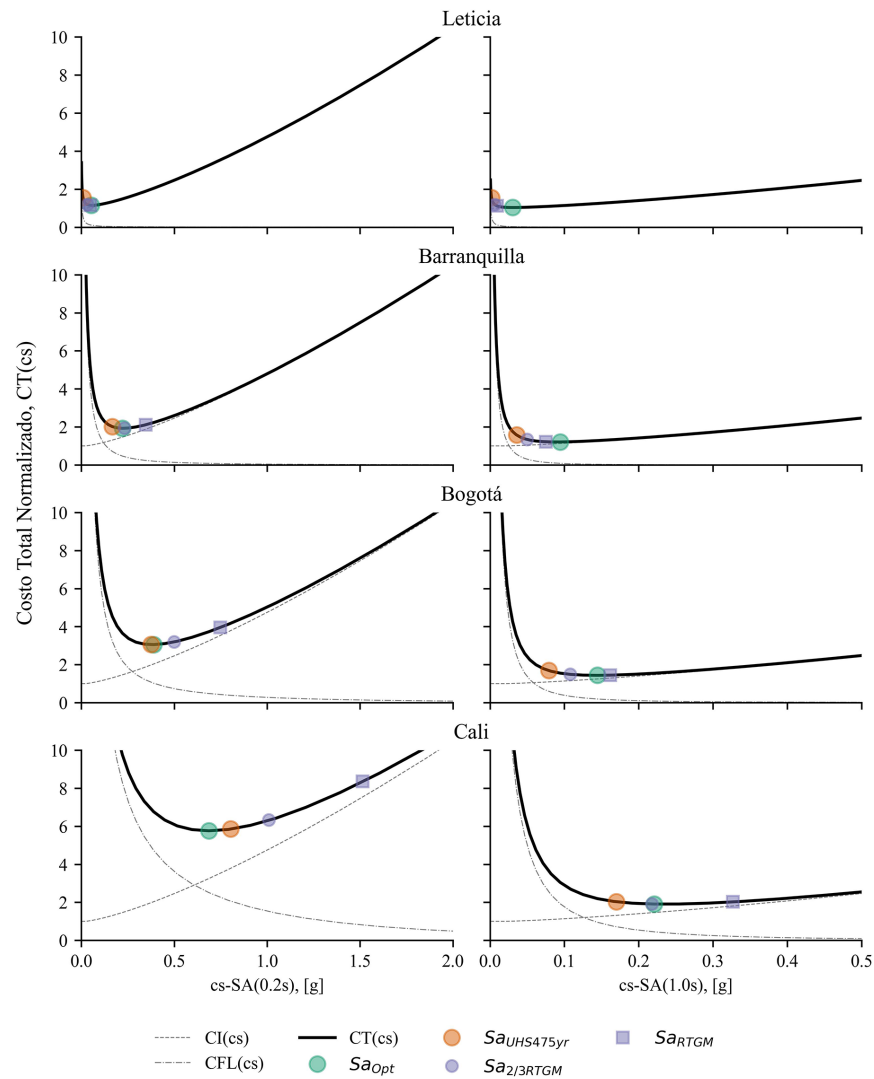


Figura 1. Costo total normalizado y cs calculados para las ciudades seleccionadas.

a ser menos conservadores. En este caso en particular, Sa_{OPT} de manera general, conduce a menores probabilidades de colapso y además menores valores de CT. Lo anterior puede observarse en que $Sa_{2/3 RTGM}$ está asociado con valores mayores de CT(cs), con una mediana de 5.1%, y a probabilidades de colapso que superan 150%, con una mediana de 92.4%.

4. Conclusiones y discusión

Las metodologías basadas en riesgo para la definición coeficientes sísmicos de diseño, aunque son prácticas presentan diferentes desafíos en su implementación, como por ejemplo la definición de los diferentes parámetros requeridos en su formulación. Un ejemplo de ello es la función de capacidad a colapso necesaria para calcular $Sa_{2/3 RTGM}$, o las funciones de

costo utilizadas en la estimación de Sa_{OPT} , las cuales pueden ser específicas para determinadas tipologías estructurales o ajustarse a diferentes condiciones socioeconómicas. De hecho, al incorporar información particular sobre el comportamiento estructural o sobre funciones de costo para tipologías específicas, podría generarse una colección de mapas de cs en lugar de un único valor genérico. Asimismo, las funciones de costo pueden adaptarse a diferentes contextos socioeconómicos, por ejemplo mediante la consideración de distintos valores de S_L (Bernal & Cardona, 2021). A pesar de estas limitaciones, ambas metodologías han mostrado un buen desempeño en la estimación de cs .

Aunque la definición de cs mediante diseño óptimo y mediante RTGM responde a enfoques distintos, es posible comparar ambos métodos en un sitio con amenaza conocida en términos de métricas asociadas al riesgo. Al contrastar las probabilidades de colapso, se observó que $Sa_{2/3 RTGM}$ tiende a ser más conserva-

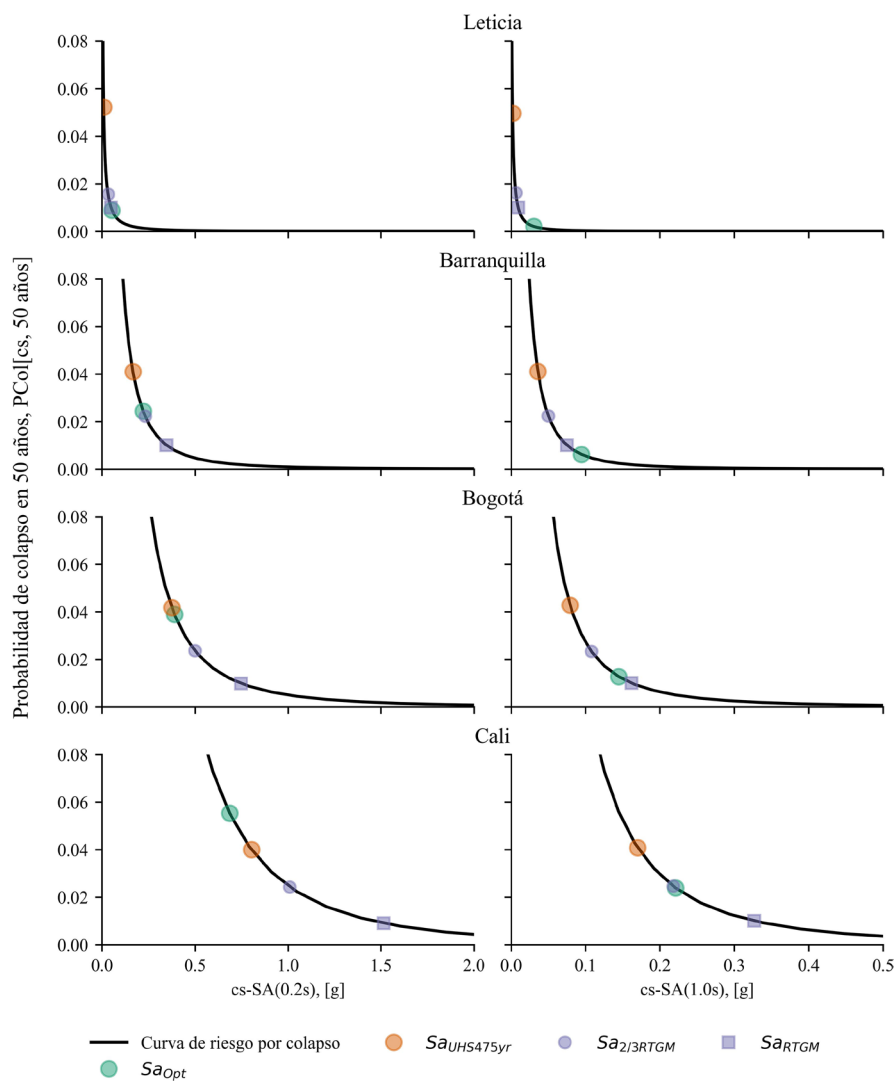


Figura 2. Probabilidad de colapso y cs para las ciudades seleccionadas.

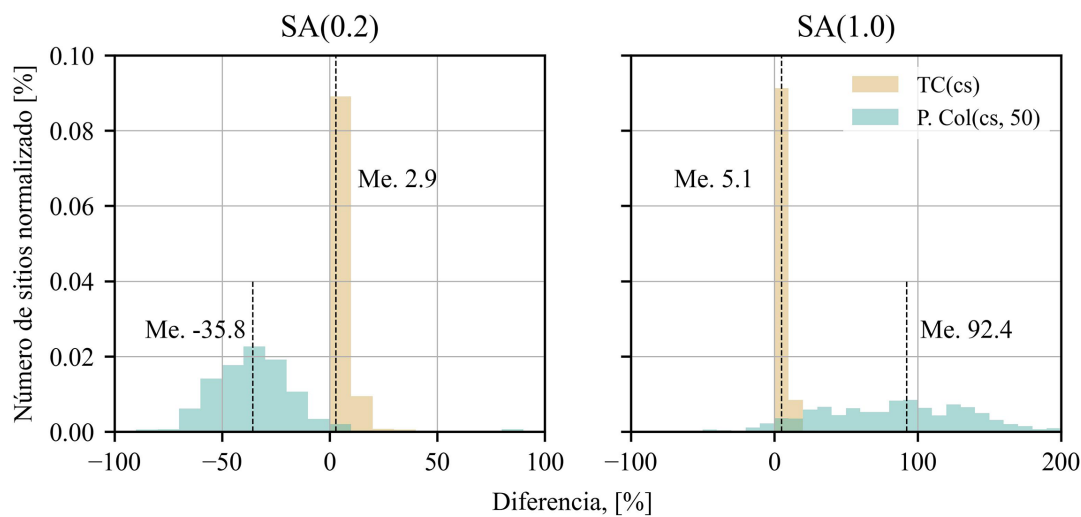


Figura 3. Comparación de metodologías basadas en riesgo para $Sa(0.2s)$ y $Sa(1.0s)$.

dor en zonas de mayor amenaza, mientras que Sa_{OPT} conduce a mayores cs cuando la amenaza es baja. Este comportamiento, ya documentado por Ordaz *et al.* (2017) mediante curvas de amenaza paramétricas genéricas y comparando Sa_{OPT} y Sa_{RTGM} , se evidencia también en la Figura 3, donde la diferencia en la probabilidad de colapso muestra tendencias opuestas para $Sa(0.2s)$ y $Sa(1.0s)$, reflejando sus distintos niveles de aceleración espectral ($Sa(0.2s) \gg Sa(1.0s)$). Aunque no es correcto comparar directamente $Sa(0.2s)$ y $Sa(1.0s)$ por representar medidas de intensidad distintas, su inclusión permite explorar cómo las metodologías responden a valores aritméticamente diferentes de amenaza, dado que tanto $CT(cs)$ como la fragilidad genérica utilizada en RTGM dependen únicamente del valor numérico de la intensidad y no de la ordenada espectral específica.

Adicionalmente, se observó que la probabilidad de colapso es altamente sensible al valor de cs , mientras que las variaciones en $CT(cs)$, fueron mucho menores al comparar las distintas metodologías. Resultados similares han sido reportados para Europa (Gkimprxis *et al.*, 2020), principalmente debido a la forma relativamente plana de las funciones de costo en la vecindad de su valor mínimo. Este hecho sugiere que el diseño óptimo podría utilizarse para definir una “zona óptima” más que un valor óptimo único (Ordaz *et al.*, 2017).

Los resultados respaldan una estrategia en la cual cs se defina como la envolvente entre Sa_{OPT} y $Sa_{2/3 RTGM}$, eligiendo siempre el valor mayor en cada sitio. Este enfoque reduce el riesgo de colapso esperado con un impacto mínimo en el costo total esperado, coherente con la existencia de una zona óptima en la función $CT(cs)$. Incluir el análisis económico como variable secundaria permite aumentar la seguridad estructural en los casos en que Sa_{OPT} resulte más conservador, e incluso obtener beneficios económicos. En síntesis:

- $cs = Sa_{OPT}$ si $Sa_{OPT} > Sa_{2/3 RTGM}$, lo cual incrementa la seguridad y reduce el costo total esperado.
- $cs = Sa_{2/3 RTGM}$ si $Sa_{2/3 RTGM} \geq Sa_{OPT}$, lo que permite aumentar el nivel de seguridad con un incremento bajo en $CT(cs)$.

Si bien los enfoques de costo óptimo y de tasa de colapso uniforme suelen considerarse excluyentes, los resultados muestran cómo pueden emplearse de manera complementaria para fundamentar normas sismorresistentes orientadas simultáneamente a la seguridad y la eficiencia. Bajo esta lógica, en zonas de amenaza alta tendería a seleccionarse $Sa_{2/3 RTGM}$, aumentando la seguridad con un incremento relativamente menor de $CT(cs)$ frente a Sa_{OPT} ; mientras que en zonas de amenaza baja, Sa_{OPT} permitiría aumentar la seguridad y reducir $CT(cs)$.

Desde el punto de vista del riesgo esperado, lo anterior es equivalente a sugerir que Sa_{OPT} debería ser seleccionada siempre que su probabilidad de colapso no sea superior a la obtenida por $Sa_{2/3 RTGM}$, o de la metodología objetivo. Lo anterior permite

optimizar la función de costo total ($CT(cs)$), siempre que el nivel de riesgo esperado no sea excedido.

Además, los resultados del [Anexo A](#) permiten incluir dentro de la envolvente el valor de Sa_{NSR10} cuando sea necesario bajo la misma precisa anterior. Esto responde a la preocupación existente sobre posibles disminuciones de la demanda sísmica en futuras actualizaciones normativas.

Finalmente, aunque el uso de un modelo de amenaza distinto generaría valores de cs diferentes para cada metodología, la evidencia indica que los hallazgos principales deberían mantenerse: (1) $CT(cs)$ es estable en la vecindad del valor óptimo, y (2) en sitios con mayor amenaza, RTGM tiende a estimar valores de cs mayores que el diseño óptimo, mientras que en sitios de baja amenaza ocurre lo contrario.

5. Limitaciones y trabajos futuros

Los resultados presentados se basan en metodologías simplificadas que emplean funciones de costo y modelos de fragilidad genéricos para Colombia. Por ello, futuros estudios deberían comparar las metodologías considerando la capacidad última de edificaciones diseñadas con los valores de cs derivados de cada enfoque. Trabajos como el de Parra García (2024), que evalúan el impacto de alternativas propuestas para la actualización de la NSR-10, permitirían obtener un panorama más detallado del efecto real del parámetro cs en una revisión normativa.

La evaluación realizada se fundamenta en supuestos adoptados por diversos autores, cuyas principales limitaciones incluyen:

- Aunque la función de costos utilizada fue desarrollada para el contexto colombiano y empleada en estudios nacionales, esta se construyó considerando únicamente edificios de concreto de dos pisos.
- Aunque la metodología RTGM ha sido adoptada en distintos países, los parámetros utilizados corresponden a la calibración realizada para Estados Unidos, basada en edificaciones en un contexto distinto al colombiano. Su regionalización podría lograrse mediante una reestimación del factor 1.5 para obtener la capacidad de diseño a partir del MCE_R , o mediante la definición de una probabilidad de colapso coherente con la capacidad de diseño sin un factor adicional, que permita mantener la premisa de una probabilidad de colapso esperada constante para todo el territorio.

Estas limitaciones abren la discusión sobre la necesidad de incorporar distintos arquetipos estructurales en la construcción de modelos de costo para la metodología de diseño óptimo, así como la importancia de regionalizar los supuestos del método RTGM al contexto colombiano.

Finalmente, aunque al utilizar modelos de amenaza diferentes se esperaba encontrar hallazgos similares, trabajos futuros podrían evaluar el impacto de diferentes modelos de amenaza en Colombia para la definición de coeficientes sísmicos de diseño utilizando las diferentes metodologías, reconociendo que son el principal input en el proceso.

6. Datos y recursos

Las curvas de amenaza calculadas para definir los parámetros de demanda sísmica siguiendo diferentes metodologías fueron calculadas utilizando el modelo de amenaza sísmica del Servicio Geológico Colombiano desarrollado en OpenQuake engine, disponible para libre descarga en el sitio web <https://amenazasismica.sgc.gov.co/>.

Los cálculos siguiendo la metodología RTGM fueron realizados utilizando la herramienta rtgmpy desarrollada por el USGS (Andrew J Makdisi *et al.*, n.d.), disponible en el sitio web: <https://code.usgs.gov/ghsc/erp/erp-rtgm-calculator>.

Los resultados obtenidos en términos de probabilidad de colapso, demanda sísmica y costo total normalizado se presentan en el archivo tipo excel [anexo](#).

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8. Declaración de conflicto de intereses

Los autores declaran que no tienen ningún potencial conflicto de intereses con respecto a la investigación, autoría o publicación de este artículo.

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Vertical Electrical Sounding Technique for Assessing the Quaternary Aquifer Vulnerability to Contamination in the Semi-Arid Khanasser Valley Region, Northern Syria

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Abstract

The aim of this paper is to evaluate the vulnerability of groundwater to contamination by adapting aquifer vulnerability index (AVI) approach, based mainly on the hydraulic conductivity (K) of the aquifer and overburden layers' thickness (h). The technique of vertical electrical sounding (VES) with the configuration of Schlumberger was applied to model the Quaternary aquifer and its overburden layers in the Khanasseer Valley area in Northern Syria. According to AVI classification, 5.88% of the study area is hugely polluted, 67.00% highly polluted, 23.53% moderately polluted, and 2.94% lowly polluted. Several hydro-geoelectrical parameters which affect the Aquifer Vulnerability Index (AVI) (such as anisotropy (λ) of the subsurface hydrogeological layers, thickness (h_{Overb}), resistivity (ρ_{Overb}), hydraulic conductivity (K), and hydraulic resistance (C) of the protecting layers) are statistically analyzed. Different mutual empirical relationships between the above parameters are established through analyzing their statistical correlation matrix. The derived empirical relationships highlight the mutual hydrological processes and the lithological connectivity nature between the study Quaternary aquifer and its overlaying layers. The obtained results highlighted the importance of safeguarding groundwater resources, and outlined resource allocation to protect the aquifer zones, for decision-makers. This was the first time that AVI approach is applied in Syria, and can be consequently extended to other Syrian aquifers. AVI can be also applied worldwide to estimate the conditions dominating the aquifer's protectivity in semi-arid regions.

Key words: aquifer vulnerability index, hydraulic conductivity, hydraulic resistance, Semi-arid Khanasser valley, Syria.

Resumen

El objetivo de este trabajo es evaluar la vulnerabilidad del agua subterránea a la contaminación mediante la adaptación del enfoque del índice de vulnerabilidad de acuíferos (AVI), basado principalmente en la conductividad hidráulica (K) del acuífero y el espesor (h) de las capas de sobrecarga. Se aplicó la técnica de sondeo eléctrico vertical (VES) con configuración Schlumberger para modelar el acuífero cuaternario y sus capas de sobrecarga en el área del valle de Khanasseer, en el norte de Siria. De acuerdo con la clasificación AVI, el 5.88% del área de estudio presenta contaminación muy alta, el 67.00% alta, el 23.53% moderada y el 2.94% baja. Se analizaron estadísticamente varios parámetros hidro-geoeléctricos que afectan el índice de vulnerabilidad del acuífero (AVI), tales como la anisotropía (λ) de las capas hidrogeológicas del subsuelo, el espesor (h_{Overb}), la resistividad (ρ_{Overb}), la conductividad hidráulica (K) y la resistencia hidráulica (C) de las capas protectoras. Se establecieron diferentes relaciones empíricas mutuas entre estos parámetros mediante el análisis de su matriz de correlación estadística. Las relaciones empíricas obtenidas destacan los procesos hidrológicos asociados y la conectividad litológica entre el acuífero cuaternario del área de estudio y sus capas suprayacentes. Los resultados obtenidos resaltan la importancia de salvaguardar los recursos de agua subterránea y orientan la asignación de recursos para proteger las zonas del acuífero, lo cual resulta relevante para la toma de decisiones. Este es el primer estudio en el que se aplica el enfoque AVI en Siria, por lo que puede extenderse a otros acuíferos del país. Asimismo, el AVI puede aplicarse a nivel mundial para estimar las condiciones que controlan la capacidad de protección de los acuíferos en regiones semiáridas.

Palabras clave: índice de vulnerabilidad de acuíferos, conductividad hidráulica, resistencia hidráulica, valle semiárido de Khanasser, Siria.

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1. Introduction

The contaminations originating from the surface affect the groundwater stored in the aquifers (Ikpe *et al.*, 2021). The anthropogenic activities negatively affect the groundwater quality due to poor waste disposal management, the leakages from the surface and underground storage tanks, mining activities, and latrines, sewage from oil spillage, and the movement of leachates from dumpsites into subsurface hydrogeological units (Oseji *et al.* 2018).

The hydrogeological aquifer systems are well protected from surface contamination and pollution when the overlaying earth layers above an aquifer have suitable hydrological conditions, regarding their resistivities, thicknesses, and hydraulic conductivities.

The aquifer overburden layers act as natural boundaries to filter percolating surface contaminated fluids, and the measure of such an ability determines the aquifer protectivity characteristics (Adeniji *et al.* 2014).

The protectivity of the underlying hydrogeological aquifer is considerably affected by some critical factors, which are the thickness, porosity, grain size, hydraulic conductivity, and anisotropy of the overburden-protecting layers (Mogaji *et al.*, 2011; Adeniji *et al.* 2014; Ekanem *et al.*, 2020; Ekanem *et al.*, 2021; Ikpe *et al.*, 2022; Asfahani, 2023a; Asfahani 2023b).

The high resistivity and high hydraulic conductivity of the permeable overlaying layers of sand and gravel facilitate the easy movement of the surface fluid contaminants and their infiltration into the aquifer system. On the contrary, the low hydraulic conductivity and low resistivity of the impervious overburden layers of clay and shale retard and slow the infiltration rate of the surface contaminants into the subsurface, such as the protectivity of the aquifer is improved considerably (Adeniji *et al.* 2014; Ayuk 2019; Ekanem *et al.* 2021; Asfahani 2023a; Asfahani 2023b).

Electrical resistivity technology, with its different approaches and different configurations, particularly the *VES* one, has been largely practiced in solving and characterizing different groundwater and hydrological problems related to aquifer potentiality, and contamination, by locating vulnerable zones, migration and the extent of contamination (Ebong *et al.*, 2014; Obiora *et al.*, 2016; Laouini *et al.* 2017; Eyankware, 2019; Oli *et al.*, 2020; Ekwe *et al.*, 2020; Eyankware *et al.* 2020a, b, & 2021; Eyankware *et al.*, 2022).

The aquifer vulnerability conditions of a given region can be easily determined by using the vertical sounding technique (*VES*), and the fast and simple aquifer vulnerability index *AVI* approach (Stempvoort *et al.*, 1993; Obiora and Ibuot, 2020; Ossai *et al.*, 2020).

The conductivity of the most contaminants is much higher than the conductivity of natural groundwater, where such pro-

nounced conductivity contrast enables an easy identification of contamination plumes by using geoelectrical methods, particularly the *VES* one. The *VES* technique can be used to describe the aquifer hydrogeological units in detail and detect their contaminant plume.

The overburden-protective capacity of an aquifer is controlled by several geoelectrical parameters, which are the resistivity (ρ_{Over}), thickness (h_{Over}), the anisotropy of the subsurface hydrogeological layers (λ), and the hydraulic conductivity (K) of the overburden layers.

The modeling of the influence of those parameters through analyzing their quantitative results by the *AVI* approach allow us to characterize and describe the protected aquifer areas and determine the contamination conditions surrounding the study aquifer. The mutual hydrological processes and the lithological connectivity between the studied aquifer and its overlaying layers can be quantitatively estimated by developing and establishing specific empirical relationships between the different related hydro-geophysical parameters.

The direct focus on determining the protectivity conditions and the contamination of the Quaternary aquifer in the semi-arid Khanasser Valley region, Northern Syria is the originality of this work through the application of both the *VES* technique and the aquifer vulnerability index *AVI* method.

The quantitative modeling of *VES* and *AVI* results allows determining the hydrogeological connectivity conditions between the Quaternary aquifer and its overlaying layers. The different geoelectrical parameters affecting the aquifer protectivity and its contamination are discussed, documented, and compared with other new geoelectrical contamination approaches (Asfahani 2023a; Asfahani 2023b). The new geoelectrical research works oriented towards determining the protectivity and the contamination of the aquifers, recently carried out, are undertaken in Syria for the first time (Asfahani 2023a; Asfahani 2023b).

The main goals of this research are therefore the following:

1. To apply the integrated electrical resistivity (*VES*) technique and the *AVI* approach to estimate the Quaternary aquifer susceptibility to surface contamination, and to locate the possible contaminated vulnerable zones in the study area;
2. To analyze the different geoelectrical parameters influencing and affecting the vulnerability to contamination conditions, by applying the statistical correlation matrix;
3. To follow the different spatial variations of those parameters in the study region;
4. To derive different empirical equations between the analyzed parameters in 2.

2. Hydrogeology of the Khanasser Valley

Khanasser Valley region is one of the integrated research sites of the International Center for Agriculture in Arid Dry Areas (ICARDA) National Resource Management Program. The choice of this site location was oriented basically towards addressing the different problems related to the marginal dryland environments. The dynamics and diversity of the natural resources and livelihoods, poverty, and the relatively easy accessibility to the study area make the Khanasser region a prime preferable candidate (Asfahani, 2007). The vulnerability to contaminations in

the semi-arid regions is an important critical matter, where the geoelectrical researches are mainly concentrated on locating the areas of acceptable contamination ranges for fresh, drinkable groundwater sites.

Khanasser Valley is located approximately 70 km southeast of Aleppo City (Figure 1), and situated between two hills, Jabal Al Hoss in the west and Jabal Shbeith in the east. The drain of the northern and southern parts of the valley is towards Jaboul salt lake and the Adami depression respectively, as indicated by figures (1 and 2).

Three aquifers exist in the semi-Khanasser Valley region to extract groundwater. The deepest one related to the upper

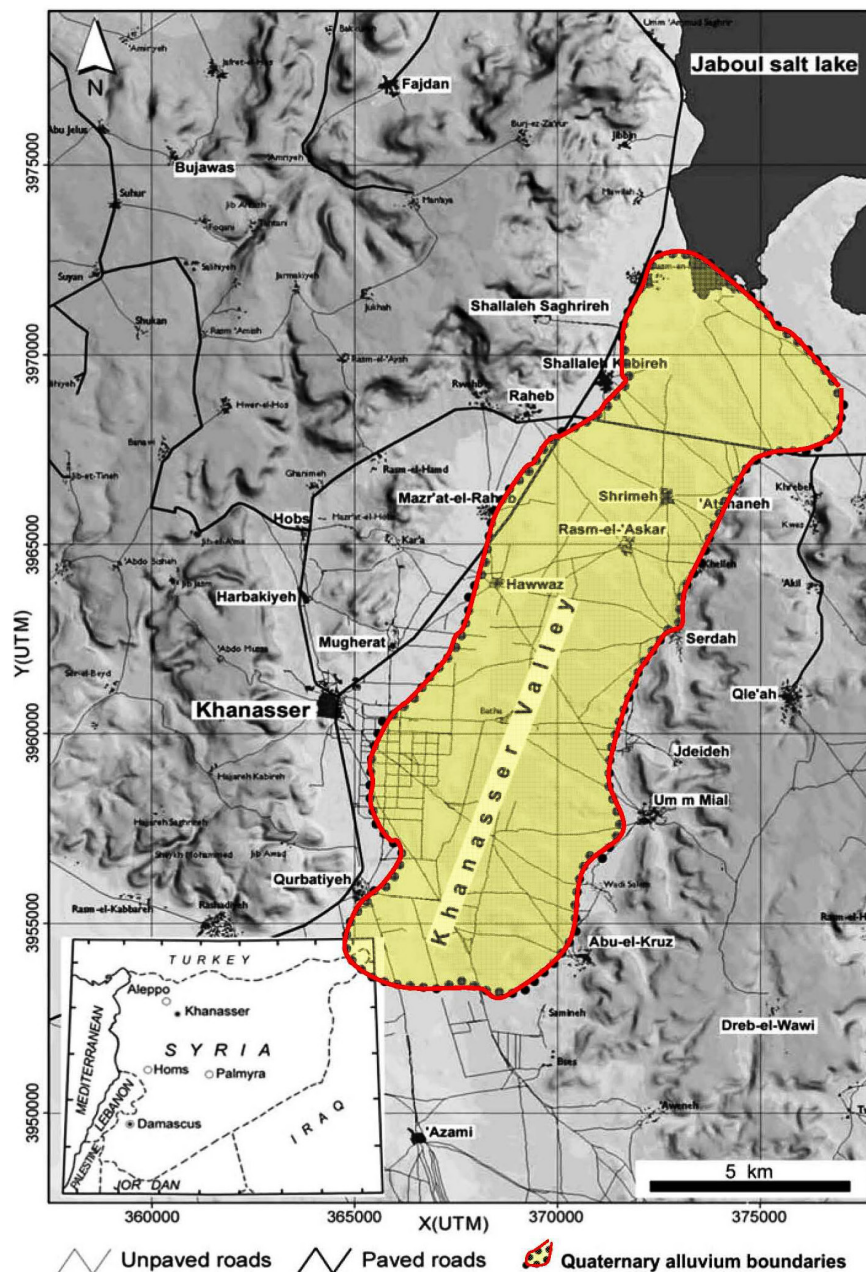


Figure 1. Location of the Khanasser Valley study region, Northern Syria.

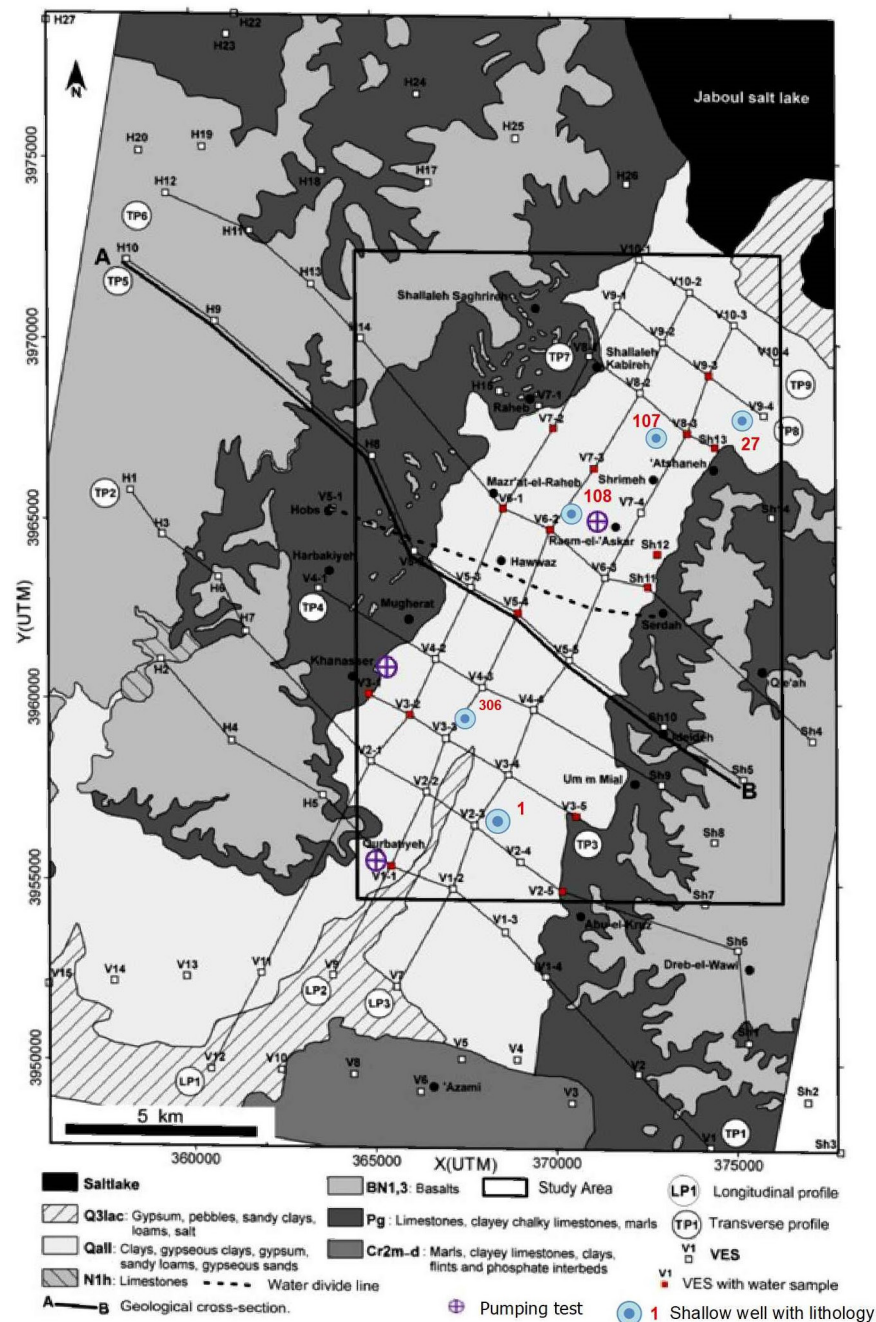


Figure 2. The VES points locations, on the geological map of the Khanasser Valley and its surroundings (After Ponikarov, 1964).

Cretaceous is 400 m under the ground level. Low-productive aquifer of Paleocene-Lower Eocene limestone is found above the Maestrichtian (ACSAD, 1984). The average hydraulic conductivity (k) of this aquifer is equal to 0.0054 m/day (Schweers *et al.*, 2002). The Paleogene strata of about 50 m of Paleocene and lower Eocene in the central part of the Khanasser valley are not sufficiently thick over the Maestrichtian formation. The Quaternary aquifer, located near the surface and covered by the alluvial and colluvial sediments of about 10 m is the most transmissive hydrological structure in the study area.

The rainwater, the infiltrating runoff, and the subsurface flow from the Jabal Shbeith and Jabal Al Hoss slopes provide the direct recharge for this aquifer.

3. Methodology

3.1. VES technique

The electrical resistivity sounding technique is applied to

measure the subsurface resistivity distribution in the study Khanasser region, Northern Syria. Thirty-four (34) vertical electrical soundings (VES) points are measured by using Schlumberger electrode array.

The electrical current (I) is injected into the earth by two electrodes (A and B), while the generated potential differences (ΔV) is measured by two potential electrodes (M and N) as indicated by Figure 3-a.

The Indian resistivity meter ($DDRI$) directly measures the apparent resistance ($\Delta V/I$) of the layers the electrical current penetrates. The apparent resistivity was thereafter evaluated through using the following equation (Dobrin, 1988):

$$\rho_a = \frac{2\pi}{\frac{1}{AM} - \frac{1}{BM} - \frac{1}{AN} + \frac{1}{BN}} \frac{\Delta V}{I} \quad (1)$$

The half-current electrode spacing $AB/2$ are between 3.0 and 500 m, and the half-potential electrode spacing $MN/2$ are between 0.25 and 20 m. The increasing of the electrode spacing $AB/2$ about a fixed point allows the establishment of the complete field apparent resistivity curve in this point ($\rho_a = f(AB/2)$). The field apparent resistivity curve is thereafter quantitatively interpreted by the inversion WINRESIST software of Velpen 2004 in order to obtain the final ID corrected optimum model, which verifies as well the goodness of fit between the field resistivity curve and the final theoretical regenerated model (Zohdy, 1989; Zohdy and Bisdorf, 1989).

Figure 3-b shows the field work during VES measurements in the Khanasser Valley region.

Figure 4-a indicates the snapshot WINRESIST for evaluating the theoretical inverted model, while Figure 4-b indicates the final corresponding VES resist graph display.

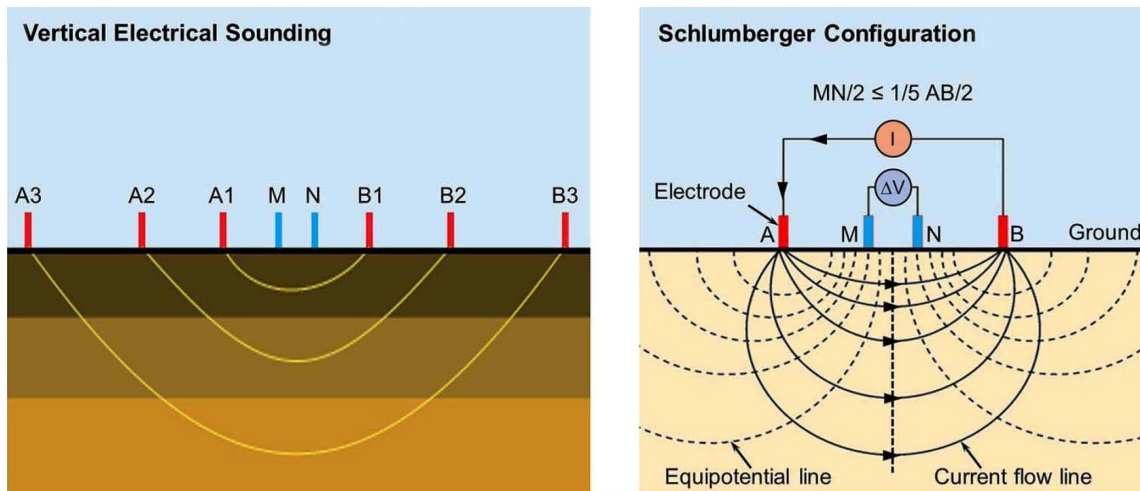


Figure 3 (a). VES Schlumberger configuration and its field operation in the field (Othman *et al.*, 2022).



Figure 3 (b). Field VES technique.

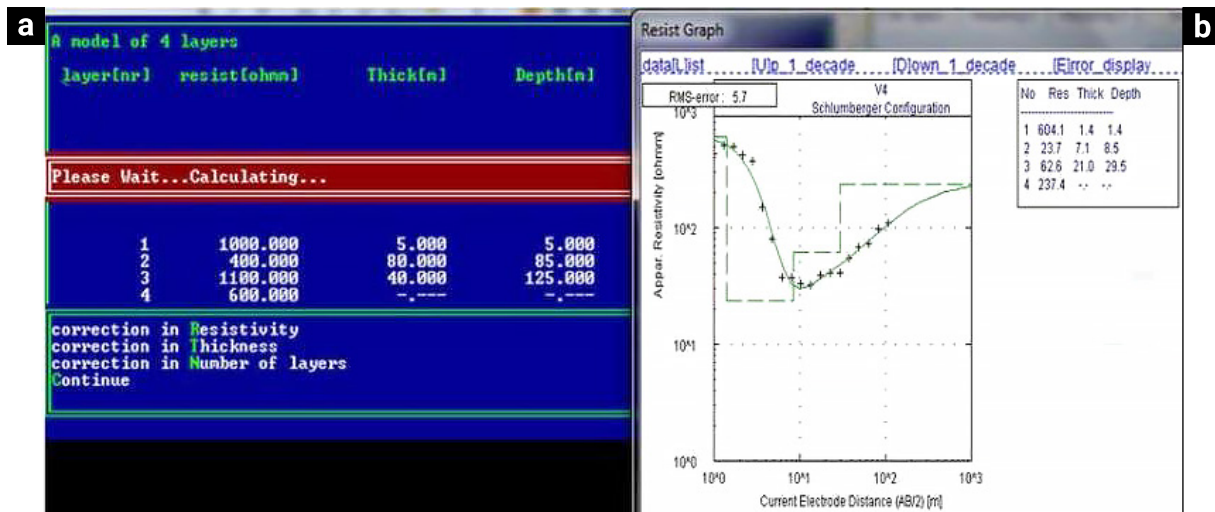


Figure 4. (a) A snapshot WINRESIST window during its running . (b) Final VES resist graph display.

The final optimized model includes the depth, thickness and actual resistivity of the traversed layers under the study VES point.

The two fundamental first-order geo-electric indices parameters of layer thickness (h) and resistivity (ρ) are used for interpreting the geoelectrical models to characterize the stratified subsurface lithological units under each studied VES location. The computation of both the hydraulic conductivity (K) and the hydraulic resistance (C) of the aquifer overburden layers are based on using (h) and (ρ).

3.2. Hydraulic conductivity (K)

The behavior of the vulnerability overburden protective layers and their hydraulic conductivities are assessed by using the following empirical equation, already proposed and applied for characterizing the alluvial aquifer in the Saharanpur area of India (Singh, 2005):

$$K = 0.0002 * e^{0.0897 * \rho} \quad (2)$$

where K (m/day) is the hydraulic conductivity and ρ ($\Omega.m$) is the overburden aquifer resistivity layer. This hydraulic conductivity parameter describes the groundwater movements through the porous and fractured nature of the subsurface alluvial rocks in the study area.

4. Aquifer vulnerability index (AVI)

The AVI approach, proposed by Stempvoort *et al.* (1993), is used herein to characterize and compute the overburden aquifer

vulnerability's hydraulic resistance (C). The parameter (C) expressed in days is evaluated through the parameters of vertical hydraulic conductivity K (m/day) and thickness h (m) of the layers overlaying the aquifer layer as follows (Stempvoort *et al.*, 1993):

$$C = \sum_{i=1}^n \frac{h_i}{K_i} = \frac{h_1}{K_1} + \frac{h_2}{K_2} + \dots + \frac{h_n}{K_n} \quad (3)$$

where h_i is thickness and K_i is the hydraulic conductivity of each covering layer.

The logarithm of the hydraulic resistance ($\log C$) is also evaluated to measure the AVI of the overburden layers to the vertical flow of fluid, which expresses the average travel time of a contaminant from the surface to the subsurface aquifer. The relationship between the hydraulic resistance (C) and AVI is shown in Table 1 according to Stempvoort *et al.* (1993).

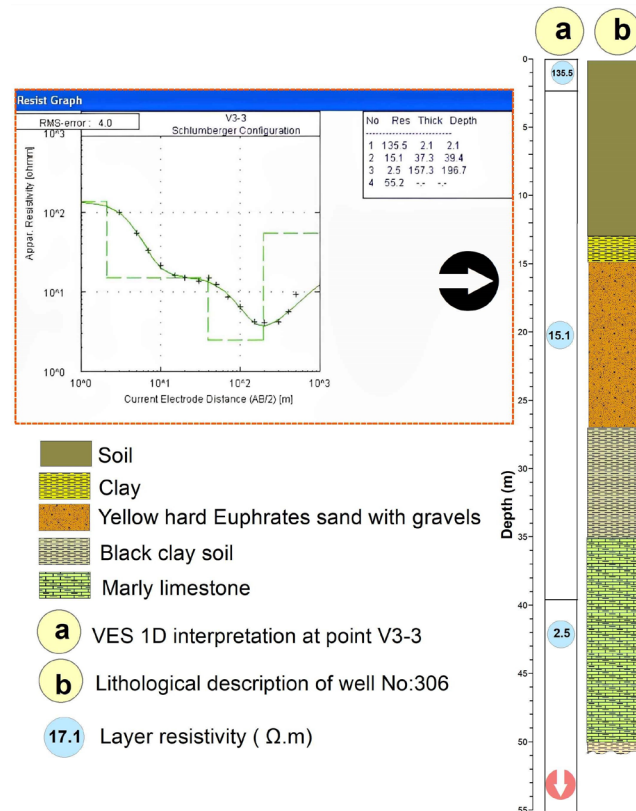
5. Results and discussion

The inversion WINRESIST software of Velpen 2004 is used to quantitatively interpret the thirty-four field apparent resistivity curves (VES) points in the Khanasser study region. The available lithological description of well No. 306 located close to V3-3 point of QH geoelectrical curve type, with its quantitative interpretation (ID) is shown in Figure 5.

The Rammel Aswad, composed of alluvial gravels and sand is the source of the shallow Quaternary aquifer in the study region, where its high thickness gives high transmissivity and yields. The large changes of Rammel Aswad are responsible on the large

Table 1. Standard values for *Log C* and *AVI* ratings (Stempvoort *et al.*, 1993).

Hydraulic Resistance <i>C</i> (day)	<i>Log C</i> (day)	Vulnerability (<i>AVI</i>)
0-10	<1	Extremely high
10-100	1-2	High
100-1000	2-3	Moderate
1000- 10000	3-4	Low
> 10000	>4	Extremely low

**Figure 5.** Lithology description of Well No: 306 with quantitative VES interpretation of V3-3 point.

variation in productivity and yields of wells vertically and laterally, from place to place even in very short distances (Asfahani, 2016).

The VES locations with high overburden thickness indicate areas of high protective capacity. The equivalent averaged overburden thickness (*hoverb*) ranges between 1.1m and 28.9m, with an average of 5.33m, as shown in Figure 6.

The equivalent averaged overburden resistivity (*poverb*) in the study region ranges between 1.5 Ω.m and 539 Ω.m with an average of 64 Ω.m as indicated in Figure 7.

Equation 2 is used to compute the hydraulic conductivity (*K*) of the overburden layers, where its variation ranges between 0.002 m/day and 32.64 m/day with an average of 1.59 m/day (Table 3). The spatial variations of the (*K*) in the study region are shown in Figure 8.

The hydraulic resistance (*C*), considered as the most critical parameter in quantifying groundwater vulnerability, is computed according to equation 3. It is based on the thickness and hydraulic conductivity of the layers above the Quaternary aquifer in the study Khanasser area. *C* varies between 0.55 and 1659.59 days with an average of 146.68 days (Table 3). The *Log C* ranges between -0.26 and 3.22 days with an average of 0.63 days (Table 3). The *Log C* variation with the VES locations is shown in Figure 9, while its spatial variations in the study region are shown in Figure 10. The capacity of the overburden alluvial rocks to retard and prevent fluid infiltration into the subsurface aquifer is a good indication of its protective capacity.

The influences of the two thickness (*hoverb*) and resistivity (*poverb*) parameters on the *Log C* are shown in Figure 11 (a, and b),

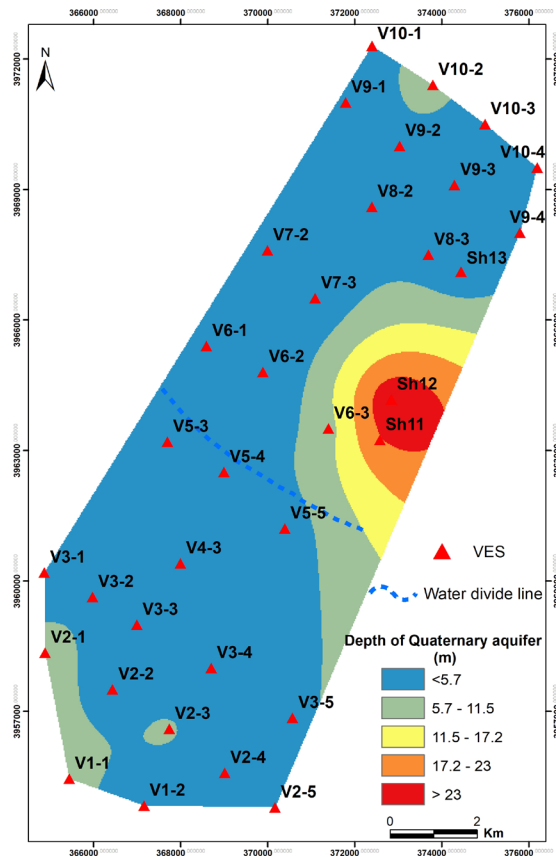


Figure 6. Quaternary aquifer overburden thickness of in the Khanasser valley region (Asfahani, 2023a)

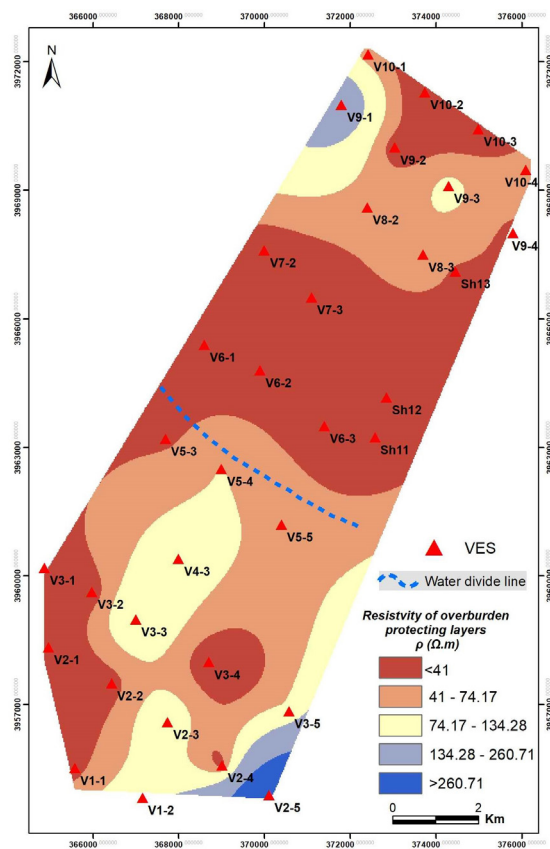


Figure 7. Quaternary aquifer overburden resistivity in the Khanasser valley region.

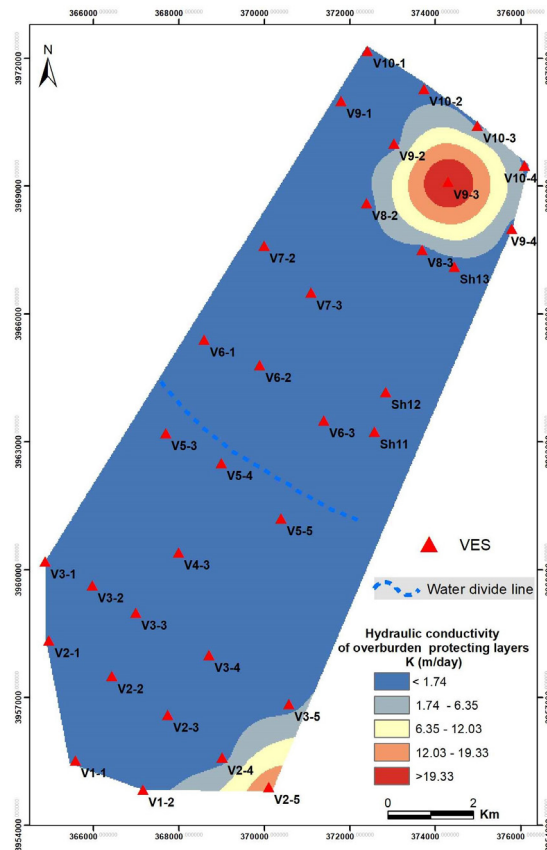


Figure 8. Hydraulic conductivity (K) of the overburden protecting layers of the aquifer Quaternary in the Khanasser valley region.

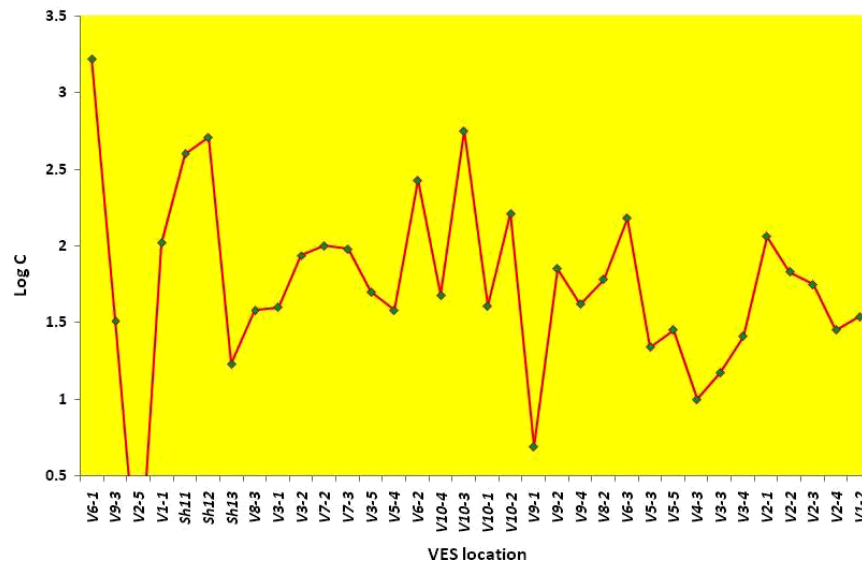


Figure 9. Variation of Log C with the thirty-four VES location points in the study area.

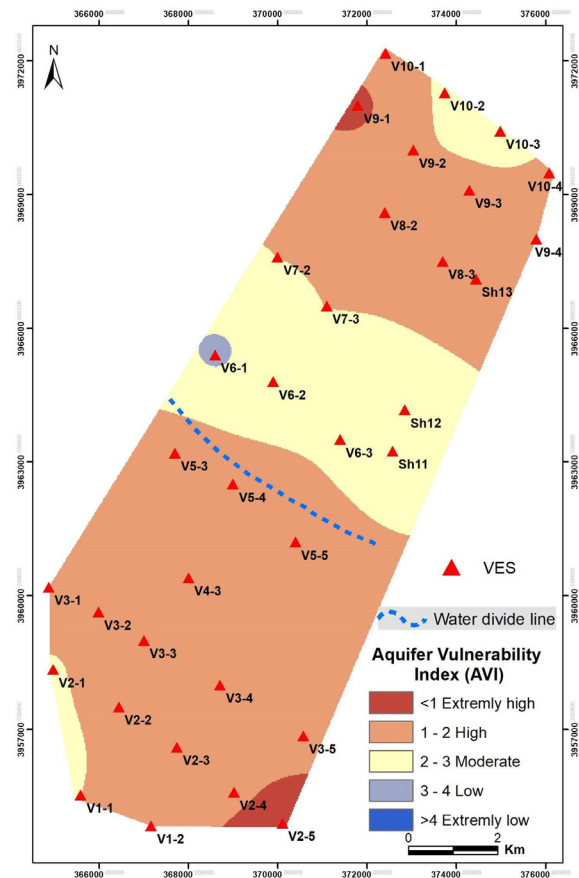


Figure 10. Spatial variations of AVI in the study Khanasser region.

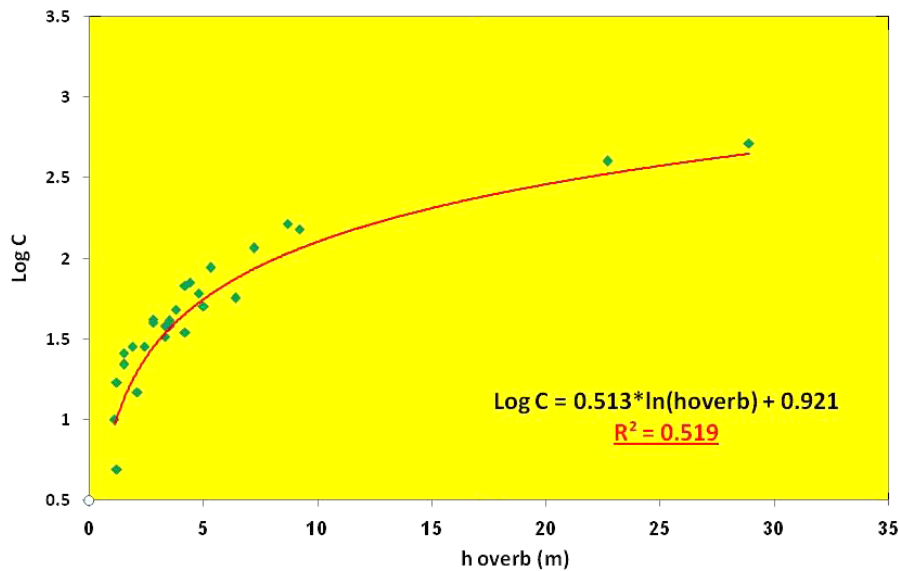


Figure 11(a). The empirical relationship between $\log C$ and $(h \text{ over } b)$ in the study area.

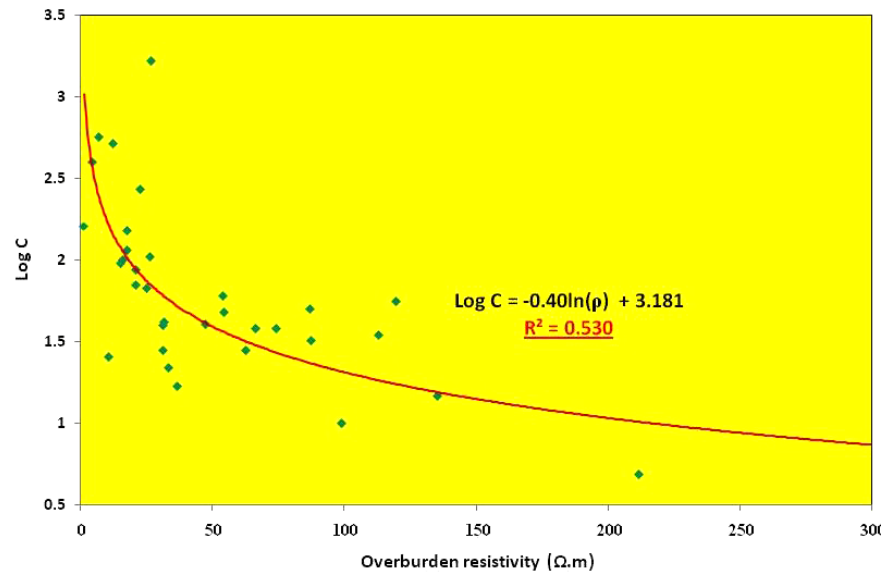


Figure 11(b). The empirical relationship between $\text{Log } C$ and (ρ_{overb}) resistivity in the study region.

where two empirical relationships are established between the $\text{Log } C$ and h_{Overb} ρ_{overb} of the aquifer Quaternary as follows:

$$\text{Log } C = 0.513 \cdot \ln(h_{\text{overb}}) + 0.921 \quad (R^2 = 0.519) \quad (4)$$

$$\text{Log } C = -0.40 \ln(\rho_{\text{overb}}) + 3.181 \quad (R^2 = 0.530) \quad (5)$$

The variations of $\text{Log } C$ with the hydraulic conductivity (K) of the overburden layers are shown in Figure 12, where a decreasing tendency is obtained between them, as much K is bigger, as much $\text{Log } C$ is more minor.

The hydraulic conductivity (K) of the overburden layers is related to the anisotropy of the study region (Asfahani, 2023a; Asfahani, 2023b), as attested by Figure 13.

Figure 13 indicates three trends between K and λ , that reflect different hydraulic systems in the study area. Those exponential trends are quantified by the following three regression equations:

$$K \text{ (m/day)} = 0.007e^{2.713\lambda} \quad (R^2 = 0.961) \quad (6)$$

$$K \text{ (m/day)} = 0.007e^{2.041\lambda} \quad (R^2 = 0.963) \quad (7)$$

$$K \text{ (m/day)} = 0.016e^{0.898\lambda} \quad (R^2 = 0.99) \quad (8)$$

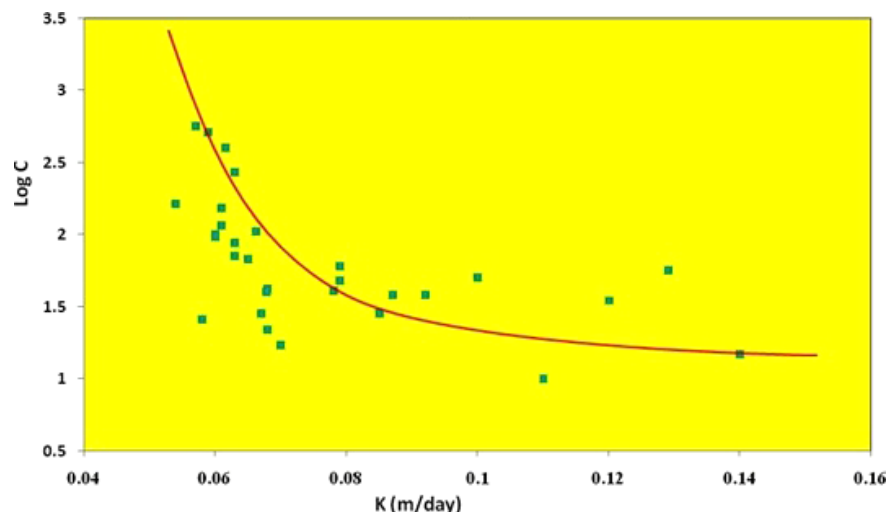


Figure 12. Variations of $\text{Log } C$ with K parameter in the study region.

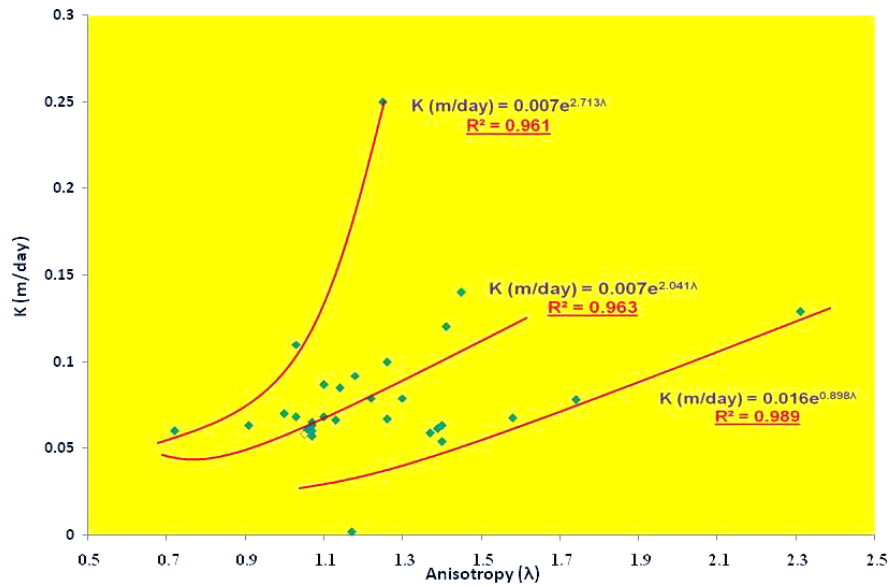


Figure 13. Different relationship trends between anisotropy (λ) and hydraulic conductivity (K) in the study area.

The variations of h_{Over} , ρ_{Over} , K , C , $\log C$, λ , and OPC for the measured thirty-four *VES* points are shown in Table 2.

Based on the relationship between (C), ($\log C$), and the aquifer vulnerability index (*AVI*) indicated in Table 1 (Stempvoort *et al.*, 1993), the thirty-four *VES* locations in the Khanasser area are classified as follows (Table 2):

The rating of (*AVI*) is exceptionally high in the *VES* (V2-5 and V9-1).

The rating of (*AVI*) is high in the *VES* (V9-3, Sh13, V8-3, V3-1, V3-2, V7-2, V7-3, V3-5, V5-4, V10-4, V10-1, V9-2, V9-4, V8-2, V5-3, V5-5, V4-3, V3-3, V3-4, V2-2, V2-3, V2-4, and V1-2).

The rating of (*AVI*) is moderate in the *VES* (V2-2, Sh11, Sh12, V6-2, V10-3, V10-2, V6-3, and V2-1).

The rating of (*AVI*) is low in the *VES* (V6-1).

The overburden protective capacity (*OPC*) of the aquifer Quaternary in the study area has been already modeled by applying the following equation (Asfahani, 2023a; Asfahani, 2023b):

$$OPC (\Omega^{-1}) = \sum_{i=1}^n \frac{h_i}{\rho_i} = \frac{h_1}{\rho_1} + \frac{h_2}{\rho_2} + \dots + \frac{h_n}{\rho_n} \quad (9)$$

where ρ_i is the resistivity and h_i is thickness of each covering layer.

It has been indicated, according to the classification of Heintz (1976), that as much the longitudinal conductance (Ω^{-1}) of the overburden protecting layers is bigger, as much the *OPC* is bigger (Asfahani, 2023a).

Figure 14 shows a good positive concordance between the

results of both (*OPC*) and *AVI* techniques, where the correlation coefficient R^2 of 0.60 is obtained for them. The equation between *OPC* and $\log C$ has the following form:

$$\log C = 0.270 \cdot \ln(OPC) + 2.267 \quad (R^2 = 0.60) \quad (10)$$

The correlation matrix indicated in Table 3 shows the different relationships between ($\log C$), and the thickness, resistivity, hydraulic conductivity, anisotropy (λ), and (*OPC*) of the overburden layers.

An acceptable correlation is shown in Table 3 between h_{Overb} and $\log C$ (0.56), overburden resistivity and $\log C$ (-0.75), and K and $\log C$ (-0.34). Table 4 summarizes the statistical results of the different treated parameters related to the measured thirty-four *VES* points in the study area.

This paper discusses the influence of those different parameters in affecting the protectivity of the aquifer Quaternary from the fluid contaminations originated in the study area. The different geoelectrical results thus obtained in this paper are important and help the decision makers for locating the effective protected groundwater area in the study region.

6. Conclusion

The aquifer vulnerability index (*AVI*) methodology with using the (*VES*) technique is undertaken to assess the aquifer

Table 2. Values of geoelectrical, hydrological, and vulnerability parameters for the measured thirty-four VES points.

<i>VES Location</i>	<i>ρ_{Over}</i>	<i>h_{Over}</i>	<i>K</i>	<i>C</i>	<i>Log C</i>	<i>λ</i>	<i>OPC</i>
V6-1	26.8	3.7	0.002	1659.59	3.22	1.17	0.14
V9-3	87.6	3.3	32.64	32.3594	1.51	1.12	0.037
V2-5	539	3.9	18.93	0.54954	-0.26	1.85	0.012
V1-1	26.4		0.0662	104.713	2.02	1.13	-
Sh11	4.8	22.7	0.0616	398.107	2.6	1.39	3.26
Sh12	12.5	28.9	0.0589	512.861	2.71	1.37	4.57
Sh13	36.7	1.2	0.07	16.9824	1.23	1	0.033
V8-3	66.5	3.3	0.087	38.0189	1.58	1.1	0.05
V3-1	31.5	2.8	0.0678	39.8107	1.6	1.58	0.09
V3-2	21.1	5.3	0.063	87.0964	1.94	0.91	0.6
V7-2	16		0.06	100	2	1.07	0.37
V7-3	15.4		0.06	95.4993	1.98	0.72	0.37
V3-5	87	5	0.1	50.1187	1.7	1.26	0.057
V5-4	74.4	3.5	0.092	38.0189	1.58	1.18	0.047
V6-2	22.6		0.063	269.153	2.43	1.07	0.76
V10-4	54.5	3.8	0.079	47.863	1.68	1.22	0.07
V10-3	7.2		0.057	562.341	2.75	1.07	2.5
V10-1	47.45	3.5	0.078	40.738	1.61	1.74	0.094
V10-2	1.5	8.7	0.054	162.181	2.21	1.4	13.75
V9-1	212	1.2	0.25	4.89779	0.69	1.25	0.006
V9-2	21	4.4	0.063	70.7946	1.85	1.4	0.21
V9-4	31.7	2.8	0.068	41.6869	1.62	1.1	0.09
V8-2	54	4.8	0.079	60.256	1.78	1.3	0.09
V6-3	18	9.2	0.061	151.356	2.18	1.06	1.29
V5-3	33.5	1.5	0.068	21.8776	1.34	1.03	0.045
V5-5	63	2.4	0.085	28.1838	1.45	1.14	0.04
V4-3	99	1.1	0.11	10	1	1.03	0.01
V3-3	135.5	2.1	0.14	14.7911	1.17	1.45	0.015
V3-4	10.8	1.5	0.058	25.704	1.41	1.05	0.14
V2-1	18	7.2	0.061	114.815	2.06	1.06	0.49
V2-2	25.4	4.2	0.065	67.6083	1.83	1.07	0.23
V2-3	119.6	6.4	0.129	56.2341	1.75	2.31	0.061
V2-4	31.5	1.9	0.067	28.1838	1.45	1.26	0.06
V1-2	113	4.2	0.12	34.6737	1.54	1.41	0.04

Quaternary protectivity in the semi-arid Khanasser Valley region of northern Syria. The inversion WINRESIST computer software program is used to quantitatively interpret the measured thirty-four VES points in terms of *ID* structure, to obtain the final geoelectrical inverted optimized models for the treated VES points. The different geoelectrical parameters and their influences on the aquifer protectivity and contamination conditions are well determined. This work also discusses the effects of the geoelec-

trical parameters controlling the overburden protective capacity of the aquifer Quaternary by analyzing the results obtained by the AVI approach with its related *Log C*. Those parameters are the thickness (*hOver*), the resistivity (*ρ_{Over}*), the hydraulic conductivity (*K*) of the overburden protecting layers, and the anisotropy of the subsurface hydrogeological layers (*λ*). It is found that as the layers covering the aquifer are thinner, and their hydraulic conductivities are higher, the aquifer will be

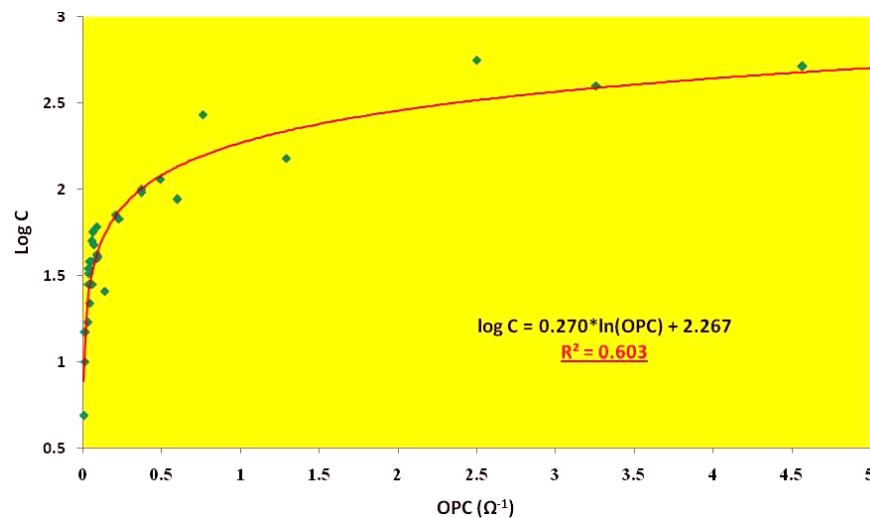


Figure 14. Empirical regression relationship between *OPC* and *Log C* in the study area.

Table 3. Correlation matrix between the *hOverb*, *ρOverb*, *K*, *λ*, *OPC* and (*Log C*) in the study area.

Variables	<i>ρOverb</i>	<i>λ</i>	<i>Log C</i>	<i>OPC</i>	<i>hOverb</i>	<i>K</i>
<i>ρOverb</i>	1	0.44	-0.75	-0.21	-0.21	0.48
<i>λ</i>		1	-0.16	0.08	0.15	0.1
<i>Log C</i>			1	0.35	0.56	-0.34
<i>OPC</i>				1	0.47	-0.09
<i>hOverb</i>					1	-0.082
<i>K</i>						1

Table 4. Statistical results of the treated geoelectrical parameters in the study region.

Statis	<i>hOver</i> (m)	<i>Over</i> (Ω.m)	<i>K</i> (m/day)	<i>C</i> (day)	<i>Log C</i>	<i>OPC</i> (Ω ⁻¹)	<i>λ</i>
Min	1.1	1.5	0.002	0.55	-0.26	0.006	0.72
Max	28.9	539	32.64	1659.59	3.22	13.75	2.31
AV	5.33	64	1.59	146.68	1.74	0.87	1.24
SD	6.1	95	6.37	299.88	0.63	2.49	0.29

increasingly vulnerable to pollution. The correlation matrix of the geoelectrical parameters with the different mutual empirical equations already established clearly indicate the considerable influence of those parameters (*hOverb*, *ρOverb*, *K*, and *λ*) on the spatial distribution of the *Log C* in the study region. The derived empirical relationships between the different analyzed hydro-geophysical parameters are essential to understand both the mutual hydrological processes and the lithological connectivity nature between the study aquifer Quaternary and its overlaying layers. This paper provides useful geoelectrical information, which help in locating the effective protected groundwater

area in the semi-arid Khanasser Valley region in Syria. The results obtained in this paper allow decision makers to assess management scenarios and coordinate surface and groundwater resources effectively. As such, the *VES* technique with the *AVI* methodology developed in this article helps the decision-makers for locating the polluted and protected aquifer zones. It can be practiced successfully to characterize other similar hydro-geological context in Syria, and worldwide outside of the Khanasser region. The *AVI* approach as described above is practiced herein for the first time in Syria, and can be easily extended to cover and deal with other Syrian aquifers to determine their

protectivity and contamination conditions. The AVI approach can be also applied worldwide to evaluate the protection conditions surrounding an aquifer in similar semi-arid regions.

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9. Data availability

The datasets related to this research paper are available with the author; however, accessing these data or making them available to others upon a reasonable request requires special permission from the Syrian Atomic Energy Commission.

10. Declarations

Conflict of interest: The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this.

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An innovative weighted fuzzy soft set-based model for multi-criteria groundwater quality assessment in urban areas: A case study of Agartala, India

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Abstract

This study presents an innovative weighted fuzzy soft set-based multi-criteria decision-making model ($\mathfrak{B}$ -model) for evaluating groundwater quality and identifying contamination sources in urban settings, with a case study in Agartala, Tripura, North-East India. Rapid urbanization and anthropogenic pressures have significantly impacted groundwater quality, demanding advanced methodologies for effective assessment and management. The proposed model incorporates ten critical groundwater quality parameters (GWQP—pH, electrical conductivity, iron concentration, dissolved oxygen, total hardness, total alkalinity, total dissolved solids, calcium, magnesium, and turbidity), transformed into fuzzy soft sets for comprehensive analysis. Groundwater samples were systematically collected from ten strategic locations across Agartala Municipal Corporation during three distinct seasons: pre-monsoon (March–May), monsoon (June–September), and post-monsoon (October–November) of 2023–2024. The analysis revealed seasonal variations in groundwater quality, with notable degradation during the pre-monsoon season due to reduced aquifer recharge and increased evaporation, while monsoon improvements were limited, primarily influenced by rainfall dilution. Specific areas consistently exhibited high pollution levels, highlighting localized contamination sources and elevated health risks. The model's weighted pollution scores enabled precise identification of pollution sources, facilitating targeted intervention strategies. This research underscores the potential of fuzzy soft set-based approaches for robust groundwater quality assessment and emphasizes their integration into sustainable water management practices and urban planning to mitigate contamination risks in rapidly urbanizing regions like Agartala. Comparative analyses with existing methods validate and underscore the advantages of our approach.

Key words: Fuzzy set, Multi-Criteria Decision-making, Soft Set, Groundwater risk assessment, Water resource management, Environmental Management.

Resumen

Este estudio presenta un innovador modelo de toma de decisiones multicriterio basado en conjuntos difusos suaves ponderados (modelo $\mathfrak{B}$) para evaluar la calidad de las aguas subterráneas e identificar las fuentes de contaminación en entornos urbanos, con un estudio de caso en Agartala, Tripura, noreste de la India. La rápida urbanización y las presiones antropogénicas han afectado significativamente la calidad de las aguas subterráneas, lo que exige metodologías avanzadas para su evaluación y gestión eficaces. El modelo propuesto incorpora diez parámetros críticos de calidad de las aguas subterráneas (GWQP: pH, conductividad eléctrica, concentración de hierro, oxígeno disuelto, dureza total, alcalinidad total, sólidos disueltos totales, calcio, magnesio y turbidez), transformados en conjuntos difusos suaves para un análisis integral. Las muestras de aguas subterráneas se recolectaron sistemáticamente en diez ubicaciones estratégicas de la Corporación Municipal de Agartala durante tres estaciones distintas: premonzón (marzo–mayo), monzón (junio–septiembre) y posmonzón (octubre–noviembre) de 2023–2024. El análisis reveló variaciones estacionales en la calidad de las aguas subterráneas, con un deterioro notable durante la estación premonzónica debido a la reducción de la recarga de los acuíferos y al aumento de la evaporación, mientras que las mejoras observadas durante el monzón fueron limitadas y estuvieron influenciadas principalmente por la dilución causada por las precipitaciones. Determinadas áreas mostraron de manera constante altos niveles de contaminación, destacando fuentes localizadas de contaminación y elevados riesgos para la salud. Las puntuaciones ponderadas de contaminación obtenidas mediante el modelo permitieron una identificación precisa de las fuentes de contaminación, facilitando estrategias de intervención específicas. Esta investigación destaca el potencial de los enfoques basados en conjuntos difusos suaves para una evaluación sólida de la calidad de las aguas subterráneas y enfatiza su integración en prácticas sostenibles de gestión del agua y planificación urbana para mitigar los riesgos de contaminación en regiones de rápida urbanización como Agartala. Los análisis comparativos con métodos existentes validan y destacan las ventajas de nuestro enfoque.

Palabras clave: Conjunto difuso, Toma de decisiones multicriterio, Conjunto suave, Evaluación del riesgo de las aguas subterráneas, Gestión de los recursos hídricos, Gestión ambiental.

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1. Introduction

Groundwater is an essential resource, particularly in urban areas where surface water is often limited or contaminated. In rapidly developing cities such as Agartala, Tripura, the pressure from urban expansion, industrial activities, and agriculture has escalated, intensifying groundwater demand and raising significant concerns about its sustainability. To address these challenges, this study applies a weighted fuzzy soft set-based approach—a method rooted in fuzzy set theory by Zadeh (1965)—that effectively handles the uncertainties and complexities inherent in environmental data. This model is particularly well-suited for multi-criteria decision-making (MCDM), where various interdependent factors influence outcomes, enhancing its flexibility for tasks like groundwater quality assessment. We employ this model to evaluate groundwater quality in Agartala, focusing on identifying pollution sources and associated health risks, thus supporting more targeted management efforts. Fuzzy logic-based assessments have shown promise in environmental contexts. For instance, Patel and Chitnis (2022) utilized fuzzy methods to assess the Sabarmati River's water quality in Gujarat, considering climate and industrial impacts. Similarly, Kumar and Krishna (2021) developed a geospatial water quality index for coal mining regions, demonstrating the adaptability of fuzzy approaches in complex pollution assessments. Building on these methods, this study offers a novel framework for groundwater risk assessment, providing valuable insights into sustainable water management strategies in urbanizing regions like Agartala.

As urban centers expand, they face mounting challenges from improper waste management, industrial runoff, and excessive groundwater extraction, all of which degrade water quality and pose significant risks to public health. This is especially true for Agartala, the capital of Tripura in North-East India, where rapid urban development has heightened the urgency for effective groundwater quality monitoring and risk assessment systems. Traditional assessment methods often struggle to capture the inherent uncertainties and complexities of urban groundwater systems, making it difficult to accurately identify pollution sources and assess the overall risk. A fuzzy logic-based approach offers a powerful and flexible solution in response to these challenges. Fuzzy logic provides a more nuanced assessment by converting precise measurements into fuzzy numbers, allowing for a better representation of the uncertainty and variability in groundwater quality data. This approach proves particularly useful in urban environments, where groundwater systems are highly dynamic, and pollution sources are often diffuse and complex. Recent advancements in integrating fuzzy logic with decision-making models and machine learning algorithms have further enhanced

the capacity to comprehensively evaluate groundwater quality. These advanced methodologies offer the ability to identify pollution sources more precisely and provide insights into potential health risks. For instance, Mallick *et al.* (2021) applied index-based methods to assess groundwater quality in Saudi Arabia, highlighting the utility of these approaches in arid regions for drinking and irrigation purposes. Milovanovic (2007) examined pollution sources along the Axios/Vardar River in Southeastern Europe, illustrating the significant impact of urbanization and industrial activities on water bodies. In India's Shivalik region, Mittal *et al.* (2021) conducted a hydrochemical analysis and health risk assessment, providing key insights into the health impacts of groundwater contamination. Ram *et al.* (2021) integrated the WQI with a GIS framework to offer a spatial perspective on groundwater contamination, demonstrating the value of combining geospatial techniques with WQI for managing urban groundwater resources. Rango *et al.* (2012) investigated the health effects of groundwater quality, particularly focusing on fluoride contamination in the Main Ethiopian Rift, highlighting the critical need for targeted interventions in regions facing high contamination risks. This study builds on such research by employing a fuzzy logic-based groundwater risk assessment framework to identify pollution sources in urban areas like Agartala, providing a novel and more accurate approach for managing groundwater contamination in rapidly urbanizing environments.

In parallel, soft set theory, introduced by Molodtsov (1999), offers a complementary framework for decision-making under uncertainty, providing flexibility in defining decision parameters. The soft set is particularly suited for addressing real-world decision-making problems involving incomplete or uncertain information, making it a valuable tool in groundwater risk assessments. While other mathematical models, such as interval-valued fuzzy sets, fuzzy sets, and rough sets, are used to handle uncertainty, each has its limitations. In contrast, soft set theory provides a more adaptable framework, allowing for greater flexibility in parameter selection, which is crucial when assessing groundwater pollution in urban environments with complex contamination sources. Molodtsov's pioneering work laid the foundation for soft set theory's broad applicability across disciplines, including environmental management, probability theory, game theory, and operations research. The versatility of soft set theory in handling uncertain data makes it ideal for evaluating groundwater quality in dynamic urban systems. Further contributions by Maji *et al.* (2003) extended the soft set theory to include operations like subsets, complements, unions, and intersections, making it more practical for addressing multi-criteria decision-making MCDM problems in environmental studies. Maji *et al.* (2002) further demonstrated soft set's potential in real-world decision-making

problems, a significant step forward in applying soft set theory to complex environmental challenges. Subsequent research by Ali *et al.* (2009) and Alcantud and Santos-García (2017) expanded the use of soft set theory in various decision-making contexts, particularly where evidence is insufficient or ambiguous. Chen *et al.* (2020) extended the soft set theory by introducing generalized vague N-soft sets, offering sophisticated techniques for decision-making in highly uncertain situations. These advancements highlight soft set theory's increasing relevance for environmental uncertainty scenarios, such as groundwater risk assessments in urban areas. By integrating fuzzy logic with soft set theory, this study leverages both approaches to provide a more comprehensive framework for identifying pollution sources in groundwater, addressing the challenges posed by data uncertainty and enabling more informed decision-making for urban water quality management.

Integrating soft set and fuzzy set theories has led to the development of fuzzy soft sets (FSS), which are particularly valuable for decision-making in uncertain and imprecise conditions, such as those encountered in groundwater quality assessments. Maji *et al.* (2001) first introduced the concept of fuzzy soft sets, and their application has since expanded across various fields, proving effective in handling complex decision-making problems with ambiguous information. In the context of groundwater risk assessment, FSSs offer a powerful framework for dealing with uncertainty, making them ideal for evaluating pollution sources in urban areas like Agartala. FSSs enable a nuanced approach to managing imprecise data, especially when multiple groundwater quality parameters are involved, such as pH, electrical conductivity, iron concentration, and dissolved oxygen. Roy and Maji (2007) laid the foundation for using FSS in decision-making problems by developing a framework based on fuzzy soft sets, which has since inspired further advancements. Feng *et al.* (2010) expanded the approach by introducing weighted fuzzy soft sets, allowing adaptability in handling diverse uncertainties and prioritizing decision-maker preferences. This weighted approach is particularly useful in groundwater assessments where different parameters may carry varying significance levels depending on the local pollution sources. Das and Granados (2021) contributed a group decision-making framework based on FSSs, incorporating weighted score functions to facilitate collective decision-making in complex environmental scenarios. Bhardwaj and Sharma (2021) presented an innovative uncertainty measure utilizing fuzzy soft set theory, further enhancing the ability to manage uncertainty in decision-making problems.

Groundwater contamination in urban areas has become a critical concern, driven by industrial discharge, agricultural runoff, and inadequate waste management practices. Conventional methods for assessing groundwater quality often struggle with

environmental data's inherent uncertainties and complexities. To address these challenges, an innovative weighted fuzzy soft set-based approach offers a powerful framework for pollution source identification and risk assessment. This approach, leveraging the strengths of fuzzy soft sets, enables a nuanced analysis by effectively handling diverse and uncertain data, thereby enhancing the accuracy and reliability of groundwater quality assessments. By applying this method, decision-makers comprehensively understand pollution sources and associated health risks, allowing for targeted interventions and improved urban groundwater management. Recent developments in fuzzy soft set theories, such as the fuzzy parameterized intuitionistic fuzzy soft multiset theory, have proven instrumental in handling complex environmental decision-making problems by enhancing data interpretability and accuracy (Das and Granados, 2022). In 2022, Das, Granados, and Bhattacharya (2022) explored novel operations on fuzzy soft sets and their applications in decision-making processes. The authors comprehensively analyze these operations, highlighting their potential to enhance decision-making frameworks across various fields. This work contributes to the growing knowledge in fuzzy set theory and its practical implications for addressing complex problems. Furthermore, IFP-intuitionistic multi-fuzzy N-soft sets have shown potential in dealing with hesitant and uncertain information, further strengthening decision-making models (Das and Granados, 2023). The synergy between fuzzy logic and machine learning allows for improved accuracy in predictions and more dynamic analysis of groundwater risks, as demonstrated in similar applications of fuzzy controllers in complex environmental systems (Darvish Falehi and Torkaman, 2023). Additionally, recent work on weighted neutrosophic soft multisets further underscores the value of advanced fuzzy techniques in refining decision-making processes, particularly in multi-criteria evaluations (Granados and Das, 2023). Das *et al.* (2023) introduced the concept of weighted hesitant bipolar-valued fuzzy soft sets, which provide a more nuanced framework for evaluating alternatives. This research aims to build on these foundational studies by offering an innovative, data-driven solution to one of the most pressing environmental issues in urban settings.

Urbanization and industrialization have significantly affected environmental dynamics, especially in rapidly developing cities, posing serious challenges to groundwater quality. The rapid expansion of urban areas often intensifies pressures on groundwater resources due to inadequate waste management, industrial runoff, and over-extraction, which threaten water quality. In such environments, robust groundwater monitoring systems are critical, as groundwater serves as a vital resource for urban and agricultural water supplies. Traditional methods of groundwater quality assessment often struggle to handle the complexities of

uncertain, imprecise, and multi-dimensional data inherent in these dynamic systems. To overcome these limitations, advanced analytical methods, such as fuzzy logic-based approaches, are emerging as effective tools for comprehensive and accurate water quality assessments. Recent studies have highlighted the growing trend of integrating Machine-learning (ML) techniques with fuzzy logic-based decision-making models to enhance water quality assessment and management. For instance, Adimalla (2021) utilized the entropy weighted water quality index (EWQI) and pollution index of groundwater (PIG) to evaluate drinking water quality, emphasizing the need for sophisticated methods in diverse environmental settings. Similarly, Ahmed *et al.* (2021) demonstrated the potential of ML techniques in analyzing water quality indices and assessing pollution levels, providing a more nuanced approach to understanding groundwater contamination. Water Quality Index (WQI) models have been widely applied to evaluate surface and groundwater consistency and safety. The WQI developed by Brown *et al.* (1970) provides a comprehensive metric that combines several water quality parameters into a single index, offering a clear overview of water quality status. However, such methods may fall short of capturing the uncertainties and complexities of groundwater systems in urban areas. By incorporating fuzzy logic into these models, researchers can better address the imprecise nature of environmental data. Fuzzy logic is particularly useful in urban groundwater management, where pollution sources are varied and dynamic. In groundwater risk assessment, the fuzzy logic-based approach goes beyond traditional WQI models, allowing for a more flexible evaluation of pollution levels by converting crisp data into fuzzy values that capture the inherent uncertainties in environmental monitoring. Using the Canadian Council of Ministers of the Environment (CCME) Water Quality Index, Wagh *et al.* (2017) categorized groundwater suitability in the Kadva River basin of Maharashtra, India, across pre-monsoon and post-monsoon seasons. Their study revealed that intensive agricultural activities and anthropogenic influences significantly impacted groundwater quality, aligning with findings from other regions where urban and agricultural pressures degrade water resources. Similarly, Galal Uddin *et al.* (2017) extensively evaluated groundwater quality near the Rooppur Nuclear Power Plant in Bangladesh, identifying critical pollution parameters. These studies underscore the importance of advanced methods for water quality monitoring, as traditional approaches may not capture the full spectrum of contamination sources and risks. In urban areas, factors such as land-use changes, industrial development, and climate variability complicate groundwater quality assessments. Miller and Hutchins (2017) reviewed the impacts of urbanization and climate change on flooding and water quality in the UK, synthesizing knowledge to address

emerging challenges in urban water resource management. Using the water quality index, Patel *et al.* (2020) investigated how increasing industries and urban areas affected the Sabarmati River in Gujarat. Their work, along with Shah and Joshi's (2017) assessment of the Sabarmati River's WQI in Gujarat, highlights the significant environmental pressures faced by urban water systems. Hutchins *et al.* (2018) explored the integrated effects of climatic stressors and future land-use changes on ground and surface water in the upper Thames River basin in the UK. Recently, Das *et al.* (2025b) developed a fuzzy MCDM model for examining human influences on urban river water quality is one of their noteworthy contributions to environmental MCDM. This research is extended in 2025 with weighted hesitant fuzzy soft set and fuzzy soft set models for rating water pollution and a case study applying fuzzy soft MCDM model to assess pollution levels in the Gomati and Haora Rivers (Das *et al.*, 2024a; 2025a). This study, and similar research point to the growing importance of combining advanced modeling techniques like fuzzy logic with environmental monitoring to manage the increasing risks to water quality. These innovative methods enable a more holistic assessment of pollution sources, particularly in urban areas where traditional monitoring systems may be insufficient. The application of fuzzy logic-based approaches in groundwater risk assessment offers a promising solution to the challenges posed by urbanization and industrialization. By allowing for a more flexible and accurate water quality evaluation, these methods provide valuable tools for managing water resources in complex urban environments, ensuring sustainable water management practices, and safeguarding public health.

Groundwater quality is shaped by various physical, chemical, and biological factors, collectively known as groundwater quality parameters (GWQPs). When groundwater quality is compromised, it poses risks to human health, ecosystems, and economic stability. This makes continuous monitoring and assessment of groundwater essential for ensuring a safe water supply and promoting sustainable resource management. Traditional assessment methods, which rely on crisp measurements and fixed standards, often fall short when addressing environmental data's inherent uncertainties and fluctuations. To address these limitations, this study employs an innovative weighted fuzzy soft set-based approach, enabling a more nuanced assessment of groundwater quality by transforming crisp data into fuzzy soft sets. This methodology better captures the uncertainty and variability in groundwater quality, supporting more flexible and informed decision-making for water resource management.

In this study, we focus on ten critical GWQPs: pH, electrical conductivity, iron concentration, dissolved oxygen, total hardness, total alkalinity, total dissolved solids, calcium, magnesium, and turbidity. The selection of these ten critical groundwater

quality parameters was based on their comprehensive ability to represent the chemical, physical, and biological characteristics of groundwater across varied land use types. These parameters are widely recognized indicators of water quality that reflect both natural geochemical processes and anthropogenic influences such as industrial activities, agricultural runoff, and domestic waste disposal. For instance, pH and electrical conductivity provide insights into water's acidity and overall ionic content, while heavy metals like iron indicate contamination from industrial or urban sources. Parameters such as total hardness, calcium, and magnesium relate to mineral dissolution from soil and rock formations, important for understanding background water quality. Dissolved oxygen and turbidity help assess biological activity and particulate contamination. By including this diverse set of parameters, the study ensures a holistic evaluation of groundwater quality that captures the effects of different land uses—residential, commercial, agricultural, and industrial—thereby enabling accurate identification of contamination sources and assessment of health risks. Groundwater samples were collected from ten strategic locations within the urban areas of Agartala during pre-monsoon, monsoon, and post-monsoon seasons to capture seasonal variations. By applying weighted fuzzy soft sets to analyze this data, we develop a comprehensive view of temporal and spatial fluctuations in groundwater quality, identifying specific sources of contamination through weighted pollution scores (ϖ -scores). These findings underscore the urgent need for enhanced groundwater management strategies in urban environments, particularly in rapid urbanization and climate variability. This research contributes crucial insights into health risks associated with groundwater contamination, offering valuable information for policymakers, urban planners, and stakeholders involved in water resource management. This study aims to guide future policy initiatives and research toward reducing pollution risks and ensuring long-term water security by highlighting the necessity of sustainable groundwater management. Additionally, the study emphasizes the potential for integrating Machine-learning algorithms with fuzzy soft set-based frameworks to strengthen continuous groundwater quality monitoring in urban areas. This integration enhances the capacity of urban management practices to mitigate contamination risks effectively, fostering sustainable and adaptive strategies for water resource management.

The structure of this chapter is organized as follows: Section 2 details the tools and techniques used for data collection and analysis, including an overview of the study area, groundwater sampling procedures, and the application of the weighted fuzzy soft set-based approach. Section 3 provides a comprehensive assessment of groundwater quality in Agartala City, utilizing the weighted fuzzy soft set methodology to identify contamination

sources and assess associated risks. Section 4 presents an in-depth analysis of the weighted pollution scores (ϖ -scores) to evaluate groundwater quality and highlight critical areas of concern. Section 5 represents the ranking of groundwater sampling stations. Section 6 offers a comparative analysis with existing methods, highlighting the advantages of our approach. Finally, Section 7 concludes with key findings and offers recommendations for future research and policy actions aimed at sustainable groundwater management in urban areas.

2. Materials and methods

This section outlines the materials and methodologies employed in assessing groundwater quality in Agartala using an innovative weighted fuzzy soft set-based approach for pollution source identification and risk assessment. It includes details on the study area, data collection procedures, and the implementation of the weighted fuzzy soft set methodology to evaluate groundwater quality and identify contamination sources, offering insights into groundwater suitability and associated risks.

2.1. Study area

The study was conducted at ten carefully chosen locations within the Agartala Municipal Corporation in West Tripura District (Table 1; Figure 1). This selection aimed to capture a representative and detailed picture of groundwater quality in Agartala, with a specific focus on high-risk zones prone to pollution due to rapid urbanization and human activities. Agartala, the capital of Tripura, has a subtropical monsoon climate characterized by hot, humid summers, a significant monsoon season with approximately 2,000 mm of annual rainfall, and mild winters. Seasonal weather variations in the city affect groundwater recharge patterns, with the majority of recharge occurring during the monsoon season through rainwater infiltration.

The ten sampling sites were distributed to cover areas with different land-use profiles and reflect various environmental conditions, including residential, commercial, and industrial zones. These sites included high-density residential neighborhoods, bustling commercial districts, and industrial zones known for higher waste discharge. Additionally, some sites were located near agricultural land, where chemical fertilizers and pesticides could contribute to contamination. The diverse land-use patterns around these locations allowed the study to comprehensively assess the groundwater contamination sources and levels across different urban landscapes within Agartala.

Geographically, the study area is situated between longitudes 91.2433°E and 91.2660°E and latitudes 23.7914°N to

Table 1. Sampling stations for groundwater quality assessment in Agartala, Tripura, including location and coordinates

Sample No.	Sampling stations	Location	Coordinates
α_1	Arundhuti Nagar	Agartala, Tripura	23.8162°N, 91.2493°E
α_2	Golbazar Market	Agartala, Tripura	23.8265°N, 91.2855°E
α_3	Shibnagar	Agartala, Tripura	23.8304°N, 91.3030°E
α_4	Battala Market	Agartala, Tripura	23.8283°N, 91.2671°E
α_5	Banamalipur	Agartala, Tripura	23.8367°N, 91.2869°E
α_6	Lake Chowmuhan Market	Agartala, Tripura	23.8419°N, 91.2797°E
α_7	Gurkhabasti	Agartala, Tripura	23.8554°N, 91.2827°E
α_8	Agartala Government Medical College	Agartala, Tripura	23.8603°N, 91.2927°E
α_9	Ushabazar	Agartala, Tripura	23.88610N, 91.24330E
α_{10}	Maharaja Bir Bikram Airport	Agartala, Tripura	23.89140N, 91.24380E

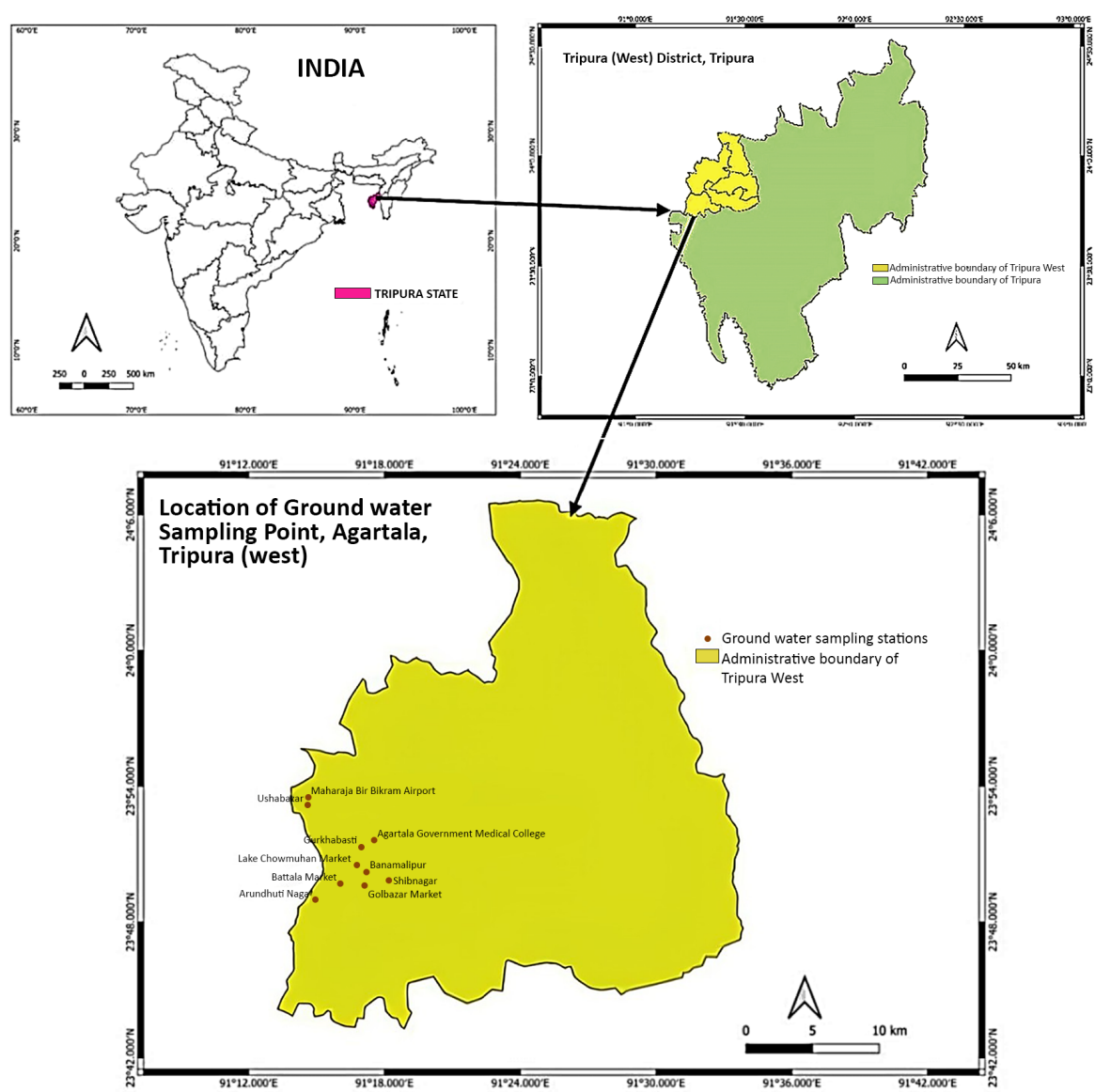


Figure 1. The study area within Agartala Municipal Corporation, Tripura.

23.9075°N. This area is primarily characterized by undulating plains with pockets of hilly terrain, along with valleys that naturally facilitate drainage. The Agartala's unique terrain and drainage system play a significant role in groundwater movement and pollutant dispersal. Rainwater runoff and inadequate waste disposal and unregulated industrial discharges enable pollutants to percolate into the groundwater system, especially in low-lying valley areas.

The population density in Agartala is among the highest in Tripura, with approximately 988,192 residents (as per the 2011 census) residing within a 984 km² area. The city's rapid urban expansion is fueled by increasing residential, industrial, and commercial activities, which collectively contribute to substantial environmental pressures on groundwater resources. Industrial areas, especially those involving small and medium enterprises, often discharge untreated wastewater into nearby drainage systems, exacerbating groundwater contamination. Residential zones contribute to groundwater pollution through domestic sewage, improperly managed waste disposal, and occasional leachate from landfills.

2.2. Hydrogeological Characteristics and Sampling Details

2.2.1. Aquifer Types and Depths

The study area in Agartala primarily features shallow alluvial and weathered fractured aquifers typical of the region's undulating plains and valley systems. The predominant aquifer types at each sampling site are as follows:

- **Residential and Commercial Zones:** Predominantly shallow, unconfined alluvial aquifers with a water table generally located between 5 to 15 meters below ground surface (BGS). The unsaturated zone thickness varies from 3 to 10 meters depending on local topography and soil cover.
- **Industrial Zones:** These areas mostly overlay weathered fractured bedrock aquifers with deeper water levels, ranging from 10 to 25 meters BGS. The unsaturated zone here tends to be thinner (approximately 2 to 6 meters) due to localized excavation and surface disturbances.
- **Agricultural and Peri-Urban Areas:** Characterized by unconfined alluvial aquifers with water tables generally between 3 to 12 meters BGS, and unsaturated zone thicknesses of 4 to 9 meters.

The typical well depths for groundwater extraction across these sites range from 15 to 35 meters, ensuring access to saturated zones for water supply.

2.2.2. Sampling Depth and Procedure

Groundwater samples were collected primarily at the well-head following standard purging protocols to obtain representative water from the saturated zone at or near the static water level. In some cases, sampling was conducted at depths slightly below the water table within the well bore to ensure minimal surface contamination influence. No surface runoff or shallow soil moisture samples were taken, ensuring that the analyses reflect true groundwater quality.

2.2.3. Contaminant Mobility and Geochemical Considerations

The ability of contaminants to reach groundwater depends on their chemical nature and interaction with the geological environment:

- **Conservative Contaminants:** Nitrates are highly mobile and persist through the unsaturated zone with minimal attenuation, making them reliable indicators of agricultural runoff or sewage infiltration. Their presence is thus closely monitored, especially near agricultural and densely populated residential areas.
- **Reactive Contaminants:** Phosphates, oils, fats, and many heavy metals exhibit strong adsorption, precipitation, or biodegradation within the soil and unsaturated zone, limiting their mobility. These contaminants tend to accumulate near the surface or in soil layers, and only reach groundwater under specific hydrogeological conditions, such as fractured rock or areas with thin unsaturated zones.

Additionally, the distance from the coastal zone influences salinity intrusion risks and contaminant dispersion, although Agartala's inland location reduces the likelihood of saltwater intrusion.

2.2.4. Health Risk Implications

Understanding contaminant type, concentration, and exposure pathway is critical for assessing health risks:

- **Acute (Short-Term) Exposure:** Typically linked to pathogens, organic contaminants, and high nitrate levels, which can cause immediate health effects such as gastrointestinal illness, methemoglobinemia ("blue baby syndrome"), or poisoning.
- **Chronic (Long-Term) Exposure:** Includes low-level, prolonged exposure to heavy metals, fluoride, and other

toxic substances that may cause cancer, neurological disorders, or developmental issues.

The study's sampling strategy ensures that the groundwater quality data reflect the actual exposure risk to consumers relying on well water, facilitating accurate health risk assessments and mitigation planning.

2.2.5. Rationale for selecting Agartala as the study area

The selection of Agartala as the focal point of this study was based on several key factors:

2.2.5.1. Natural Factors:

- **Geological Composition:** The geological makeup of an area significantly influences groundwater quality. For example, regions rich in limestone typically display elevated hardness levels due to higher concentrations of calcium and magnesium.
- **Weathering and Erosion:** Natural processes such as weathering and erosion can release essential minerals and salts into groundwater systems, potentially affecting their quality.
- **Precipitation and Recharge:** Rainfall plays a critical role in groundwater dynamics by diluting existing contaminants and replenishing aquifers, leading to fluctuations in contaminant concentrations over time.

2.2.5.2. Anthropogenic (Human-Induced) Factors:

- **Agricultural Activities:**
 - **Pesticides and Fertilizers:** The application of agrochemicals in farming can lead to significant groundwater contamination, primarily from nitrates, phosphates, and residual pesticides.
 - **Irrigation Practices:** Excessive irrigation may result in soil salinization, negatively affecting groundwater quality by increasing salinity levels.
- **Industrial and Urban Activities:**
 - **Industrial Waste Disposal:** Improper disposal practices of industrial waste can introduce heavy metals and toxic chemicals into groundwater systems.
 - **Urban Runoff:** Stormwater runoff from urban areas can carry pollutants such as oils, greases, and heavy metals into groundwater, further degrading its quality.
- **Sewage and Wastewater:**
 - **Leaking Septic Systems:** Inadequately managed

septic systems can contaminate groundwater with pathogens, nitrates, and other harmful pollutants.

- **Untreated or Poorly Treated Wastewater:** Insufficient treatment of wastewater can introduce harmful bacteria, viruses, and chemicals into the groundwater supply.
- **Landfills:**
 - Poorly managed landfills produce leachate—a toxic liquid containing harmful chemicals and heavy metals—that can seep into the soil and potentially reach groundwater. The likelihood and extent of groundwater contamination depend largely on the thickness of the unsaturated zone and the depth of the groundwater table; thicker unsaturated zones and deeper water levels generally provide greater natural attenuation, reducing contaminant mobility and risk.
- **Deforestation and Land Use Changes:**
 - **Soil Erosion:** Deforestation increases soil erosion by removing vegetation cover, leading to greater sediment runoff and elevated turbidity in groundwater recharge areas. The impact on groundwater quality depends significantly on the depth of the groundwater table—shallower water tables are more vulnerable to sediment infiltration, while deeper groundwater may be less immediately affected due to natural filtration through the unsaturated zone.
- **Over-Extraction of Groundwater:**
 - **Saltwater Intrusion:** In coastal areas, excessive groundwater extraction can lead to saltwater intrusion, raising salinity levels in freshwater aquifers.
 - **Lowering of the Water Table:** Over-pumping groundwater resources can result in a lowered water table, concentrating contaminants like arsenic and fluoride in remaining water supplies.
- **Climate Change:**
 - **Changes in Precipitation Patterns:** Variability in rainfall can significantly impact groundwater recharge rates and the concentration of contaminants in groundwater.
 - **Temperature Variations:** Increasing temperatures can alter groundwater chemistry by affecting evaporation rates and altering precipitation patterns, impacting recharge and contaminant levels.

This study employs an innovative weighted fuzzy soft set-based approach for groundwater pollution source identification and risk assessment in urban areas. This methodology effectively captures the uncertainty and variability inherent in groundwater

quality data, by integrating various groundwater quality parameters through a weighted fuzzy soft set framework.

Water samples were systematically collected from selected sites across Agartala City, and physicochemical parameters were analyzed. The results were compared against established national and international water quality standards, facilitating the identification of areas in urgent need of improved groundwater management and protection measures. This approach not only enhances the accuracy of groundwater quality assessments but also assists in pinpointing specific pollution sources, thereby providing essential insights for policymakers and urban planners engaged in sustainable water resource management. The study aims to contribute to more effective strategies for mitigating groundwater pollution risks and ensuring long-term water security in urban environments through this innovative framework.

2.3. Method

In this section, we will establish the foundational concepts necessary for understanding the Weighted Fuzzy Soft Set-Based Approach employed for groundwater pollution source identification and risk assessment in urban areas. By introducing key ideas such as weighted fuzzy sets, soft sets, and fuzzy soft sets, we will highlight their critical role in developing our innovative framework. These concepts are essential for effectively managing uncertainty and imprecision in decision-making processes related to groundwater quality analysis.

Let V represent a universal set, or the initial universe, consisting of all possible objects under consideration. The power set of V , denoted as $P(V)$, refers to the set containing all possible subsets of V . Meanwhile, E represents a set of parameters that describe various aspects or attributes of the elements within V .

2.3.1. Fuzzy Sets

A fuzzy set (Zadeh, 1965), as introduced by Zadeh in 1965, extends the classical notion of a set by allowing partial membership, meaning that elements of the set can belong to it with varying degrees. In contrast to traditional binary logic, where an element is either in or out of a set, fuzzy sets permit a gradual assessment of membership using a membership function, which assigns each element a value between 0 and 1.

A fuzzy set Z over a universe V is expressed as $Z = \{(o, \mu_Z(o)) : o \in V\}$, where $\mu_Z: V \rightarrow [0, 1]$ is the membership function, representing the degree of membership for each element $o \in V$. Here, the value $\mu_Z(o)$ indicates how strongly element o belongs to the fuzzy set Z . For example, if $\mu_Z(o) = 0$, the element does not belong to the set at all, whereas if $\mu_Z(o) = 1$, it fully belongs to the set. Intermediate values between 0 and 1 capture

partial membership, providing a powerful way to represent vague or uncertain information.

Fuzzy sets allow for the representation of varying degrees of membership across different groundwater quality parameters, enabling us to assign importance to each parameter based on its relevance to pollution assessment. This is particularly useful in situations where certain factors may have a greater impact on groundwater quality than others, facilitating a more nuanced analysis. The set of all possible fuzzy sets on V is denoted by $FS(V)$.

2.3.2. Soft Sets

A soft set (Molodtsov, 1999) is a mathematical tool for dealing with uncertainty, originally introduced to provide a flexible and simplified framework for addressing vague data, where the information may not be entirely clear or precise. The formal structure is based on the relationship between parameters and subsets of a universe of discourse.

A soft set over a universe V is defined as a couple (F, E) , where F is a function $F: E \rightarrow P(V)$. This function associates each parameter in the set E with a specific subset of V . In simpler terms, for each parameter $p \in E$, the mapping $F(p)$ identifies a subset of elements in V to which the parameter is applicable. This formalizes the idea of associating each parameter with relevant data, while also accommodating uncertainty, as the subsets may not be precisely defined.

Soft sets provide a flexible mathematical framework for dealing with uncertainties associated with groundwater pollution sources. By incorporating various parameters and their associated relationships, soft sets enable us to represent complex decision-making scenarios without the need for fixed membership grades, which is particularly advantageous in the context of environmental assessments.

2.3.3. Fuzzy Soft Sets

Fuzzy soft sets (Maji et al., 2001) combine the flexibility of soft sets with the nuanced membership grading of fuzzy sets. By allowing parameters to be associated with fuzzy sets rather than crisp subsets of V , FSSs offer an enhanced framework for modeling problems with multiple levels of uncertainty and imprecision.

A couple (F, E) is said to be an FSS over a universe V , where $F: E \rightarrow FS(V)$ a function that assigns a fuzzy set to each parameter in P . In this setup, for each parameter $p \in E$, the corresponding fuzzy set $F(p)$ provides a degree of membership for each element in V , reflecting the extent to which the element

satisfies or is related to the parameter p . This structure enables the incorporation of both parameter-based uncertainty (through soft sets) and gradual membership (through fuzzy sets), making FSSs well-suited for complex decision-making scenarios where data is not only uncertain but also fuzzy in nature.

To better understand the concepts, consider an example where V is a set of wells, and E represents various parameters related to water quality, such as pH level, pollution, and temperature. Each parameter in E (e.g., "acceptable pH range") can be associated with a fuzzy set over V , where the membership function indicates how well each well satisfies the given condition. The fuzzy soft set then provides a comprehensive and flexible model for assessing water quality, accounting for both uncertainty in the parameters and the fuzziness of the data. Fuzzy soft sets integrate the advantages of both fuzzy sets and soft sets, allowing for a comprehensive representation of uncertainties in groundwater quality data. This approach enhances our ability to model the interactions between different GWQPs, leading to a more robust evaluation of pollution sources and risks.

By integrating these foundational concepts, our proposed weighted fuzzy soft set-based approach establishes a robust framework that effectively tackles uncertainty, complexity, and multi-criteria decision-making, paving the way for future applications in groundwater pollution source identification and risk assessment in urban areas.

Central to this framework is the introduction of the weighted score function ϖ for fuzzy soft sets. This innovative function enables us to quantify the impact of various groundwater quality parameters (GWQPs) on pollution assessment, allowing for a more nuanced evaluation of groundwater contamination levels. The $\mathfrak{B}$ -model harnesses this concept to serve as an effective water pollution rating system, systematically assessing the risks associated with different pollution sources.

The application of the ϖ function within the $\mathfrak{B}$ -model facilitates the aggregation of data from multiple GWQPs, leading to a comprehensive understanding of groundwater quality in urban environments. This approach not only enhances our capability to identify pollution sources but also assists in prioritizing intervention strategies based on the severity of contamination. By employing this method, we aim to provide actionable insights for policymakers and stakeholders in their efforts to mitigate groundwater pollution and promote sustainable resource management.

2.3.4. Weighted Fuzzy Soft Set

A weighted fuzzy soft set (WFSS) incorporates an additional weight function into the fuzzy soft set structure. Formally, a weighted fuzzy soft set is defined as a triple (F, E, ϖ) , where:

- (F, E) is a FSS as described above.

- $\varpi: E \rightarrow [0,1]$ is a weight function that assigns a weight to each parameter $e \in E$, reflecting the relative importance or significance of that parameter in the decision-making or assessment process.
- For each parameter $p_k \in E$, the associated weight is $\varpi_k = \varpi(p_k)$, where ϖ_k lies between 0 and 1. This weight scales the influence of the fuzzy membership values associated with that parameter.

A WFSS allows for the incorporation of both fuzzy set theory, which deals with uncertainty and gradation of membership, and weighted soft set theory, which introduces the concept of relative importance or priority among attributes. This combination enables more nuanced and context-specific modeling and analysis, particularly in decision-making processes where attributes may carry varying degrees of significance. The WFSS framework incorporates the notion of relative importance among parameters, making it particularly useful in cases where attributes have different levels of significance.

2.4. Weighted water pollution score function

Consider (F, E, ϖ) to be a weighted fuzzy soft set over V , where ϖ_k is the weight assigned to each parameter $e_k \in E$. The mapping $\varpi: E \rightarrow [0,1]$ assigns a weight to each parameter e_k , in such a way that $\varpi_k = \varpi(e_k)$.

The weighted water pollution score function W for (F, E, ϖ) is defined as:

$$W(s) = \frac{\sum_{k=1}^m [\varpi(e_k) \times \mu_{F(e_k)}(s)]}{\sum_{k=1}^m \varpi(e_k)}, e_k \in E \text{ and } \forall s \text{ in } V \quad (1)$$

- s represents a specific location in the dataset.
- e_k refers to individual GWQPs such as pH, TDS, etc.
- $\mu_{F(e_k)}(s)$ is the fuzzy membership function, which provides a value between 0 and 1, representing the degree to which the sample meets ideal conditions for parameter e_k . A value of 0 indicates the ideal condition, while a value of 1 indicates the worst condition.
- $\varpi(e_k)$ represents the weight assigned to parameter e_k , reflecting its importance in the overall water quality assessment.

2.4.1. Interpretation of W :

- The weighted pollution score W provides a composite score that reflects the overall pollution level for a particular location or sample. A score near 0 (zero) indicates excellent water quality, while a score approaching 1 (one) signifies poor water quality.

- By adjusting the weights $\varpi(e_k)$, the model can emphasize certain parameters more than others. This flexibility is essential because the significance of different GWQPs can vary depending on local environmental conditions or specific water use cases (e.g., drinking, irrigation, industrial use).

This innovative approach is applied within the $\mathfrak{B}$ -model to evaluate groundwater contamination resulting from urbanization and anthropogenic activities. By integrating these weighted fuzzy soft sets into our analysis, we enhance the identification of pollution sources and conduct a thorough risk assessment, ultimately guiding effective groundwater management strategies in urban settings.

2.5. Weighted fuzzy soft set based MCDM model ($\mathfrak{B}$ -model)

The $\mathfrak{B}$ -model is developed to assess groundwater contamination through an innovative approach that leverages weighted fuzzy soft sets. This model is structured to evaluate the sources of groundwater pollution, particularly focusing on impacts from urbanization and anthropogenic activities. The methodology employs the principles of fuzzy set theory, soft sets, and weighted fuzzy soft sets to compute a comprehensive score for water quality.

The following steps outline the $\mathfrak{B}$ -model, which integrates these concepts to facilitate the identification of pollution sources and assess the associated risks effectively:

Step 1: Define the sampling stations, GWQPs, and expert groups.

Identify key elements needed for the analysis: sampling stations, GWQPs, and expert opinions.

- **Sampling Stations** $S = \{\alpha_1, \alpha_2, \alpha_3, \dots, \alpha_n\}$: These are the physical locations where groundwater samples are collected for the study. Each station represents a unique site that is being monitored for contamination levels.
- **Groundwater Quality Parameters** $P = \{\beta_1, \beta_2, \beta_3, \dots, \beta_m\}$: These are the specific factors (e.g., pH, dissolved oxygen, total dissolved solids) that are used to evaluate the quality of groundwater. Each parameter has a distinct role in identifying contamination, especially from urbanization and human anthropogenic activities.
- **Expert Group** $E = \{e_1, e_2, e_3, \dots, e_q\}$: Experts in the field (such as environmental scientists, hydrologists, and public health professionals) are involved in providing their opinions on the data, ensuring that the results are validated by experience and domain knowledge.

Step 2: Collect crisp data summaries from experts.

Gather precise, non-fuzzy (crisp) measurements of GWQPs from each sampling station.

- **Crisp Data Summaries** $DT = \{dt_1, dt_2, dt_3, \dots, dt_q\}$: These are the raw numerical values collected by experts for each GWQP at each station. For example, at a given station, the pH value might be 7.5, and the total dissolved solids might be 300 mg/L.
- These crisp values represent the initial observations and are essential for later steps in converting them into a fuzzy soft set framework, which can incorporate uncertainty in the data.

Step 3: Enter the standard and ideal values of GWQPs.

Incorporate regulatory standards or ideal values for each GWQP as a benchmark.

- **Standard and Ideal Values**: Regulatory agencies (such as the World Health Organization or local environmental protection agencies) provide guidelines for acceptable levels of each GWQP. For instance, the ideal pH for drinking water might be between 6.5 and 8.5.
- These values are necessary to define fuzzy membership functions in the next step, which will measure how far the observed data deviates from the ideal or standard values.

Step 4: Define fuzzy membership functions for GWQPs.

Convert the crisp data from Step 2 into fuzzy data by defining membership functions for each GWQP.

- **Fuzzy Membership Function** $\mu_{pt_k}: \mathbb{R} \rightarrow [0, 1]$: A fuzzy membership function is created for each water quality parameter $pt_k \in P$. It maps the real-valued data (e.g., pH = 7.5) to a fuzzy value between 0 and 1, where:
 - A value close to 1 indicates that the GWQP is far from ideal (poor water quality).
 - A value close to 0 means the GWQP is near the ideal range (good water quality).
- For example, a pH of 6.5 might map to a membership value of 0.1 (indicating good quality), while a pH of 9 might map to a value of 0.9 (indicating poor quality).

Step 5: Assign weights to each GWQP.

Define the relative importance of each GWQP by assigning weights.

- **Weight Function**: This function assigns a weight to each GWQP $\beta_k \in P$, where $\varpi_k = \varpi(\beta_k)$, $k = 1, 2, 3, \dots, m$. The weight is a value between 0 and 1, indicating how critical that parameter is in determining overall water quality.

- For example, if total dissolved solids are more important than pH in determining groundwater contamination, it might be assigned a higher weight (e.g., $\varpi_{\text{TDS}} = 0.7$) compared to pH (e.g., $\varpi_{\text{pH}} = 0.3$).

This step allows for prioritization, where more significant parameters contribute more heavily to the final score.

Step 6: Convert crisp data into WFSSs.

Combine the crisp data, membership functions, and weights to form weighted fuzzy soft sets (WFSSs).

- The crisp data summaries from Step 2, along with the fuzzy membership functions from Step 4 and weights from Step 5, are now integrated to create WFSSs for each expert.
- These WFSSs (ψ_1, P, ϖ) , (ψ_2, P, ϖ) , $(\psi_3, P, \varpi), \dots, (\psi_q, P, \varpi)$ represent the final fuzzy representations of the water quality data, incorporating both fuzziness (due to uncertainty in measurements) and weights (to reflect the importance of different parameters).

Step 7: Calculate the weighted score for every data collection site.

Calculate the ϖ -score, which represents the overall groundwater quality at every data collection site.

- The ϖ -score $\Omega_{\varpi}(t)$ is calculated for every data collection site t using the following formula:

$$\Omega_{\varpi}(t) = \frac{\sum_{k=1}^m [\varpi(\beta_k) \times \Omega(\mu_{\Psi(\beta_k)}(t))]}{\sum_{k=1}^m \varpi(\beta_k)}, \beta_k \in P \text{ and } \forall t \text{ in } S \quad (2)$$

- This formula computes a weighted average of the fuzzy membership values, taking into account the importance of each parameter (via the weights). It provides a single score for each station, which can be used to compare groundwater quality across all sampling locations.

Step 8: Interpret the ϖ -score.

Assess the groundwater quality at each station based on the ϖ -score.

- A lower ϖ -score (closer to 0) indicates that the water quality at a particular sampling station is good, meaning that the contamination levels are low.
- A higher ϖ -score (closer to 1) indicates poor water quality, suggesting significant contamination.
- This final step helps identify which sampling stations

have safe water and which ones require intervention for sustainable management strategies.

The $\mathfrak{B}$ -model methodically transforms raw water quality data into a fuzzy decision-making framework, accounting for uncertainties and varying levels of importance among parameters. By computing weighted scores for each sampling station, the model provides a robust system for assessing groundwater contamination and identifying areas with degraded water quality. This algorithm enables a nuanced assessment of groundwater contamination, particularly in urban environments affected by urbanization and human anthropogenic activities, and aids in the development of sustainable management strategies.

The flowchart Figure 2 outlines the systematic steps of the $\mathfrak{B}$ -model designed to assess groundwater quality, specifically addressing contamination arising from urbanization and anthropogenic activities in Agartala, Tripura, India. Each step emphasizes the integration of an innovative weighted fuzzy soft set-based approach with multi-criteria decision-making principles, facilitating a thorough evaluation of groundwater pollution sources and associated risks. This structured methodology combines expert insights with empirical data, ensuring a nuanced understanding of groundwater contamination levels. By systematically identifying and quantifying pollution sources, the $\mathfrak{B}$ -model serves as a valuable tool for guiding effective groundwater management strategies tailored to the specific challenges faced in urban environments. The results derived from this model provide critical information for policymakers and stakeholders aiming to mitigate pollution and protect vital water resources in urban areas.

3. Assessment of groundwater contamination in Agartala City

In this segment, we undertake a comprehensive assessment of groundwater contamination levels in Agartala City, West Tripura, utilizing an innovative weighted fuzzy soft set-based approach specifically designed for identifying pollution sources and conducting risk assessments in urban areas. This methodology is not only crucial for understanding the dynamics of groundwater quality but also plays a vital role in facilitating informed, knowledge-based decision-making. Through this approach, we aim to develop effective strategies that mitigate pollution, ensuring the safety and quality of groundwater resources, and thereby safeguarding public health and environmental integrity.

The $\mathfrak{B}$ -model is established as a multi-criteria decision-making framework that seamlessly integrates soft set and fuzzy set theories. Within this framework, the weighted fuzzy soft set

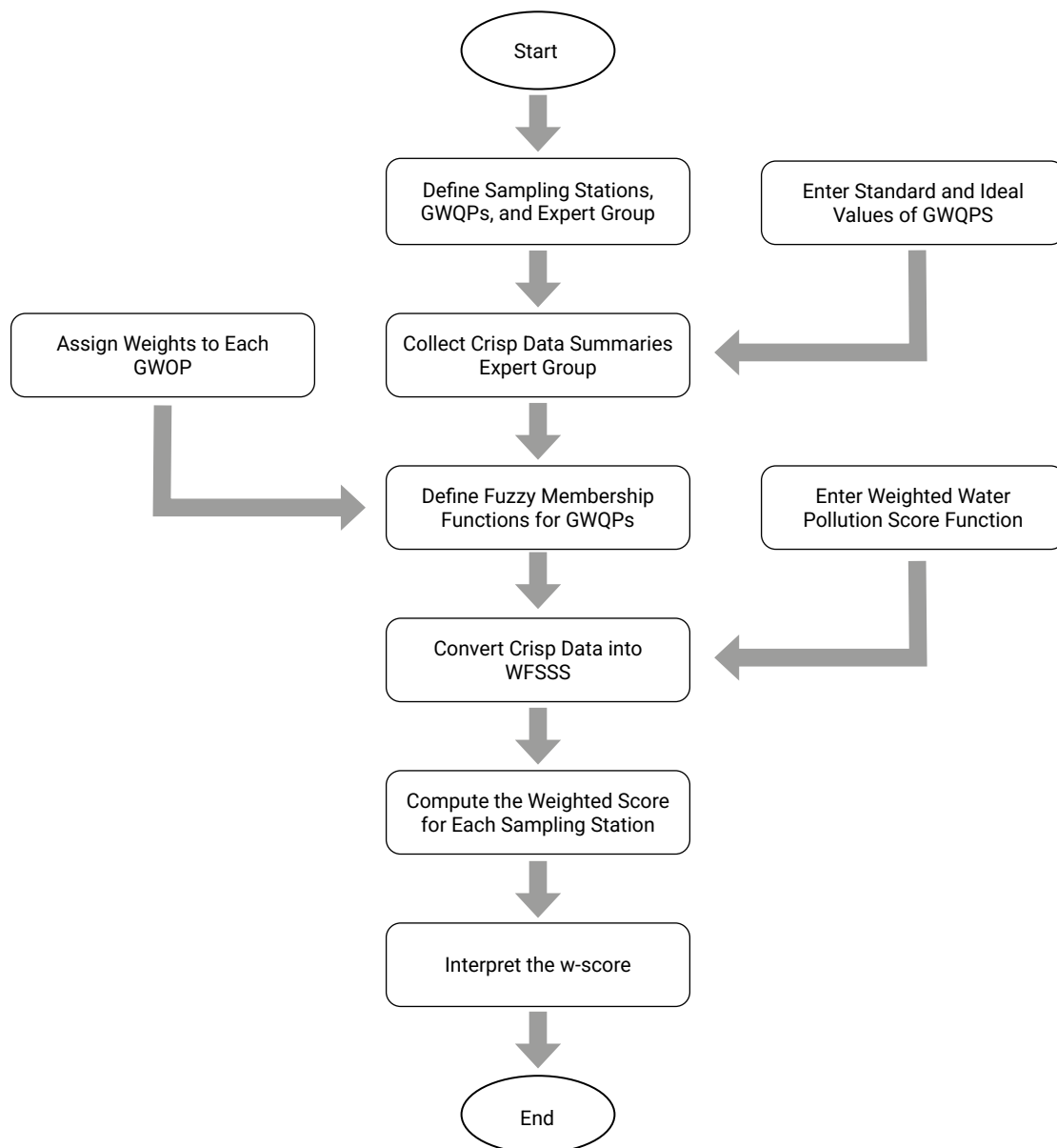


Figure 2. Flowchart for $\mathfrak{B}$ -model: Groundwater Quality Assessment.

score (ϖ -score) functions as the primary indicator of groundwater quality. A ϖ -score approaching zero signifies excellent groundwater quality, reflecting minimal contamination, while a score nearing one indicates substantial contamination levels. This model adeptly aggregates multiple groundwater quality parameters, assigns relative weights to each parameter, and produces a comprehensive single parametric value that encapsulates the overall groundwater quality. By allowing for the nuanced interpretation of these scores, the model effectively highlights the critical parameters that influence water safety.

For this study, ten strategically selected groundwater sampling locations across Agartala City were chosen, as illustrated in Figure 1 and detailed in Table 1. These sites were selected based

on several criteria, including population density, proximity to urban settlements, and potential sources of contamination. The coordinates of the sampling sites were meticulously recorded using a Garmin eTrex Vista Cx GPS device, ensuring precise location mapping. Samples were collected during the 2023-2024 period, covering different seasonal variations: pre-monsoon, monsoon, and post-monsoon, which are essential for understanding temporal fluctuations in water quality.

Each water sample was collected in triplicate using 1.5-liter polypropylene bottles. To prevent contamination, these bottles were pre-washed with a 10% hydrochloric acid (HCl) solution and thoroughly rinsed with the sample water at the time of collection. The study focused on ten key GWQPs that are critical for evaluating the

impacts of urbanization and anthropogenic activities on groundwater quality. These parameters include pH, Electrical Conductivity, Iron, Dissolved Oxygen (DO), Total Hardness, Total Alkalinity, Total Dissolved Solids, Calcium, Magnesium, and Turbidity. The selection of these parameters was based on their relevance to urban pollution sources and their potential health impacts.

To ensure the reliability and accuracy of the results, all sampling and analysis procedures adhered to the established guidelines outlined by the American Public Health Association (APHA, 2005). The groundwater quality data collected from the ten selected locations were analyzed across the three distinct seasons, with seasonal summaries presented in Tables 2, 3, and 4. This detailed seasonal analysis is vital for capturing the variations in groundwater quality that can occur due to changing climatic conditions and human activities.

The obtained values were meticulously compared to the recommended water quality standards established by the World Health Organization (WHO, 2011), which are summarized in Table 5. This comparison serves as a benchmark for evaluating the degree of contamination and identifying critical areas requiring

immediate attention. The results of this thorough analysis provide invaluable insights into the extent of groundwater contamination arising from urbanization and anthropogenic activities.

Furthermore, these findings underscore the pressing need for sustainable management strategies aimed at addressing groundwater pollution effectively. By identifying specific sources of contamination and understanding their impacts on groundwater quality, stakeholders can implement targeted interventions, regulatory measures, and community awareness programs to protect this vital resource. Ultimately, the innovative approach outlined in this study not only enhances our understanding of groundwater dynamics but also contributes to the development of sustainable practices that can mitigate pollution and safeguard public health in urban environments.

Let $S = \{s\alpha_1, s\alpha_2, s\alpha_3, s\alpha_4, s\alpha_5, s\alpha_6, s\alpha_7, s\alpha_8, s\alpha_9, s\alpha_{10}\}$ represent the set of sampling stations within Agartala City, as specified in Table 1. The set P represents the GWQPs being considered, and it is defined as follows:

$$P = \{\beta_1, \beta_2, \beta_3, \beta_4, \beta_5, \beta_6, \beta_7, \beta_8, \beta_9, \beta_{10}\}.$$

Table 2. Crisp data summaries of GWQPs for the pre-monsoon season.

S	β_1	β_2	β_3	β_4	β_5	β_6	β_7	β_8	β_9	β_{10}
$s\alpha_1$	6.40	115	1.5	5.4	40	135	180	20	35	3.6
$s\alpha_2$	6.70	125	1.8	5.2	45	130	170	25	40	3.7
$s\alpha_3$	6.95	130	2.0	5.0	50	140	185	30	45	3.5
$s\alpha_4$	6.10	135	1.2	5.3	55	125	160	35	50	3.8
$s\alpha_5$	6.55	120	1.7	5.1	60	145	190	40	55	3.3
$s\alpha_6$	6.75	110	1.3	5.5	65	150	200	45	60	3.4
$s\alpha_7$	6.85	105	1.6	5.6	70	160	210	50	65	3.2
$s\alpha_8$	6.00	130	1.4	5.8	75	170	220	55	70	3.9
$s\alpha_9$	6.50	120	1.9	5.7	80	155	195	60	75	3.6
$s\alpha_{10}$	6.05	115	1.1	5.9	85	140	170	65	80	3.7

Table 3. Crisp data summaries of GWQPs for the monsoon season.

S	β_1	β_2	β_3	β_4	β_5	β_6	β_7	β_8	β_9	β_{10}
$s\alpha_1$	6.60	120	1.4	5.2	32	119	170	15	30	3.4
$s\alpha_2$	6.85	110	1.9	5.3	38	122	180	20	35	3.7
$s\alpha_3$	6.00	125	2.5	5.6	43	145	190	25	40	3.9
$s\alpha_4$	6.90	130	2.2	5.7	48	152	200	30	45	3.5
$s\alpha_5$	6.55	120	1.7	5.5	51	155	210	35	50	3.4
$s\alpha_6$	6.75	115	1.3	5.0	56	160	220	40	55	3.6
$s\alpha_7$	6.85	105	1.6	5.8	62	172	195	45	60	3.1
$s\alpha_8$	6.00	130	1.4	5.7	68	155	180	50	65	3.0
$s\alpha_9$	6.70	125	1.8	5.6	74	141	160	55	70	3.2
$s\alpha_{10}$	6.75	115	2.0	5.5	80	130	140	60	75	3.5

Table 4. Crisp data summaries of GWQPs for the post-monsoon season.

S	β_1	β_2	β_3	β_4	β_5	β_6	β_7	β_8	β_9	β_{10}
$s\alpha_1$	6.50	110	1.3	5.2	34	134	173	21	33	3.6
$s\alpha_2$	6.75	117	1.8	5.5	39	145	182	27	41	3.2
$s\alpha_3$	6.90	113	1.5	5.9	44	162	191	31	47	3.4
$s\alpha_4$	6.85	124	1.2	5.8	49	177	183	35	51	3.3
$s\alpha_5$	6.60	127	1.1	5.2	53	187	210	47	53	3.2
$s\alpha_6$	6.85	124	1.7	5.4	57	179	202	45	63	3.5
$s\alpha_7$	6.90	131	2.5	5.7	62	117	163	50	65	3.8
$s\alpha_8$	6.05	120	3.1	5.5	67	129	128	55	71	3.9
$s\alpha_9$	6.70	125	1.5	5.6	72	121	139	63	75	3.6
$s\alpha_{10}$	6.85	119	1.4	5.1	77	133	132	65	83	3.7

Table 5. Standard and ideal values of the GWQPs according to WHO.

P	Parameter name	Standard value	Ideal value	Recommending agencies
β_1	pH	6.5-8.5	7	WHO (2011)
β_2	Electrical Conductivity (mho/cm)	250	0	WHO (2011)
β_3	Fe (mg/l)	1	0.3	WHO (2011)
β_4	Dissolved Oxygen (mg/l)	5.00	14.6	WHO (2011)
β_5	Total Hardness(mg/l)	500	0	WHO (2011)
β_6	Total Alkalinity (mg/l)	200	0	WHO (2011)
β_7	Total Dissolved Solids (mg/l)	500	0	WHO (2011)
β_8	Calcium (mg/l)	75	0	WHO (2011)
β_9	Magnesium (mg/l)	50	0	WHO (2011)
β_{10}	Turbidity (mg/l)	5	0	WHO (2011)

This set contains the ten key GWQPs under evaluation. The data summaries of these parameters, collected from the ten selected sampling stations across different seasons, are provided in Tables 2, 3, and 4. Additionally, the ideal and standard values for each of the GWQPs are outlined in Table 5.

To calculate the weight α_i for each GWQP $p_i \in P$, we use the following formula:

$$\alpha_i = \frac{1}{V_i}$$

where V_i represents the recommended standard value of the i -th GWQP, $p_i \in P$. For example, the standard value for pH (denoted by β_1) is taken to be 8.5, meaning $V_1 = 8.5$.

Using this formula, the weights α_i allocated to each of the GWQPs in P have been determined as follows:

$$\varpi = \{\alpha_1 = \alpha(\beta_1) = 0.118; \alpha_2 = \alpha(\beta_2) = 0.004; \alpha_3 = \alpha(\beta_3) = 1; \alpha^4 = \alpha(\beta_4) = 0.2; \alpha_5 = \alpha(\beta_5) = 0.002; \alpha_6 = \alpha(\beta_6) = 0.005; \alpha_7$$

$$= \alpha(\beta_7) = 0.002; \alpha_8 = \alpha(\beta_8) = 0.013; \alpha_9 = \alpha(\beta_9) = 0.02; \alpha_{10} = \alpha(\beta_{10}) = 0.2\}.$$

The relative-weights assigned to the GWQPs provide a quantitative measure of the importance of each parameter in evaluating groundwater quality. These weights, combined with the crisp data collected from the sample stations, enable a comprehensive assessment of the groundwater quality in Agartala City.

In this study, crisp numbers are converted into triangular, left-open, and right-open fuzzy numbers. Triangular fuzzy numbers are defined by three parameters: the lower limit a , the peak b , and the upper limit c . The membership function of a triangular fuzzy number $T(a, b, c)$ is defined as follows:

$$\mu_T(x) = \begin{cases} \frac{b-x}{b-a}; & \text{when } a \leq x \leq b \\ \frac{x-b}{c-b}; & \text{when } b \leq x \leq c \\ 1 & \text{otherwise} \end{cases}$$

Where:

- a is the lower bound,
- b is the peak or most likely value,
- c is the upper bound.

Right-open fuzzy numbers have a membership function that is 1 for all values less than a certain point and gradually decreases to 0 for values greater than that point. Conversely, **left-open fuzzy numbers** have a membership function that is 1 for all values greater than a certain point and gradually decreases to 0 for values less than that point.

Drawing from the ideal and standard values of the GWQPs listed in Table 5, we develop fuzzy membership functions to represent the different levels of conformity or deviation of each GWQP relative to the recommended thresholds. These fuzzy membership functions provide a method to quantitatively evaluate how closely the recorded values for each parameter align with the ideal or acceptable benchmarks.

1. **pH:** The pH level of water reflects its acidity or alkalinity, essential for aquatic life. The triangular fuzzy number captures uncertainty around ideal pH values, defined by the membership function:

$$\mu_{\beta_1}(x) = \begin{cases} \frac{7.0-x}{7.0-6.5}; & \text{when } 6.5 \leq x \leq 7.0 \\ \frac{x-7.0}{8.5-7.0}; & \text{when } 7.0 \leq x \leq 8.5 \\ 1; & \text{otherwise} \end{cases}$$

2. **Electrical conductivity:** Electrical conductivity (EC) is a key parameter reflecting the ability of water to conduct electrical current, which correlates with the concentration of dissolved salts. The membership function for EC is defined as:

$$\mu_{\beta_2}(x) = \begin{cases} \frac{x-0}{250-0}; & \text{when } 0 \leq x \leq 250 \\ 1; & \text{when } x \geq 250 \end{cases}$$

This indicates that the ideal EC value is up to 250 $\mu\text{S/cm}$, after which the membership function remains constant at 1. EC values above this threshold suggest a higher concentration of dissolved ions, which may affect water quality.

3. **Fe:** Iron (Fe) concentration in water is another critical parameter, especially in determining water's potability. The membership function for Fe is given by:

$$\mu_{\beta_3}(x) = \begin{cases} \frac{x-0.3}{1-0.3}; & \text{when } 0.3 \leq x \leq 1 \\ 1; & \text{otherwise} \end{cases}$$

This function describes the acceptable Fe concentration range from 0.3 to 1 mg/L. The membership function equals 1 for Fe concentrations within this range, reflecting the safe levels for water consumption. Higher concentrations may indicate potential contamination, affecting human and aquatic health.

4. **Dissolved oxygen:** Dissolved oxygen is critical for the survival of aquatic organisms. The right-open fuzzy number reflects full membership for lower oxygen levels, tapering off as oxygen increases:

$$\mu_{\beta_4}(x) = \begin{cases} \frac{14.6-x}{14.6-5}; & \text{when } 5 \leq x \leq 14.6 \\ 1; & \text{when } x \leq 5 \\ 0; & \text{when } x \geq 14.6 \end{cases}$$

5. **Total hardness:** Total hardness refers to the concentration of calcium and magnesium ions in water. The left-open fuzzy number signifies that higher hardness levels are more acceptable for certain uses:

$$\mu_{\beta_5}(x) = \begin{cases} \frac{x-0}{300-0}; & \text{when } 0 \leq x \leq 300 \\ 1; & \text{when } x \geq 300 \end{cases}$$

6. **Total alkalinity:** Total alkalinity represents the water's capacity to neutralize acids, which is crucial for maintaining stable pH levels. The left-open fuzzy number emphasizes the importance of higher alkalinity values:

$$\mu_{\beta_6}(x) = \begin{cases} \frac{x-0}{200-0}; & \text{when } 0 \leq x \leq 200 \\ 1; & \text{when } x \geq 200 \end{cases}$$

7. **Total dissolved solid:** Total dissolved solids indicate the overall concentration of dissolved substances in water. The left-open fuzzy number captures the significance of lower TDS levels for water quality:

$$\mu_{\beta_7}(x) = \begin{cases} \frac{x-0}{500-0}; & \text{when } 0 \leq x \leq 500 \\ 1; & \text{when } x \geq 500 \end{cases}$$

8. **Calcium:** Calcium levels affect water hardness and aquatic life. The left-open fuzzy number suggests that higher calcium concentrations are beneficial within certain limits:

$$\mu_{\beta_8}(x) = \begin{cases} \frac{x-0}{75-0}; & \text{when } 0 \leq x \leq 75 \\ 1; & \text{when } x \geq 75 \end{cases}$$

9. **Magnesium:** Magnesium (Mg) is an essential nutrient for aquatic life and plays a significant role in various biological processes. The membership function for magnesium concentration is defined as:

$$\mu_{\beta_9}(x) = \begin{cases} \frac{x-0}{50-0}; & \text{when } 0 \leq x \leq 50 \\ 1; & \text{when } x \geq 50 \end{cases}$$

This function indicates that magnesium concentrations up to 50 mg/L are considered ideal, with the membership function remaining at 1 for any values above this threshold. Higher magnesium concentrations can enhance water quality but may also indicate potential sources of pollution, affecting the overall health of aquatic ecosystems.

10. **Turbidity:** Turbidity is a measure of the cloudiness or haziness of water, primarily caused by suspended particles. It is an important indicator of water quality, influencing light penetration and photosynthesis in aquatic environments. The membership function for turbidity is defined as:

$$\mu_{\beta_{10}}(x) = \begin{cases} \frac{x-0}{5-0}; & \text{when } 0 \leq x \leq 5 \\ 1; & \text{when } x \geq 5 \end{cases}$$

This indicates that turbidity levels up to 5 NTU (Nephelometric Turbidity Units) are acceptable, with the membership

function remaining at 1 for turbidity values above this threshold. Increased turbidity can negatively affect aquatic life and reduce water clarity, impacting photosynthesis and habitat quality.

After establishing fuzzy membership functions for each of the GWQPs and considering the associated weight ϖ , the crisp data summaries of the GWQPs are transformed into FSSs (ψ, P, ϖ) , (φ, P, ϖ) , and (σ, P, ϖ) . These fuzzy soft sets capture the relationship between the GWQPs and their fuzzy membership values while accounting for the importance (weight) of each parameter. The corresponding ϖ -score $\Omega_{\varpi}(\alpha_i)$ for each sample station $\alpha_i \in S$ is provided in Tables 6, 7, and 8. These tables showcase how the fuzzy soft sets and the ϖ -scores reflect the degree of water quality at each sampling station, with the weights applied to emphasize the influence of certain parameters on the overall assessment.

4. Detailed result analysis of groundwater quality ϖ -scores

In this section, we discuss the detailed result analysis of groundwater quality ϖ -scores across different seasons. The seasonal variations in physicochemical parameters and their impact on the overall water quality indices are evaluated to understand the temporal changes in groundwater quality for drinking purposes.

4.1. Pre-monsoon analysis

During the pre-monsoon period, groundwater quality is generally poor across all sampling stations. The ϖ -scores range from approximately 0.883325 to 0.956557, indicating high levels of contaminants due to low recharge rates and higher evaporation. This period sees the concentration of pollutants as water

Table 6. WFSS (ψ, P, ϖ) representation of GWQPs for the pre-monsoon season including corresponding ϖ -scores.

S	β_1	β_2	β_3	β_4	β_5	β_6	β_7	β_8	β_9	β_{10}	ϖ -score
	0.118	0.004	1	0.2	0.002	0.005	0.002	0.013	0.02	0.2	
α_1	1	0.46	1	0.958	0.08	0.675	0.36	0.27	0.7	0.72	0.944504
α_2	0.6	0.50	1	0.979	0.09	0.650	0.34	0.33	0.8	0.74	0.921355
α_3	0.1	0.52	1	1	0.1	0.700	0.37	0.40	0.9	0.7	0.883325
α_4	1	0.54	1	0.969	0.11	0.625	0.32	0.47	1	0.76	0.956557
α_5	0.9	0.48	1	0.990	0.12	0.725	0.38	0.53	1	0.66	0.939664
α_6	0.5	0.44	1	0.948	0.13	0.750	0.40	0.60	1	0.68	0.907270
α_7	0.3	0.42	1	0.938	0.14	0.800	0.42	0.67	1	0.64	0.886515
α_8	1	0.52	1	0.917	0.15	0.850	0.44	0.73	1	0.78	0.955499
α_9	1	0.48	1	0.927	0.16	0.775	0.39	0.80	1	0.72	0.949293
α_{10}	1	0.46	1	0.906	0.17	0.700	0.34	0.87	1	0.74	0.949405

Table 7. WFSS (φ, P, ϖ) representation of GWQPs for the monsoon season including corresponding ϖ -scores.

S	β_1 0.118	β_2 0.004	β_3 1	β_4 0.2	β_5 0.002	β_6 0.005	β_7 0.002	β_8 0.013	β_9 0.02	β_{10} 0.2	ϖ -score
$\mathbf{s}\alpha_1$	0.8	0.48	1	0.980	0.064	0.595	0.34	0.20	0.6	0.68	0.925002
$\mathbf{s}\alpha_2$	0.3	0.44	1	0.969	0.076	0.610	0.36	0.27	0.7	0.74	0.895391
$\mathbf{s}\alpha_3$	1	0.50	1	0.938	0.086	0.725	0.38	0.33	0.8	0.78	0.951692
$\mathbf{s}\alpha_4$	0.2	0.52	1	0.927	0.096	0.760	0.40	0.40	0.9	0.70	0.881760
$\mathbf{s}\alpha_5$	0.9	0.48	1	0.948	0.102	0.775	0.42	0.47	1	0.68	0.936540
$\mathbf{s}\alpha_6$	0.5	0.46	1	1	0.112	0.800	0.44	0.53	1	0.72	0.918692
$\mathbf{s}\alpha_7$	0.3	0.42	1	0.917	0.124	0.860	0.39	0.60	1	0.62	0.880824
$\mathbf{s}\alpha_8$	1	0.52	1	0.927	0.136	0.775	0.36	0.67	1	0.60	0.932901
$\mathbf{s}\alpha_9$	0.6	0.50	1	0.938	0.148	0.705	0.32	0.73	1	0.64	0.909432
$\mathbf{s}\alpha_{10}$	0.5	0.46	1	0.948	0.160	0.650	0.28	0.80	1	0.70	0.911106

Table 8. WFSS (σ, P, ϖ) representation of GWQPs for the post-monsoon season including corresponding ϖ -scores.

S	β_1 0.118	β_2 0.004	β_3 1	β_4 0.2	β_5 0.002	β_6 0.005	β_7 0.002	β_8 0.013	β_9 0.02	β_{10} 0.2	ϖ -score
$\mathbf{s}\alpha_1$	1	0.440	1	0.979	0.068	0.670	0.346	0.28	0.66	0.72	0.946661
$\mathbf{s}\alpha_2$	0.5	0.468	1	0.948	0.078	0.725	0.364	0.36	0.82	0.64	0.897737
$\mathbf{s}\alpha_3$	0.2	0.452	1	0.906	0.088	0.810	0.382	0.41	0.94	0.68	0.877064
$\mathbf{s}\alpha_4$	0.3	0.496	1	0.917	0.098	0.885	0.366	0.47	1	0.66	0.885068
$\mathbf{s}\alpha_5$	0.8	0.508	1	0.979	0.106	0.935	0.420	0.63	1	0.64	0.929763
$\mathbf{s}\alpha_6$	0.3	0.496	1	0.958	0.114	0.895	0.404	0.60	1	0.70	0.896608
$\mathbf{s}\alpha_7$	0.2	0.524	1	0.927	0.124	0.585	0.326	0.67	1	0.76	0.892347
$\mathbf{s}\alpha_8$	1	0.480	1	0.948	0.134	0.645	0.256	0.73	1	0.78	0.958449
$\mathbf{s}\alpha_9$	0.6	0.500	1	0.938	0.144	0.605	0.278	0.84	1	0.72	0.920198
$\mathbf{s}\alpha_{10}$	0.3	0.476	1	0.990	0.154	0.665	0.264	0.87	1	0.74	0.907145

levels drop, which results in poorer water quality. The lack of dilution and higher rates of extraction during this time contribute significantly to the elevated ϖ -scores, signalling that the water quality is at its lowest.

4.2. Monsoon analysis

In the monsoon period, the ϖ -scores show some improvement, with values ranging from about 0.880824 to 0.951692. This slight improvement is attributed to the dilution effect caused by heavy rainfall, which increases water volumes and reduces the concentration of contaminants. However, the improvement is not substantial enough to change the overall classification from poor to good quality. The continuous input of fresh rainwater helps to dilute some of the contaminants, but the presence of surface runoff can still introduce pollutants into the groundwater system.

4.3. Post-monsoon analysis

During the post-monsoon period, ϖ -scores again reflect poor water quality, with values ranging from roughly 0.877064 to 0.958449. The scores are quite similar to those in the pre-monsoon period, indicating that the quality of groundwater does not significantly improve post-monsoon. The slight variations in scores can be due to the settling of contaminants and reduced but ongoing agricultural runoff. The period sees stabilized water levels but still carries the accumulated effects of contaminants from the previous months.

The monsoon period shows a slight improvement in groundwater quality compared to the pre-monsoon period. This improvement is primarily due to the dilution effect of increased rainfall, which helps to lower the concentration of pollutants. However, the introduction of surface runoff during heavy rains can still introduce new contaminants. The post-monsoon period

does not show significant improvement over the monsoon period. The slight decline or stabilization in water quality scores indicates that while the recharge from the monsoon helps maintain water levels, the settling of particles and continuing urbanization and anthropogenic activities keep the quality poor. Throughout the year, groundwater quality remains consistently poor, with only minor improvements during the monsoon period. This suggests that factors such as continuous contamination sources, inadequate dilution during non-rainy periods, and ineffective natural filtration are contributing to the persistently poor water quality.

The analysis of ϖ -scores across different periods reveals that groundwater quality is generally poor regardless of the season. The monsoon period provides a brief improvement due to dilution, but this is not sufficient to ensure good water quality. Effective measures, including continuous monitoring, pollution control, and sustainable water management practices, are essential to address the underlying causes of contamination and improve groundwater quality throughout the year.

5. Ranking of sampling stations according to ϖ -scores in each season

Based on the provided ϖ -scores, here are the rankings of the sampling stations for pre-monsoon, monsoon, and post-monsoon periods (Table 9). Stations are ranked from best to worst groundwater quality, with lower ϖ -scores indicating better quality.

5.1. Summary of Rankings

Pre-Monsoon: Station 7 has the best quality, while Station 4 has the worst.

Monsoon: Station 7 has the best quality, while Station 3 has the worst.

Post-Monsoon: Station 3 again has the best quality, while Station 8 has the worst.

5.2. Overall Analysis

Best stations across seasons: Station 7 generally performs well, ranking highest in both pre-monsoon and post-monsoon periods.

Worst stations across seasons: Stations 4 and 8 consistently rank among the lowest across different seasons, indicating persistent issues with water quality.

This ranking provides a clear view of which sampling stations require more attention and intervention to improve groundwater quality.

6. Comparative Analysis of Water Quality Assessment Models

Groundwater quality assessment is critical for sustainable water resource management and public health. Various water quality assessment models have been developed to evaluate contamination levels, each with its own methodology, sensitivity, and classification criteria. In this study, we compare the Canadian Council of Ministers of the Environment (CCME) Water Quality Index (WQI), Brown's WQI (1970), and the proposed ϖ -score model for groundwater quality evaluation. This comparison provides insights into seasonal variations and highlights differences in quality ratings, emphasizing their significance in environmental planning and pollution control.

6.1. Overview of Water Quality Indices

6.1.1. Brown et al. (1970) WQI

- One of the earliest models for water quality assessment.
- Uses a weighted sum of multiple water quality parameters.
- Provides a single composite score to represent overall quality.
- Highly stringent in evaluating pollution, often classifying water as very poor when contamination is even slightly above acceptable limits.
- Useful for assessing the necessity of water treatment measures before consumption.

6.1.2. Canadian Council of Ministers of the Environment (CCME) WQI (2001)

- Developed as a standardized tool for assessing aquatic ecosystem health.
- Uses a fuzzy logic-based mathematical formula to determine water quality.
- Classifies water into five categories: Excellent, Good, Fair, Marginal, and Poor based on scope (number of parameters failing), frequency (frequency of failure), and amplitude (extent of failure).
- More flexible than Brown's WQI and often provides a less strict classification of water quality.

6.1.3. Proposed ϖ -Score Model

- A novel model developed to address seasonal variations and site-specific contamination.
- Uses a fuzzy multi-criteria decision-making approach that integrates expert opinions, uncertainty, and the weighted

importance of different water quality parameters.

- Designed to offer a more adaptive assessment, particularly for highly variable groundwater quality conditions.
- Aligns closely with Brown's WQI in being more conservative in quality assessment.

6.2. Seasonal Variations in Water Quality Assessments

The assessment of water quality across different seasons provides critical insights into how climatic and environmental factors influence groundwater contamination. Tables 9, 10 and 11 present the rankings for water quality across pre-monsoon, monsoon, and post-monsoon periods using the three models.

6.2.1. Pre-Monsoon Season

- ϖ -score model indicates poor groundwater quality with high contamination levels due to low recharge rates, increased evaporation, and pollutant concentration.
- Brown WQI classifies the water as very poor, emphasizing the need for treatment before usage.

- CCME WQI gives slightly better results, classifying the water as marginal to fair, indicating frequent impairments but slightly more optimistic compared to Brown's model.

The spatial distribution of water quality across various sampling points during the pre-monsoon season is visually represented in Figures 3(a), 3(b), and 3(c), corresponding respectively to the $\mathfrak{B}$ -model, Brown WQI, and CCME WQI.

6.2.2. Monsoon Season

- All three models show a slight improvement in water quality due to the dilution effect of rainfall.
- ϖ -score model still classifies groundwater quality as poor but acknowledges a minor improvement.
- Brown WQI remains highly conservative, rating the water as very poor, indicating that despite dilution, surface runoff introduces new pollutants.
- CCME WQI provides a more moderate assessment, classifying most locations in the fair category, reflecting its less stringent criteria.

Table 9. Ranking of groundwater sampling stations according to ϖ -scores.

Seasons	Best optimal choice	Ranking according to good quality
Pre-monsoon	$s\alpha_7$	$s\alpha_7 \gg s\alpha_3 \gg s\alpha_6 \gg s\alpha_2 \gg s\alpha_5 \gg s\alpha_1 \gg s\alpha_9 \gg s\alpha_{10} \gg s\alpha_8 \gg s\alpha_4$
Monsoon	$s\alpha_7$	$s\alpha_7 \gg s\alpha_4 \gg s\alpha_2 \gg s\alpha_9 \gg s\alpha_{10} \gg s\alpha_6 \gg s\alpha_1 \gg s\alpha_8 \gg s\alpha_5 \gg s\alpha_3$
Post-monsoon	$s\alpha_3$	$s\alpha_3 \gg s\alpha_4 \gg s\alpha_7 \gg s\alpha_6 \gg s\alpha_2 \gg s\alpha_{10} \gg s\alpha_9 \gg s\alpha_5 \gg s\alpha_1 \gg s\alpha_8$

Table 10. Ranking of groundwater sampling stations according to Brown Water Quality index.

Seasons	Best optimal choice	Ranking according to good quality
Pre-monsoon	$s\alpha_{10}$	$s\alpha_{10} \gg s\alpha_4 \gg s\alpha_6 \gg s\alpha_8 \gg s\alpha_1 \gg s\alpha_7 \gg s\alpha_5 \gg s\alpha_2 \gg s\alpha_9 \gg s\alpha_3$
Monsoon	$s\alpha_6$	$s\alpha_6 \gg s\alpha_8 \gg s\alpha_1 \gg s\alpha_7 \gg s\alpha_5 \gg s\alpha_9 \gg s\alpha_2 \gg s\alpha_{10} \gg s\alpha_4 \gg s\alpha_3$
Post-monsoon	$s\alpha_5$	$s\alpha_5 \gg s\alpha_4 \gg s\alpha_1 \gg s\alpha_{10} \gg s\alpha_3 \gg s\alpha_9 \gg s\alpha_6 \gg s\alpha_2 \gg s\alpha_7 \gg s\alpha_8$

Table 11. Ranking of groundwater sampling stations according to CCME Water Quality index.

Seasons	Best optimal choice	Ranking according to good quality
Pre-monsoon	$s\alpha_{10}$	$s\alpha_{10} \gg s\alpha_4 \gg s\alpha_6 \gg s\alpha_8 \gg s\alpha_1 \gg s\alpha_7 \gg s\alpha_5 \gg s\alpha_2 \gg s\alpha_9 \gg s\alpha_3$
Monsoon	$s\alpha_6$	$s\alpha_6 \gg s\alpha_8 \gg s\alpha_1 \gg s\alpha_7 \gg s\alpha_5 \gg s\alpha_2 \gg s\alpha_9 \gg s\alpha_{10} \gg s\alpha_4 \gg s\alpha_3$
Post-monsoon	$s\alpha_5$	$s\alpha_5 \gg s\alpha_4 \gg s\alpha_1 \gg s\alpha_{10} \gg s\alpha_9 \gg s\alpha_3 \gg s\alpha_6 \gg s\alpha_2 \gg s\alpha_7 \gg s\alpha_8$

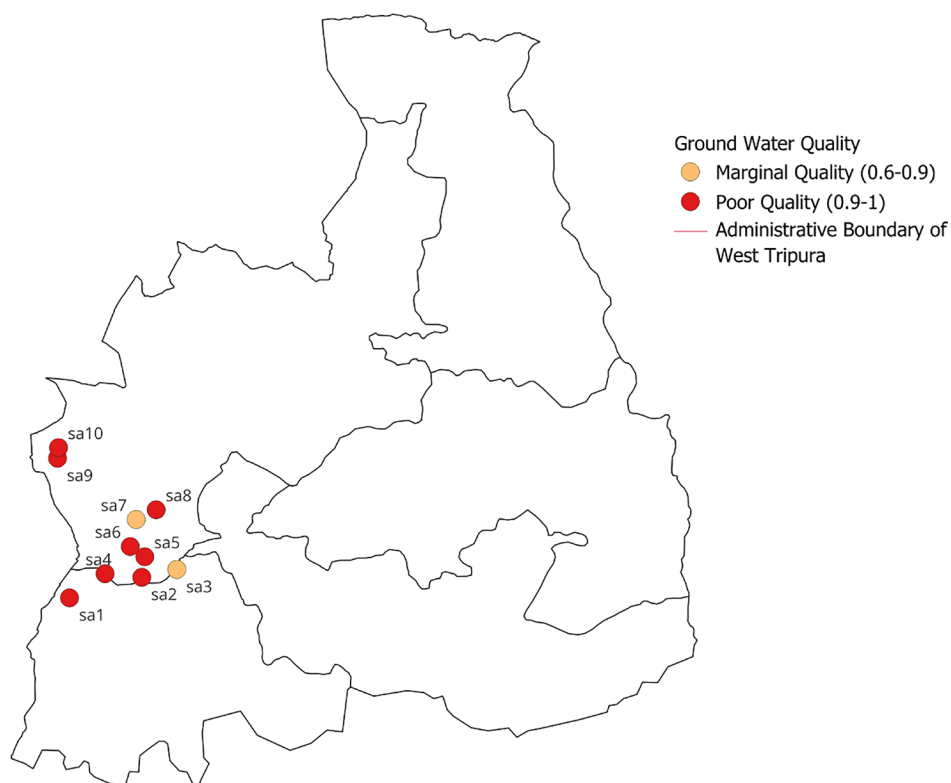


Figure 3(a). Ground water quality in pre-monsoon as per WFSS based 3-model in different water sampling points.

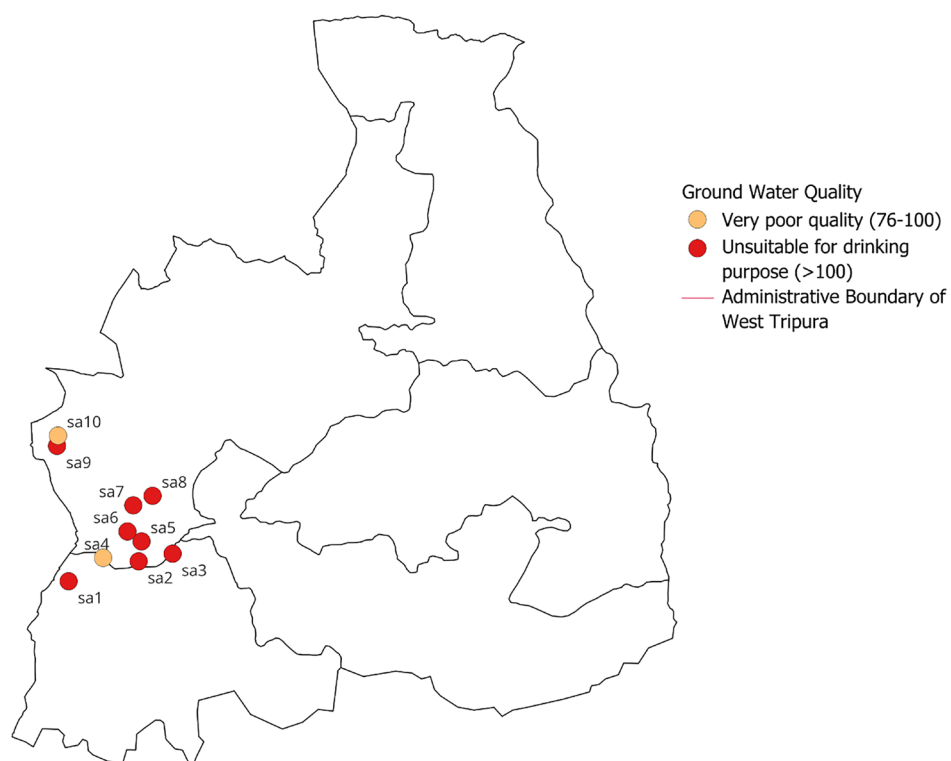


Figure 3(b). Ground water quality in pre-monsoon as per Brown WQI in different water sampling points.

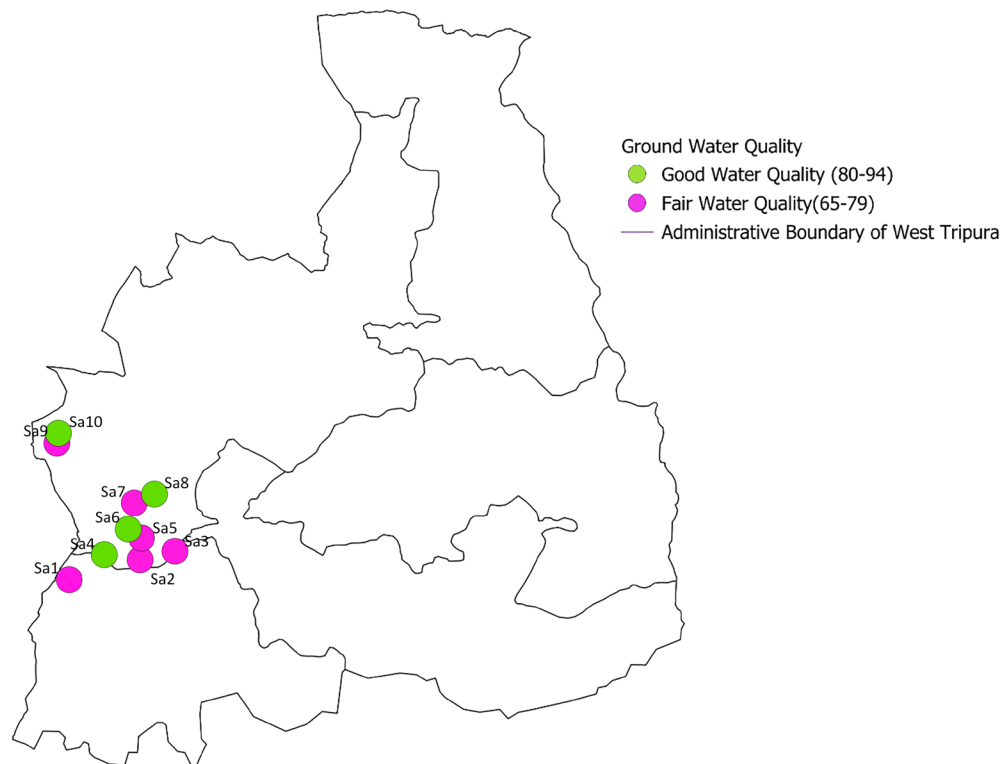


Figure 3(c). Ground water quality in pre-monsoon as per CCME WQI in different water sampling points.

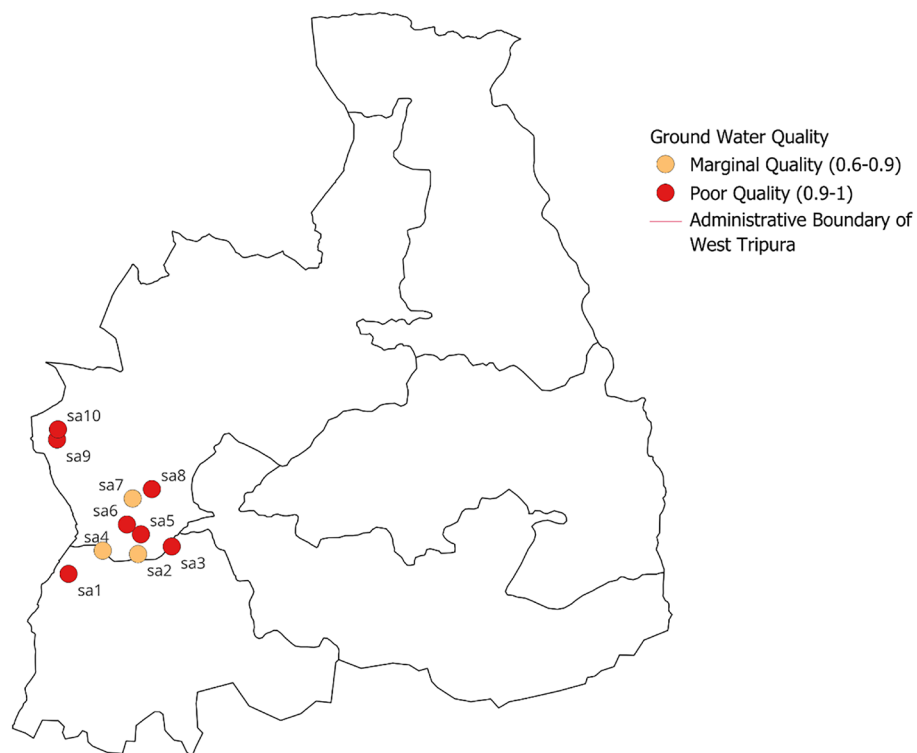


Figure 4(a). Ground water quality in monsoon as per WFSS based $\mathfrak{B}$ -model in different water sampling points.

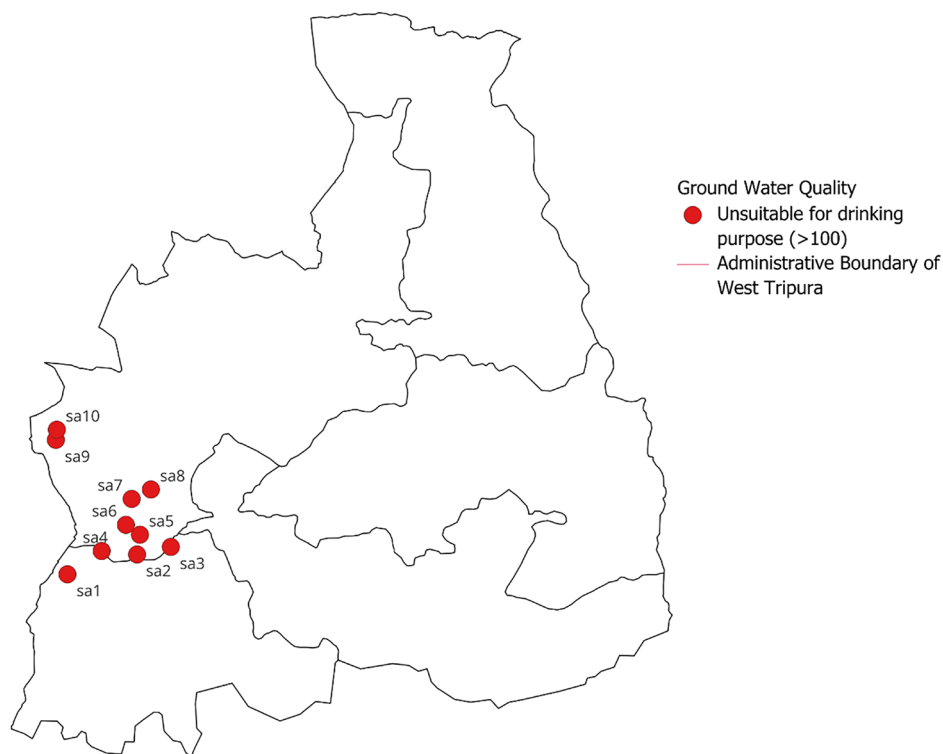


Figure 4(b). Ground Water Quality in Monsoon as per Brown WQI in Different Water Sampling Points.

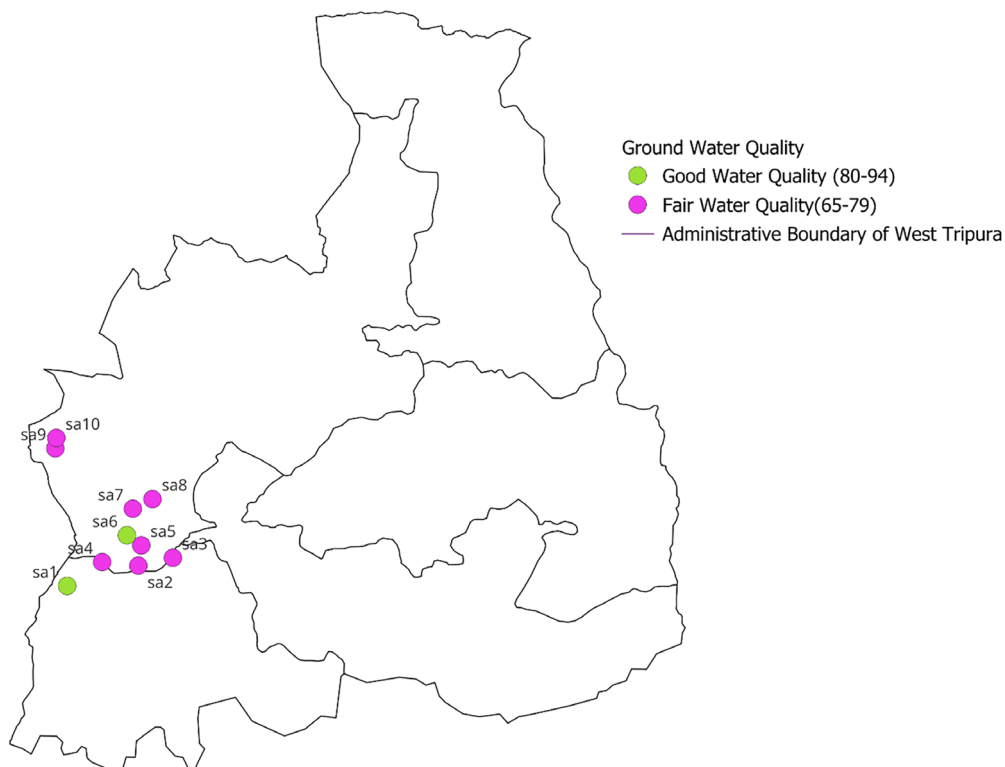


Figure 4(c). Ground Water Quality in Monsoon as per CCME WQI in Different Water Sampling Points.

Figures 4(a), 4(b), and 4(c) show the groundwater quality at different locations during the monsoon season, as measured by the WFSS-based $\mathfrak{B}$ -model in 4(a), Brown WQI in 4(b), and CCME WQI in 4(c), clearly comparing how each method rates the water quality.

6.2.3. Post-Monsoon Season

- $\mathfrak{w}$ -score model and Brown WQI indicate a return to poor quality, similar to pre-monsoon levels.
- CCME WQI gives better scores, rating water as fair to good at some locations.
- The minor improvement noted across models is likely due to settling of suspended solids and reduced urban runoff. However, agricultural runoff and anthropogenic activities continue to degrade quality, leading to persistent contamination.

Figures 5(a), 5(b), and 5(c) show groundwater quality at different locations during the post-monsoon season, as evaluated by the WFSS-based $\mathfrak{B}$ -model in 5(a), Brown WQI in 5(b), and CCME WQI in 5(c), highlighting how each method reflects changes in water quality after the monsoon.

6.3. Comparative Analysis of Model Sensitivity

1. Brown’s WQI is the most stringent and sensitive model, categorizing water quality as very poor in most cases. This suggests that even minor pollution levels significantly impact the final rating, making it highly useful for identifying critical pollution hotspots and emphasizing preventative water treatment measures.
2. CCME WQI provides a more balanced evaluation by considering scope, frequency, and amplitude of contamination. It tends to classify water less severely than Brown’s model, indicating that it tolerates minor exceedances in pollutant levels. This model is useful for regulatory compliance and general water resource management.
3. The $\mathfrak{w}$ -score model aligns more with Brown’s strin-

gent classification, reflecting significant contamination concerns across all seasons. Unlike Brown’s WQI, however, it incorporates expert assessments and a fuzzy decision-making approach, making it more adaptive to site-specific conditions. This model is beneficial for targeted groundwater management interventions in urban areas.

6.4. Implications for Groundwater Management

- Brown’s WQI suggests that aggressive treatment measures are required before groundwater use, reinforcing the need for immediate pollution control interventions.
- CCME WQI, while more moderate, still indicates that groundwater is frequently impaired, requiring regular monitoring and long-term pollution management strategies.
- The $\mathfrak{w}$ -score model highlights the importance of seasonal variations, indicating that groundwater contamination is persistent, requiring continuous monitoring rather than seasonal interventions.

The comparative analysis of these models highlights their strengths and limitations in evaluating groundwater quality. Brown’s WQI is highly stringent, making it useful for identifying pollution hotspots but sometimes overly restrictive. CCME WQI provides a more flexible assessment, making it useful for broader environmental monitoring. The $\mathfrak{w}$ -score model aligns more closely with Brown’s WQI but integrates fuzzy decision-making techniques, making it a more adaptive and insightful tool for site-specific water management.

The choice of an appropriate water quality index should depend on the specific water management objectives. If the goal is a highly conservative pollution assessment, Brown’s WQI is suitable. If a general regulatory framework is needed, CCME WQI is appropriate. However, for detailed groundwater quality assessment in urban environments with complex pollution sources, the $\mathfrak{w}$ -score model offers the best balance between strict evaluation and adaptive decision-making. The key comparative findings of Brown WQI, CCME WQI, and the $\mathfrak{w}$ -score model across different seasons are summarized in Table 12.

Table 12. Summary of Comparative Findings.

Model	Pre-Monsoon Rating	Monsoon Rating	Post-Monsoon Rating	Sensitivity to Pollution	Best Use Case
Brown WQI (1970)	Very Poor	Very Poor	Very Poor	Highly sensitive (strictest)	Critical pollution hotspot identification
CCME WQI (2001)	Marginal - Fair	Fair	Fair - Good	Moderately sensitive (more forgiving)	General water management and policy
$\mathfrak{w}$ -Score Model	Poor	Poor	Poor	Adaptive & conservative	Site-specific groundwater quality monitoring

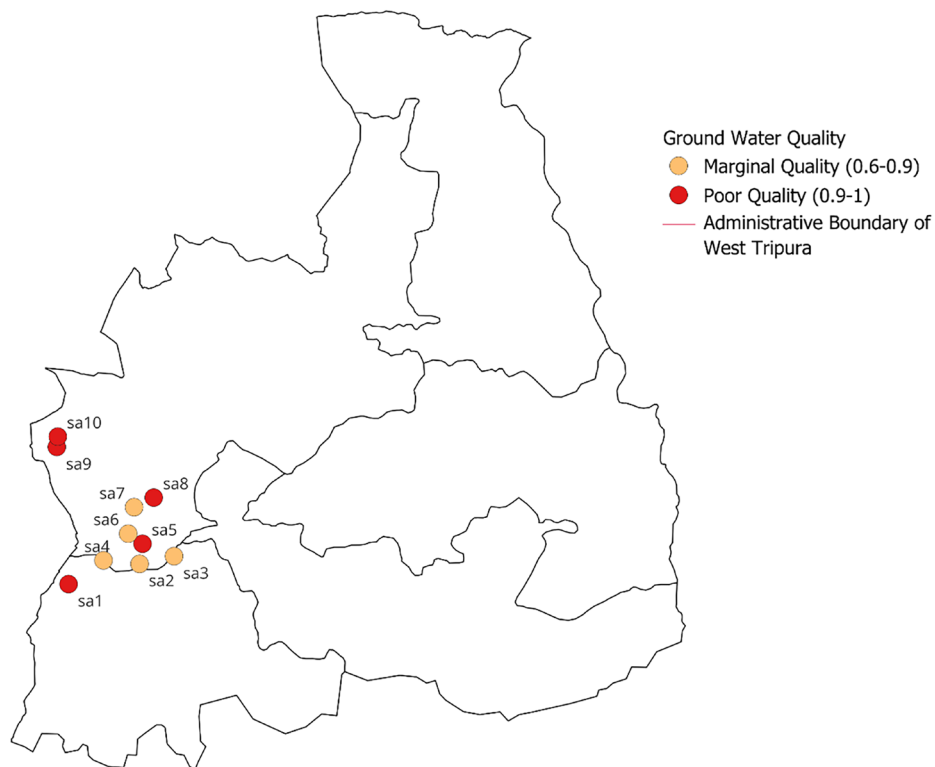


Figure 5(a). Ground water quality in post-monsoon as per WFSS based 3-model in different water sampling points.

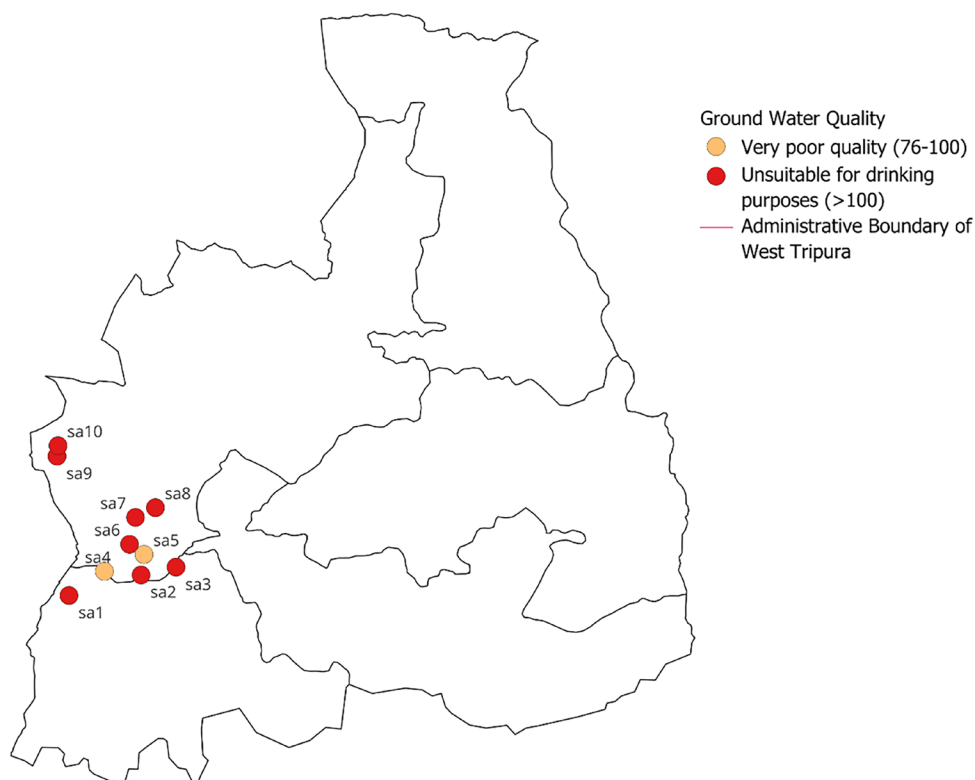


Figure 5(b). Ground Water Quality in Post- Monsoon as per Brown WQI in Different Water Sampling Points.



Figure 5(c). Ground Water Quality in Post- Monsoon as per CCME WQI in Different Water Sampling Points.

7. Conclusions

This study introduces an innovative weighted fuzzy soft set-based approach, known as the $\mathfrak{B}$ -model, for groundwater pollution source identification and risk assessment in urban areas. This pioneering methodology provides a refined and adaptable framework for analyzing water contamination, particularly in rapidly urbanizing environments like Agartala. The novelty of this research lies in its integration of weighted fuzzy soft set theory with a multi-criteria decision-making algorithm to calculate pollution scores. This integration facilitates a nuanced evaluation of groundwater quality across different seasons while effectively capturing the inherent uncertainties in environmental data. Such an approach is crucial for understanding the multifaceted impacts of urbanization and industrialization on groundwater resources.

The findings of this study highlight the ongoing challenges regarding groundwater quality in Agartala, with the most severe contamination levels observed during the pre-monsoon season. During this time, reduced water recharge coupled with increased evaporation exacerbates pollutant concentrations. Although the monsoon season provides some relief through dilution from rainfall, the overall improvements in water quality are insufficient to meet acceptable standards. The application of the weighted fuzzy

soft set-based MCDM model in groundwater quality assessment, as demonstrated here, reinforces the growing consensus on the necessity of advanced analytical tools for effective environmental management and decision-making.

Future research should aim to expand the capabilities of the $\mathfrak{B}$ -model by incorporating real-time data from environmental sensors, thereby enhancing its predictive power and allowing for dynamic assessments of groundwater quality. Additionally, exploring advanced machine learning algorithms, such as deep learning techniques, could further improve the accuracy of pollution predictions generated by the $\mathfrak{B}$ -model. It is equally important to investigate the socio-economic implications of groundwater quality degradation, considering its potential impacts on public health and local economies. Interdisciplinary research that integrates hydrology, data science, and urban planning will provide a holistic approach to addressing the environmental challenges associated with rapid urbanization.

The results and methodologies developed in this study are applicable to similar environmental challenges faced by other rapidly urbanizing cities worldwide. The $\mathfrak{B}$ -model is versatile and can be adapted to tackle a wide array of environmental issues, including air pollution, soil contamination, and surface water quality assessments. Its capacity to manage uncertainty

and synthesize diverse datasets positions it as a valuable tool for policymakers and urban planners charged with managing natural resources in complex and dynamic environments. By offering a systematic and data-driven approach to environmental monitoring, the $\mathfrak{B}$ -model can inform the development of targeted interventions, ensuring that the most vulnerable areas receive the attention and resources necessary for sustainable groundwater management and pollution mitigation.

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Ethical approval: Any of the authors did not conduct any human or animal experiments for this publication.

Conflict of Interest: The authors declare that they have no conflict of interest regarding the publication of this manuscript.

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Estudio hidrogeofísico para determinar la vulnerabilidad intrínseca y la capacidad protectora del acuífero de San Agustín Texcaltitlán, Estado de México

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Abstract

In this study, the hydrogeophysical investigation of the San Agustín Texcaltitlán aquifer, municipality of Tenancingo, State of Mexico, was carried out to determine the intrinsic parameters such as porosity (n) and vertical hydraulic conductivity (K_v) by granulometric analysis, the variation of the water level was measured in wells and the thickness (h) of the strata of the unsaturated and saturated zone was determined using the Vertical Electrical Sounding (VES) method and Schlumberger electrical resistivity array (ρ). The objective was to determine and zone the intrinsic vulnerability to groundwater contamination by anthropogenic sources with the AVI method, which defines the hydraulic resistance (C) and the protective capacity of the aquifer with the ICE method, from the longitudinal unitary conductance (S), with the geoelectrical method of the VES. Both methods only require two parameters, K_v , and the thickness h of the layers that constitute the non-saturated zone (NSZ), respectively. The data of 20 VES acquired were interpreted with the iterative computer program Interpex IX1D. The results obtained indicate that the porosity of the NSZ is 0.36-0.40 and the vertical hydraulic conductivity is 6-15 m/d, obtained with the empirical formula of Slitcher. From 20 VESs performed, 5 to 7 layers were detected for the aquifer system with resistivity values of 10-3,600 ohm-m and variable thicknesses, which were used to calculate the variations in hydraulic resistance (C), giving values of 0.4-6.0 (days) indicating low to high vulnerability, longitudinal conductance (S) and transverse resistance (R), known as Dar Zarrouk parameters, gave values of 0.2-6.0 Ω^{-1} , indicating low to high protection capacity and 1,000-26,000 (ohm-m²), indicating areas of low to high infiltration capacity, respectively. Finally, the conceptual model of hydrogeological functioning of the Texcaltitlán aquifer system was developed.

Key words: water resources, hydraulic conductivity, vulnerability, hydraulic resistance (C), longitudinal conductance (S).

Resumen

En este estudio se llevó a cabo la investigación hidrogeofísica del acuífero de San Agustín Texcaltitlán, municipio de Tenancingo Estado de México, para determinar los parámetros intrínsecos como la porosidad (n) y la conductividad hidráulica vertical (K_v) por análisis granulométrico; se midió la variación del nivel del agua en norias y se determinó el espesor (h) de los estratos de la zona no saturada y saturada empleando el método del Sondeo Eléctrico Vertical (SEV) y el arreglo Schlumberger de resistividad eléctrica (ρ). El objetivo consistió en determinar y zonificar la vulnerabilidad intrínseca a la contaminación del agua subterránea por fuentes antropogénicas con el método AVI, que define la resistencia hidráulica (C) y la capacidad protectora del acuífero con el método ICE, a partir de la conductancia longitudinal unitaria (S), con el método geoeléctrico del SEV. Ambos métodos solo requieren de dos parámetros, la K_v y el espesor h de las capas que constituyen la zona no saturada (ZNS), respectivamente. Los datos de 20 SEV adquiridos se interpretaron con el programa de computadora iterativo Interpex IX1D. Los resultados obtenidos indican que la porosidad de la ZNS es de 0.36-0.40 y la conductividad hidráulica vertical de 6-15 m/d, obtenida con la fórmula empírica de Slitcher. De 20 SEV realizados, se detectaron de 5 a 7 capas para el sistema acuífero con valores de la resistividad de 10-3,600 ohm-m y espesores variables, que se utilizaron para calcular las variaciones de la resistencia hidráulica (C), dando valores de 0.4-6.0 (días) indicando baja a alta vulnerabilidad, la conductancia longitudinal (S) y la resistencia transversal (R), conocidos como parámetros de Dar Zarrouk, arrojaron valores de 0.2-6.0 (Ω^{-1}), indicando baja a alta capacidad de protección y de 1,000-26,000 (ohm-m²), indicando zonas de baja a alta capacidad de infiltración, respectivamente. Finalmente, se elaboró el modelo conceptual de funcionamiento hidrogeológico del sistema acuífero de Texcaltitlán.

Palabras clave: recursos hídricos, conductividad hidráulica, vulnerabilidad, resistencia hidráulica (C), conductancia longitudinal (S).

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1. Introducción

El crecimiento no controlado y el desarrollo humano en el Estado de México, conllevan un aumento en las presiones sobre los ecosistemas, en particular sobre los recursos hídricos superficiales y subterráneos en el acuífero de San Agustín Texcaltitlán, municipio de Tenancingo, Estado de México. El aumento de la temperatura y la disminución de la precipitación que se presentan en la región, por los cambios climáticos, dan lugar a una disminución de los recursos hídricos disponibles y a un aumento de las necesidades de agua para consumo humano, para los cultivos de temporal y de riego (Cai *et al.*, 2024; Olivera *et al.*, 2024; Tolimir *et al.*, 2024). Además, las actividades antropogénicas, de cultivo, ganaderas y piscícolas (cría de trucha), han contribuido a la contaminación de los recursos hídricos superficiales y subterráneos como se observó en campo. En consecuencia, se producirá una mayor demanda de agua subterránea y, por lo tanto, los acuíferos se someten a una mayor presión (Rusli *et al.*, 2023; Borowiecka *et al.*, 2024; Mustafa y Mawlood, 2024). El agua subterránea constituye un recurso esencial en las regiones húmedas, que se caracterizan por presentar una marcada variabilidad temporal y espacial en la disponibilidad de los recursos hídricos (Bourmada *et al.*, 2024; Ferreira *et al.*, 2024). Por ello, es muy importante realizar una caracterización integrada de los recursos hídricos subterráneos y evaluar su potencial hidráulico, la vulnerabilidad a la contaminación del agua subterránea y su capacidad de protección por fuentes antropogénicas de acuerdo con la problemática del área de estudio, ya que hay una dependencia mucho mayor del agua subterránea; que se considera de buena calidad, menos contaminada y menos vulnerable a la contaminación que el agua superficial, asociada en mayor intensidad con los efectos del cambio climático de los recursos hídricos (Baig *et al.*, 2023; Aladeboyeje *et al.*, 2024; Cai *et al.*, 2024; Etuk *et al.*, 2022; Loganathan y Sathiyamoorthy, 2024; Sarrazin *et al.*, 2024). Sin embargo, cuando los acuíferos presentan comunicación hidráulica con la superficie del suelo, el agua subterránea puede ser vulnerable a la contaminación proveniente de fuentes superficiales. La capacidad de las capas suprayacentes o zona no saturada (ZNS), para retardar y filtrar los fluidos percolantes que ingresan en la superficie del terreno, es una medida de su capacidad protectora del acuífero. Así, a la capa de la ZNS del acuífero se le ha denominado como la capa protectora del acuífero. Por otro lado, se ha aceptado ampliamente que la conductividad hidráulica (K) de un material del subsuelo disminuye con el aumento de la resistividad (Fatoba *et al.*, 2014). De acuerdo a Alao y Dogara (2018), la evaluación de la capacidad protectora del agua subterránea contra la contaminación superficial, aplicando el método del

Índice de Vulnerabilidad Acuífera (AVI, por su sigla en inglés, Stempvoort *et al.*, 1992) y el método geoeléctrico del índice de la capacidad eléctrica (ICE) (Abdulrazzaq *et al.*, 2020), es una función tanto de la conductividad hidráulica, de la conductancia longitudinal (S), como del espesor de la capa protectora. De acuerdo a la indexación con los métodos AVI e ICE, de áreas que presentan alta vulnerabilidad del agua subterránea, facilitará una mejor gestión del agua subterránea. También, se ha observado que una cubierta del acuífero gruesa y una baja conductividad hidráulica dan como resultado una menor susceptibilidad del acuífero a la contaminación. Por lo tanto, las áreas con bajos niveles de vulnerabilidad del acuífero generalmente tienen valores hidráulicos bajos y alta conductancia longitudinal. Por lo anterior, la amenaza para un acuífero generalmente aumentará si el sistema hidrogeológico no tiene una buena capa protectora. Se trata entonces, de garantizar a la comunidad de San Agustín, Texcaltitlán, que disponga de agua potable e higiénica, para una buena salud y garantizar un desarrollo sostenible de la población.

El término vulnerabilidad de las aguas subterráneas, hace referencia específicamente a las propiedades intrínsecas e inherentes del suelo que determinan la facilidad de contaminación de las aguas subterráneas en forma natural o por actividades humanas antropogénicas (Foster, 1987; Stempvoort *et al.*, 1992; Vrba y Zaporozec, 1994; Aller *et al.*, 1987; George *et al.*, 2024). El término tiene sus inicios de empleo en Europa. Foster *et al.*, (2013) lo define como “la susceptibilidad de un acuífero a que se contamine el agua subterránea debido al impacto de las actividades humanas”; finalmente Civita y De Maio (2004), señalan que la vulnerabilidad intrínseca, es la “probabilidad de infiltración y percolación de líquidos y soluciones acuosas de nutrientes a través de la zona no saturada”. La vulnerabilidad a la contaminación de las aguas subterráneas, se encuentra en función del tipo de contaminantes, ya que cada sustancia se comporta de manera distinta, dependiendo de los parámetros fisicoquímicos y sus relaciones con los componentes del sitio llamada “vulnerabilidad específica” (Duda *et al.*, 2024; Gharchae *et al.*, 2024).

La evaluación de la vulnerabilidad intrínseca se realiza por diferentes métodos tales como el Índice de Vulnerabilidad del Acuífero (AVI, por su sigla en inglés), que permite determinar las zonas de riesgo a la contaminación de un acuífero (Baig *et al.*, 2023; George *et al.*, 2025).

En la literatura existe una variedad de métodos para determinar la vulnerabilidad a la contaminación de un acuífero como DRASTIC, GOD, SINTAX, entre otros (Duijvenbooden, *et al.*, 1987; Foster y Hirata, 1988; Stempvoort *et al.*, 1992, Vrba y Zaporozec, 1994; Civita, y De Maio, 1997), en función de las características hidrogeológicas de una zona y los datos

disponibles. En este estudio, se aplicó el método del Índice de Vulnerabilidad Acuifera (AVI, Stempvoort *et al.*, 1992), ya que es relativamente sencillo y rápido de aplicar, permite una evaluación de la vulnerabilidad intrínseca y tiene una base física mínima, que requiere de sólo dos parámetros, el espesor (h_i) y la conductividad hidráulica vertical (K_{vi}) de los estratos que sobreyacen el nivel freático, que pueden obtenerse de información de pozos existentes, sondeos geofísicos u otros estudios hidrogeológicos rutinarios, lo que reduce la necesidad de trabajo en campo adicional complejo o costoso.

Sin embargo, en el área de estudio solo se cuenta con un pozo que no tiene información y para obtener valores representativos de la conductividad hidráulica (K_v), se empleó el análisis granulométrico utilizando las fórmulas empíricas de Breyer y Schlichter para su estimación (Vukovic y Soro, 1992; Odong, 2008) y emplearlos en el método AVI.

Cabe mencionar, que en el área de estudio solo existe un pozo de bombeo que abastece a la comunidad de San Agustín y no cuenta con información. Bajo esta situación y como es de esperarse, si no se tiene otro tipo de información como de *SEV*, los resultados finales pueden no ser representativos de la totalidad del acuífero, dando lugar a un escenario de alta incertidumbre, es decir, la perforación de un pozo proporciona información de la litología real (arcilla, limo, arena, grava, roca), los espesores reales en un punto y los parámetros hidráulicos de la transmisividad y el coeficiente de almacenamiento, mediante pruebas de bombeo, que solo describen la vecindad inmediata del pozo, ignorando la heterogeneidad del acuífero a mayor escala. Además, no se puede determinar con certeza la ubicación de los límites impermeables como (barreras) o zonas de recarga (ríos, presas), lo que lleva a errores en la predicción del descenso del nivel freático a largo plazo. Los *SEV* realizados cercanos a un pozo permiten asociar los valores de resistividad (ohm-m) con los materiales geológicos reales encontrados en la perforación mediante el proceso de calibración en la inversión geofísica, cuando se cuenta con información del pozo. Sin embargo, se realizaron una serie de 16 Sondeos Eléctricos Verticales (*SEV*) distribuidos espacialmente en diferentes zonas del acuífero, que es una ventaja crucial que permite mitigar estas limitaciones al proporcionar información indirecta del subsuelo, trazando perfiles geoelectrónicos y mapas de contorno, para delimitar la geometría, profundidad y espesor del acuífero en toda la zona de estudio, no solo donde se encuentra el pozo, ya que ayuda a identificar zonas de baja resistividad o si el agua es de mala calidad, si el acuífero se acuña o si hay un cambio en la litología a medida que se alejan del pozo y son de mucha utilidad para identificar los sitios para una nueva perforación y el diseño del pozo. En general, el uso de técnicas geofísicas en superficie no invasivas aumenta significativamente la rentabilidad de una investigación

de aguas subterráneas (Kelly y Mares, 1993).

Las técnicas geoelectricas se utilizan ampliamente para detectar la zona saturada de un acuífero, la vulnerabilidad intrínseca y las zonas protectoras de un acuífero a la contaminación antropogénica con el método del índice de la capacidad eléctrica (ICE) (Abdulrazzaq *et al.*, 2020), mediante los parámetros de segundo orden de Dar Zarrouk, de la resistencia transversal ($T = R_T$) y la conductancia longitudinal (S) llamados así por Maillet (1947). La técnica del sondeo eléctrico vertical (*SEV*) con configuración Schlumberger, es la más eficaz para la investigación de aguas subterráneas. Además, la aplicación de la técnica del *SEV*, es apropiada para mapear el potencial de un acuífero y en la localización de sitios para perforación de pozos y exploración de las aguas subterráneas.

En San Agustín Texcaltitlán, Estado de México, el deterioro de la calidad del agua subterránea se debe principalmente a las actividades agrícolas, ganaderas y domésticas, por la recarga del riego de retorno, la descarga de aguas residuales domiciliarias a los ríos o arroyos y la disminución de la recarga subterránea natural, como entrada principal de agua al acuífero a través de la zona no saturada (ZNS), que, dependiendo de los tiempos de tránsito y materiales geológicos, pueden afectar a la zona saturada (ZS). En condiciones naturales, la calidad del agua subterránea depende del contenido de sales disueltas, de la calidad del agua de recarga, de la litología del subsuelo, de la velocidad de flujo del agua subterránea, de su relación con otros acuíferos y con el agua superficial.

En esta zona se aplican abonos orgánicos en seco (estiércol de vacunos, bovinos, aves de corral, etc.) tradicionalmente en forma manual, para evitar la entrada de organismos patógenos al subsuelo para el cultivo de maíz en San Agustín, Texcaltitlán. Sin embargo, no se cuenta con un procedimiento apropiado de almacenamiento de estos abonos, ya que se acumulan en montones en los corrales o en los campos agrícolas al aire libre, constituyendo una fuente puntual de contaminación al agua, aire y suelo; para posteriormente aplicarlos directamente en el suelo agrícola, esparciéndolos en el terreno, dando lugar a una fuente de contaminación difusa.

En la zona de estudio no se reportan investigaciones sobre la evaluación de los recursos hídricos y de la vulnerabilidad del acuífero. La mayoría de los estudios se enfocan en el acuífero del Valle de Toluca (Franco-Plata, 2002; Garfias *et al.*, 2017); donde aplicaron el método DRASTIC, SIG y simulación numérica, para delimitar nuevas zonas a proteger en un ambiente aluvial que, de contaminarse, la calidad del agua subterránea puede deteriorarse en un tiempo menor a 50 años, identificando que las zonas presentan de baja a muy alta vulnerabilidad. Por otro lado, un estudio en Villa Guerrero (Velázquez-Zepeda, *et al.*, 2017), en una zona dedicada a la floricultura, con el

método SINTACS, donde se indica que los mayores niveles de vulnerabilidad específica se presentaron en el centro del municipio, debido al tipo de unidades hidrogeológicas y, finalmente un estudio en Temascaltepec sobre el riesgo de un acuífero por residuos mineros con un método multicriterio y zonas de protección (Valle-González, 2021), para la protección de fuentes prioritarias de agua subterránea, indicando como fuentes de alta prioridad de protección el socavón de Guadalupe.

Sin embargo, dada la tendencia que se tiene a nivel nacional sobre el uso de los recursos hídricos, los problemas sobre la calidad y disponibilidad de agua son un problema que se ha venido agravando debido al aumento acelerado de la contaminación antropogénica de los cuerpos de agua, susceptibles de servir como fuente de abastecimiento (Romero y Romero, 2020; Adame y Cubero, 2024).

Por lo anterior, los parámetros que determinan la vulnerabilidad intrínseca y la capacidad de protección del acuífero son principalmente el espesor (h_i) de las capas que constituyen la ZNS, la conductividad hidráulica (K_i) y la resistividad eléctrica (ρ_i), respectivamente. Por lo que, el objetivo de este estudio consiste en emplear los índices de susceptibilidad de las capas hidrogeológicas a la vulnerabilidad intrínseca con el método AVI y la capacidad de protección del acuífero con el método geoelectrico del índice de la capacidad eléctrica (ICE) para detectar y categorizar aquellas capas geoelectricas de alta permeabilidad y porosidad (materiales aluviales) que permiten el acceso de agua de lluvia o contaminantes, que atraviesen la capa de suelo y la ZNS hasta alcanzar el acuífero principal y, para elaborar finalmente un modelo conceptual preliminar de funcionamiento hidrogeológico del acuífero de San Agustín Texcaltitlán, en el municipio de Tenancingo, Estado de México.

2. Experimental

2.1. Localización del área de estudio

El poblado de Texcaltitlán, municipio de Tenancingo en el Estado de México, representa el 6% del territorio estatal cubriendo una extensión territorial es de 142.45 km². Se localiza en las últimas estribaciones del Nevado de Toluca, en el Eje Volcánico Transmexicano (EVTM), entre las coordenadas proyectadas UTM $X_{\min} = 399,000$, $X_{\max} = 402,000$ de longitud oeste y $Y_{\min} = 2,090,000$, $Y_{\max} = 2,096,000$ de latitud norte, a una altitud promedio de 2,380 m.s.n.m., limita al norte con Temascaltepec, al sur con Sultepec y Almoloya de Alquisiras, al este con Coatepec de Harinas y al oeste con San Simón de Guerrero y Tejupilco. Cuenta con 33 localidades y una población total de 15,824 habitantes (INEGI, 2009). La zona de estudio seleccionada, se ubica en la parte central del municipio de San

Agustín Texcaltitlán, abarcando las comunidades de San José, San Agustín, San Miguel, Santa María y Cabecera municipal, cubriendo una superficie de 1.1 km², Figura 1.

Se realizó un recorrido de acuerdo al mapa de la geología que aflora la zona de estudio (Figuras 1 y 2), para la toma de muestras de suelo, a una profundidad de 30 a 50 cm excavados con pala, que constituye la capa de suelo y el horizonte A, logrando recolectar 6 muestras y su ubicación se registró mediante un sistema de posicionamiento global (GPS, Garmin 62s). Las muestras de suelo recolectadas se secaron primero al aire y luego se pasaron por una serie de tamices (No. 4, 10, 20, 30, 40, 50, 100, 200, 324, 400 y charola), para su análisis en granulométrico en el laboratorio de Hidrogeología de la UAM-Lerma. Las muestras de suelo se analizaron con base en la Norma Oficial Mexicana NOM-021-SEMARNAT-2000 (SEMARNAT 2002), que establece las especificaciones de fertilidad, salinidad y clasificación de suelos, en sus apartados AS-01 (preparación de la muestra), AS-02 (pH medido en agua) y AS-09 (determinación de la textura del suelo), con el propósito de clasificar los suelos por tipo textural y determinar los parámetros hidráulicos como contenido de humedad (w), la porosidad (n), el rendimiento específico (S_y), así como, estimar el valor de la conductividad hidráulica vertical (K_v), mediante las fórmulas empíricas de Breyer y Schlichter (Vukovic y Soro, 1992; Odong, 2008) y utilizarla con el método AVI. Además, se indican la ubicación de las norias, el pozo de la comunidad y de los sondeos eléctricos verticales (SEV) realizados. Los datos usados en este estudio cubren una superficie de 1.1 km².

2.1.1. Referente geológico

El municipio de Texcaltitlán se localiza en la zona fisiográfica llamada “Sierra Madre del Sur” en el Eje Volcánico Transmexicano (EVTM). Es una región que consiste en una franja de rocas tipo andesita, brecha volcánica, basalto y tobas; correspondientes al periodo terciario y cuaternario, así como materiales piroclásticos (Atlas-T2, 1981; SGM, 2013). Las rocas del terciario son en su gran mayoría volcánicas (ígneas extrusivas intermedias, ácidas y básicas), las cuales cubren discordantemente tanto a las rocas sedimentarias del Cretácico como a las rocas metamórficas del Triásico (Figura 2). De este periodo afloran también rocas sedimentarias continentales (areniscas y conglomerados) que en ocasiones yacen directamente sobre las rocas metamórficas y en otras, lo hacen sobre rocas ígneas extrusivas intermedias (andesíticas). Del Cuaternario existen rocas volcánicas de tipo basáltico que, por sus estructuras bien conservadas, evidencian la actividad volcánica reciente. Estas estructuras se presentan al sureste del municipio de Texcaltitlán hasta los límites con el municipio de Amatepec. También, se encuentran los depósitos aluviales que rellenan los valles de los ríos que drenan hacia la cuenca del Río Balsas (Atlas-T2, 1981). Los sedimentos lacus-

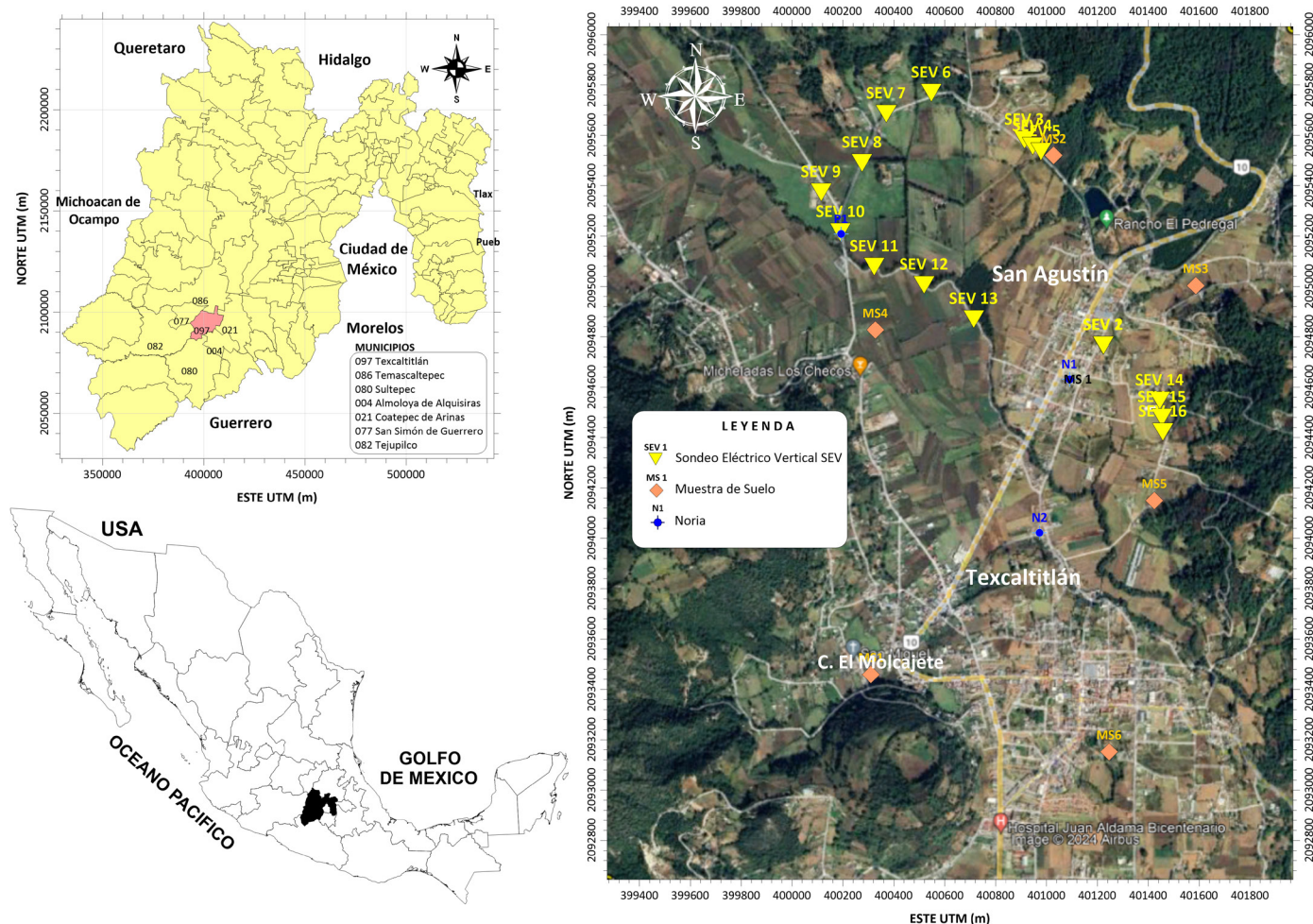


Figura 1. Mapa de la ubicación geográfica del municipio de Texcaltitlán, mostrando la ubicación de las estaciones de SEV (SEV1-SEV16), los sitios de muestreo de suelo para análisis granulométrico (MS1-MS6), las norias (N1-N2) y el Pozo (P1).

tres y aluviales intercalados con materiales clásticos de origen volcánico se presentan en los valles del municipio. El acuífero correspondiente al Valle de Texcaltitlán, está constituido por materiales piroclásticos de cenizas volcánicas, materiales de origen aluvial y lacustre, con un gran porcentaje de arenas y conglomerados, rodeado por un relieve montañoso en una zona de influencia al noreste del volcán Nevado de Toluca (Xinantécatl), que se caracteriza por presentar manantiales naturales y alta humedad, el escurrimiento de los arroyos perenes la Gavia y Palo Seco, entre otros escurrimientos intermitentes locales. En general, las formaciones geológicas que rodean al valle de Texcaltitlán, consisten en grandes y pequeños cerros formados de rocas que fueron arrojadas mediante la erupción del Nevado de Toluca, algunas de estas elevaciones tienen forma de volcán como el Cerro de la Joya y El Molcajete y otros de forma cónica como El Cerro del Tejocote, El Calvario, El Cerrito del Caballito y la cabecera municipal que también está asentada en un cerro.

2.1.2. Hidrología

El municipio de Texcaltitlán forma parte de la región hidrológica del Cutzamala, pertenece a la subcuenca del Río Balsas RH18Gf del Río San Agustín y el Arroyo Palo Seco. El municipio está constituido por seis riachuelos y un río principal (Río San Agustín). Los arroyos que pasan por esta región nacen de los deshielos del Nevado de Toluca y otros que se originan en el cerro de La Gavia al noroeste de San Agustín, estos arroyos unen sus aguas en la comunidad de San Agustín y dan origen al río para continuar su cauce hacia Almoloya de Alquisiras, que de acuerdo con los lugares por los que va pasando recibe varios nombres como; Río de San Agustín, La Gavia, de Venta Morales, de la Cruz Verde, de la Rosita, de Santa María y el Ojo de Agua (Figura 3). En el municipio existen 5 manantiales que abastecen de agua a gran parte de la población (H. Ayuntamiento de Texcaltitlán, 2019).

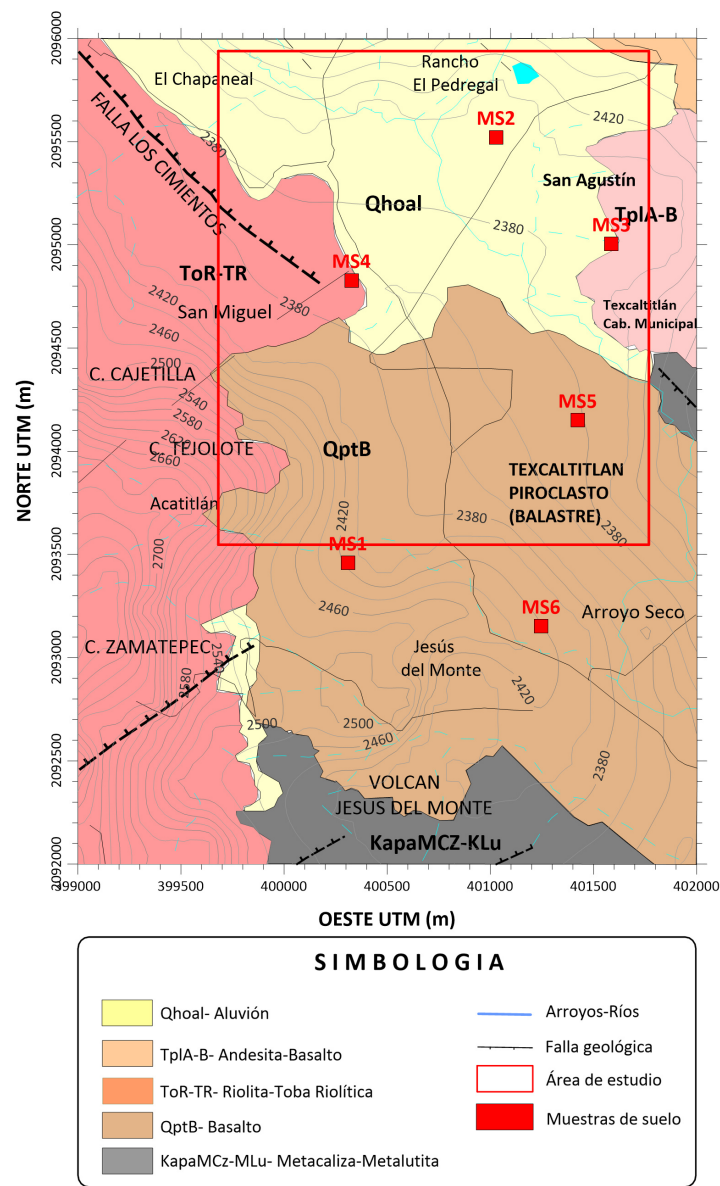


Figura 2. Esquema geol3gico de las rocas que afloran en el municipio de Texcaltitlán, Estado de México.

2.2. Métodos de análisis

2.2.1. Evaluación del Índice de Vulnerabilidad Acu3fera (AVI)

La vulnerabilidad acu3fera se define como la prontitud con la que un acu3fero libre determinado es probable de contaminarse (Estrada *et al.*, 2013). Depende de las características hidr3ulicas de las capas (espesor y conductividad hidr3ulica de las capas), que cubren un acu3fero libre, denominadas capas protectoras (Sendr3s *et al.*, 2023). Las características hidr3ulicas como la porosidad (*n*) y la conductividad hidr3ulica (*K*), se determinaron a partir del análisis granulométrico de muestras de suelo utilizando fórmulas empíricas (Odong, 2008, Fallico *et al.*, 2010). En la

zona de San Agustín, la capa de suelo (arcillo limo-arenoso), puede definirse como la capa protectora que protege al acu3fero subyacente. Las aguas residuales que son descargadas sin ningún tratamiento a los cauces principales (Río San Agustín y Río Palo Seco), pueden percolar e infiltrarse a través de la capa protectora (arcilla con limo y arena) dando lugar a la recarga de agua subterránea y contaminar el acu3fero granular. Por lo tanto, la vulnerabilidad del acu3fero está estrechamente relacionada con la textura de la capa de arcilla heterogénea y la conductividad hidr3ulica, donde la presencia de lentes de arena o limo pueden actuar como una ventana hidr3ulica o zona vulnerable por donde los contaminantes pueden ingresar y filtrarse para alcanzar el nivel freático (Edwards *et al.*, 2022).

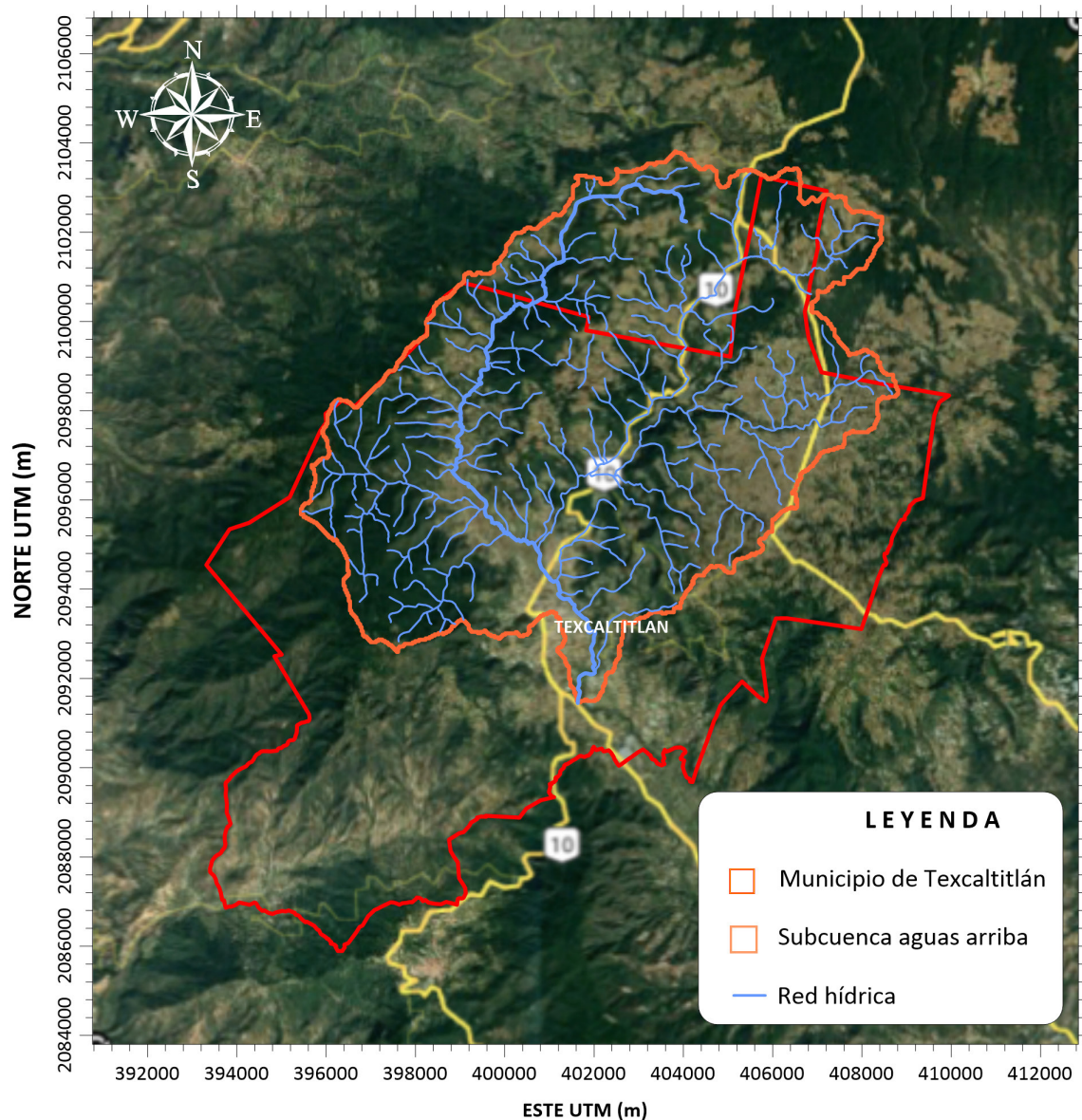


Figura 3. Microcuenca del Río San Agustín y red hidrográfica de Texcaltitlán.

La evaluación de la vulnerabilidad acuífera es una herramienta importante para definir el impacto ambiental de la contaminación antropogénica, para dar un uso sustentable del agua subterránea a escala local o regional (Kirsch y Hinsby, 2007). Es posible utilizar varios métodos para evaluar la vulnerabilidad de los acuíferos como DRASTIC (Aller, *et al.*, 1987), SINTACS (Civita y De Maio 1997, 2004; Kirlas *et al.*, 2022), GOD (Foster, 1988), AVI (Stempvoort, 1992), la Conductividad Eléctrica Integrada (IEC) del método geoelectrico (Sendrós *et al.*, 2023), entre otros, en función del entorno hidrogeológico de la zona de interés y de los datos disponibles. En este estudio se utilizaron dos métodos, el Índice de Vulnerabilidad de los Acuíferos (AVI), que es un método ampliamente utilizado para evaluar la vulnerabilidad de los acuíferos a los contaminantes

superficiales y el método de la Conductividad Eléctrica Integrada (IEC, por su siglas en inglés), denominada como Índice de la Capacidad Eléctrica (ICE) o índice de protección basado en la geofísica (IPG).

El índice AVI es un método para evaluar la vulnerabilidad de acuíferos mediante la resistencia hidráulica (C), determinado por el paso del flujo vertical a través de los distintos materiales de la zona no saturada (ZNS), que sobreyacen al acuífero libre, indicando el tiempo aproximado que le toma atravesar la zona no saturada (Kalinski *et al.*, 1993; Ducci y Sellerino, 2022; Sendrós *et al.*, 2023). La resistencia hidráulica (C) cuantifica la vulnerabilidad del acuífero mediante la ecuación (1):

$$C = \sum_{i=1}^n \frac{h_i}{K_{Vi}} \quad (1)$$

donde, C es la resistencia hidráulica total (en días o años), que sólo requiere de dos parámetros, h_i , el espesor de cada estrato de la zona no saturada al nivel freático (en m) y la K_{vi} , que es la conductividad hidráulica vertical de cada estrato del subsuelo (en m/d). Por lo que, una protección eficaz de un acuífero libre, está garantizada por las capas protectoras con suficiente espesor y baja conductividad hidráulica, que proporcionan un largo tiempo de residencia del agua que se infiltra. De esta manera, el resultado obtenido permite definir que, a mayor resistencia hidráulica, menor será el grado de vulnerabilidad del acuífero estudiado, Tabla 1 (Stempvoort, 1992).

En este estudio, la conductividad hidráulica (K_v) se calculó mediante el análisis del tamaño de partícula de muestras de la capa de cobertura de suelo en un intervalo de 30 a 50 cm de profundidad, utilizando fórmulas empíricas que relacionan K_v con el coeficiente de uniformidad (U) y la porosidad (n). El área de estudio presenta características granulométricas y texturales muy similares a las del material para el que las fórmulas empíricas utilizadas fueron calibradas originalmente, cubriendo un amplio intervalo de valores del diámetro de las partículas de 0.01 a 5 mm y se utilizan en este estudio como una estimación preliminar, por la falta de datos de pozos (sólo existe un pozo y sin información) y para minimizar la incertidumbre en los valores de la conductividad hidráulica estimada. Vukovic y Soro (1992), Odong (2008), presentan varios métodos empíricos y presentan una fórmula, ecuación (2), para la porosidad:

$$n=0.255(1+0.83^U) \tag{2}$$

donde U es el coeficiente de uniformidad de las partículas y se expresa como:

$$U = \left(\frac{d_{60}}{d_{10}} \right) \tag{3}$$

donde, d_{60} y d_{10} representan el diámetro de grano en (mm) para el cual, el 60% y el 10% de la muestra, respectivamente, son más pequeños, estos valores de U entre 2.9 a 4.7, se correlacionan con la conductividad hidráulica vertical K_v para muestras ho-

mogéneas y heterogéneas. Dos de las fórmulas más comunes, son las propuestas por Breyer y Schlitcher. La fórmula de Breyer no considera la porosidad y a menudo se considera más útil para materiales heterogéneos y granos mal clasificados con un coeficiente de uniformidad entre 1 y 20 y un tamaño de grano efectivo entre 0.06 mm y 0.6 mm, se expresa como ecuación (4).

$$K = \frac{g}{v} \times 6 \times 10^{-4} \log \frac{500}{U} d_{10}^2 \tag{4}$$

La fórmula de Schlitcher es más apropiada para tamaño de grano entre 0.01 y 5 mm, para arenas bien graduadas con una mezcla amplia de tamaños de partículas, también considera la viscosidad cinemática v del agua y la gravedad g como constantes que rigen su movimiento, está dada como ecuación (5):

$$K = \frac{g}{v} \times 6 \times 10^{-4} [1 + 10(n - 0.26)] d_{10}^2 \tag{5}$$

Los valores de K para el material arenoso (10^{-5} - 10^{-1} m/s) son varios ordenes de magnitud superiores a los de las capas arcillosas (10^{-9} - 10^{-6} m/s) (Freeze y Cherry, 1979; Kirsch y Hinsby, 2007). Por lo que, en este caso la principal implicación es la imposibilidad de evaluar la heterogeneidad espacial de las propiedades del material del sitio (porosidad, permeabilidad, saturación).

2.2.2. Sondeo eléctrico vertical (SEV)

Los estudios hidrogeológicos detallados en campo hacen un amplio uso de la prospección geofísica, que es efectiva y rápida. Los métodos de prospección eléctrica de resistividad (Figura 4), estudian las variaciones del campo eléctrico (Ley de Ohm) y la distribución de la resistividad en el subsuelo, cuando una corriente eléctrica pasa a través del suelo (Keller, 1970; Orellana, 1982; Kirsch, 2009). El método de prospección eléctrica se utiliza comúnmente para estudios hidrogeológicos, mineros, geotécnicos, así como en estudios ambientales (Akeninyen *et*

Tabla 1. Relación de la resistencia hidráulica con la vulnerabilidad acuífera de acuerdo al método AVI (Prashant *et al.*, 2020).

Resistencia Hidráulica C	Log (C)	Vulnerabilidad
< 10	< 1	Extremadamente Alta
10-100	1 a 2	Muy Alta
100-1000	2 a 3	Moderadamente Alta
1000-10000	3 a 4	Baja
>10000	> 4	Extremadamente Baja

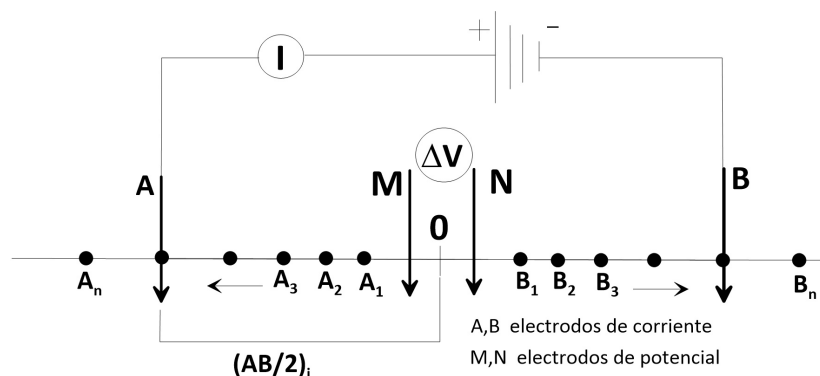


Figura 4. Arreglo de electrodos Schlumberger.

al. 2011; Romero-Ruiz *et al.*, 2019; Ugbaja y Edet, 2004). La resistividad aparente (ρ_a) del subsuelo se midió directamente, utilizando el resistivímetro Terrameter SAS 1000 de ABEM y sus accesorios. Se realizaron un total de dieciséis *SEV* utilizando la configuración tetraelectródica Schlumberger, con un espaciamiento de electrodos de corriente ($AB/2$) que varía de 2 a 500 m y un espaciamiento de los electrodos de potencial ($MN/2$) que varía de 0.50 m a 50.00 m, para alcanzar una profundidad de investigación entre 80 a 180 m.

Durante las mediciones en terreno, el resistivímetro proporciona el valor de la resistividad aparente (ρ_a), para cada separación de electrodos, que es el producto de la resistencia eléctrica (R) del terreno por un factor de proporcionalidad (K), ecuación (6):

$$\rho_a = KR = K \frac{\Delta V}{I} \quad (6)$$

donde K , es un factor geométrico que depende de la separación de electrodos y del tipo de arreglo, para el arreglo Schlumberger, se expresa como, ecuación (7):

$$K = \pi \frac{(AB)^2 - (MN)^2}{MN} \quad (7)$$

Para alcanzar una profundidad de investigación entre 80 y 150 m, dependiendo del tipo de material geológico presente en el subsuelo, la proporción entre la distancia de AB (electrodos de corriente) y la distancia MN (electrodos de potencial), varía aproximadamente entre 1/10 a 1/3 (Parasnis, 1979). Este método se ha utilizado en hidrogeología para determinar el espesor, profundidad y fronteras de un acuífero (Zohdy, 1972). La interpretación cuantitativa de las curvas suavizadas, se llevó a cabo

mediante la modelación computacional inversa con el programa IX1D, desarrollado por Vender Velpen (1988).

Para determinar de las características hidráulicas de un acuífero, se pueden establecer correlaciones empíricas entre los parámetros hidráulicos (obtenidos mediante análisis granulométrico o de pruebas de bombeo) y los parámetros eléctricos (calculados a partir de mediciones de resistividad eléctrica como el *SEV*), para obtener la transmisividad y/o la conductividad hidráulica en áreas extensas donde los datos de las pruebas de bombeo son escasos (Soupios *et al.*, 2007; Niwas y Celik, 2012; Hasan *et al.*, 2019). En este estudio, se utilizaron los parámetros de Dar-Zarrouk de la resistencia transversal (R_T) y la conductancia longitudinal (S), para obtener proporciones útiles entre los parámetros hidráulicos y eléctricos en el área de estudio. Niwas y Singhal (1981) establecieron una relación analítica entre la transmisividad (T) y la resistencia transversal (R_T), por un lado, y la transmisividad (T) y la conductancia longitudinal (S), por otro.

De acuerdo a la ley de Darcy, el caudal de fluido Q que pasa a través de un área de sección transversal, es directamente proporcional al gradiente hidráulico multiplicado por una constante de proporcionalidad k , la conductividad hidráulica y está dada por la ecuación (8)

$$Q = kAi \quad (8)$$

y de la ley de Ohm, que establece que la densidad de corriente eléctrica J en un punto, es directamente proporcional al campo eléctrico E , multiplicado por una constante de proporcionalidad σ , la conductividad eléctrica, inversa de la resistividad eléctrica ρ , dada como:

$$J = \sigma E \quad (9)$$

Niwas y Singhal (1981) combinaron la ecuación (8) con la resistencia transversal (R_T) y la conductancia longitudinal, para obtener la siguiente ecuación, respectivamente,

$$T = k\sigma R_T = \frac{kS}{\sigma} \tag{10}$$

2.2.3. Parámetros de Dar Zarrouk (*T* y *S*)

Los parámetros de Dar Zarrouk, la resistencia Transversal *T* ($\Omega\cdot m^2$) y la Conductancia Longitudinal *S* (Ω^{-1} o Siemens), son propiedades geoelectricas integrales que caracterizan a un conjunto de capas horizontales en el subsuelo definidas por sus espesores (*h_i*) y resistividad (*ρ_i*). Mailett (1947) estudió la ambigüedad al problema inverso del *SEV*, llamado *equivalencia*, que resolvió proponiendo dos parámetros que llamó de Dar Zarrouk (*T* y *S*). Se definen con respecto a una columna o prisma rectangular cuadrado de un medio geológico estratificado, con bases cuadradas y caras laterales rectangulares de lado igual a la unidad de longitud (1 m, es decir largo 1 m y ancho 1 m), con eje perpendicular a la orientación de las capas que atraviesa todas las capas del medio estratificado de espesor *H(m)*. Suponiendo que el prisma es atravesado por una corriente eléctrica que fluye perpendicularmente a la estratificación, las *n* capas se comportaran como conductores en serie, por lo que sus resistencias se suman. Así, resulta la resistencia transversal total *T* ($\Omega\cdot m^2$), de la base a la superficie del terreno. Mientras que la conductancia longitudinal *S*, donde la corriente fluye paralelamente a la estratificación, la resistencia del prisma que corresponde a la capa *n* y tomando su inversa, la conductancia, se obtiene la conductancia longitudinal *S* para las *n* capas, que tienen un papel importante en la interpretación de los *SEV* (Orellana, 1966, 1982; Zohdy, 1972; Henriet, 1976). Posteriormente, otros autores (Niwas y Singhal, 1985; Singh *et al.*, 2004; Mondal *et al.*, 2017), han estudiado la importancia de los parámetros de Dar Zarrouk para obtener información de las propiedades hidrogeológicas y de la capacidad de protección de un acuífero libre.

La resistencia total (Ωm^2) del flujo de corriente perpendicular a las *n*-capas geoelectricas, es la suma de las resistencias de cada capa y está dada como ecuación (11):

$$T = R_T = \sum_{i=1}^n h_i \rho_i = h_1 \rho_1 + h_2 \rho_2 + h_3 \rho_3 + \dots + h_n \rho_n \tag{11}$$

La resistividad transversal media o equivalente para el conjunto de *n*-capas estratificadas, se define como, ecuación (12):

$$\rho_t = \frac{T}{H} \tag{12}$$

Donde *H*= $\sum h_i$, es el espesor total del conjunto de las *n*-capas en la sección geoelectrica. Si la corriente fluye paralelamente a la estratificación, la conductancia longitudinal (ohm^{-1} o siemens), se expresa como, ecuación (13):

$$S = \sum_{i=1}^n \frac{h_i}{\rho_i} = \frac{h_1}{\rho_1} + \frac{h_2}{\rho_2} + \frac{h_3}{\rho_3} + \dots + \frac{h_n}{\rho_n} \tag{13}$$

La resistividad longitudinal media o equivalente para el conjunto de *n*-capas estratificadas, se define como, ecuación (14):

$$\rho_l = \frac{H}{s} \tag{14}$$

Para definir la heterogeneidad y anisotropía de un medio, Mailett propuso la pseudo-anisotropía que se expresa numéricamente como, ecuación (15):

$$\lambda = \sqrt{\frac{\rho_t}{\rho_l}} \tag{15}$$

Debido a que las observaciones de la resistencia hidráulica (*C*) depende del espesor (*h_i*) de las capas sobre el sistema satu-

Tabla 2. Índice de la conductancia longitudinal (capacidad protectora) (Oladapo y Akin-torinwa, 2007).

Conductancia longitudinal S (mhos)	Índice de la capacidad protectora	Clase de vulnerabilidad
>10	Excelente	Extremadamente baja
5-10	Muy buena	Muy Baja
0.7-4.5	Buena	Baja
0.2-0.69	Moderada	Moderada
0.1-0.19	Débil	Alta
< 0.1	Pobre	Muy alta

rado y de los tipos de materiales geológicos que se encuentran por arriba de él; en un medio poroso, la resistencia hidráulica es función del contenido de arcilla (a mayor arcillosidad mayor resistencia hidráulica) y esta influye directamente en la resistividad eléctrica de los sedimentos granulares (a menor arcillosidad menor resistencia eléctrica), por lo que Kalinski *et al.*, (1993), proponen como alternativa sustituir la resistencia hidráulica por la resistividad o resistencia eléctrica, la que puede determinarse de forma relativamente fácil aplicando métodos de prospección geoelectrica con el método del *SEV*.

Es evidente la similitud entre las ecuaciones (1 y 10) de la resistencia hidráulica (C) del método AVI y de la conductancia longitudinal (S), respectivamente. La resistencia hidráulica (C) de una capa protectora depende de la porosidad efectiva para materiales arenosos o areno-gravosos de textura gruesa y en el contenido de arcilla para materiales de textura fina. Ambos parámetros dependen de la resistividad eléctrica de los materiales (Kirsch, 2006). En este caso, la conductividad hidráulica (K_i), puede relacionarse con la resistividad (ρ_i) o la conductividad eléctrica (σ_i) para calcular la resistencia hidráulica (C), denominada Índice de la Capacidad Eléctrica (ICE) o Índice de Protección basado en la Geofísica (IPG) (Casas *et al.*, 2008), específicamente con el método geoelectrico del *SEV*. Por lo que, Índice de la Capacidad Eléctrica (ICE) puede utilizarse para evaluar la vulnerabilidad del acuífero mediante la ecuación (16):

$$ICE = \sum_{h=ST}^{h=NP} \frac{h_i}{\rho_i} = \sum_{i=1}^n h_i \times \sigma_i \quad (16)$$

donde: h_i es el espesor de cada capa que se encuentra desde la superficie del terreno (ST) hasta el nivel freático (NF) expresada en metros (m) y ρ_i es la resistividad eléctrica (ohm-m) de las capas que se encuentran entre la superficie del terreno y el nivel freático.

Los parámetros anteriores se utilizaron para detectar las zonas protectoras y el grado de vulnerabilidad de las aguas subterráneas que circulan en un acuífero libre (Tabla 2). Por lo tanto, para una formación geológica gruesa de baja resistividad, tendrán una mayor protección de los contaminantes que provienen desde la superficie del terreno, es decir, el flujo de corriente horizontal es dominante y la conductancia longitudinal (S) es mayor y viceversa, si en la primera capa no hay arcilla, el flujo de corriente vertical es dominante y la resistencia eléctrica transversal (T), proporciona información de las capas permeables, es decir, de aquellas zonas favorables para la infiltración o recarga natural (Henriet, 1976; Oladapo *et al.*, 2007; Casas *et al.*, 2008).

2.3. Análisis de las características hidrogeológicas de la capa de suelo y nivel freático

La capa superficial de suelo, que depende de la evolución geológica compleja de una región, juega un papel importante en el estudio de vulnerabilidad del agua subterránea a la contaminación, a través de la interacción del ciclo hidrológico y la dinámica del agua de percolación en la zona no saturada y la recarga de agua subterránea y migración de solutos en el subsuelo (Freeze, 1979; Tóth, 1999). La interacción está determinada en parte por las condiciones climatológicas, el escurrimiento de agua superficial y las características del medio poroso. El análisis y evaluación de esta interacción, está controlado por las propiedades del suelo como la textura, litología, propiedades hidráulicas, contenido de humedad y materia orgánica (Segal *et al.*, 2008; Thomas *et al.*, 2017).

Se recolectaron 6 muestras de suelo en sitios predefinidos en el área de estudio, se pesaron *in situ* y se dejaron secar al aire libre en el laboratorio de hidrogeología de la UAM Lerma. Posteriormente, se disgregaron y se tamizaron con un juego de mallas (#4, 10, 20, 40, 50, 100, 200, 325, 400 y charola), para obtener las curvas granulométricas y clasificar los suelos por su textura de acuerdo a la nomenclatura FAO. También, son útiles para determinar la porosidad, la conductividad hidráulica y el coeficiente del rendimiento específico S_y .

El contenido de humedad gravimétrica, w (%), se determinó con la ecuación (17):

$$w = \frac{(M_{sh} - M_{ss})}{M_{ss}} = \left(\frac{M_{sh}}{M_{ss}} - 1 \right) * 100 \quad (17)$$

donde M_{sh} , es la masa de suelo húmedo recolectada en campo, M_{ss} el peso seco o masa de suelo secado al aire libre y w (%) el contenido de humedad gravimétrica.

2.4. Evaluación de la fluctuación del nivel de agua

La recarga (R , L/T) se estimó por medio de la fluctuación del nivel del freático aplicable para acuíferos libres (Healy y Cook, 2002). Fue necesario realizar un registro del nivel freático 2 veces por día y hacer una estimación del almacenamiento específico (S_y) de la zona de fluctuación del nivel freático, asumiendo que el agua que llega al nivel freático, pasa a integrarse al flujo subterráneo y que la evapotranspiración desde el nivel freático, el aporte al flujo regional subterráneo y otras salidas o entradas al sistema acuífero son nulas. El S_y puede entenderse como la diferencia entre la porosidad total y la capacidad de almacenamiento en sus poros, donde se presenta el flujo de agua

por gravedad o zona no saturada (ZNS) y se considera igual a la porosidad efectiva (n_e). Por lo que, la recarga del acuífero se calcula como la ecuación (18):

$$R(t_j) = S_y * \Delta H(t_j) \quad (18)$$

donde $R(t_j)$ es la recarga entre los tiempos t_0 y t_j (tiempo al inicio y al pico del ascenso del nivel de agua, respectivamente), S_y es el almacenamiento específico (adimensional) y, $\Delta H(t_j)$ es el ascenso del nivel freático hasta el pico atribuido a la recarga (L).

De acuerdo con Weinzettel *et al.*, (2005), la respuesta del nivel freático a los eventos de recarga es muy rápida debido a su poca profundidad, a la existencia de trayectorias preferenciales del flujo, al comportamiento del flujo tipo pistón sobre la matriz porosa y a que el agua contenida en los poros por arriba del nivel freático, no es la misma que acaba de infiltrarse; es agua que esta previamente en los poros y es empujada por el agua reciente que ingresa, por lo que ésta no debe recorrer hasta el nivel freático para que se aprecie su ascenso con éste.

3. Resultados y discusión

3.1. Curva de distribución granulométrica

Previo al análisis granulométrico se obtuvo el contenido gravimétrico de humedad w (%). La humedad del suelo es un parámetro crítico que define el exceso o déficit de agua para las plantas y su movilidad en el subsuelo. En la Tabla 3 se indica el número de muestra asociada al peso de la muestra húmeda colectada en campo, M_{sh} , masa de suelo húmedo, peso seco M_{ss} , o masa de suelo secado al aire libre, w % contenido de humedad gravimétrica calculada con la ecuación (14).

Se obtuvo que en los sitios de las muestras M2 y M6, presentan mayor humedad, indicando que son zonas donde puede presentarse la dispersión y transporte con mayor facilidad de contaminantes no reactivos, como iones cloruros o nitratos, debido a que son disueltos y transportados por el agua de lluvia a niveles inferiores del subsuelo. El agua de lluvia o superficial, se infiltra a través de las capas protectoras incorporándose a la recarga del agua subterránea.

Del análisis granulométrico para cada muestra de suelo, se construyó la curva de distribución granulométrica (Figura 5) en un gráfico semi-logarítmico, d (mm) vs % que pasa la malla #4 de donde se obtienen los diámetros d_{10} , y d_{60} para obtener el coeficiente de uniformidad (U), estimar el valor de la porosidad (n , %) y la conductividad hidráulica (K , m/d) de acuerdo a las fórmulas empíricas de Slitcher y Breyer (Tabla 4).

De la Figura 5 se observa que las curvas de distribución granulométrica, corresponden con arenas bien graduadas, con contenido de arcilla, limo y grava fina, predominando arena fina a gruesa en un intervalo de tamaño de partícula entre 0.4 a 5 mm. En la Tabla 4 se presentan los valores obtenidos del coeficiente de uniformidad U entre 2.9 a 4.7, a partir de los diámetros de partícula d_{10} , y d_{60} .

3.2. Estimación de la conductividad hidráulica de campo (K_f)

El coeficiente de conductividad hidráulica por el método de Slitcher y Breyer se obtuvo para cada muestra analizada con base a las curvas granulométricas acumuladas. Con la fórmula empírica de Schlitcher, se obtuvieron valores de 6.6 (7.64×10^{-3} cm/s) a 14.8 (2.53×10^{-1} cm/s) m/d y un promedio de 10.86 m/d (1.3×10^{-2} cm/s), mientras que con la fórmula de Breyer se obtuvieron valores de 22.9 (2.6×10^{-2} cm/s) a 49.7 (5.7×10^{-2} cm/s) m/d, con un promedio de 36.3 (4.2×10^{-2} cm/s) m/d (Tabla 5), que se correlaciona con material arenoso.

3.3. Almacenamiento específico (S_y)

El almacenamiento específico se puede visualizar como el coeficiente de porosidad efectiva para drenaje (n_e), donde la porosidad total (n) se derivó de la relación empírica con el coeficiente de uniformidad de grano (U) y se obtuvo un valor promedio del rendimiento específico (S_y) de 0.3733, asociado con un material arenoso.

3.4. Evaluación de la fluctuación del nivel de agua

La evaluación del nivel del agua en un acuífero libre, permitió obtener información del ascenso y/o descenso del nivel del agua (Δh), con respecto al tiempo, para un periodo de 21

Tabla 3. Porcentaje de humedad en las muestras de suelo.

	Número de muestra					
	M1	M2	M3	M4	M5	M6
M_{sh} (g)	2000	2000	2000	2000	2000	2000
M_{ss} (g)	1700	1490	1725	1720	1715	1415
w (%)	17.65	34.23	15.94	16.28	16.62	41.34

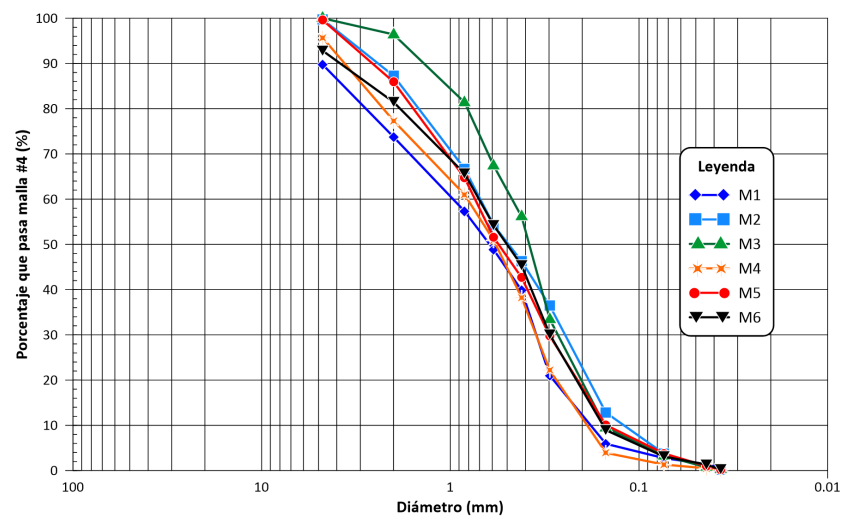


Figura 5. Curva de distribución granulométrica de seis muestras de suelo.

Tabla 4. Valores de los diámetros d_{10} , d_{60} y U (mm).

Muestra	d_{10} (mm)	d_{60} (mm)	U
M1	0.22	1.0	4.5
M2	0.15	0.70	4.7
M3	0.17	0.48	2.9
M4	0.21	0.80	4.0
M5	0.17	0.73	4.4
M6	0.17	0.73	4.4

Tabla 5. Resultados de K_v por el método Slitcher y Breyer (m/día).

Muestra	K (m/día) Slitcher	K (m/día) Breyer
M1	14.7	49.7
M2	6.6	22.9
M3	11.5	30.6
M4	14.8	46.5
M5	9.1	29.9
M6	8.4	28.1

días, en dos norias de la zona y en el Río San Agustín, así como un valor estimado de la recarga hacia el acuífero libre. En el vaciado de un acuífero libre, la porosidad efectiva es igual al almacenamiento específico, que es el volumen de agua cedido por unidad de volumen de material acuífero, drenado por un descenso del nivel freático. En la noria 1, que tiene una profundidad de 6.5 m de profundidad presenta un abatimiento de 0.04 m/d, la noria 2 con 2.0 m de profundidad de 0.037 m/d y el Río San Agustín de 0.013 m/d. De aquí, que se obtuvo un valor de la recarga para cada zona de 0.015 m/d, 0.014 m/d y 0.005 m/d, respectivamente.

3.5. Evaluación de la vulnerabilidad acuífera con el método AVI

Este método cuantifica la vulnerabilidad por la resistencia hidráulica al flujo vertical del agua a través de las capas protectoras (arcillas). Los valores de K_v para el material arenoso (10^{-5} - 10^{-1} m/s), son de varias magnitudes superiores a las de las capas arcillosas (10^{-8} - 10^{-6} m/s), por lo que, para la resistencia hidráulica, se presentan capas de arena con presencia de arcilla. Como K_v tiene unidades de longitud/tiempo (m/s o m/d), la dimensión de C es el tiempo. De acuerdo con Van Stempvoort *et al.* (1992), esto se puede utilizar como una estimación aproximada

del tiempo de viaje vertical del agua a través de las capas de la zona no saturada, aunque no se consideran parámetros importantes que controlan el tiempo de viaje como el gradiente hidráulico y la difusión.

En la Figura 6 se muestra el mapa del índice de vulnerabilidad acuífera AVI, obtenido a partir de los valores de los espesores de la zona no saturada obtenidos de los *SEV* y de los valores de la conductividad hidráulica del método de Slitcher para la primera capa de cobertura de suelo, dando como resultado valores de la resistencia hidráulica *C* de 0.4 a 6.0 días. Los valores de 0.4 a 1.4 días, indican que en la zona centro-sur existe una baja vulnerabilidad a la contaminación del agua subterránea, mientras que en la zona norte presenta una moderada vulnerabilidad de 2.2 a 3.2 días y alta vulnerabilidad en la zona poniente, donde se ubica el pozo municipal y en la zona norte en el *SEV* 3, a un lado del río, con valores de 4.2 a 6.0 días.

Cabe mencionar, que los datos medidos en la zona sur y suroeste se encuentran dispersos, debido a restricciones de acceso, ya que son terrenos privados y no se tuvo acceso, lo que genera importantes incertidumbres al extrapolar los resultados en zonas con fuertes variaciones laterales. Las técnicas de interpolación de

datos de la vulnerabilidad acuífera y distribución de la resistividad como Kriging Ordinario, el Inverso de la Distancia Ponderada (IDW) y el de mínima curvatura, son herramientas geoestadísticas más utilizadas para estimar valores en áreas no muestreadas a partir de datos puntuales (como pozos o *SEV*) y son fundamentales para construir mapas de vulnerabilidad (DRASTIC, GOD, SINTACS, AVI, ICE, entre otros) y evaluar la susceptibilidad a la contaminación de un acuífero. En este estudio, el algoritmo de Kriging Ordinario, implementado en Surfer 25, que es un interpolador exacto o de suavizado, debido a su capacidad para modelar la estructura de autocorrelación espacial y proporcionar estimaciones insesgadas con varianza mínima, resultó ser el más apropiado, ajustando un variograma esférico, para definir la estructura de la covarianza espacial de los datos, asignando pesos a los vecinos más cercanos basado en la distancia y dirección, para mapear la vulnerabilidad del acuífero en estudio al estimar valores en áreas no muestreadas basándose en datos puntuales, que incorpora la anisotropía y las tendencias subyacentes de forma eficiente en aquellas zonas con fuertes variaciones laterales de las condiciones geológicas. Por lo que, la falta de datos puede subsanarse mediante mediciones geofísicas adicionales con *SEV* en los huecos.

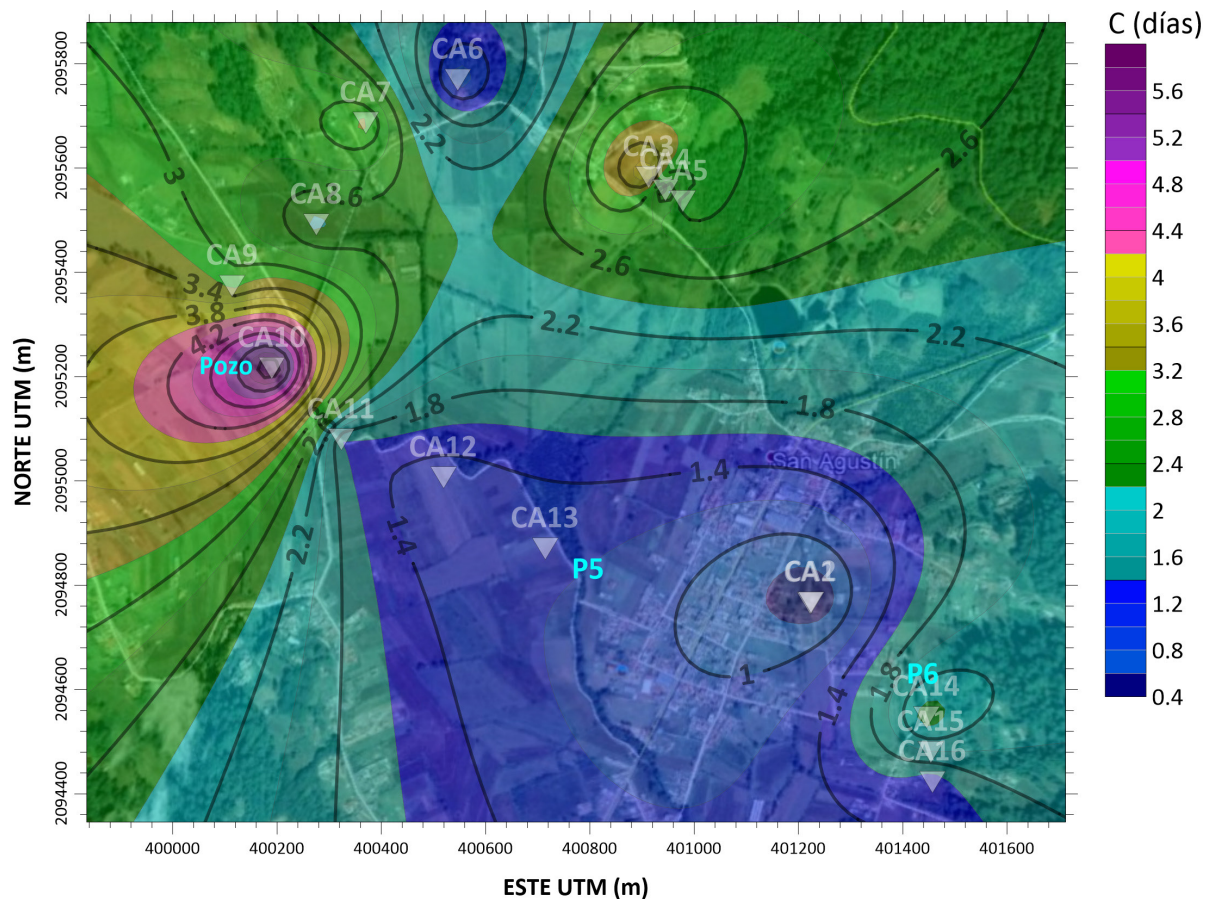


Figura 6. Mapa de la distribución de la resistencia hidráulica (AVI), de la zona de estudio.

3.6. Análisis geoelectrico de los SEV

El estudio hidrogeofísico ambiental con el método geoelectrico del SEV, se llevó a cabo para evaluar la secuencia litológica en el Valle de San Agustín, Texcalyacac Estado de México, el grado de vulnerabilidad y la capacidad protectora del acuífero libre con el método ICE (conductancia longitudinal, S).

En la Figura 7 se muestra el mapa del Valle de San Agustín, Texcaltitlán y la delimitación de la zona de estudio, así como la ubicación de los SEV, sobre caminos y sitios donde fue posible tener acceso. Para este estudio, se realizaron 16 SEV nombrados como SEV1, SEV 2, SEV 3,..., SEV 16, distribuidos a lo largo de 6 perfiles con el arreglo de electrodos tipo Schlumberger.

3.6.1. Curvas de SEV

Los resultados de la inversión geofísica de datos de resistividad aparente para dos estaciones de SEV se presentan en la Figura 8, se obtuvieron modelos de capas para cada una de las estaciones de SEV y los valores de los espesores de cada capa y su resistividad verdadera, que se integraron en mapas

y perfiles para configurar los espesores y resistividad de la litología del subsuelo, para calcular los parámetros de Dar Zarrouk como la Conductancia Longitudinal (S), la Resistencia Transversal (T), la resistividad longitudinal, la resistividad transversal y el coeficiente de anisotropía (λ), utilizando las formulas apropiadas.

En general, se detectaron 6 y 7 capas geoelectricas o unidades litológicas, con diferentes tipos de curvas en el área de estudio y se caracterizó por valores de espesor y resistividad variables. El espesor de la capa superficial del suelo presenta valores entre 0.48 a 1.15 m y la resistividad de la capa varía de 8 a 1253 Ωm . El espesor de la segunda capa tiene valores entre 0.7 y 6.7 con una resistividad que varía de 10 a 62 Ωm , lo que indica que la composición del material es de arcilla, laterita, arcilla arenosa y arena arcillosa. Los valores del espesor de la tercera capa oscilan entre 1.2 y 16.0 m y resistividad de 5 a 167 Ωm , lo que indica la presencia de arcilla y material arenoso con grava y matiz limo arcillosa con contenido de humedad. La cuarta capa presenta un espesor variable de 1.4 a 38.8 m y una resistividad de 6 a 59 Ωm . La quinta capa muestra un espesor variable de 5.2 a 37.4 m y resistividad de 4 a 244 Ωm , indicando la presencia de arcilla y

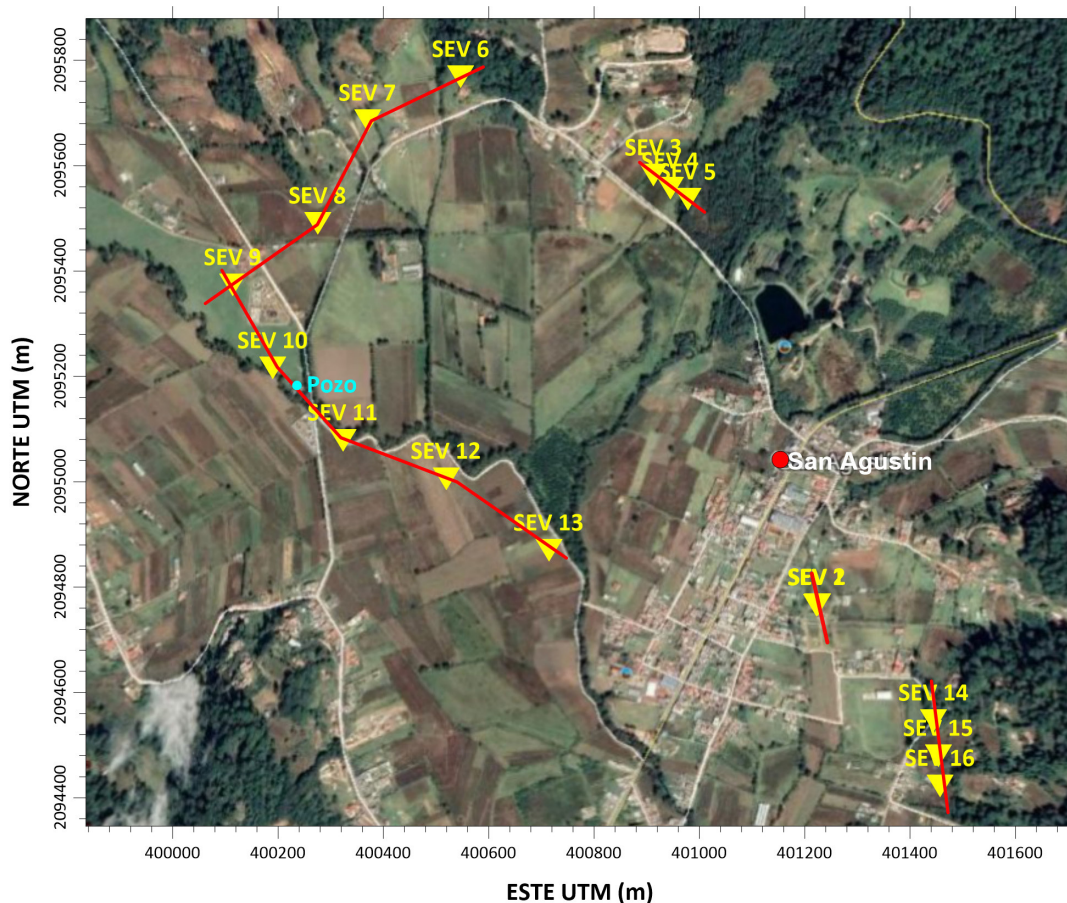


Figura 7. Localización de los puntos de SEV.

arena con grava y matriz limo arcillosa. La sexta capa presenta un espesor variable de 6.8 a 80.7 m y resistividad de 7 a 307 Ω m, indicando la presencia de arcilla y material alterado areno arcilloso. La séptima capa fue la última detectada con espesor no identificado (se considera de valor infinito) y resistividad de 7 a 2,769 Ω m, indicando presencia de arcilla o agua mineralizada y roca ígnea compacta y/o fracturada.

Los parámetros de las capas (resistividad y espesor verdaderos) obtenidos de la interpretación cuantitativa con el programa IX1D, se resumen en la Tabla 6, que brinda como resultado los mapas de distribución de la resistividad los cortes geoelectricos en cada punto investigado.

3.6.2. Mapas geoelectricos de la distribución de la resistividad en el subsuelo

En la Figura 9, se muestra la distribución de la resistividad aparente a diferente profundidad (0.8, 2.5, 4.0 y 7.0 m) en la zona de estudio. Las zonas que presentan menor resistividad (<10 Ohm-m), son materiales asociados a grano fino (arcillas), limos (< 20 Ohm-m), indican zonas de baja infiltración y de conductividad hidráulica. Las zonas que presentan altos valores de resistividad indican zonas de mayor infiltración, asociadas con materiales de grano medio a grueso (> 20 a < 250 Ohm-m) como arenas (medias, gruesas) y gravas de moderada a alta conductividad hidráulica. Las zonas que presentan valores de la resistividad > 250 y < 1,000 Ohm-m, también se asocia con materiales permeables (grava y roca ígnea alterada o fracturada). Por ultimo las zonas que presentan valores de resistividad mayores a 1,000 Ohm-m se asocian a roca compacta.

3.6.3. Perfiles geoelectricos

Perfil 1. Este perfil corre de suroeste a este en el área de estudio indicada, se trazó correlacionando los tres sondeos eléctricos verticales, CA1, CA2 y CA17, la distancia entre cada sondeo es 3 metros y el perfil tiene una longitud de 12 metros. La sección geoelectrica se ha construido según la interpretación cuantitativa de los SEVs, revelando la presencia de siete capas o unidades (U) en los tres SEVs, las cuales se describen a continuación (Figura 10). Se detecta a lo largo del perfil, la presencia de resistividad eléctrica entre 50 a 1000 ohm-m, se observa que a mayor profundidad disminuye la resistividad. El primer intervalo que va de los 0 a 1.5 metros de profundidad, se asocia con la presencia de arena y grava, de 1.5 a 6 metros; el tipo de material se asocia a conglomerados en el SEV 1, de los 6 a 12 metros con material de arena media a gruesa y arena limosa. A una profundidad de 10 m se presenta material arcillo limoso.

Perfil 2. Este perfil corre de Noroeste a Sureste en el área de estudio indicada, se trazó correlacionando los tres sondeos eléctricos verticales, SEV3, SEV4 y SEV5, la distancia es entre cada SEV es de 20 metros, creando un perfil de análisis de 60 metros (Figura 11). Se detecta a lo largo del perfil la presencia de resistividad eléctrica entre 3,800 a > 200 ohm-m, se observa que a mayor profundidad mayor resistividad, la menor resistividad en encuentra sobre los SEVs 4 y 5. El material asociado con las primeras capas (de 0 20 metros de profundidad) es de tipo arenoso desde granos finos a gruesos y en ese mismo intervalo se encuentran los conglomerados para después (profundidad de 20 a 100 metros) encontrar roca alterada en la parte del SEV 3.

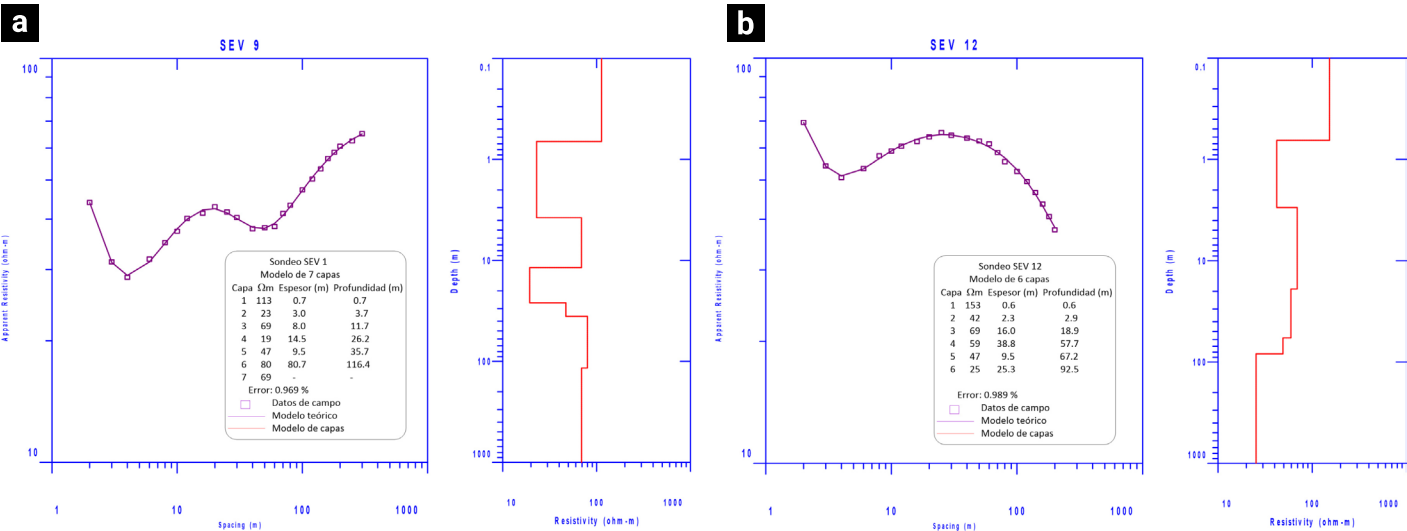


Figura 8. Curva tipo HKHKH obtenida de la inversión del SEV 9 y curva tipo HKHK obtenida de la inversión del SEV 12.

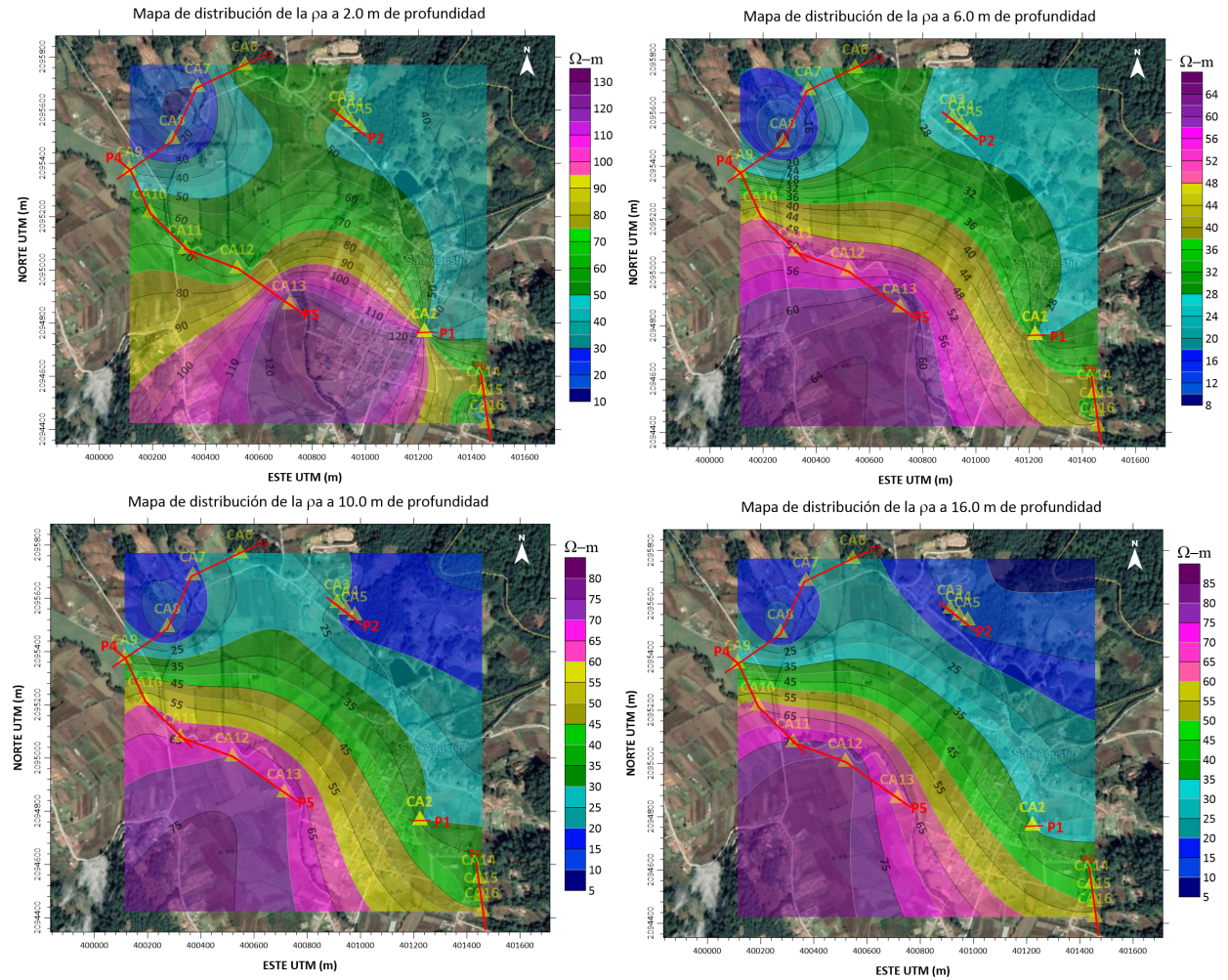


Figura 9. Distribución de la resistividad verdadera para diferentes profundidades.

Tabla 6. Resumen de parámetros geoelectrónicos obtenidos de la inversión de datos con IX1D de los SEV, para el cálculo de los parámetros de Dar Zarrouk.

No.SEV	Resistividad de las capas ($\Omega\text{-m}$)								Espesor de las capas (m)							
	ρ_1	ρ_2	ρ_3	ρ_4	ρ_5	ρ_6	ρ_7	ρ_8	h_1	h_2	h_3	h_4	h_5	h_6	h_7	h_8
SEV 1	1253	52	23	104	8				0.5	1.0	2.7	3.6	inf			
SEV 2	8	30	73	17	90	7			0.6	1.5	3.4	4.1	inf			
SEV 3	50	62	15	34	4	308	3769		0.5	1.0	2.8	4.2	16.7	18.7	inf	
SEV 4	27	39	19	15	4	14	17	174	0.6	1.2	1.7	2.4	8.2	11.8	49.5	inf
SEV 5	19	24	13	6	5	7	72	37	0.5	1.2	1.2	3.1	8.3	6.8	50.3	inf
SEV 6	126	47	53	19	11	27	7	682	0.6	1.2	1.8	6.5	5.2	12.8	29.4	inf
SEV 7	13	16	24	14	24	13	42	389	13.0	1.4	3.2	8.5	11.0	23.3	20.8	inf
SEV 8	160	10	5	17	73	12	61	44	0.5	0.9	2.9	1.7	8.1	20.1	41.1	inf
SEV 9	113	23	69	19	47	80	69		0.6	3.2	8.0	14.5	9.5	80.7	inf	
SEV 10	107	27	88	49	73	28	74	197	0.8	1.8	3.1	6.1	10.4	26.3	116	inf
SEV 11	125	40	167	33	119	12			0.7	3.6	5.1	14.3	37.4	inf		
SEV 12	153	42	69	60	49	25			0.6	2.3	16.0	38.8	25.3	inf		
SEV 13	162	35	93	50	94	23	240		1.2	2.0	3.0	4.5	10.4	55.6	inf	
SEV 14	131	41	66	40	199	83	19	160	1.2	6.7	5.6	9.7	24.2	13.5	75.7	inf
SEV 15	18	23	18	43	244	97	51	68	0.5	1.1	2.8	1.4	12.3	10.2	122.2	inf
SEV 16	90	43	93	33	213	62	225	23	0.7	2.6	2.8	7.0	14.7	38.4	87.7	inf

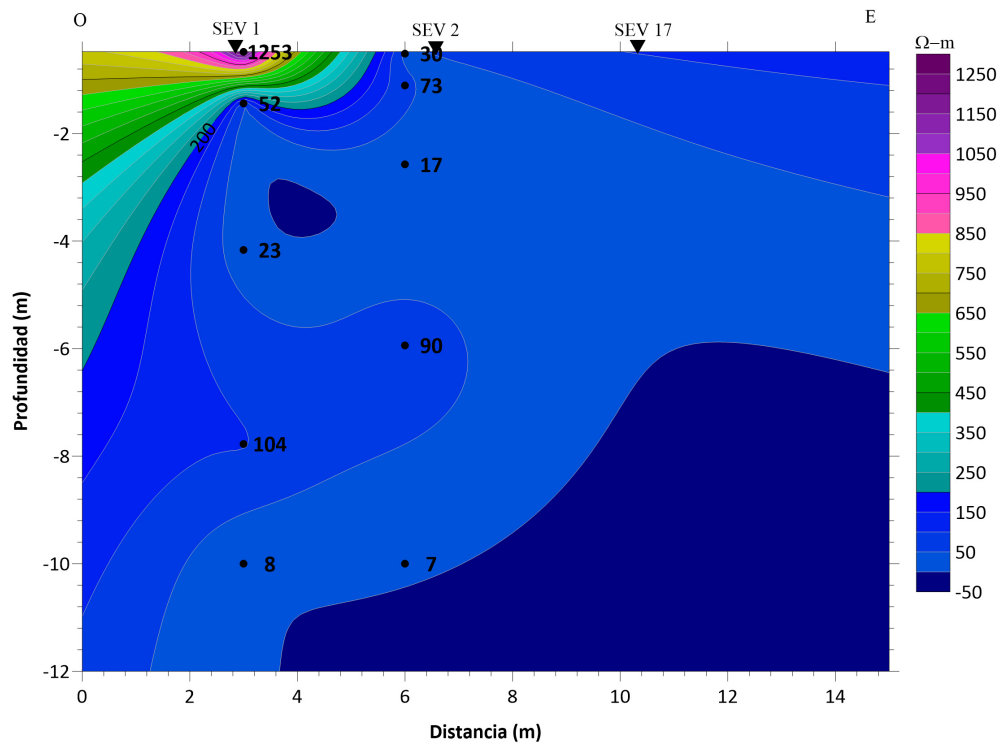


Figura 10. Perfil geoelectrico 1 de iso-resistividad verdadera.

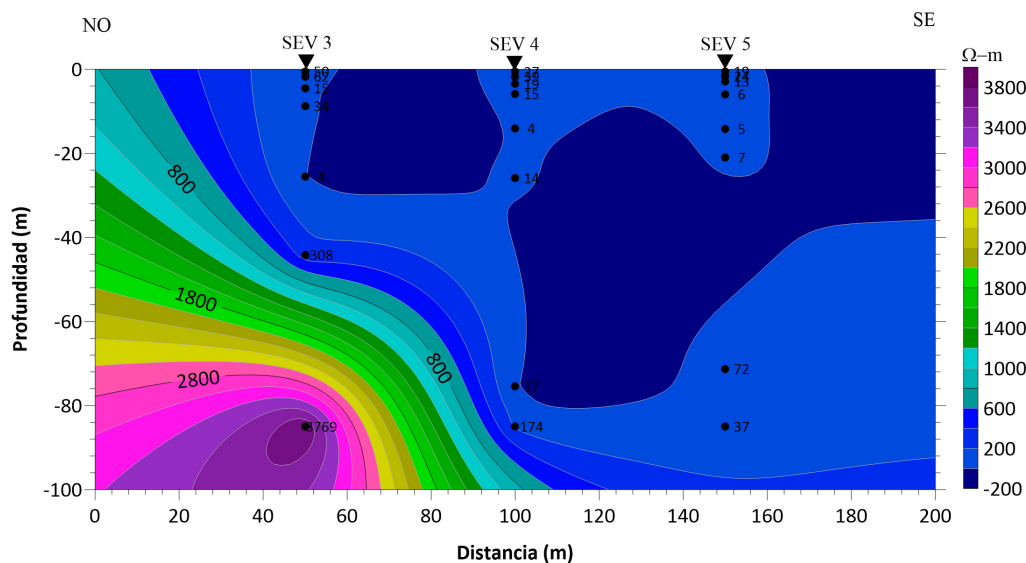


Figura 11. Perfil geoelectrico 2 de iso-resistividad verdadera.

Perfil 3. Este perfil corre de Noreste a Suroeste en el área de estudio indicada, se trazó correlacionando los cuatro sondeos eléctricos verticales, CA6, CA7, CA8 y CA10, la distancia es entre cada *SEV* es de 200 metros, creando un perfil de análisis de 700 metros (Figura 12). Se detecta a lo largo del perfil la presencia de resistividad eléctrica entre 700 a > 30 ohm-m, se observa que a mayor profundidad mayor resistividad, la menor resistividad se encuentra sobre los *SEVs* 8 y 10. El material asociado con las primeras capas (de 0 a 100 metros de profundidad)

es de tipo limo-arenoso fino. En el segundo intervalo de 100 a 160 metros de profundidad se presenta material conglomerado y de 160 a +200 metros hay roca alterada.

Perfil 4. Este perfil corre de Noreste a Suroeste en el área de estudio indicada, se trazó correlacionando los tres sondeos eléctricos verticales, SEV9, SEV10, y SEV11, la distancia es entre cada *SEV* es de 200 metros, creando un perfil de análisis de 500 metros (Figura 13). Se detecta a lo largo del perfil la presencia de resistividad eléctrica entre 180 a > 30 ohm-m, en este perfil la

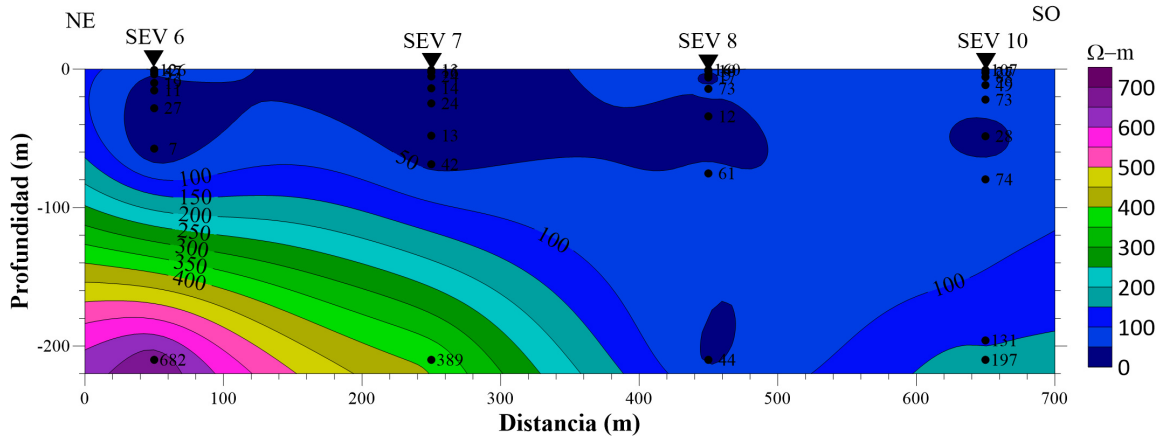


Figura 12. Perfil geoelectrico 3 de iso-resistividad verdadera.

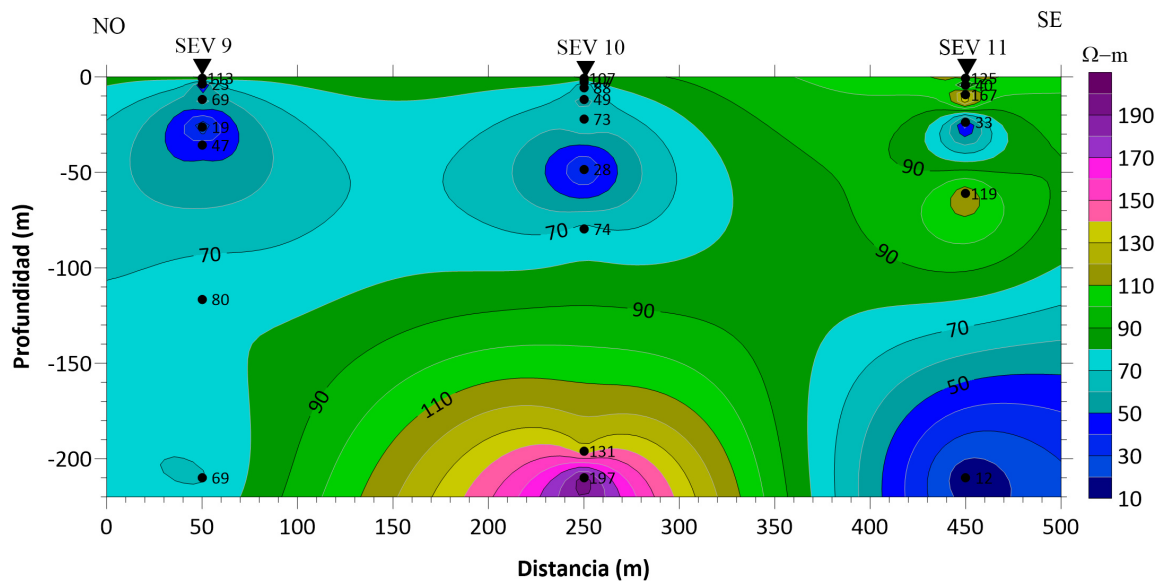


Figura 13. Perfil geoelectrico 4 de iso-resistividad verdadera.

resistividad no tiene un patrón de orden para las profundidades y, por lo tanto, el tipo de material asociado se encuentra distribuido a lo largo de éste. El color morado a más de 200 metros de profundidad se asocia con material rocoso alterado y conglomerados, el color verde y azul se asocia con arenas gruesas y limos.

Perfil 5. Este perfil corre de Noroeste a Sureste en el área de estudio indicada, se trazó correlacionando los tres sondeos eléctricos verticales SEV11, SEV 12 y SEV13. La distancia es entre cada SEV es de 200 metros, creando un perfil de análisis de 500 metros (Figura 14). Se detecta a lo largo del perfil la presencia de resistividad eléctrica entre 250 a > 30 ohm-m, del lado izquierdo sobre el SEV 11 se observa que la resistividad va de mayor a menor conforme a la profundidad, por el contrario, en el SEV 12 la resistividad va de menor a mayor. A una profun-

didad de 50 metros se puede encontrar material de tipo limo y arena fina, de 50 a más de 100 metros material de arena gruesa y conglomerados, así como, roca. Alterada.

Perfil 6. Este perfil corre de Noroeste a Sureste en el área de estudio indicada, se trazó correlacionando los tres sondeos eléctricos verticales SEV14, SEV15 y SEV16.

La distancia es entre cada SEV es de 60 metros, creando un perfil de análisis de 200 metros (Figura 15). Se detecta a lo largo del perfil valores de resistividad eléctrica entre 30 a 250 ohm-m, a una profundidad de 40 metros se puede encontrar material tipo limo, arena fina y gruesa, en menor espesor conglomerados, a una profundidad de 40 a 100 metros se detectaron conglomerados y arenas gruesas, de 100 a 180 metros material arenoso, conglomerados y roca alterada.

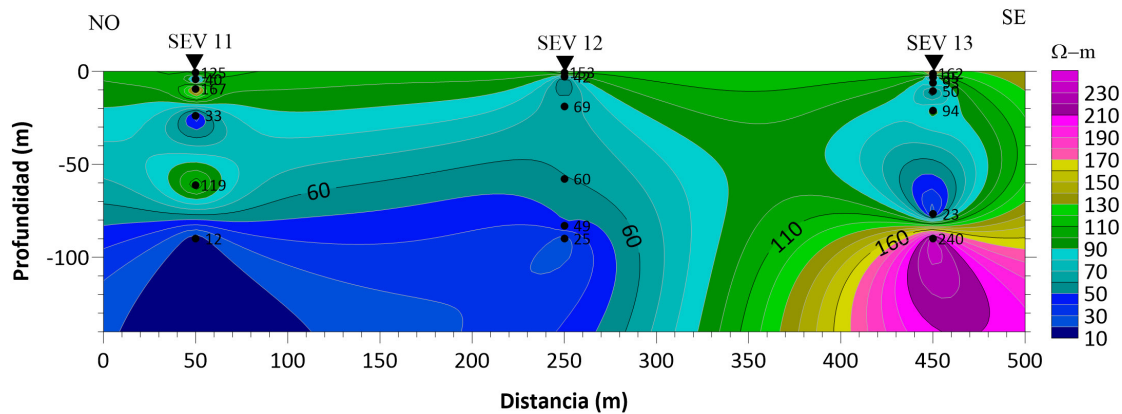


Figura 14. Perfil geoelectrico 5 de iso-resistividad verdadera.

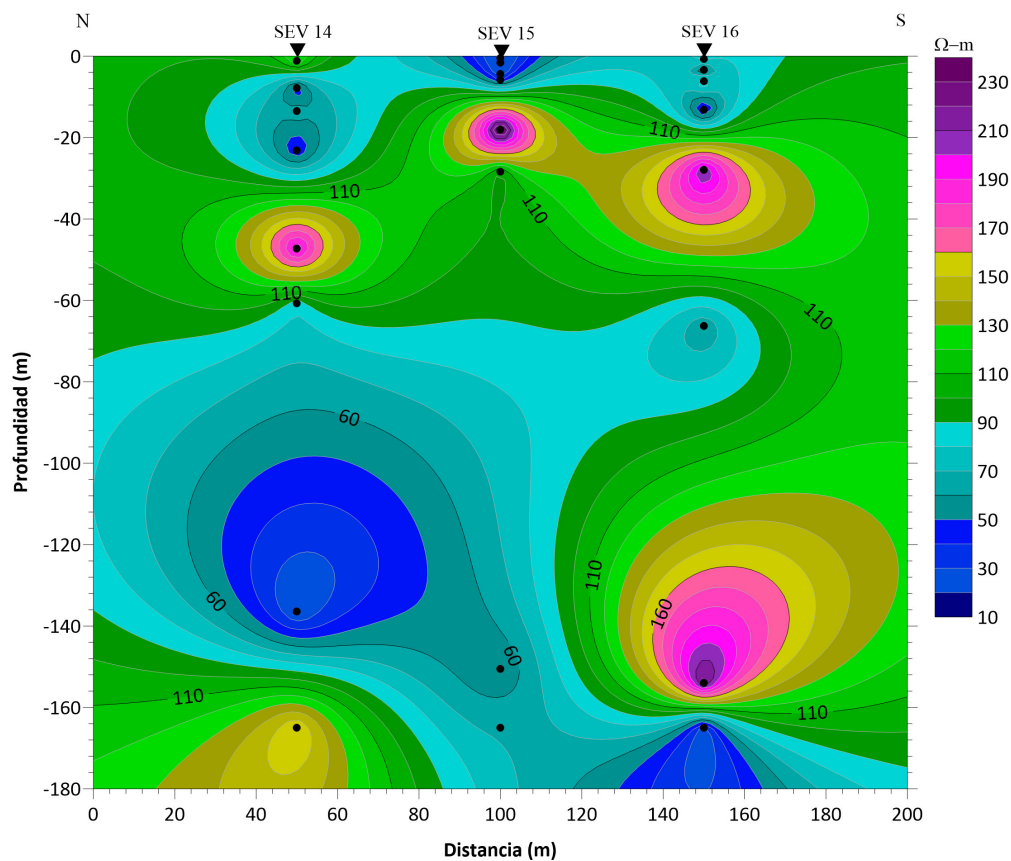


Figura 15. Perfil geoelectrico 6 de iso-resistividad verdadera.

3.6.4. Mapa de la conductancia longitudinal

La conductancia longitudinal (ohm^{-1} o Siemens) es un parámetro que permite cuantificar la capacidad de protección y el grado de vulnerabilidad de un acuífero, en función de las capas suprayacentes y que conforman la zona no saturada. Para identificar las zonas que mejor protección brindan al agua subterránea se presenta el mapa de conductancia longitudinal (Figura 16), en el que se identifican 5 zonas y sus correspondientes valores.

Valores menores a $1.2 \Omega^{-1}$, indican baja capacidad de protección y vulnerabilidad alta, valores entre 1.2 y $2.2 \Omega^{-1}$ la capacidad protectora y la vulnerabilidad es moderada, valores entre 2.2 y $3.2 \Omega^{-1}$ representan una capacidad protectora y vulnerabilidad media, valores entre 3.2 y $4.0 \Omega^{-1}$ muestran una capacidad protectora y vulnerabilidad baja, finalmente, a valores mayores a 4 indican una capacidad protectora muy alta y una vulnerabilidad muy baja.

Las áreas con valores más bajos de S (alta vulnerabilidad) se ubican en la parte sureste de la zona de estudio, en los límites

entre las localidades de San Agustín y San José, esta zona no está habitada. Sin embargo, se concentra una zona extensa de cultivo. Los valores más altos de S (vulnerabilidad baja), se presentan en la parte norte de la zona de estudio, en la colonia cruz verde de la localidad de San Agustín. En general el mapa indica que gran parte de la zona de estudio y los ríos que atraviesan el poblado y el pozo activo, se encuentran en el intervalo de protección media a baja y vulnerabilidad media a alta.

3.6.5. Mapa de distribución de la Resistencia Transversal

La resistividad eléctrica transversal (T) (Figura 17) de AVI se calculó para las capas que conforman la zona saturada, a partir del nivel piezométrico. El resultado se presenta en el mapa de resistencias transversales con tres subconjuntos, menores a $5,000 \Omega m^2$, valores entre $5,000$ y $9,000 \Omega m^2$ y valores superiores a $14,000 \Omega m^2$. Los valores más altos para este parámetro se ubican al sur y sureste de la zona de estudio.

3.7. Modelo conceptual

Como resultado de la exploración geoelectrica con el método del SEV , mediante la inversión de datos geoelectricos medidos en

campo con el programa IX1D, proporcionaron un modelo de capas del subsuelo y sus espesores del sistema acuífero de San Agustín Texcaltitlán, Estado de México, para integrar un modelo conceptual hidrogeológico preliminar de un sector al suroriente del Valle de Toluca, de 2 km^2 , se plantea a partir del análisis conjunto de la información geológica, hidrogeológica y particularmente de la geofísica (hidroestratigrafía), todos ellos indicadores del comportamiento del flujo y la hidráulica subterránea (Figura 18). El modelo hidrogeológico conceptual preliminar, es por tanto un paso importante durante el desarrollo e implementación de esquemas de planeación y aprovechamiento óptimo de los recursos hídricos subterráneos, así como un elemento importante en el proceso de la modelación numérica del flujo y transporte de contaminantes (Anderson *et al.*, 2017). Para la integración del modelo conceptual del acuífero libre de San Agustín Texcaltitlán, se consideraron los siguientes elementos: Condiciones de frontera, geomorfología, hidrología e hidrogeología.

3.7.1. Condiciones de frontera

Frontera horizontal: Al noreste en la localidad de San Agustín, se encuentran rocas volcánicas con profundidad variable. Al sur se encuentra una alternancia de materiales piroclásticos de

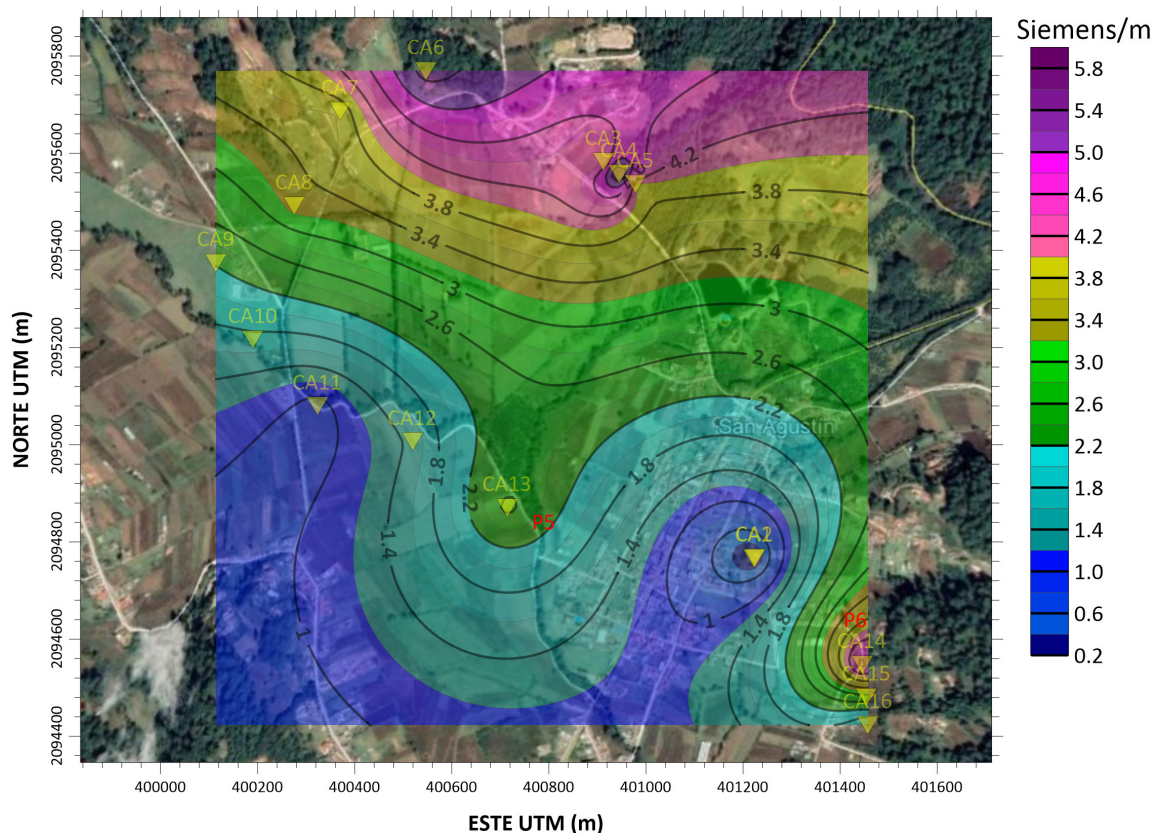


Figura 16. Mapa de distribución de la conductancia longitudinal (S) en (Siemens) y zonificación de la vulnerabilidad intrínseca.

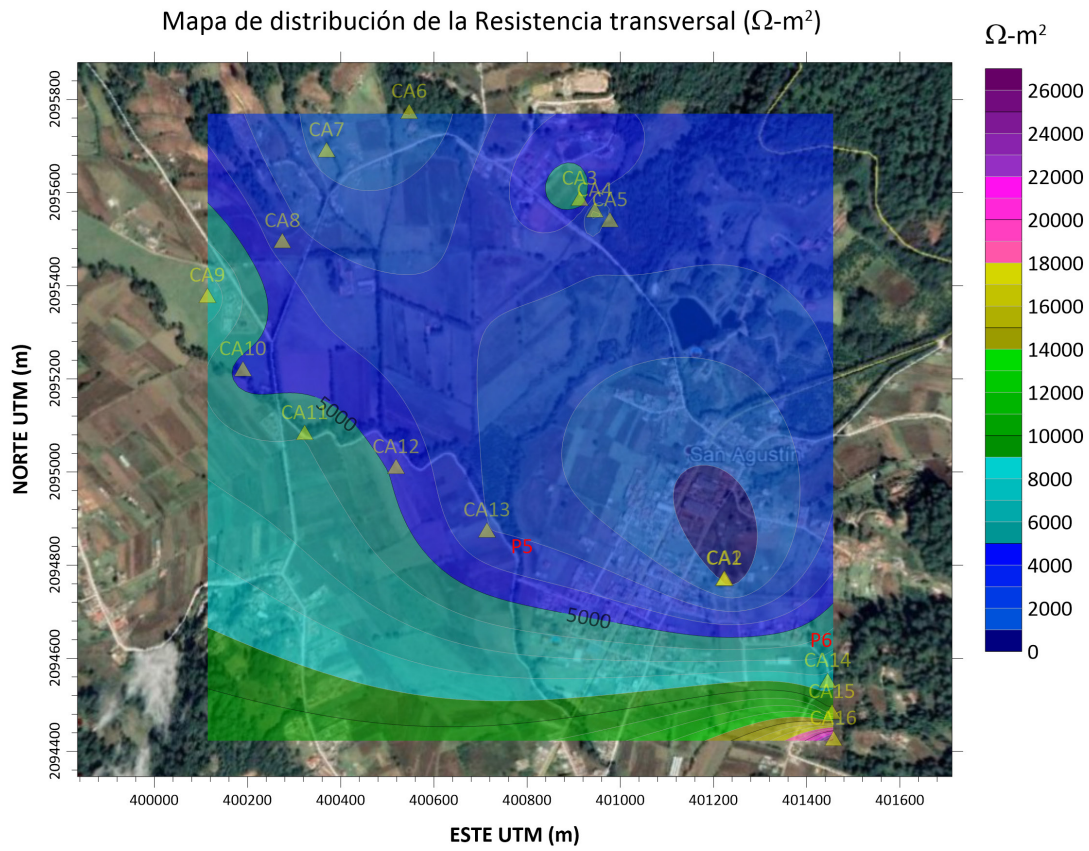


Figura 17. Mapa de distribución de la resistencia transversal ($\Omega\text{ m}^2$).

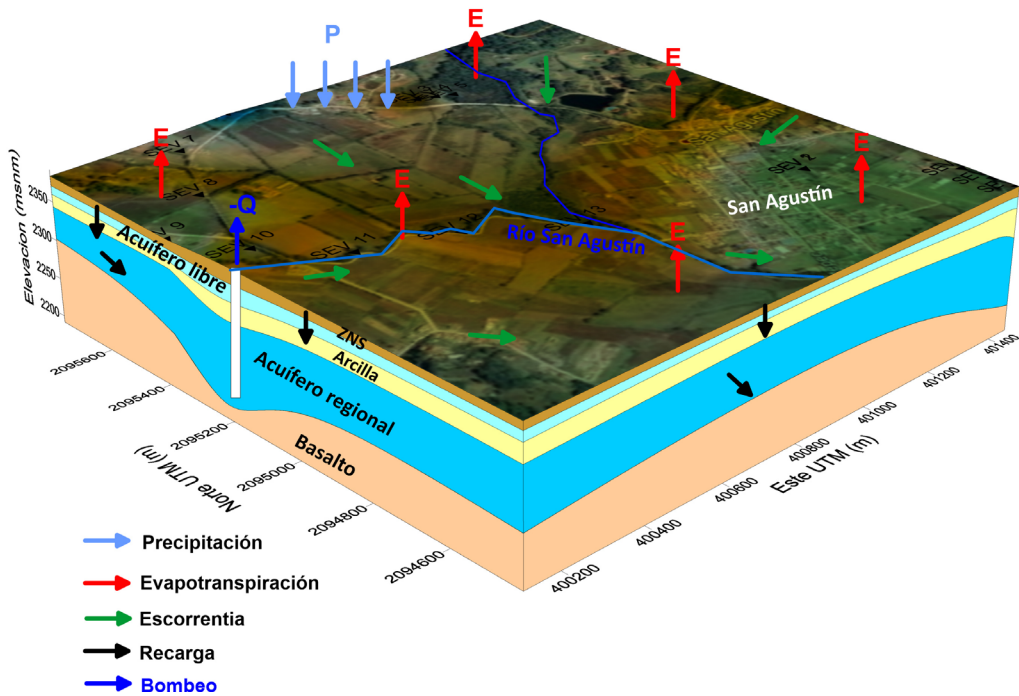


Figura 18. Modelo conceptual del área de estudio.

espesor variable y se asocia como una frontera de carga constante. Al oriente y poniente el flujo de ladera de las estribaciones del Nevado de Toluca y el proveniente del Río San Agustín, que se define como niveles de carga variable.

Frontera vertical: Se encuentran sedimentos aluviales del reciente, interestratificados con material aluvial, piroclastos y conglomerado, de espesor variable. Tienen alta permeabilidad y distribución variable, predominando en toda el área de estudio. El acuífero libre granular, es un sistema multicapa, con espesor promedio de 100 m.

Entradas: En este caso, se consideran como entradas: (1) la recarga horizontal al acuífero proveniente del poniente, por el norte el flujo del Río San Agustín; (2) la recarga vertical natural.

Salidas: Entre éstas se encuentran: (1) La recarga horizontal natural hacia el sureste, (2) La evaporación y la evapotranspiración y, (3) Por el bombeo de un pozo ubicado aproximadamente a 1 km del poblado de San Agustín.

3.7.2. Geomorfología

El área de estudio en general presenta un terreno suavemente ondulado con un gradiente de 0.5, dentro de un valle con orientación NW-SE. Los sedimentos aluviales son los que rellenan el valle.

3.7.3. Hidrogeología

Se elaboró un modelo conceptual preliminar de acuerdo a la integración de los sondeos eléctricos verticales (*SEV*) medidos en campo, que proporcionaron un modelo de capas del subsuelo y datos litológicos, que constituye un método altamente eficaz y rentable para definir las unidades hidroestratigráficas en entornos complejos que se presentan tanto en un acuífero aluvial libre (no confinado) como uno confinado. Los *SEV* proporcionan perfiles de resistividad eléctrica (profundidad, espesor y resistividad) del subsuelo, mientras que los datos litológicos de los sondeos calibran estas señales eléctricas con los materiales geológicos específicos (por ejemplo, arcilla, arena, grava, y roca). El sistema acuífero está formado por material sedimentario de relleno reciente (Cuaternario) con niveles freáticos someros, del orden de los 2.5 a 6 m en promedio, de moderada a alta conductividad hidráulica y heterogénea. De los resultados obtenidos, se infiere que la base del acuífero se correlaciona con la presencia de basalto alterado, que aflora al noreste y sur del área de estudio. De los resultados obtenidos, se infiere que la base del acuífero se correlaciona con la presencia de basalto alterado con valores de resistividad entre 400 y 800 ohm-m, que aflora al noreste y sur del área de estudio. De acuerdo a la metodología del *SEV*, la separación de electrodos de corriente fue 2 a 500 m, para alcan-

zar una profundidad de investigación de 80 a 180 m, de acuerdo a la geología del subsuelo, como se indica en la Sección 2.1.1. El área de estudio pertenece hidrogeológicamente a la Cuenca de Amacuzac, al norte por la Sierra del Nevado de Toluca. La microcuenca está caracterizada por un invierno frío con lluvias y un verano caluroso con lluvias. La precipitación media anual alcanza los 1,035 mm/año.

4. Conclusiones

Uno de los principales problemas recurrentes de la calidad del agua subterránea del acuífero de Texcaltitlán es la salinidad. La presencia de iones cloruros y sodio, se presentan en la zona de estudio. Los suelos en el área de estudio son principalmente de tipo arenosos de textura media a gruesa y presencia de arcilla, con una porosidad efectiva de 0.36 a 0.4 y conductividad hidráulica de 6 a 15 m/d. En la zona existe un pozo perforado aproximadamente a 100 m, que abastece a la población. De acuerdo a los valores de los parámetros fisicoquímicos que están por debajo del límite de la norma oficial mexicana, el agua es de buena calidad, pero propensa a contaminarse con el tiempo. El uso del método geoelectrico de resistividad en superficie, se considera una herramienta apropiada y de bajo costo, para estudiar las características resistivas del subsuelo y detectar las unidades hidroestratigráficas en el subsuelo de la zona de estudio. El procesamiento computacional de los resultados permitió generar mapas y secciones geoelectricas, revelando el espesor de las capas y su profundidad, con sus respectivos valores de resistividad. Con respecto a la evaluación de la capacidad protectora de la cobertura con AVI, se obtuvieron valores de la resistencia hidráulica *C* de 0.4 a 6.0 días. Los valores indican que en la zona centro-sur y en la zona poniente existe alta vulnerabilidad a la contaminación del agua subterránea, mientras que en la zona norte hay una moderada vulnerabilidad. En general, la zona de estudio presenta de buena a regular capacidad protectora contra la infiltración de fluidos o lixiviados al acuífero subyacente, sólo se detectaron zonas puntuales, donde las capas superficiales al acuífero presentan elevados valores de infiltración como la zona poniente. Con los datos del estudio geoelectrico analizados e interpretados. Se elaboró un modelo conceptual preliminar de acuerdo a la integración de los sondeos eléctricos verticales (*SEV*) medidos en campo, que proporcionaron un modelo de capas del subsuelo y datos litológicos, que constituye un método altamente eficaz y rentable para definir las unidades hidroestratigráficas en entornos complejos que se presentan tanto en un acuífero aluvial libre (no confinado) como uno confinado. Los *SEV* proporcionan perfiles de resistividad eléctrica (profundidad, espesor y resistividad) del subsuelo, mientras que los datos litológicos de los sondeos

calibran estas señales eléctricas con los materiales geológicos específicos (por ejemplo, arcilla, arena, grava, y roca).

Como resultado de la exploración geoeléctrica con el método del *SEV*, mediante la inversión de datos geoeléctricos medidos en campo e interpretados con el programa IX1D, proporcionaron un modelo de capas del subsuelo y sus espesores del sistema acuífero de San Agustín Texcaltitlán, Estado de México, para integrar un modelo conceptual hidrogeológico preliminar de un sector al suroriente del Valle de Toluca. Además, se puede indicar que las inferencias pueden significar que el modelo es válido solo bajo condiciones específicas o contextos restringidos en el sitio estudiado. Finalmente, se puede indicar que, la recarga del acuífero es moderadamente lenta por la presencia de material arcilloso en la zona no saturada, lo que generará una baja tasa de recarga en el sitio.

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Comparative Study of Atmospheric Particulate Matter Size Distribution in East and West Tehran, Iran

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Abstract

In order to investigate the particle size distribution pattern of atmospheric suspended particles in Tehran, simultaneous sampling was conducted at six stations located in the western (ST1 to ST3) and eastern (ST4 to ST6) halves of the city. Mass concentrations were measured across nine size fractions ranging from particles larger than 11 μm to those smaller than 0.4 μm . The results indicated that at the western stations, the highest mass concentrations were mainly observed in the coarser particle fractions (11-7 μm and $\geq 11 \mu\text{m}$), with maximum values of 19.6 and 16.3 $\mu\text{g.m}^{-3}$ recorded at ST2 and ST1, respectively. This pattern suggests the dominance of mechanical sources and road dust resuspension in the western part of the city. In contrast, the eastern half of Tehran exhibited an increasing trend in concentration within the finer fractions (less than 2.1 μm), with the highest value measured at ST6 in the <0.4 μm fraction (18.7 $\mu\text{g.m}^{-3}$). Additionally, in the 0.7-0.4 μm and 2.1-1.1 μm ranges, eastern stations showed higher concentrations compared to the western stations. This shift in size distribution pattern-from coarse-particle dominance in the west to fine-particle dominance in the east-may be attributed to differences in land use, traffic density, combustion-related sources, as well as topographic conditions and prevailing wind patterns across Tehran. Overall, the findings indicate a greater contribution of combustion-related and secondary fine particles in the eastern half, whereas the western half appears to be more influenced by primary sources and coarse particle resuspension. These results highlight the importance of region-specific management strategies for effective control of particulate matter pollution in the megacity of Tehran.

Key words: Atmospheric Particulate Matter, Particle Size Distribution, Urban Air Quality, Spatial Variation.

Resumen

Para investigar el patrón de distribución del tamaño de las partículas atmosféricas suspendidas en Teherán, se realizó un muestreo simultáneo en seis estaciones ubicadas en las mitades occidental (ST1 a ST3) y oriental (ST4 a ST6) de la ciudad. Se midieron las concentraciones de masa en nueve fracciones de tamaño que iban desde partículas mayores de 11 μm hasta aquellas menores de 0.4 μm . Los resultados indicaron que en las estaciones occidentales, las concentraciones de masa más altas se observaron principalmente en las fracciones de partículas más gruesas (11-7 μm y $\geq 11 \mu\text{m}$), con valores máximos de 19.6 y 16.3 $\mu\text{g.m}^{-3}$ registrados en ST2 y ST1, respectivamente. Este patrón sugiere el predominio de fuentes mecánicas y la resuspensión de polvo de la carretera en la parte occidental de la ciudad. En contraste, la mitad oriental de Teherán exhibió una tendencia creciente en la concentración dentro de las fracciones más finas (menos de 2.1 μm), con el valor más alto medido en ST6 en la fracción <0.4 μm (18.7 $\mu\text{g.m}^{-3}$). Además, en los rangos de 0.7-0.4 μm y 2.1-1.1 μm , las estaciones orientales mostraron concentraciones más altas en comparación con las estaciones occidentales. Este cambio en el patrón de distribución de tamaño, del predominio de partículas gruesas en el oeste al predominio de partículas finas en el este, puede atribuirse a las diferencias en el uso del suelo, la densidad del tráfico, las fuentes relacionadas con la combustión, así como las condiciones topográficas y los patrones de viento predominantes en Teherán. En general, los hallazgos indican una mayor contribución de partículas finas secundarias y relacionadas con la combustión en la mitad oriental, mientras que la mitad occidental parece estar más influenciada por fuentes primarias y la resuspensión de partículas gruesas. Estos resultados resaltan la importancia de las estrategias de gestión específicas de la región para el control efectivo de la contaminación por material particulado en la megaciudad de Teherán.

Palabras clave: material particulado atmosférico, distribución del tamaño de las partículas, calidad del aire urbano, variación espacial.

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1. Introduction

Despite industrial advancements in recent years, improvements in air quality have stalled not only in less developed countries but also in many regions worldwide, and this trend continues at an alarming rate. This situation has led to the formation of “black clouds” of urban atmospheric pollution, exacerbating atmospheric stability issues. Such conditions have contributed to an increase in hospital visits by patients suffering from asthma, Chronic Obstructive Pulmonary Disease (COPD), and cardiovascular diseases, as well as a rise in the consumption of chemical medications (Kelly *et al.*, 2015). Rapid urbanization has also resulted in elevated concentrations of fine and coarse particulate matter in the air, making this phenomenon one of the most critical environmental challenges of the century in developing countries (Zweifel *et al.*, 2009; Thompson *et al.*, 2013). Daily human exposure to particles emitted from fossil fuel combustion in both mobile and stationary sources, as well as particles originating from heating systems and cooking processes in confined spaces, poses significant health risks (WHO, 2013b). Research on pregnant women exposed to prolonged PM_{2.5} has shown that post-delivery, biological complications and long term disturbances in overall neonatal health emerge. Low birth weight and preterm birth are among these adverse outcomes (Ritz *et al.*, 2008; Sapkota *et al.*, 2012; Proietti *et al.*, 2013). Limited studies have addressed the health effects associated with residing in areas where individuals are continuously exposed to traffic related pollutants. However, some research has identified air pollution as a novel risk factor for type 2 diabetes mellitus (T2DM), with strong evidence linking these effects to NO₂ exposure (Raaschou-Nielsen *et al.*, 2013; Puett *et al.*, 2011a; Puett *et al.*, 2011b; Kramer *et al.*, 2010; Ranft *et al.*, 2009; Guxens and Sunyer, 2012). In the United States, Pope *et al.*, 2009, evaluated data collected from 51 cities over an extended period between 1980 and 2000, as provided by the American Cancer Society, regarding long-term exposure to PM_{2.5}. They reported that the implementation of air quality regulations and the subsequent reduction in PM_{2.5} concentrations between 1980 and 2000 contributed to an overall increase of approximately 2.7 years in life expectancy among the affected populations (Pope *et al.*, 2009).

Recently, findings from the Swiss Study on Air Pollution and Lung Diseases in Adults (SAPALDIA) were published concerning air pollution and respiratory disease in adults. According to this report, in eight communities surveyed in 1991 and again in 2002, the annual mean PM₁₀ concentration decreased by 5-6 µg.m⁻³. This reduction in particulate levels was associated with a corresponding decline in the annual rate of lung function deterioration (Downs *et al.*, 2007). These studies, along with other

research, have examined the relationship between long-term air pollution exposure and mortality (Katsouyanni *et al.*, 2001; Hoek *et al.*, 2002; Filleul *et al.*, 2005). It is noteworthy that, today, air pollution has surpassed drinking water contamination as a primary environmental concern and has become a leading cause of premature mortality in recent years (Leoeule *et al.*, 2012; Krewski *et al.*, 2009). According to the World Health Organization's latest report in 2012, approximately 3.7 million people in urban and rural open air environments died as a result of air pollution (WHO, 2014). Additionally, in recent years, mortality associated with low concentrations of particulate matter (PM) has also been significant (Ostro *et al.*, 2006; Naess *et al.*, 2007; Crouse *et al.*, 2012; Meister *et al.*, 2012). These findings indicate that, alongside the scarcity of potable water, air pollution has emerged as a major global environmental challenge in recent years (OECD, 2014). Schindler *et al.* (2009) reported that reductions in symptoms such as regular cough, chronic cough with phlegm, wheezing, and shortness of breath may be associated with decreases in particulate matter (PM) concentrations (Schindler *et al.*, 2009). In a separate study conducted in Switzerland on nine cohorts of children between 1992 and 2001, a link was observed between reductions in ambient PM₁₀ concentrations and improvements in respiratory health, including decreased incidence of chronic cough, bronchitis, common colds, mild nocturnal dry coughs, and pulmonary inflammation (Bayer-Oglesby *et al.*, 2005). The results suggest that health improvements can occur to some extent following reductions in particulate matter concentrations. However, with current knowledge, it is not possible to definitively identify individual characteristics or sources with regard to their health effects. Moreover, no specific source or concentration of particulate matter can be considered entirely without adverse effects. Nonetheless, the pathogenic potential of particulate matter may operate through various mechanisms (EPA, 2009; WHO, 2013a; HEI, 2013a). Components with direct adverse effects on health have been identified through extensive research, including large-scale studies such as the WHO REVIHAAP Project (Review of Evidence on Health Aspects of Air Pollution) and other systematic investigations in this field (WHO, 2013a; HEI, 2013a; WHO, 2012; HEI, 2010; HEI, 2013b). These components include chemical constituents such as black carbon (BC), organic carbon (OC), secondary inorganic particles, particle size (coarse and ultrafine), and sources (e.g., road traffic). Furthermore, research indicates that short-term exposure to black carbon can be more hazardous than exposure to PM₁₀ or PM_{2.5}, although black carbon alone cannot be considered solely responsible for adverse effects. Some researchers suggest that these particles in the atmosphere, as indicators of primary combustion related to traffic (such as organic compounds), are relatively less harmful compared to overall particulate mass (WHO, 2012).

Organic carbon (OC) is a complex and heterogeneous mixture of primary and secondary airborne particles. Given common combustion sources, OC can co-occur with black carbon. Therefore, assessing the potential toxicity of specific OC compounds is challenging, as there is insufficient evidence to distinguish between the toxicity of primary versus secondary OC particles. Nevertheless, studies have demonstrated associations between OC exposure and respiratory disorders as well as cardiovascular events (Kim *et al.*, 2008; Kim *et al.*, 2012; Hildebrandt *et al.*, 2009; Ito *et al.*, 2011; Son *et al.*, 2012; Zanobetti and Schwartz, 2009; Ostro *et al.*, 2010). Long-term exposure to OC has been linked to ischemic cardiovascular diseases and, ultimately, increased mortality (Anderson *et al.*, 2010). Epidemiological evidence also indicates that short-term exposure to sulfate is associated with cardiovascular and respiratory mortality, as well as hospital admissions for heart and lung conditions (Kim *et al.*, 2012; Ito *et al.*, 2011).

Moreover, studies have reported physiological changes in the heart, including ventricular dysfunction and endothelial impairment, correlated with daily sulfate exposure (Anderson *et al.*, 2010; Bind *et al.*, 2012).

Epidemiological data indicate that short-term exposure to coarse particles (2.5–10 μm) significantly impacts cardiovascular and respiratory health, including premature mortality (Meister *et al.*, 2012; Peng *et al.*, 2008; Atkinson *et al.*, 2010; Mann *et al.*, 2010; Oiu *et al.*, 2012). Systematic reviews present varying conclusions regarding the health effects of fine particulate matter ($\text{PM}_{2.5}$) (EPA, 2009; Brunekreef and Forsberg, 2005; EPA, 2013). Research on the long-term impact of coarse particles on public health is limited, and cardiovascular mortality or morbidity linked to these particles has not been widely reported (Puett, 2011b). However, toxicological evidence shows that coarse particles can act as carriers for toxic substances, similar to $\text{PM}_{2.5}$ (Graff *et al.*, 2009; Wegesser *et al.*, 2008). Limited data and insufficient studies contribute to the scarcity of findings regarding coarse particulate matter, due in part to differences in deposition and inhalation mechanisms. Ultrafine particles ($<0.1 \mu\text{m}$) exhibit unique properties, including a strong tendency to agglomerate and form composite particles, rendering them more toxic than $\text{PM}_{2.5}$ or coarse particles. Beyond particle size and penetration into the respiratory tract, ultrafine particles have highly active surfaces that can adsorb toxic chemicals, penetrate internal organs, remain airborne for extended periods, and travel long distances. Given their significant potential health impacts in humans and animals, research on ultrafine particles is limited, with studies such as those conducted by the Health Effects Institute (HEI) providing valuable insights (HEI, 2013b). Epidemiological investigations consistently demonstrate strong adverse effects of ultrafine particles (Ruckerl *et al.*, 2011; Weichenthal, 2012). HEI findings

suggest that current evidence on the health impacts of ultrafine particles can be considered indicative of the primary pathways through which $\text{PM}_{2.5}$ exerts its harmful effects (HEI, 2013b).

Toxicological studies have demonstrated that the patterns of deposition, resuspension, and particle transport play a critical role in environmental perturbation processes (Kreyling *et al.*, 2010). Considering the prevalence of diesel engines and the use of diesel fuel for powering buses and taxis in many industrialized countries, it is well-established that these engines emit significantly higher particulate matter compared to gasoline engines equipped with three catalytic converters. Diesel engine exhaust particles (DEPs) release substantial quantities of particulate matter into the atmosphere in most major cities worldwide (Quality of Urban Air Review Group, 1996). The toxicological characteristics, particle size, and chemical and surface properties of these exhaust-generated particles are noteworthy, with approximately 80% of DEP particles having an aerodynamic diameter of less than 1 μm . Notably, DEPs possess a highly adsorptive carbon core, which facilitates the deep lung transport of active metal oxides and polycyclic aromatic hydrocarbons.

In addition to traffic density, health impacts are influenced by proximity to transportation corridors as well as the condition of both light and heavy diesel vehicles (Janssen *et al.*, 2003; Gowers *et al.*, 2012). In 2012, the International Agency for Research on Cancer (IARC) classified diesel engine exhaust as a carcinogenic agent, providing evidence of its association with lung cancer and limited evidence linking it to bladder cancer (IARC, 2012). Although most research has focused on diesel exhaust and roadside health effects, non-exhaust sources also constitute a significant subject for investigation (Van der Gon, *et al.*, 2013). Particles generated from tire wear on heavily trafficked roads are gradually emerging as a health concern, potentially surpassing exhaust emissions in significance, with some evidence indicating associations with cardiovascular and pulmonary problems (Riediker *et al.*, 2004; Gottipolu *et al.*, 2008; Gasser *et al.*, 2009; Mantecca *et al.*, 2009). Given the sensitivity of this issue, the siting of critical and densely populated areas has always been a fundamental principle in public health considerations, and this principle now significantly influences urban planning and growth patterns. Tehran, as one of the major cities facing severe air pollution challenges globally, experiences hazardous air quality on many days of the year, particularly during cold periods associated with temperature inversion events. Moreover, due to its geographical setting, topography, and prevailing wind directions, addressing this issue and implementing preventive and control measures is crucial.

Given the high risk of inhaling atmospheric particles for residents in polluted areas, understanding the behavior of particulate matter in Tehran is of critical importance and must be

considered in all aspects of urban development (Oroji *et al.*, 2021). The presence of a substantial number of military facilities in the eastern and northeastern parts of Tehran, combined with the circulation and movement patterns of atmospheric pollutants, underscores the importance of assessing the region's exposure to both the quantity and quality of particulate matter. Awareness of this exposure is essential for guiding future control measures to mitigate this environmental threat. Therefore, this study aims to evaluate the threat posed by atmospheric particles in the eastern and northeastern districts of Tehran and to assess the vulnerability of residents in these areas to various particle types based on their size.

2. Materials and Methods

2.1. Geographical Location of the Study Area

Tehran is located at the southern foothills of the Alborz mountain range, geographically spanning between $51^{\circ}05'$ to $51^{\circ}53'$ E longitude and $35^{\circ}34'$ to $35^{\circ}59'$ N latitude (Berberian and Yeats, 2017) (Figure 1). The elevation of Tehran relative to mean sea

level varies from 1.700 m in the northern areas, 1.200 m in the central part, to 1.100 m in the southern regions, resulting in a general north to south slope across the city. In addition to this overall gradient, local topographical irregularities within the city influence air pollution dynamics. Tehran Province is separated from its northern neighbor, Mazandaran, by the Alborz mountain range. These elevations increase from west to east, reaching their maximum at Mount Damavand. In the eastern section, the Savadkuh and Firuzkuh mountains connect to the Shahmirzad highlands. Other notable elevations in the province include Hasanabad and Namak Mountains south of Bibi Shahrbanu, Aghaghadr in the southeast, and the Ghasr e Firoozeh highlands in the east. Plains constitute another natural feature of the province, extending from Hashtgerd to the Varamin plain. Due to their gentle slope from the northeast to the southwest, these plains provide favorable conditions for human settlement. The expansion and increasing density of urban areas in these regions reflect this suitability. Alluvial plains, forming a part of these areas, have an elevation of approximately 790 m above sea level and are considered the lowest-lying regions in the province. The climate of the province is generally temperate in mountainous areas and semi-arid in the plains. Atmospheric pressure shows

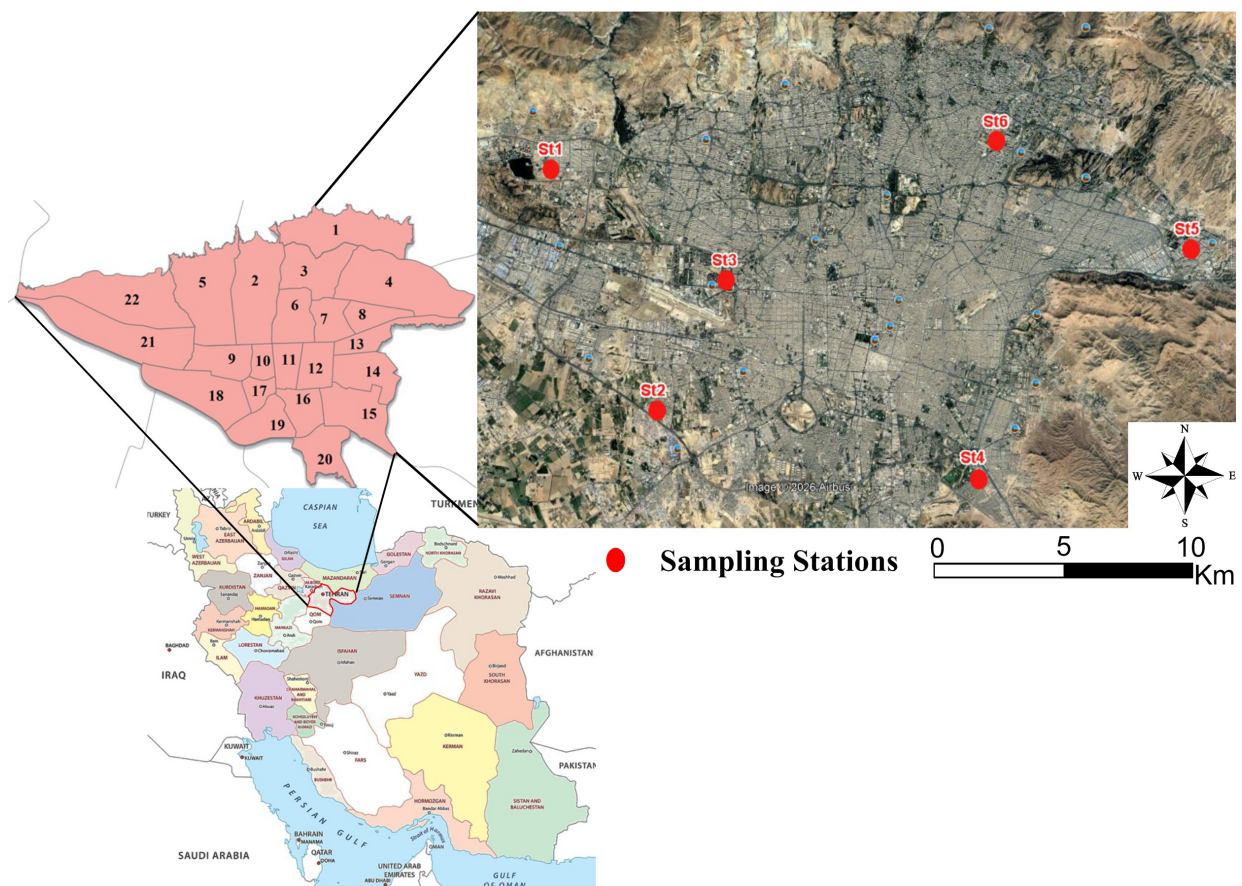


Figure 1. Geographical location of the study area and sampling stations

its maximum increase in late autumn and early winter, with the highest precipitation occurring in March (Oroji *et al.*, 2019). Therefore, the geographical and geological characteristics of the region play a significant role in controlling, stabilizing, and removing atmospheric particles and may render certain areas more vulnerable than commonly assumed.

2.2. Sampling Method

This research was conducted between 2020 and 2021. A sampling station was selected in the eastern part of Tehran (Hakimiyeh district) for sample collection. Another station was chosen in the western part of the city, in the Azadi Square area. In this study, a new and advanced sampling technique was employed to determine the concentration and aerodynamic size distribution of atmospheric particles and to assess the regional risk associated with these particulates. For this purpose, a 1 ACFM (CFM equivalent to one cubic foot per minute) ambient cascade impactor was used for particle collection. The cascade impactor operates at a constant flow rate of 28.3 L/min, supplied by a continuous vacuum pump, and consists of eight aluminum stages (Papastefanou, 2008). The stages have effective cutoff diameters of 11, 7.0, 4.7, 3.3, 2.1, 1.1, 0.7, and 0.4 μm , corresponding to stages 0, 1, 2, 3, 4, 5, 6, 7, and F, respectively. Stage 0 serves solely as the nozzle plate. Stage F comprises the collection plate of stage 7 along with a backup filter. Stages 0 through 6 include a unified air-inlet section containing 400 nozzles, while stage 7 contains 201 nozzles. The inlet diameter is approximately 3.125 inches.

The nozzle diameters decrease progressively from the upper to lower stages, ranging from 0.0625 inches in stage 0 to 0.01 inches in stage 7. Each stage is equipped with a removable stainless-steel or glass collection substrate (3.25 inches in diameter). The outlet section of each stage is approximately 0.75 inches larger than the collection plate, allowing non-impacted particles to bypass the plate and move to the subsequent stage (Papastefanou, 2008). The smaller nozzles increase the jet velocity sequentially across the eight stages, enabling the impaction of progressively finer particles onto the collection discs of each lower stage (Papastefanou, 2008). For this research, 6 stations including 3 points in the western part and 3 stations in the eastern part of the study area were selected for sampling. The sampling results are shown in Table 1. Sampling was carried out 3 times per month. The sampling duration for each run ranged from 72 hours to 7 days. After sampling, the collection plates were carefully weighed, and based on the mass of particles accumulated on each plate and the total volume of sampled air, the concentration and mass fraction of the particles were calculated. This procedure was repeated for each sampling event with the cascade impactor.

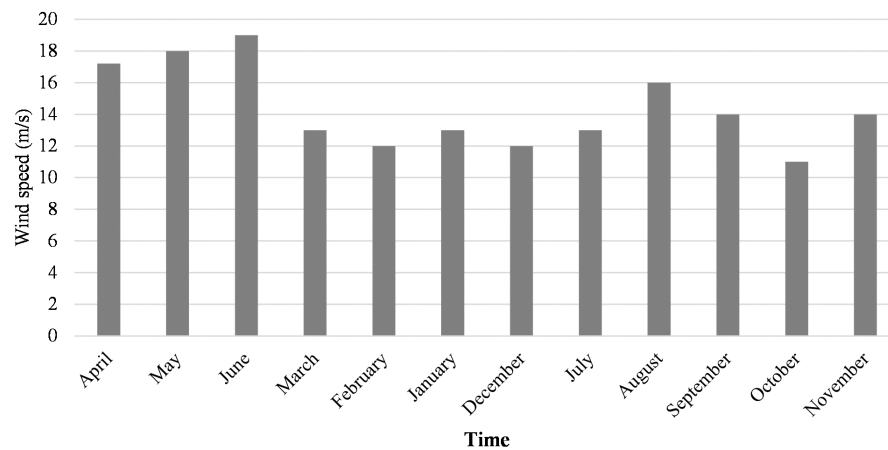
3. Results and Discussion

The highest wind speed recorded in April 2020 was 17.1 m/s with a predominant wind direction of 260°. The monthly mean of maximum wind speeds during this month reached 15.2 m/s. In May, the maximum wind speed increased to 21.7 m/s blowing from 290°, while the regional average of maximum values was 18.5 m/s. Over the study period, June showed a maximum wind speed of 16 m/s, accompanied by a regional mean maximum of 15.1 m/s. During July, August, and September, the peak wind speeds were measured at 15.1, 14.2, and 13 m/s, respectively. The corresponding regional mean maximum wind speeds were 14.4 m/s in July, 15.0 m/s in August, and 11.1 m/s in September. The prevailing wind directions for these months were recorded as 220°, 290°, and 260°, respectively. In autumn, the maximum wind speed in October reached 15.3 m/s from 260°, followed by 15.5 m/s in November from 290°, and 15 m/s in December from 210°. The regional mean maximum wind speeds for these months were 14, 14, and 13 m/s, respectively. During the winter months, maximum wind speeds showed relatively small variations, averaging 16.1 m/s, with the dominant wind direction centered around 270°. The regional mean maximum wind speeds for January, February, and March were recorded as 16, 14, and 16.4 m/s, respectively. Overall, the prevailing wind direction in the Hakimiyeh (East area) during the evaluation period was westerly (west to east), representing 25% of all recorded winds. In total, 38% of the winds observed in Tehran in 2020 were within the directional sector spanning northwest to southwest. The findings indicate that winds exceeding 6 m/s blowing from the west occur more frequently in spring than in other seasons. Additionally, during summer, while westerly winds remain dominant, southeastern winds also appear with notable frequency. These observations confirm that the highest proportion of winds stronger than 6 m/s from the west occurs in spring. Furthermore, in summer, despite the continued dominance of westerly winds, southeastern flows also contribute significantly. Monthly variations in wind speed for the sampling station are presented in Figure 2.

The results of particle size distribution measurements at three stations: Azadi (ST3), Chitgar (ST1), and Tehransar (ST2) in the western half of Tehran show that the mass distribution pattern of particles largely follows a relatively similar trend, but significant differences are also observed in some size ranges. In general, the highest mass concentration at all three stations is related to coarser particles (diameter greater than 11 μm); this range has the highest contribution at Chitgar station with a value of 19.6 $\mu\text{g} \cdot \text{m}^{-3}$, followed by Azadi station (18.9 $\mu\text{g} \cdot \text{m}^{-3}$) and Tehransar (15.6 $\mu\text{g} \cdot \text{m}^{-3}$). This indicates the dominant role of mechanical sources and surface dust re-emission (such as heavy traffic, construction activities, and surrounding soil surfaces) in

Table 1. Average concentration distribution of particulate matter at sampling stations.

Particle diameter (μm)	Particle concentration ($\mu\text{g.m}^{-3}$)					
	ST1	ST2	ST3	ST4	ST5	ST6
$11 \leq$	15.6	19.6	18.9	11.7	11.2	7.7
11-7	16.3	15.8	14.5	12.3	10.5	8.5
7-4.7	13.9	12.6	12.1	11.4	9.5	8.1
4.7-3.3	12.1	11.8	11.9	11.3	12.2	11.14
3.3-2.1	11.8	12.7	12.1	12.7	10.7	10.1
2.1-1.1	12.5	12.8	12	12.8	14	13.19
1.1-0.7	10.4	11.5	11.65	12.5	13.4	11.65
0.7-0.4	8.6	9.2	9.1	13.1	12.8	13.1
$0.4 \geq$	10.2	9.3	8.7	13.4	15.6	18.7

**Figure 2.** Monthly variations in wind speed across the study area.

the western half of Tehran, especially in the Chitgar area, which is affected by highways and open lands.

In the size range of 7–11 μm , the concentrations at all three stations are relatively high and close to each other (between 14.5 and 16.3 $\mu\text{g.m}^{-3}$), indicating a more uniform distribution of coarse particles over the area. Tehransar shows the highest value (16.3 $\mu\text{g.m}^{-3}$) in this range, which could be due to the impact of local traffic, construction activities, or horizontal transport of particles from adjacent areas. In the intermediate ranges (4.7–7 to 1.1–2.1 μm), the concentration changes are smaller and the values fluctuate in the range of 11 to 13 $\mu\text{g.m}^{-3}$. This relative uniformity indicates that the share of particles with a combined origin (mechanical-combustion) is almost similar at all three stations and is probably affected by the same atmospheric conditions and regional air mixing.

In the finer particle segment (diameter less than 1.1 μm), a slight decreasing trend in concentration is observed; the lowest values are in the 0.7–0.4 μm range at all three stations (be-

tween 8.6 and 9.2 $\mu\text{g.m}^{-3}$). However, in the smallest size range ($\leq 0.4 \mu\text{m}$), a relative increase is observed at Tehransar station (10.2 $\mu\text{g.m}^{-3}$), which is higher than Azadi and Chitgar. This increase could indicate a higher contribution of combustion sources (such as light and heavy vehicles, fossil fuel combustion, and secondary chemical processes in the atmosphere) at this station. In general, the particle size distribution at all three stations shows a weak multi-peaked pattern characterized by the dominance of the coarse mode, which is expected in the semi-arid climate of Tehran and under the influence of regional dust and surface re-emission.

Comparisons between stations show that Chitgar has the highest concentration in most of the coarser ranges, while Tehransar shows a higher contribution in the finer ranges (especially less than 0.4 μm). Azadi also recorded intermediate values in most of the ranges. These differences could be due to differences in land use, traffic density, proximity to highways, green spaces (such as Chitgar Park), as well as local wind flow patterns. Overall, the

results show that in the western half of Tehran, the contribution of coarse particles is significant, but the significant presence of fine and ultrafine particles also indicates the role of combustion sources and secondary processes in the composition of urban aerosols; an issue that is of particular importance from the perspective of environmental health and air quality management, because finer particles have more harmful effects on human health due to their greater ability to penetrate the respiratory tract.

The monthly average concentration of suspended particles at sampling stations for a year is shown in Table 1. The results of particle size distribution sampling at three eastern stations in Tehran, including Khavaran (ST4), Piroozi (ST5), and Hakimieh (ST6), indicate a dominant pattern of concentration in fine particles and an increase in the proportion of particles with an aerodynamic diameter of less than $2.5\ \mu\text{m}$. In general, in all three stations, the trend of concentration changes from coarser particles ($\geq 11\ \mu\text{m}$) to finer particles ($\leq 0.4\ \mu\text{m}$) is increasing, indicating the dominance of combustion sources and secondary processes of particle formation in the eastern half of Tehran. The lowest concentration values are mainly observed in the range of $11\ \mu\text{m}$ and larger (7.7 to $11.7\ \mu\text{g}\cdot\text{m}^{-3}$), while the highest values are related to the smallest size fraction ($\leq 0.4\ \mu\text{m}$), reaching $18.7\ \mu\text{g}\cdot\text{m}^{-3}$, especially at Hakimieh station.

At Khavaran station, the particle distribution is relatively uniform but with a slight increase towards fine particles; the concentration has increased from $11.7\ \mu\text{g}\cdot\text{m}^{-3}$ in the range $\geq 11\ \mu\text{m}$ to $13.4\ \mu\text{g}\cdot\text{m}^{-3}$ in the range $\leq 0.4\ \mu\text{m}$. This pattern indicates a combination of local mechanical sources (urban dust and surface resuspension) and combustion sources such as traffic. The significant contribution of particles in the ranges 2.1 – 1.1 and 0.7 – $0.4\ \mu\text{m}$ (more than $12\ \mu\text{g}\cdot\text{m}^{-3}$) indicates the important role of secondary fine particles resulting from photochemical reactions in the urban atmosphere. At Piroozi station, a significant concentration is observed in particles smaller than $1.1\ \mu\text{m}$, with the highest value recorded in the range $\leq 0.4\ \mu\text{m}$ equal to $15.6\ \mu\text{g}\cdot\text{m}^{-3}$. Also, the value of $14\ \mu\text{g}\cdot\text{m}^{-3}$ in the range of 2.1 – $1.1\ \mu\text{m}$ indicates that particles in the $\text{PM}_{2.5}$ range constitute the dominant contribution. The relative decrease in the concentration in the coarser ranges (7 – $11\ \mu\text{m}$) could indicate limited local dust sources or faster deposition of these particles compared to fine particles. Overall, the pattern of Piroozi station indicates the dominance of urban combustion sources, especially heavy traffic and dense human activities in this part of the city.

At Hakimieh station, the highest concentration of particles is observed in the smallest size range ($18.7\ \mu\text{g}\cdot\text{m}^{-3}$ at $\leq 0.4\ \mu\text{m}$), which is noticeably higher than the other two stations. This indicates the accumulation of ultrafine particles and the possibility of being affected by pollutant transport, atmospheric stability conditions, and secondary particle formation processes. High

values (13.19 and $13.1\ \mu\text{g}\cdot\text{m}^{-3}$, respectively) were also recorded in the ranges of 2.1 – 1.1 and 0.7 – $0.4\ \mu\text{m}$, indicating that the size structure at this station is strongly biased towards fine particles. From a health perspective, this situation is of particular importance, as particles smaller than $1\ \mu\text{m}$ have the ability to penetrate deeply into the respiratory tract and even enter the bloodstream.

In a comparison of the three eastern stations, Hakimieh shows the highest concentration in ultrafine particles, while Khavaran has a more balanced distribution between coarse and fine particles, and Piroozi has recorded the highest concentration in the mid-range $\text{PM}_{2.5}$. In general, the dominant contribution of particles below $2.5\ \mu\text{m}$ at all three stations indicates that in the eastern half of Tehran, combustion sources (traffic, fossil fuels, and urban activities) and secondary atmospheric processes play the main role in the particulate matter load, while the contribution of coarse-grained mechanical sources is lower. This size distribution pattern can be used in pollution source analysis, modeling of particle residence time in the atmosphere, and health risk assessment, especially considering that finer particles have a longer residence time in the atmosphere and have a higher horizontal transport capability.

According to the data provided by six sampling stations (three stations in the western half and three stations in the eastern half of Tehran), statistical analysis of particle size distribution indicates a significant difference in the mass concentration pattern between the two halves of the city. At stations ST1 to ST3 (western half), the highest mass concentration is observed in the range of coarser particles ($11\ \mu\text{m}$ and 7 – $11\ \mu\text{m}$); for example, in the $11\ \mu\text{m}$ class, the concentration varies from 15.6 to $19.6\ \mu\text{g}\cdot\text{m}^{-3}$. In contrast, at stations ST4 to ST6 (eastern half), the highest concentration is recorded in the range of finer particles (less than 0.7 and especially less than $0.4\ \mu\text{m}$), such that in the $0.4\ \mu\text{m}$ and smaller class, the values have increased from 13.4 to $18.7\ \mu\text{g}\cdot\text{m}^{-3}$. This pattern indicates the dominance of coarse particles with mechanical origin (road dust, construction activities and soil resources) in the west of Tehran and the dominance of fine particles with combustion origin (heavy traffic, industrial activities and fossil fuel combustion) in the east of the city.

In terms of correlation between stations, Pearson correlation coefficients qualitatively indicate two distinct clusters in the pattern of particle size changes. The western stations (ST1–ST3) show a strong positive correlation with each other in the coarse-grained classes, such that the trend of gradual decrease in concentration with decreasing particle diameter is almost similar. In contrast, the eastern stations (ST4–ST6) have a high positive correlation in the fine-grained classes, and the trend of increasing concentration is in line with decreasing particle size at these stations. Also, a negative correlation is observed between the coarse ($\geq 7\ \mu\text{m}$) and fine ($\leq 0.7\ \mu\text{m}$) classes in all stations;

This means that as the proportion of coarse particles increases at a station, the relative proportion of fine particles decreases and vice versa. This inverse relationship indicates the dominant difference in emission sources and dynamic processes affecting particle size distribution in the two halves of the city. In general, the results of the correlation analysis show that the structure of particle size distribution in Tehran is influenced by the spatial pattern of pollutant sources, topographic conditions, and prevailing wind direction, and the western half can be described as having a coarse particle regime and the eastern half as having a fine particle regime. This statistical distinction can be a suitable basis for source apportionment analysis and for formulating targeted control policies at the regional scale of Tehran. The distribution chart of the average suspended particles collected for the sampling stations is shown in Figure 3.

The average concentration of sampling stations in the eastern and western regions of Tehran is shown in Table 2. Statistical analysis of the size-concentration distribution of suspended particles in the western half (stations 1 to 3) and eastern half of Tehran (stations 4 to 6) shows that the pattern of concentration changes in terms of particle diameter in the two parts of

the city follows a reverse trend. In western Tehran, the highest mass fraction is related to coarse particles (≥ 11 and $7-11\text{ }\mu\text{m}$) with averages of 18.03 and $15.53\text{ }\mu\text{g.m}^{-3}$, and with decreasing particle diameter, a relative decreasing trend in concentration is observed, such that the relative minimum is recorded in the range of $0.7-0.4\text{ }\mu\text{m}$ ($8.96\text{ }\mu\text{g.m}^{-3}$). In contrast, in eastern Tehran, an increasing pattern towards fine particles is observed; the highest average concentration is in the range $\leq 0.4\text{ }\mu\text{m}$ ($15.9\text{ }\mu\text{g.m}^{-3}$) and then $0.7-0.4\text{ }\mu\text{m}$ ($13\text{ }\mu\text{g.m}^{-3}$), while the share of coarser particles is relatively lower. This difference indicates the dominance of sources of mechanical origin (such as resuspended dust and construction activities) in the west and the dominance of combustion and traffic sources in the east of the city.

In terms of statistical correlation between the size distribution pattern in the two halves of the city, the Pearson correlation coefficient between the average concentrations in the west and east for different diameter classes shows a strong negative correlation (r around -0.8 to -0.9), which indicates the opposite behavior of the particle size distribution in the two parts of the city. This negative correlation indicates that whenever the mass fraction of a diameter interval increases in the west, a relative decrease

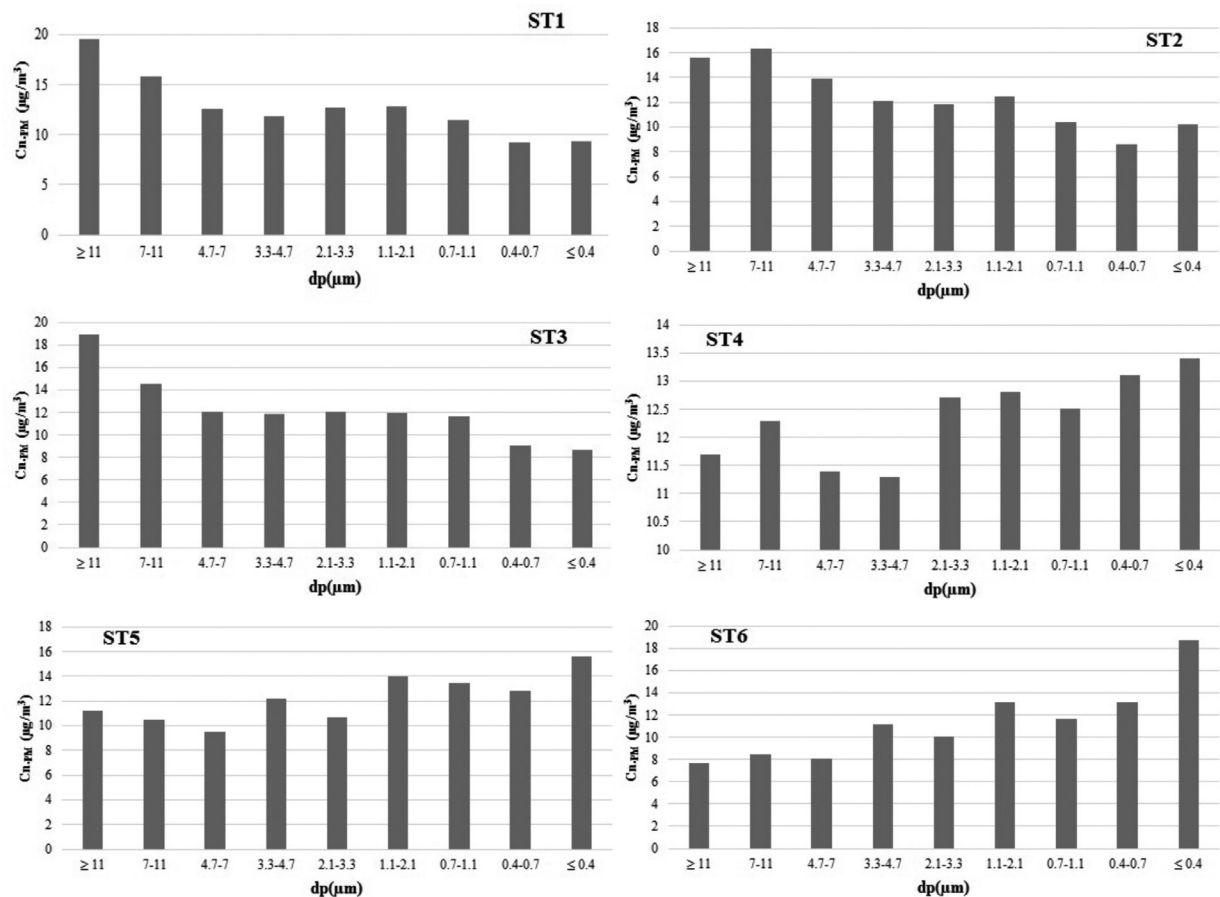


Figure 3. Distribution diagram of suspended particles collected in the study area.

Table 2. Average concentration and weight percentage of particles in the western and eastern areas of the region.

Particle diameter (μm)	Particle concentration ($\mu\text{g.m}^{-3}$)			
	Ave _{ST1-3}	W %	Ave _{ST4-6}	W %
11 $\leq$	18.03	16.02	10.2	9.47
11-7	15.53	13.8	10.43	9.68
7-4.7	12.86	11.43	9.66	8.97
4.7-3.3	11.93	10.6	11.54	10.71
3.3-2.1	12.2	10.84	11.16	10.36
2.1-1.1	12.43	11.05	13.33	12.37
1.1-0.7	11.18	9.94	12.51	11.62
0.7-0.4	8.96	7.97	13	12.06
0.4 $\geq$	9.4	8.35	15.9	14.76
	112.55	100	107.76	100

is observed in the same interval in the east, and vice versa. Also, in terms of relative contribution, in the west, about 41% of the total mass is related to particles larger than 4.7 μm , while in the east, more than 50% of the total mass is related to particles smaller than 2.1 μm . This statistical difference could be due to differences in land use patterns, traffic intensity, building density, and prevailing wind direction at the urban scale. Overall, statistical analysis of the results shows that there is a distinct spatial gradient in the particle size distribution between the west and east of Tehran, and the particle size structure in the two halves of the city differs significantly not only in terms of quantity but also in terms of correlation behavior; an issue that can be considered in modeling source identification and estimating the residence time of particles in the urban atmosphere.

The results of this study indicate that atmospheric particles emitted from both stationary and mobile sources are gradually removed through multiple processes while being transported by the prevailing winds toward the eastern and northeastern areas. Consequently, fine particles capable of remaining suspended in the air for extended periods reach these regions, exposing the residents to elevated levels of particulate pollution. Moreover, considering that particulate matter with diameters smaller than 4 μm can penetrate the trachea, bronchi, and alveolar sacs (WHO, 2012), this issue becomes particularly critical. Prolonged exposure in these areas characterized by the presence of residential, administrative, and especially military facilities may substantially increase the risk of common air pollution related diseases. This challenge may lead to the daily inhalation of soot and dispersed particles originating from the combustion of fossil fuels by both mobile and stationary sources, as well as particles produced from heating systems and indoor cooking activities in confined spaces (WHO, 2013b). Findings from previous studies on pregnant women with long term exposure to $\text{PM}_{2.5}$ demonstrate that after

childbirth, various biological complications and persistent impairments in overall infant health may emerge. Low birth weight and preterm delivery are among the documented adverse outcomes (Ritz *et al.*, 2008; Sapkota *et al.*, 2012; Proietti *et al.*, 2013).

4. Conclusion

The adverse health impacts resulting from inhalation of hazardous air pollutants such as particulate matter (PM) have been unequivocally demonstrated. Fine particulate matter has been a major subject of extensive global research over recent decades, with substantial evidence linking both short term and long term exposure to PM with increased mortality. Diesel exhaust particles are now widely recognized as carcinogenic in most studies, and the potential of air pollution to contribute to adverse birth outcomes, diabetes, neurological disorders, and impaired cognitive performance has been firmly established. Currently, no indication exists of a threshold below which exposure to PM does not lead to negative health outcomes. Recent studies provide conclusive evidence of an association between long term exposure to $\text{PM}_{2.5}$ and mortality, even when ambient concentrations are below the annual WHO Air Quality Guidelines. Moreover, the findings indicate that reducing individual exposure to $\text{PM}_{2.5}$ and PM_{10} over specified time periods can significantly enhance life expectancy and improve respiratory health. Effective air quality management and particulate matter reduction require coordinated actions across multiple sectors including environment, transportation, energy, health, and housing at regional, national, and international levels. Considering the substantial mortality burden associated with road traffic related particulate emissions, integrated improvements in urban transportation policy are essential. Reducing traffic volume and transitioning to cleaner

fuels or alternative technologies are critical priorities. Extensive research has documented the direct human exposure to airborne particulate matter and its contribution to a range of physical and psychological health disorders, emphasizing the damaging influence of atmospheric pollutants (Oroji *et al.*, 2021; Oroji *et al.*, 2019). Accordingly, the establishment of residential and administrative facilities along pathways of atmospheric pollution increases exposure risk and can exacerbate physical and mental health problems depending on occupational and environmental conditions. Therefore, implementing control programs and limiting new development projects in these high exposure zones must become central components of urban planning policies. Proper ventilation, standard heating and cooling systems, and improved quality of building infrastructure particularly doors and windows in residential, administrative, industrial, and laboratory environments constitute additional essential measures to prevent prolonged exposure to particulate matter in affected areas.

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Tropospheric Correction using PyAPS in the West Region of Venezuela

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Abstract

The subsidence of the East Coast of Lake Maracaibo-COLM in Zulia state in Venezuela is a geological event of anthropic cause with almost a century of existence. We wanted to know the current state of this event with the use of the Interferometric Synthetic Aperture Radar-InSAR technique, for this, we emphasized the need to mitigate atmospheric delays in the data, for which the ERA5 climate model with PyAPS was applied. In order to obtain accurate subsidence measurements in three oil fields located in the COLM (Tía Juana, Lagunillas and Bachaquero), whose cumulative subsidence process is approximately 5 meters between 1926 and 1986. For this study, subsidence values were estimated, for the period from 2018 to 2020, using a dataset of 157 interferometric Sentinel-1 images (79 from ascending orbits and 78 from descending orbits), which allowed the calculation of the values of displacements along the line of sight-LOS for both orbits, the tropospheric delay contribution, and the east-west and vertical components values, extracted from representative pixels with high coherence and with spatial and temporal average, having random noise component reduced, obtaining displacement values for Tía Juana, Lagunillas and Bachaquero fields respectively of: -6.4 +/- 0.8 cm/y; -7.9 +/- 1.0 cm/y and; -7.1 +/- 0.8 cm/y, for ascending mode. From 1.2 +/- 0.5 cm/y; -4.1 +/- 0.5 cm/y and; -1.8 +/- 0.3 cm/y, for descending mode. Also, by selecting representative pixels, we estimated reliable values for contribution from tropospheric delay, obtaining: -0.2 cm/y and -0.6 cm/y; -0.3 cm/y and -0.5 cm/y and; -0.4 cm/y and -0.5 cm/y. And the east-west (dE) and vertical (dU) components for the three fields, with: -6.79 cm/y and -2.94 cm/y; -3.27 cm/y and -5.19 cm/y and; -5.92 cm/y and -6.29 cm/y respectively, minimizing the risk that geometric projection errors will amplify underlying noise.

Key words: InSAR, Displacement, Subsidence, COLM, Venezuela.

Resumen

La subsidencia de la Costa Oriental del Lago de Maracaibo (COLM) en el estado Zulia, Venezuela, es un evento geológico de causa antrópica con casi un siglo de existencia. Se buscó conocer el estado actual de este evento mediante el uso de la técnica de Interferometría de Radar de Apertura Sintética (InSAR); para ello, se enfatizó la necesidad de mitigar los retrasos atmosféricos en los datos, por lo que se aplicó el modelo climático ERA5 con PyAPS. Esto con el fin de obtener mediciones precisas de la subsidencia en tres campos petroleros ubicados en la COLM (Tía Juana, Lagunillas y Bachaquero), cuyo proceso de subsidencia acumulada es de aproximadamente 5 metros entre 1926 y 1986. Para este estudio, se estimaron los valores de subsidencia para el período de 2018 a 2020 utilizando un conjunto de datos de 157 imágenes interferométricas de Sentinel-1 (79 de órbitas ascendentes y 78 de órbitas descendentes), lo que permitió calcular los valores de desplazamiento a lo largo de la línea de visión (LOS) para ambas órbitas, los valores de la contribución del retraso troposférico y los valores de las componentes este-oeste y vertical, extraídos de píxeles representativos con alta coherencia y con promedio espacial y temporal, habiendo reducido la componente de ruido aleatorio. Se obtuvieron valores de desplazamiento para los campos de Tía Juana, Lagunillas y Bachaquero, respectivamente, de: -6.4 +/- 0.8 cm/año, -7.9 +/- 1.0 cm/año y -7.1 +/- 0.8 cm/año para el modo ascendente; y de 1.2 +/- 0.5 cm/año, -4.1 +/- 0.5 cm/año y -1.8 +/- 0.3 cm/año para el modo descendente. Asimismo, mediante la selección de píxeles representativos, se estimaron valores confiables para la contribución del retraso troposférico, obteniendo: -0.2 cm/año y -0.6 cm/año; -0.3 cm/año y -0.5 cm/año y; -0.4 cm/año y -0.5 cm/año. Por último, las componentes este-oeste (dE) y vertical (dU) para los tres campos fueron de: -6.79 cm/año y -2.94 cm/año; -3.27 cm/año y -5.19 cm/año; y -5.92 cm/año y -6.29 cm/año, respectivamente, minimizando el riesgo de que los errores de proyección geométrica amplifiquen el ruido subyacente.

Palabras clave: InSAR, Desplazamiento, Subsistencia, COLM, Venezuela.

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1. Introduction

The usefulness of Synthetic Aperture Radar images for Earth observation began in the 1950s for military purposes. Its expansion into the geoscientific world began with the launch of the SEASAT civilian satellite in 1978 and with other subsequent missions (Meng *et al.*, 2024).

Geoscientists around the world have applied the Interferometric Synthetic Aperture Radar-InSAR technique in the study of crustal deformations. This tool has made it possible to improve the detection, quantification and characterization of processes, both natural, such as: aquifer dynamics, tectonic and magmatic processes, etc.; (Biggs & Wright, 2020; González, 2024; Medici *et al.* 2024; Meng *et al.* 2024) as those induced by human activities that cause movements of the surface.

One of the human activities that induces surface deformation refers to the extraction of fluids, such as: hydrocarbons and groundwater, added to constructed buildings and infrastructure on top can generate deformation and collapse of the ground. Also, the process of compactation and rearrangement of the sediments, alongside a significant reduction of pore space within subsurface layers have high contribution to the loss of surface elevation (Poland and Davis, 1969). In this context, the Interferometry Synthetic Aperture Radar-InSAR has transformed our understanding of Earth dynamics by imaging the entire Earth's surface. With the launch of the Sentinel-1 pairs, in 2014, a reliable and long-term archive of ground-based InSAR measurements is available, to support the monitoring and mitigation of soil movements from anthropogenic and/or natural sources, affecting the civil, geotechnical and structural engineering sectors (Biggs and Wright, 2020).

However, a limitation in the use of satellite radar data for the detection of crustal deformations lies in atmospheric signals (Agram *et al.*, 2013, Dogru *et al.*, 2023), which often mask actual displacement, particularly in mountainous areas (Brencher *et al.*, 2023; Dogru *et al.*, 2023).

According to Hu and Mallorquí (2019), phase noise in InSAR is classified into two types according to its origin. The first is of ionospheric origin, occurring in spectral bands such as P or L due to fluctuations in electron density between 100 and 1000 km altitude, which alters the signal path (Gray *et al.*, 2000). The second type is tropospheric delays, caused by variations in temperature, pressure, and humidity (Chen *et al.*, 2025). These delays combine a turbulent component (affecting flat and mountainous terrain, with high spatial correlation but low temporal correlation) and a stratified component (directly correlated with topography, which only distorts measurements in areas with unevenness such as hills or mountains) (Hanssen, 2001; Xiao *et al.*, 2021). The total delay is calculated according to Equation 1 by integrating the differential

hydrostatic (temperature and pressure) and differential wet (water vapor) components between the surface and the satellite elevation along the line of sight (LOS) (Equation 1, Hanssen, 2001):

$$\Delta\delta L_{\text{atm}}^{\text{InSAR}} = \frac{10^{-6}}{\cos\theta} \left[\frac{k_1 R_d}{g_m} \Delta P_{\text{diff}} + \int_{Z_{\text{surf}}}^{Z_{\text{top}}} \left(k'_2 \frac{\Delta_e}{T} k_3 \frac{\Delta_e}{T^2} \right) dz \right] \quad (1)$$

Where: θ = incident angle. $\Delta P_{\text{diff}} = P_{\text{slave}} - P_{\text{master}}$ (pressure difference between the two acquisitions). $\Delta_e = e_{\text{slave}} - e_{\text{master}}$ (vapor pressure difference between acquisitions).

$$k'_2 = k_2 - (R_d/R_v)k_1 (\approx 23.4 \text{ K/hPa})$$

The PyAPS tool (Jolivet *et al.*, 2011) calculate a Zenith Total Delay (ZTD) (Mateus *et al.*, 2015) perform a numerical integration of refractivity along the vertical profile at each grid node of the meteorological model (ERA-Interim, ERA5 in modern PyAPS), unlike many empirical models that calculate the ZTD at a single point and then multiply it by a mapping function. The single-path LOS delay is defined as (Equation 2, Jolivet *et al.*, 2011):

$$L_{\text{LOS}} = \frac{1}{\cos(\theta)} \int_{Z_0}^H (n - 1) dz \quad (2)$$

Where: θ is the local incidence angle. The term $1/\cos(\theta)$ acts as the geometric mapping factor.

One way to address the presence of turbulent and vertically stratified components in signal detection has been the development of global atmospheric models (GAM), including global and regional operational and re-analysis weather models (e.g., NARR, ERA-Interim, MERRA-2, HRES) (Cao *et al.*, 2021), a variety of research has demonstrated the potential of using GAM-based predictive corrections to mitigate tropospheric InSAR delays (Jolivet *et al.*, 2011; Kinoshita, 2021; Ulma *et al.*, 2021; Kiriu *et al.*, 2022; Chen *et al.*, 2022; Sailellah and Fukushima, 2023; Zhang *et al.*, 2023; Dogru *et al.*, 2023), these predictive approaches have become routine for correcting tropospheric delays (Cao *et al.*, 2021).

To improve the accuracy of InSAR measurements, methods such as that of Jolivet *et al.* (2011), which corrects for spatial and temporal variations of tropospheric stratification, have been proposed. This method generates tropospheric delay maps synchronized with SAR acquisitions from the ERA-Interim weather model, the transition to ERA5 (the successor from ECMWF) is particularly critical for tropical regions due to significant improvements in how the model handles the complex moisture dynamics characteristic of those environments (Hersbach *et al.*,

2020). By validating it in interferograms without deformation, it was found that removing the atmospheric signal before phase unwrapping minimizes errors in regions with complex topography.

Albino *et al.* (2020) evaluated two methods to correct atmospheric errors: the first method applying phase elevation correlations and, the second method applying global weather models, also, evaluated the ability of time series to detect deformation anomalies. For which they used a fixed threshold and the use of a cumulative sum control chart, to represent accurate deformation values, applicable to any volcano in the world.

Kinoshita (2021) developed a neutral atmospheric delay correction model for InSAR, using total zenith delay (ZTD) and horizontal gradient data from Global Navigation Satellite Systems (GNSS). Whose usefulness of the correction model was evaluated in ALOS-2 interferograms over the Kanto Plain in Japan.

Ulma *et al.* (2021) used the Correction Online GACOS to correct the tropospheric delay model of persistent backscatters in 81 Sentinel-1A images for subsidence estimation in Surabaya, Indonesia, between 2017 and 2019.

Kiriu *et al.* (2022) evaluated the performance of three numerical weather models to mitigate tropospheric lag for InSAR applications in a tropical region. Their evaluation consisted of comparing the effectiveness of models to correct for atmospheric noise in Sentinel-1 interferograms at various spatial wavelengths. This analysis was performed using variograms to measure noise reduction, and GNSS data served as a benchmark against SAR-derived tropospheric delay estimates provided by the models.

For their part, Chen *et al.* (2022) researchers from Chengdu University of Technology-China proposed a method for topography-dependent atmospheric correction based on the multilayer perceptron (MLP) neural network model that combines spatial and topographic information data, in Sentinel-1 images, applied at the Baihetan Dam. The researchers contrasted the results with those obtained in the GACOS correction and the correction of the traditional linear model, where the MLP model reduced the phase standard deviation by 64%, being an indicator of the quality of the interferograms.

In turn, Sailellah and Fukushima (2023) researchers from Tohoku University compared the performance of two tropospheric delay correction methods for InSAR, in ALOS-2 data acquired over Japan. The first method consisted of the integration of the delay along the line of sight (LOS) of the mesoscale model (MSM) of the Japan Meteorological Agency (JMA) and; the second method employed GACOS correction that applies an iterative decomposition approach.

For their part, Zhang *et al.* (2023) performed multiple data simulations that included variable elastic deformation compo-

nents. To solve the constraints problems on the weak flanks of the Common Scene Stacking (CSS) method under different deformation conditions, the researchers developed an iterative strategy. Their results indicated that the signal-to-noise ratio (SNR) is a key parameter affecting CSS performance in atmospheric phase display (APS) separation.

Dogru *et al.* (2020), seeking to overcome atmospheric effects in two of their InSAR studies, whose study areas were located in Central Anatolia between the period January 2016 and December 2018, and in East Anatolia between the period of September 2016 and December 2018 in Turkey, applied high-resolution ECMWF meteorological models together with an empirical phase elevation approach to correct the Sentinel-1 interferograms. Where the reduction of the standard deviation, being the indicative quality factor, worked better in the interferograms in descending mode for both studies.

In the present study, tropospheric correction was implemented using the PyAPS module. This tool, developed in Python 3, allows quantifying and correcting atmospheric noise of the type stratified in interferograms. The correction was made using ERA5 meteorological data on the area of interest in western Venezuela, corrected rates obtained with near 8 cm/y are more closely aligned with historical geodetic and topographic data recorded between 1926 and 1986, which showed approximately 5 meters of subsidence over 60 years. This suggests that earlier InSAR studies without correction may have produced less accurate or anomalous results due to unmitigated atmospheric interference. For the analysis, 157 Sentinel-1 interferograms were processed in the descending and ascending orbit directions, corresponding to the period 2018-2020 (Figure 1).

The ECMWF ERA5 model provides high-resolution atmospheric humidity, pressure and temperature data, essential for phase correction, of disturbances introduced by the atmosphere in the radar signal, in interferograms, for more accurate strain measurements (<https://www.ecmwf.int/en/forecasts/dataset/ecmwf-reanalysis-v5>). The ERA5 dataset provides information on the state of the global atmosphere, land and oceans. It allows the analysis of meteorological phenomena on a detailed scale, with a horizontal spatial resolution of $0.25^{\circ} \times 0.25^{\circ}$ for the atmosphere and $0.5^{\circ} \times 0.5^{\circ}$ for ocean waves, allowing the study of the evolution of the climate in the long term, with hourly estimates of a large number of atmospheric, terrestrial and oceanic variables, such as: temperature, humidity, wind, precipitation, solar radiation, etc.

Also, the model provides a deterministic correction for the stratified delay, the turbulent components are mitigated statistically through the inversion process, the linear trend estimation, and the selection of high-coherence pixels within the MintPy workflow (Yunjun *et al.*, 2019).

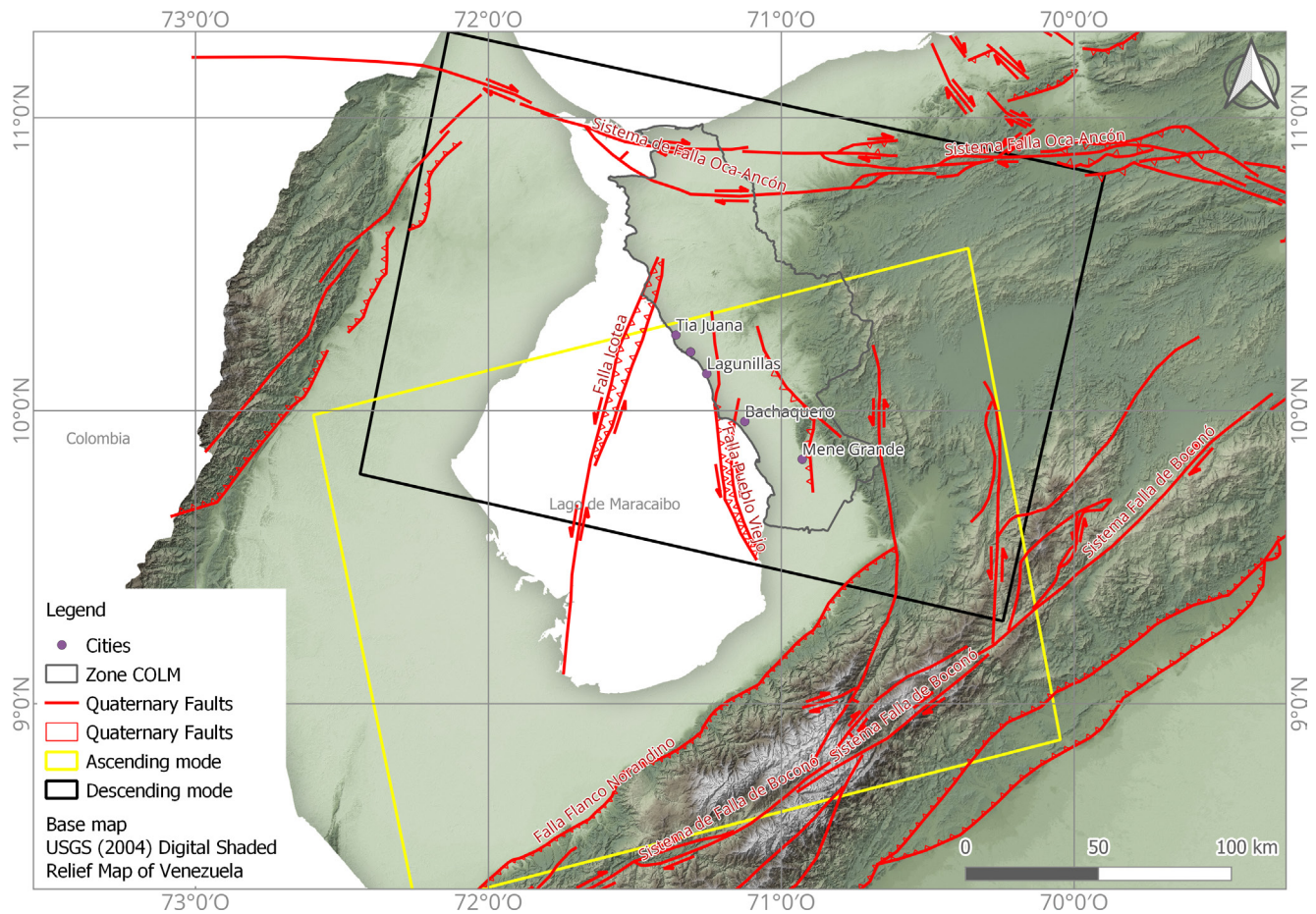


Figure 1. The frame of descending (black box) and ascending (yellow box) modes Sentinel 1 images. The area is surrounded by the fault systems of: Oca-Ancón (dextral strike-slip), Pueblo Viejo (reverse left-lateral strike-slip), Valera (left-lateral strike-slip), Icorea (reverse left-lateral strike-slip), Northern Foothills (thrust fault), Boconó (dextral strike-slip) (Audemard *et al.*, 2000).

2. Materials and Methods

The interferogram time series was generated using the ASF HyP3 (Alaska Satellite Facility's Hybrid Pluggable Processing Pipeline) platform (Hogenson *et al.*, 2020). For tropospheric correction, atmospheric data from the ERA5 model of the European Centre for Medium-Range Weather Forecasts (ECMWF), obtained through the Copernicus Climate Data Store (CDS), were used. These data were processed with the PyAPS based Atmospheric Phase Display estimation algorithm (Python), which generates differential phase delay maps caused by the stratified atmosphere to correct for radar interferograms (Yunjun *et al.*, 2019).

The selected scenes corresponded to the path/frame 171/557 in descending orbit and 4/25 in ascending orbit. For both modes, 78 pairs were generated for the descending mode and 79 pairs for the ascending mode, for the pair between January 2018 and December 2020. However, to ensure the quality of the interferograms, this study applied maximum recommended thresholds for the perpendicular baseline. The perpendicular baseline was

limited to 100 meters to mitigate the topographic strips (see Figure 2), a criterion that only one interferogram exceeded. A small baseline is less distracted by the shape of the relief and can focus on the actual movement (displacement) of the soil. In COML region keeping the $B_{\perp}$ ensures the cms of movement are real ground displacements.

The temporal resolution was set at 12 days, determined by the availability of the images for both trajectory modes. Following this selection, 157 data pairs met all criteria. These selected pairs were processed on demand in HyP3 with the GAMMA software, obtaining products such as unwrapped phase (applying an threshold of 0.6 phase filter and water mask prior to time series inversion), wrapping phase, estimated coherence, etc. Subsequently, for tropospheric correction, it was processed with MintPy (Miami InSAR Time-series software in Python) (Yunjun *et al.*, 2019), this applies inversion algorithms of Subsets of Small Baselines (SBAS) (Berardino *et al.*, 2002) and uses the ERA5 model (Jolivet *et al.*, 2011) to perform the correction of tropospheric delay in time series using PyAPS.

3. Methodology

Tropospheric correction with PyAPS was implemented through MintPy (Yunjun *et al.*, 2019) by applying phase corrections directly to the time series, which is organized as a sequence of phases ordered chronologically with respect to a master acquisition. MintPy divides time series analysis into: interferogram network inversion for raw phase time series and, removal of tropospheric delay, topographic residue, timing error, and orbital error from the raw phase time series to derive the displacement time series (Yunjun *et al.*, 2019).

Instead of directly forming a set of interferograms with a single reference, the approach of inverting a reference interferogram network offers several advantages in analysis. It minimizes temporal decorrelation, phase information is preserved, and reduces the impact of spatial uncorrelation arising from topographic variations and geometric distortions, as well as reduces the impact of APS, which are source of error in InSAR analysis, where more accurate deformation measurements are obtained. In turn, the investment technique can handle missing data points, making it more robust to data breaches. Likewise, the least-squares calculation was employed to quantify the noise level within the time series. Also, the Weighted Least Squares (WSL) is used to manage connectivity and rank deficiency, only inverting the largest connected component and generating a numInversion dataset for those pixels coherent in a few interferograms, masking out pixels that don't meet a minimum threshold of connectivity. According to the methodology developed by Yunjun *et al.* (2019) and implemented in Python, the step flow breaks down as follows (Figure 3).

The workflow described above was applied to the west region of Venezuela. As a result of InSAR processing, 157 interferograms were generated in their descending and ascending modes. Then, the velocity phase average maps from each dataset

were generated in LOS view, shown in Figures 4 and 5 for the descending and ascending datasets.

The phase of each interferogram developed is relative to an arbitrary pixel. Therefore, the algorithm references all interferograms in a common reference pixel (in black color). The reference point step selects a common reference pixel for the interferogram stack. The default approach of Mintpy is to choose a pixel with the highest spatial coherence in the stack, in this case an threshold of 0.7 was used by default (Yunjun *et al.*, 2019).

Crustal deformation, caused by natural or anthropogenic processes, presents a linear behavior in a first approximation. To quantify it, the displacement rate is estimated, calculated as the slope of the linear fit of the time series. This calculation of the estimates the displacement velocity. Interpreting the resulting values, negative values indicate that the target is moving away from the radar (subsidence in vertical deformation). Positive values indicate that the target is moving towards the radar (uplift in vertical deformation).

The estimated velocity includes an expression of its uncertainty, which is derived directly from the goodness of linear fit. This uncertainty is quantified by the standard deviation of the residuals of the adjustment made to the time series.

However, the spatial pattern of the estimated standard deviation shows the spatial correlation of noise in the time series. The uncertainty depends on the distance, and increases with increasing pixel pitch. Figures 4b and 5b show each pixel's uncertainty relative to the reference pixel.

The intersection indicates the moment when the magnitude of the displacement and its variability (standard deviation) reach a point of significant relationship (Figures 4c,d and 5c,d). This point may indicate a change in the stability of the process that generates the displacements, which may coincide with an event that disturbed the stability of the displacements, such as a geological event, or a change in the activity that produces the

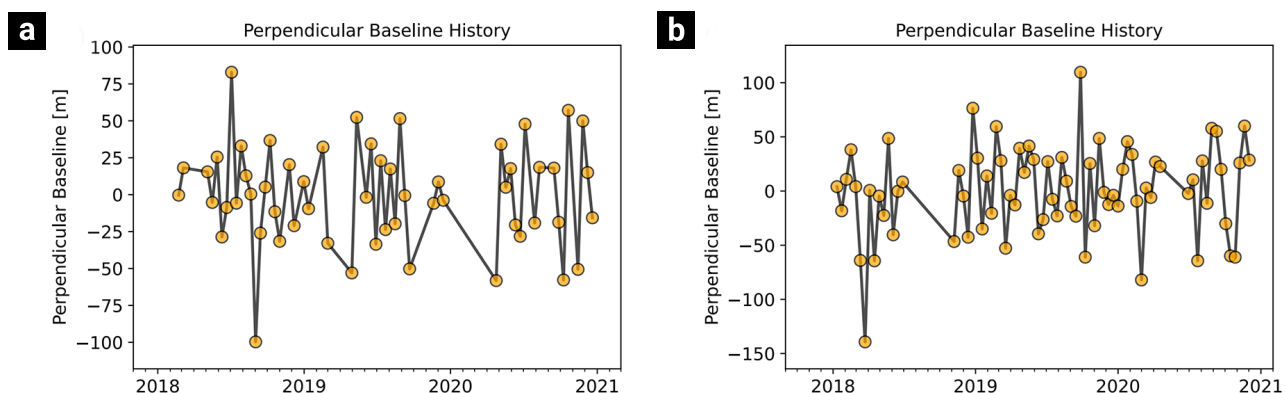


Figure 2. Baseline configuration for the 157 interferograms (a) ascending and (b) descending modes giving an overview of the network.

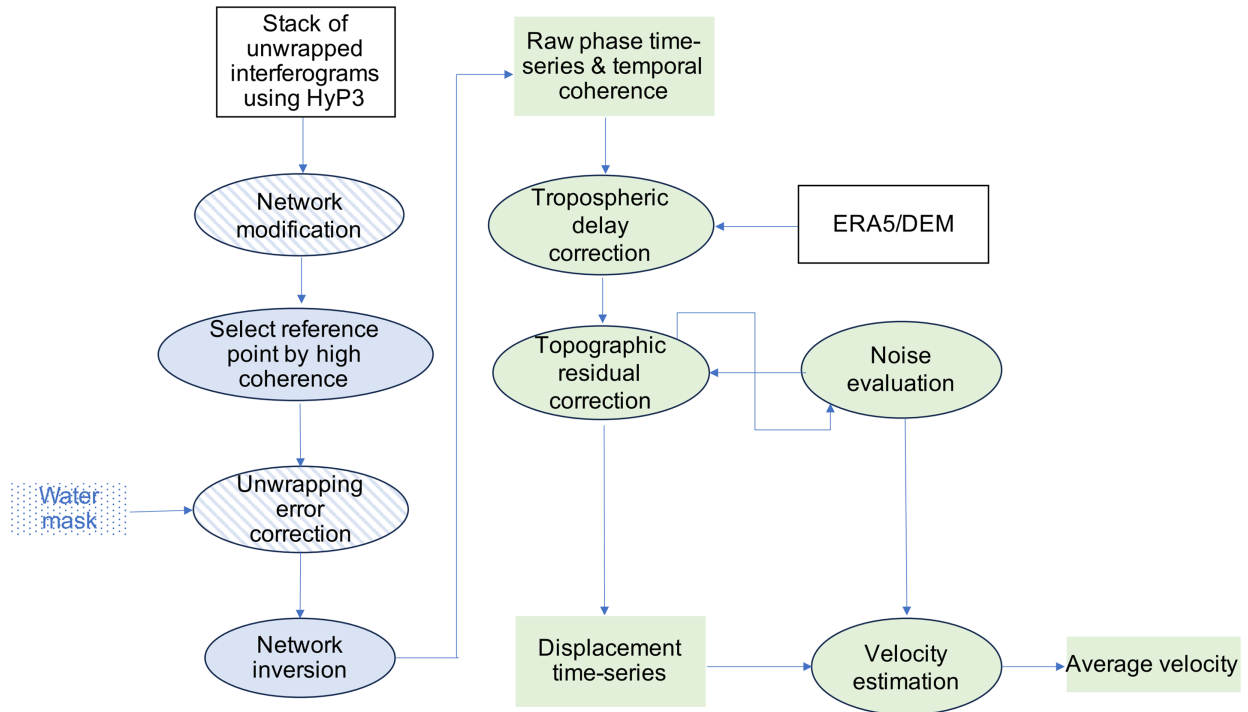


Figure 3. Flowchart adopted in this study (modified from Yunjun *et al.*, 2019).

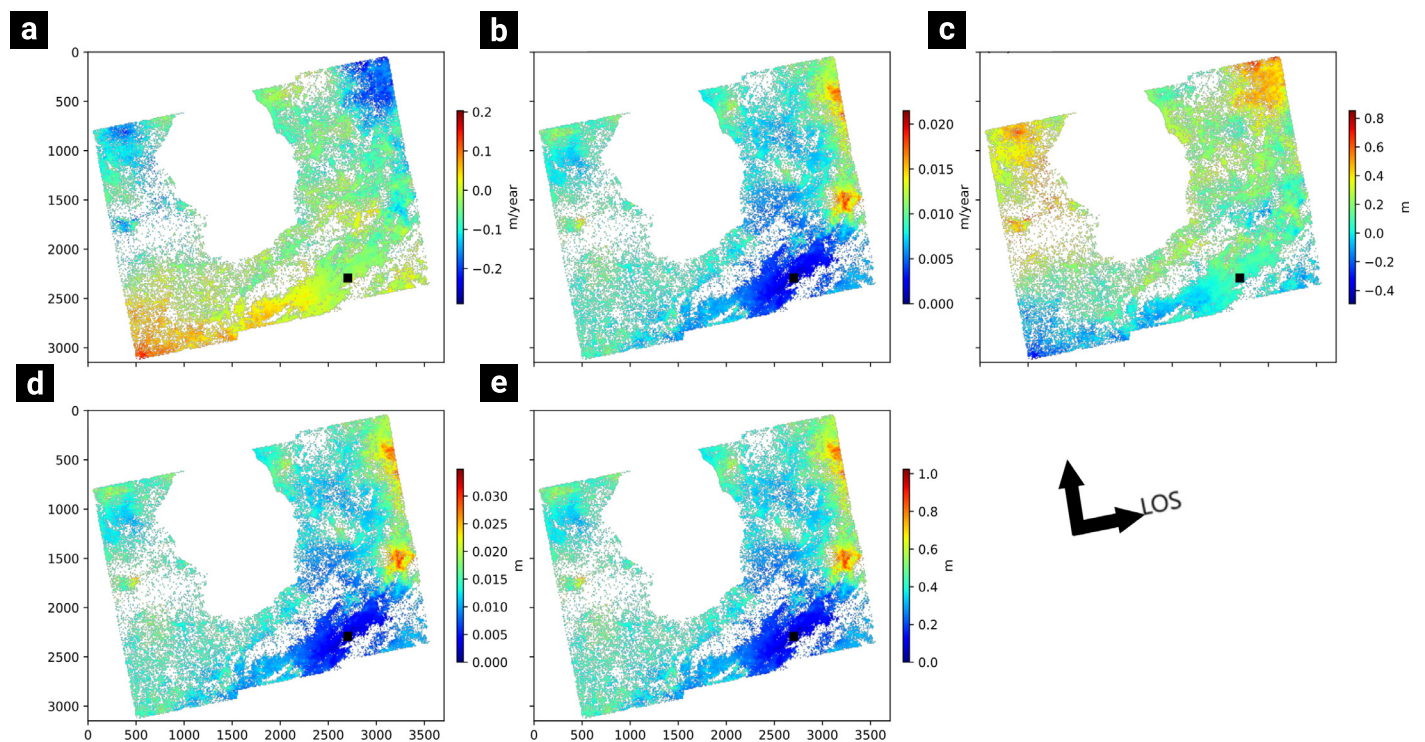


Figure 4. Annual displacement velocity for the period 2018-2019-2020 in LOS, in its ascending mode, for the west region of Venezuela (common reference pixel is given in black color) (a) velocity, (b) standard deviation of velocity, (c) intercept, (d) intercept standard deviation, (e) residue.

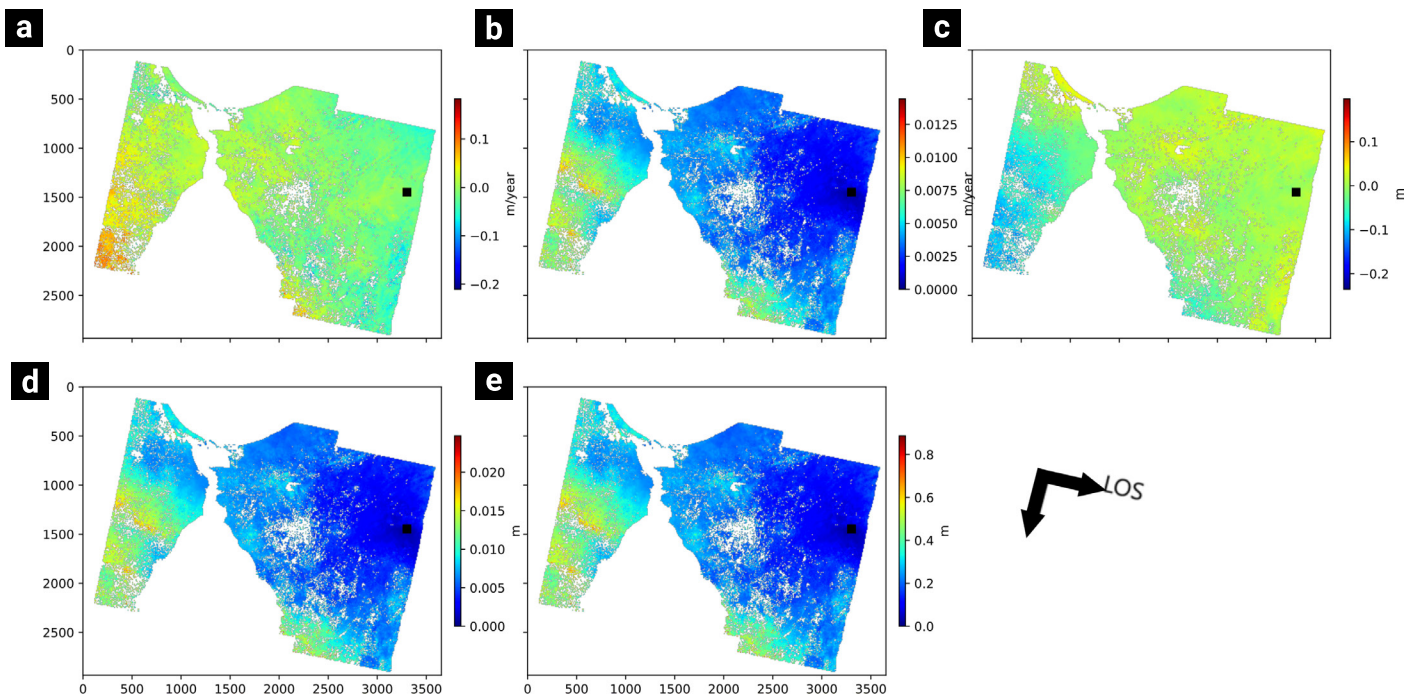


Figure 5. Annual displacement velocity for the period 2018-2019-2020 in LOS, in its descending mode, for the west region of Venezuela (common reference pixel is given in black color) (a) velocity, (b) standard deviation of velocity, (c) intercept, (d) intercept standard deviation, (e) residue.

displacements. The standard deviation quantifies the uncertainty associated with the intercept estimate. The residue provides the quality of the linear model fit, where small and random residuals indicate that the model is suitable (Figures 4e and 5e). Conversely, suppose the residuals show an increasing or decreasing trend, in that case, it suggests that the linear model may not be suitable for describing the deformation.

MintPy also calculates the temporal average of the spatial coherence of the entire stack as a possible auxiliary measure to choose reliable pixels after time series reversal, ranges from 0 to 1. Where pixels with values closer to 1 are considered reliable. For a dense network of interferograms, a threshold of 0.7 can be used (Yunjun *et al.*, 2019). The oil fields analyzed in COLM have stable infrastructure that maintain high coherence (> 0.8) regardless of the threshold. Therefore, the maximum subsidence rates reported (e.g., -7.9 cm/y) are likely very robust and insensitive to the threshold (see Figures 6 and 7).

4. Results and Discussion

The calculated phase delay is subtracted from the unwrapping interferogram to eliminate the effects of the atmosphere. It is a powerful and flexible tool for atmospheric correction of InSAR interferograms. Using high-quality data from the ERA5 model,

PyAPS enables more accurate ground deformation measurements (see Figures 8 and 9), the atmospheric data are interpolated to the geometry of the InSAR image to obtain humidity, pressure, and temperature values at each image pixel.

The Maps of VelocityStd, represented like (b) in the figures 8 and 9, is referred to trust in the calculated speed of subsidence, represents the standard deviation of the linear fit residuals, low values < 0.5 cm/y, mean the ground is moving at a very steady, predictable rate. The atmospheric noise is low, and the linear model has a perfect fit for the data. High values > 1.5 cm/y, indicate that the scatter of the points around the line is high. This is usually caused by remaining turbulent atmospheric noise, soil moisture changes, or non linear ground movement (Yunjun *et al.*, 2019).

After of the PyAPS correction the values are between 0.1 cm/y and 0.6 cm/y (see Table 1) demonstrating excellent results, between excellent and an good adjustment of the model (see Table 2) with an high confidence in the displacement rates in LOS (see Figures 8 (b) and 9 (b)).

In previous InSAR investigations for the west region of Venezuela, specifically the East Coast of Maracaibo (known by their initials in spanish as COLM), surface deformation values have been obtained in the oil fields, with high agreement with linear historical rates (Murria & Saab, 1992) suggests that non linearities were not significant enough to change the overall

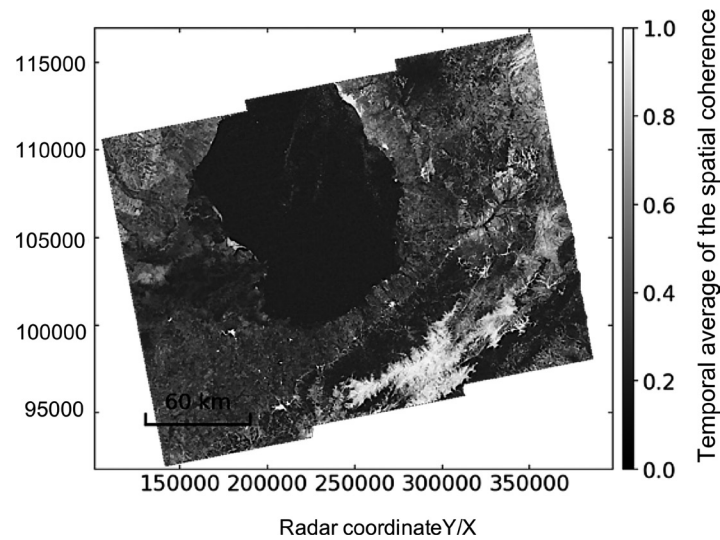


Figure 6. Average spatial coherence for the period 2018-2019-2020, in its ascending mode.

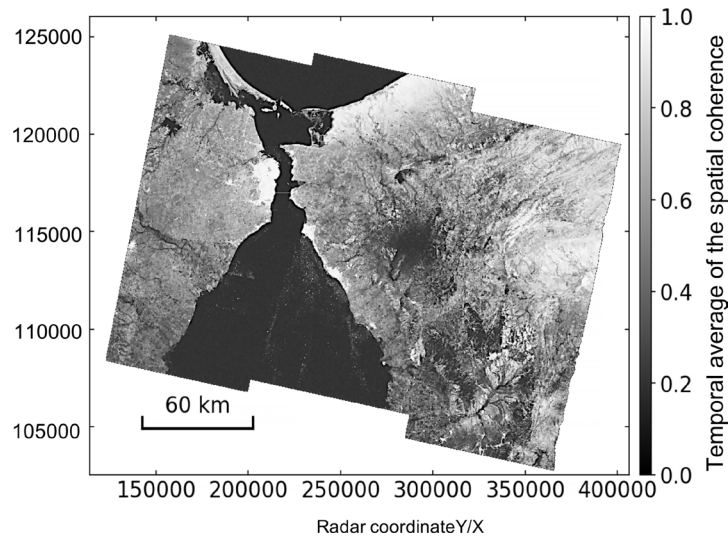


Figure 7. Average spatial coherence for the period 2018-2019-2020, in its descending mode.

interpretation of the subsidence hazard, annual velocity of displacement in LOS of the soil surface of -5.1 cm/y, -10.3 cm/y and -5.8 cm/y, respectively (Deguchi & Narita, 2015). Arenas *et al.* (2019) determined the subsidence of the COLM, using Sentinel 1 images, obtaining displacements between 2.8 cm/y and -2.8 cm/y in the areas of Cabimas, Tia Juana and Ciudad Ojeda for a period of three years. Quintana *et al.* (2021, 2025), applied the PSInSAR method for the ascending mode using 20 Sentinel-1 images, obtained displacement values in LOS ranging from -4.0 cm in the Lagunillas area, while in Ciudad Ojeda there is evidence of an uplift process of 4.5 cm/y, Tia Juana with 3.5 cm/y and Bachaquero with areas that rise towards the center of the city with 3.0 cm/y and areas that sink towards the NW with

2.0 cm/y. However, the application of atmospheric corrections in these studies was not mentioned, it can be inferred that the resulting values may be affected by atmospheric delays, causing them not to reflect the true velocity of displacements in LOS.

The estimated velocity values, obtained after the tropospheric PyAPS correction, specifically on the COLM, in LOS (in its ascending mode), for the surroundings of the Tia Juana, Lagunillas and Bachaquero fields respectively of -6.4 ± 0.8 cm/y; -7.9 ± 1.0 cm/y and; -7.1 ± 0.8 cm/y (the uncertainty is referred to a temporal measure of the unmodeled noise) (see Figures 10 through 13).

The estimation of the annual displacement velocity values in LOS (in its descending mode) for the surroundings of the

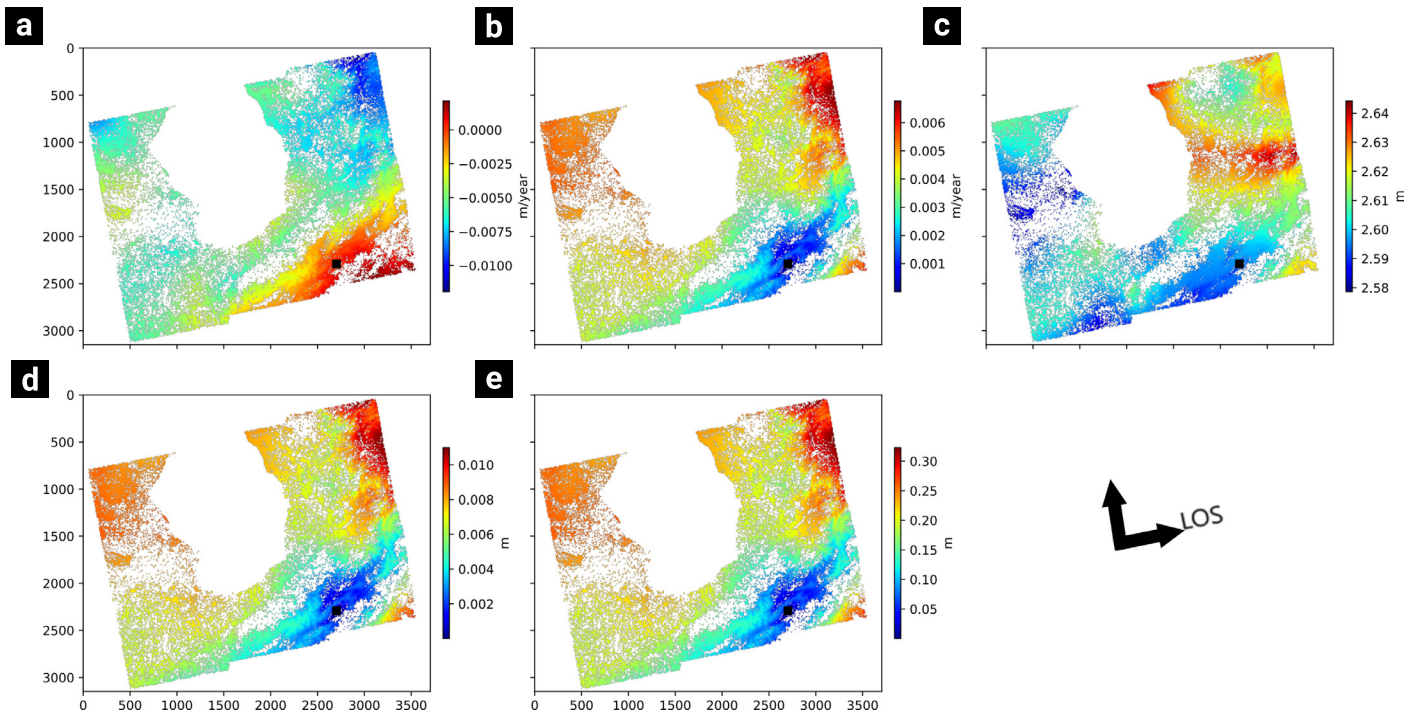


Figure 8. Displacement LOS rates after the calculated phase delay from the unwrapping interferogram for the period 2018-2019-2020 in LOS, in its ascending mode, correction based on the ECMWF ERA 5.

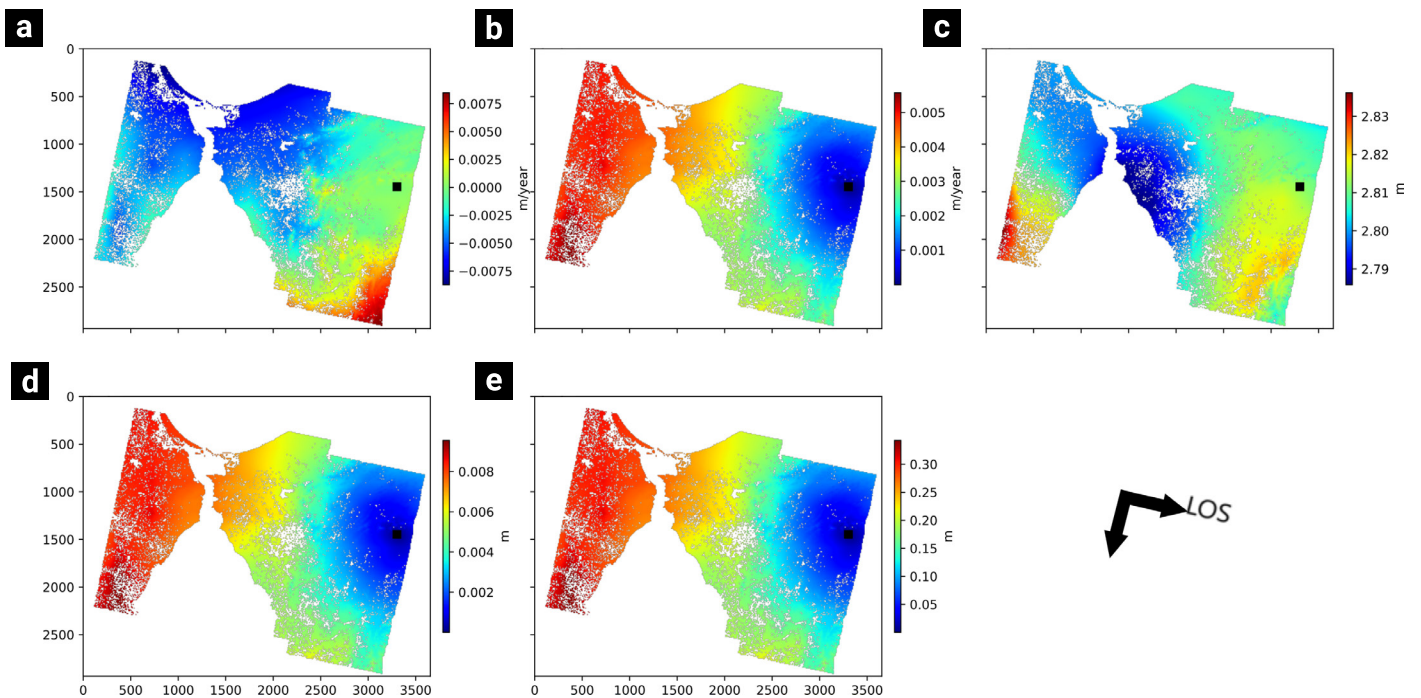


Figure 9. Displacement LOS rates after the calculated phase delay from the unwrapping interferogram for the period 2018-2019-2020 in LOS, in its descending mode, correction based on the ECMWF ERA5.

Table 1. Quantitative validation of the correction PyAPS ERA5 in COLM for the period 2018-2019-2020 based in the Maps of VelocityStd.

Maps VelocityStd		
	Before	After
Ascending	2 cm/y	0.6 cm/y
Mode	1.5 cm/y	0.5 cm/y
	1 cm/y	0.4 cm/y
	0.5 cm/y	0.3 cm/y
		0.2 cm/y
		0.1 cm/y
Descending	1.25 cm/y	0.5 cm/y
Mode	1 cm/y	0.4 cm/y
	0.75 cm/y	0.3 cm/y
	0.5 cm/y	0.2 cm/y
	0.25 cm/y	0.1 cm/y

Table 2. Qualitative validation of the correction PyAPS ERA5 in COLM for the period 2018-2019-2020.

Value Range (cm/y)	Interpretation	Meaning for the COLM study
0.0 - 0.5	Excellent	High confidence in the subsidence rates. Minimal noise.
0.5 - 1.0	Good	Standard noise levels for tropical C-band InSAR.
> 1.0	Moderate/Poor	Areas likely affected by vegetation or high atmospheric turbulence.

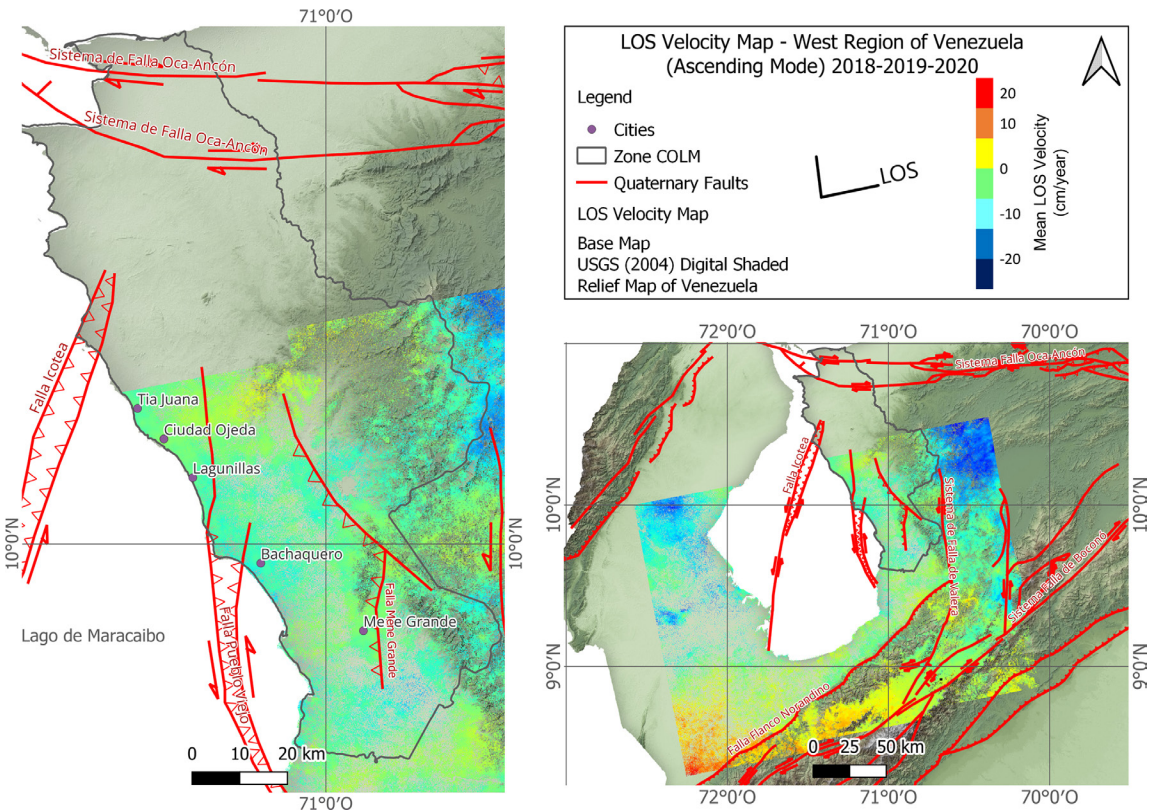


Figure 10. Annual values of displacement in LOS in the Tía Juana, Lagunillas, and Bachaquero oil fields, in ascending mode, for the period 2018-2019-2020.

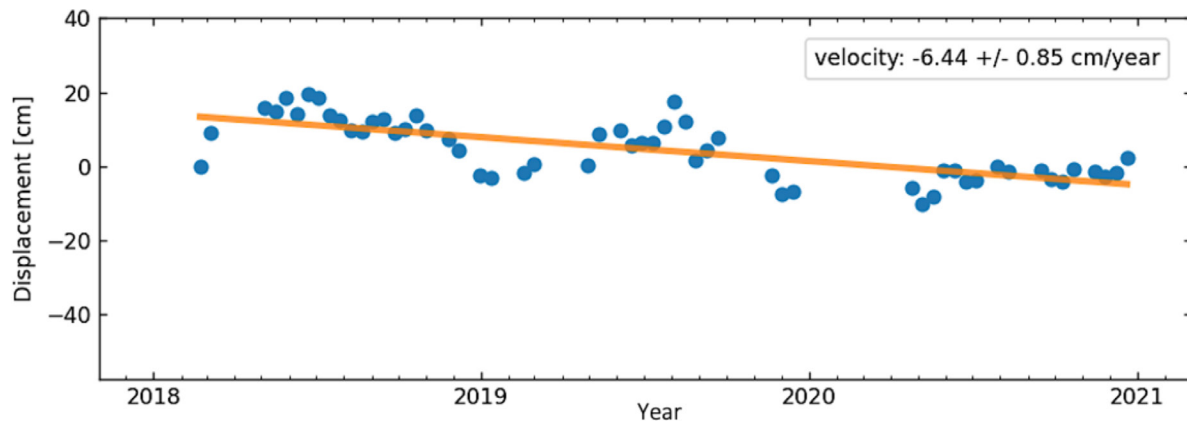


Figure 11. Displacement in LOS (cm/yr) for Tia Juana field, for the period 2018-2019-2020, in its ascending mode. The blue dots in the time series correspond to the cumulative offset values. In contrast, the orange line corresponds to the calculated trend line. The estimated values of the velocity and the uncertainties were calculated.

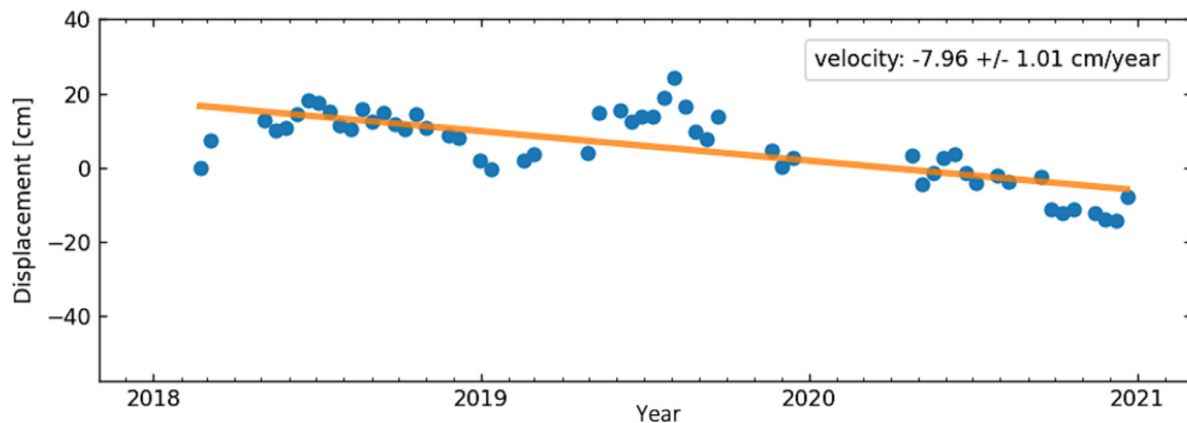


Figure 12. Displacement in LOS (cm/yr) for Lagunillas field, for the period 2018-2019-2020, in its ascending mode. The blue dots in the time series correspond to the cumulative offset values. In contrast, the orange line corresponds to the calculated trend line. The estimated values of the velocity and the uncertainties were calculated.

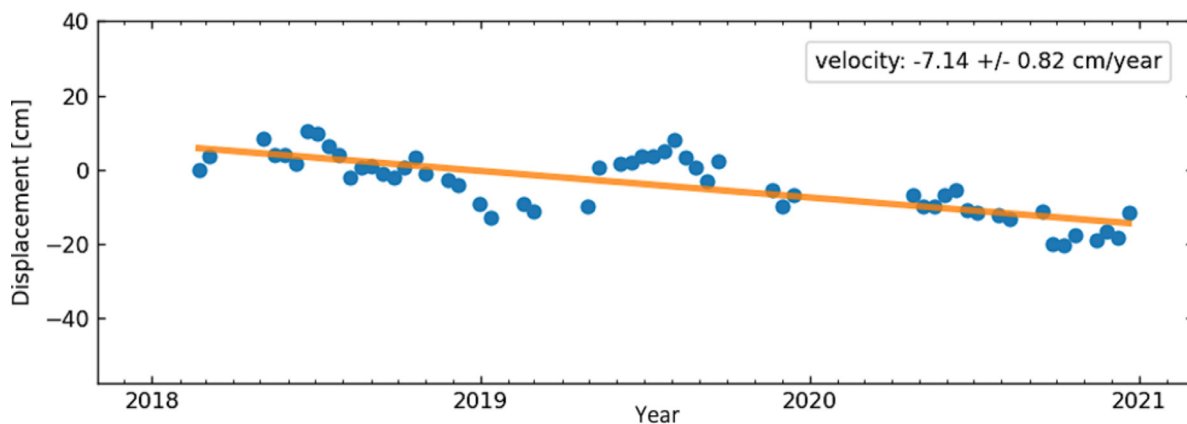


Figure 13. Displacement in LOS (cm/yr) for Bachaquero, for the period 2018-2019-2020, in its ascending mode. The blue dots in the time series correspond to the cumulative offset values, while the orange line corresponds to the calculated trend line. The estimated values of the velocity, and the uncertainties were calculated.

Tia Juana, Lagunillas and Bachaquero fields respectively of 1.2 ± 0.5 cm/y; -4.1 ± 0.5 cm/y and; -1.8 ± 0.3 cm/y (the uncertainty is referred to a temporal measure of the unmodeled noise) (see Figures 14 through 17).

The different previous studies have applied different InSAR methods, DInSAR (Differential Interferometric Synthetic Aperture Radar) compares only two radar images from different dates. The topography, using a DEM, is subtracted to see what changed on the ground. PSInSAR (Persistent Scatterer InSAR) (Ferretti *et al.*, 2001) focuses on individual targets, such as infrastructures, that maintain high stability and signal backscatter over the entire study period; it connects every image to a single master reference, making it highly effective for monitoring urban infrastructure but less dense in rural areas and, and SBAS (Small Baseline Subset) (Hamzaoui *et al.*, 2025) included natural elements, by grouping images into multiple subsets with small spatial and temporal separations (baselines), minimizes the decorrelation and allows for a denser coverage of pixels in tropical terrains, like the areas surrounding the oil fields in the COLM region (see Table 3).

Also, it was possible to estimate delay tropospheric contribution and, the east-west and vertical components values using the Equation 3, combining the Standard Deviation (Std) and, ERA5 velocities in LOS in both modes, by decomposing the vectors, obtaining the contribution rates for the deformation, and dE and dU components to the three fields (see Table 4) (Equation 3, Fialko *et al.*, 2001, Hassen, 2001, Witkowski *et al.*, 2024).

$$U_e = \frac{dLOS_{desc} \cos \theta_{asc} - dLOS_{asc} \cos \theta_{desc}}{Denom}$$

$$U_u = \frac{dLOS_{asc} (-\sin \theta_{desc} \sin \alpha_{desc}) - dLOS_{desc} (-\sin \theta_{asc} \sin \alpha_{asc})}{Denom}$$

$$Denom = \cos \theta_{asc} \sin \theta_{desc} \sin \alpha_{desc} - \cos \theta_{desc} \sin \theta_{asc} \sin \alpha_{asc}$$
(3)

Where: $dLOS_{asc}$: displacement in LOS in its ascending mode; $dLOS_{desc}$: displacement in LOS in its descending mode; θ : Incident angle; α : Angle acimut.

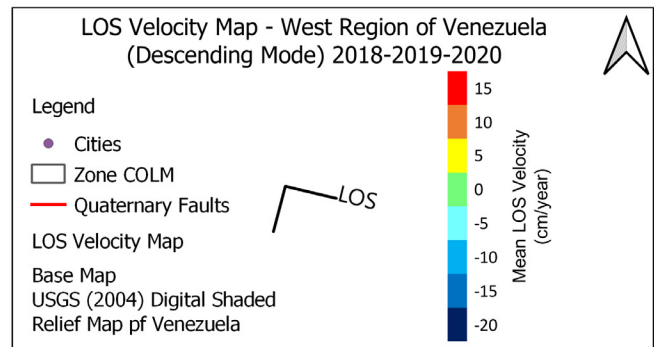
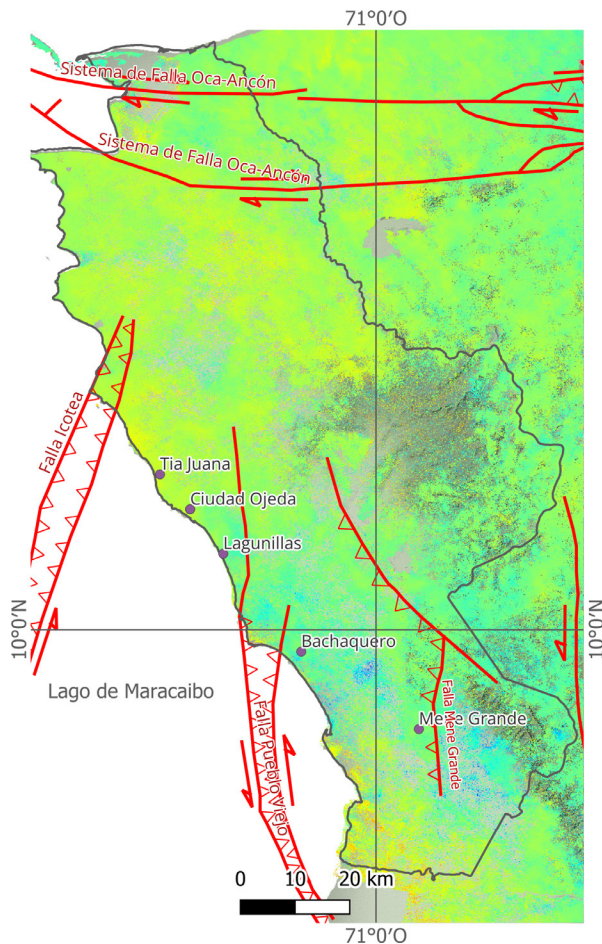


Figure 14. Annual values of displacement in LOS in the oil fields of Tia Juana, Lagunillas and Bachaquero, in descending mode, for the period 2018-2019-2020.

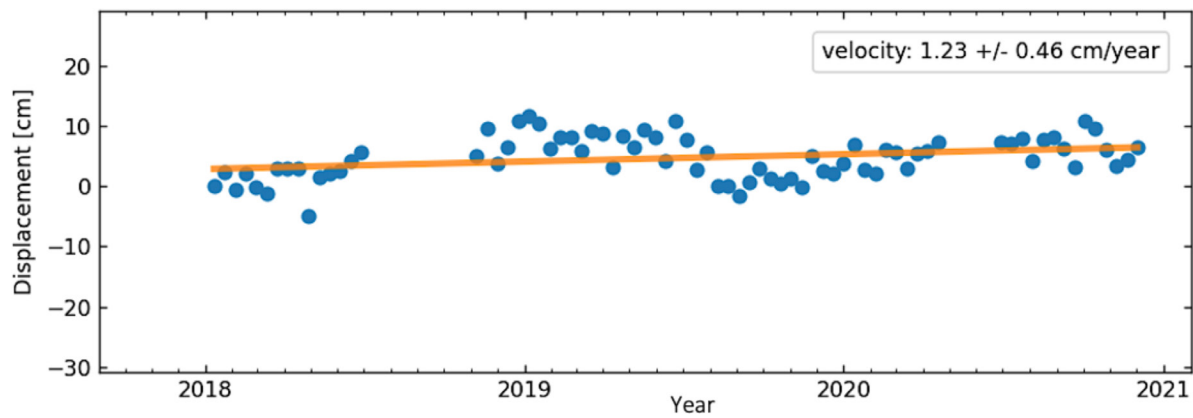


Figure 15. Displacement in LOS (cm/yr) for Tia Juana, for the period 2018-2019-2020, in its descending mode. The blue dots in the time series correspond to the cumulative offset values, while the orange line corresponds to the calculated trend line. The estimated values of the velocity, and the uncertainties were calculated.

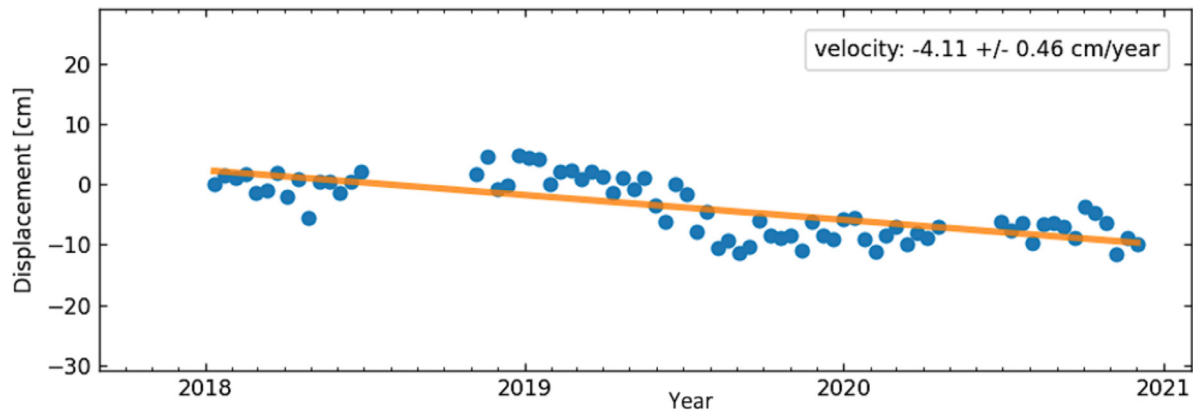


Figure 16. Displacement in LOS (cm/yr) for Lagunillas, for the period 2018-2019-2020, in its descending mode. The blue dots in the time series correspond to the cumulative offset values, while the orange line corresponds to the calculated trend line. The estimated values of the velocity, and the uncertainties were calculated.

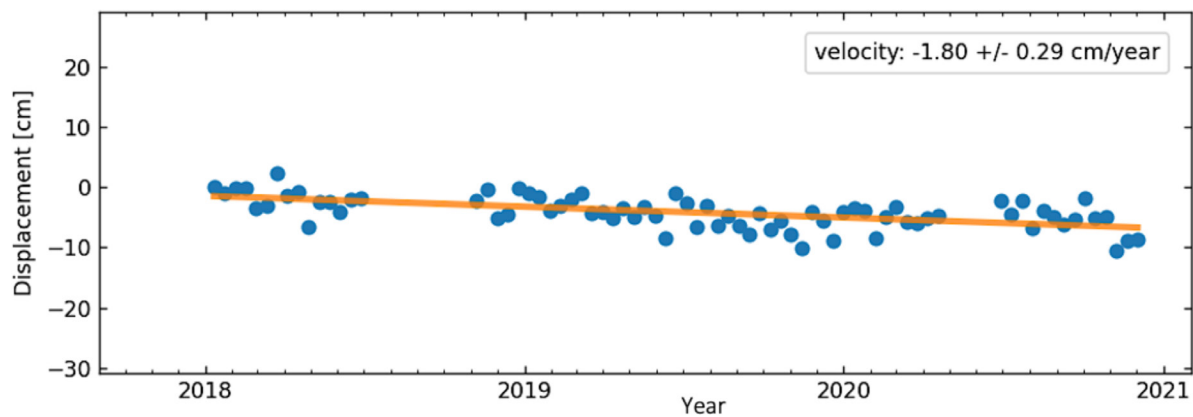


Figure 17. Displacement in LOS (cm/yr) for Bachaquero, for the period 2018-2019-2020, in its descending mode. The blue dots in the time series correspond to the cumulative offset values, while the orange line corresponds to the calculated trend line. The estimated values of the velocity, and the uncertainties were calculated.

Table 3. Comparative of values obtained in the COLM in the different studies conducted.

Zone	2021 (PSInSAR) Quintana <i>et al.</i>	2019 (DInSAR) Arenas <i>et al.</i>	2015 (DInSAR) Deguchi and Narita	2019 Arenas <i>et al.</i> (PCT 2006)
Lagunillas	- 4 cm		-10,3 cm	-3 cm
Ciudad Ojeda	4,5 cm	3 cm		5 cm
Tia Juana	3,5 cm	-3 cm	5,1 cm	-3 cm
Bachaquero	3 cm		-5,8 cm	-3 cm
Quintana <i>et al.</i> , 2026 (SBAS)				
Zone	Displacement LOS in Ascending mode		Displacement LOS in Descending mode	
Tia Juana	-6.4 cm	+/- 0.8 cm	1.2 cm	+/- 0.5 cm
Lagunillas	-7.9 cm	+/- 0.1 cm	- 4.1 cm	+/- 0.5 cm
Bachaquero	-7.1 cm	+/- 0.8 cm	- 1,8 cm	+/- 0.3 cm

Table 4. Delay tropospheric contribution and, the East and Vertical components values using the Equation 3, combining the Standard Desviation (Std) and ERA5 velocities in LOS in both modes for Tia Juana, Lagunillas and Bachaquero oil fields to the period 2018-2019-2020.

Oil Fields	Delay tropospheric contribution		East-West and Vertical Components	
	dE (east-west)	dU (up)	dE (east-west)	dU (up)
	cm/y	cm/y	cm/y	cm/y
Tia Juana	-0.2	-0.6	-6.79	-2.94
Lagunillas	-0.3	-0.5	-3.27	-5.19
Bachaquero	-0.4	-0.5	-5.92	-6.29

The North-South displacement component was neglected due to the near-polar orbit of Sentinel 1, which results in low sensitivity to North-south motion.

Although the estimated tropospheric contribution (ranging from 0.2 cm/y to 0.6 cm/y) falls within the reported uncertainty margins of the deformation rates, its systematic nature poses a risk of cumulative bias in long term monitoring. By applying the PyAPS ERA5 correction, we effectively isolated the anthropic signal from topography dependent water vapor delays, ensuring that the calculated east west (dE) and vertical (dU) components reflect true reservoir compaction rather than atmospheric artifacts. This correction is particularly critical when contextualizing current rates against the 60 year historical subsidence of 5 meters, as it prevents the artificial inflation of deformation rates by approximately 5% to 8%, thereby providing a more rigorous baseline for ongoing dike stability and flood risk assessments in the COLM.

5. Conclusions

The InSAR technique is one of many applications of Remote Sensing suited for the COLM and Occidental Region of

Venezuela studies, it solves the observational gaps inherent in traditional surveying, providing continuous monitoring, spatial density of data, and non invasive tool and cost effective for the monitoring of active oil fields without interrupting production or requiring ground access to potentially hazardous or restricted industrial zones. The methodology emphasized the atmospheric correction to tropical regions to obtain accurate values.

According to the obtained results, it is evident that the subsidence continues, specifically in the three oil fields of the COLM, with estimated LOS rates between -6 cm/y and -7 cm/y in its ascending mode and with values between -1 and -4 cm/y for Lagunillas and Bachaquero in its descending mode. However, Tia Juana presents positive values in descending mode. Also, for the estimation of the delay tropospheric contribution rates for the east and vertical components, the values between -0.2 to -0.6 cm/y and, the east-west (dE) and vertical (dU) components values for the three fields, with: -6.79 cm/y and -2.94 cm/y; -3.27 cm/y and -5.19 cm/y and; -5.92 cm/y and -6.29 cm/y respectively.

The study is further evidence of the importance of the application of atmospheric corrections when using the InSAR technique for the study of crustal deformations. When observing the values of the estimated tropospheric delay contribution, it is

evident that the rates for the east and vertical components would be masked by atmospheric effects, affecting their accuracy. While the tropospheric signal might not be statistically significant in terms of overwhelming the error bars, it is geophysically significant. In a 3 years study (2018–2020), an uncorrected 0.6 cm/y atmospheric bias would result in a 1.2 cm error in total cumulative subsidence. For a region sensitive to millimetric changes in stability, this bias is too large to ignore.

Similarly, the InSAR technique is once again validated as suitable for the measurement of displacements, aimed at establishing the behavior of the subsidence phenomenon in a given period and also allowing the determination of its spatial distribution. However, since this technique is discrete in time, it is advisable to complement the measurements with continuous monitoring of geodetic data (e.g., cGPS/GNSS), by comparing InSAR displacement at GNSS station locations, ensuring that large scale atmospheric artifacts aren't interpreted as broad regional subsidence, validate the PyAPS/ERA5 correction, and to detect subtle, non linear deformation that would otherwise be buried under the phase grass of turbulent atmospheric noise.

It is recommended to continue the study with the extension of the temporality in the East Coast of Lake Maracaibo-COLM, and to correlate these results with the GNSS studies.

In conclusion, we can point out that the subsidence rates obtained by InSAR technique in the COLM, over a time window of 3 years (01/2018-12/2020), are very similar to the rates already obtained close to 8 cm/y, over the long term (5 m in 60 years, between 1926 and 1986), by conventional geodetic or topographic methods prior to the satellite era. However, satellite measurements do not require such a long time monitoring due to their high accuracy.

Finally, this study contributes to Environmental Geology and Geomechanics in several ways, showed how fluid extraction can become the primary driver of geomorphological change, outpacing natural geological processes in the basin. The displacement rates found (–7.9 cm/y in Lagunillas) can be used by reservoir engineers to calculate compaction coefficients and pore pressure changes within the Mioceno and Eoceno formations.

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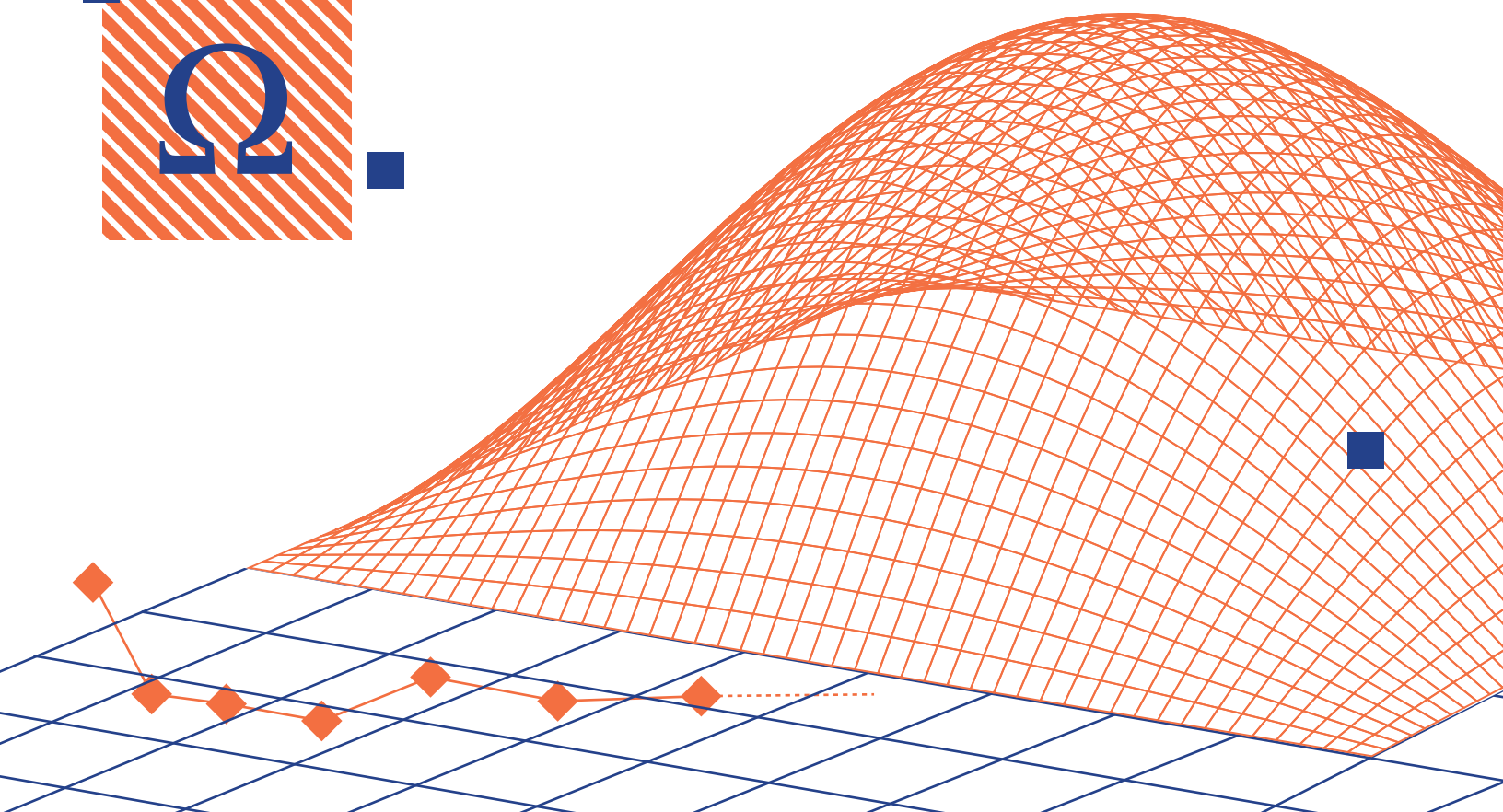
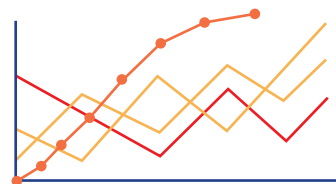
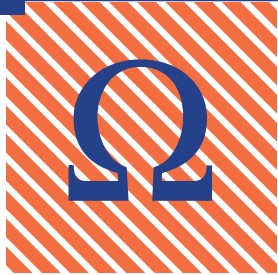
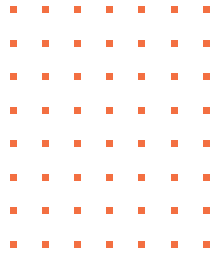


Sección especial

Geofísica Matemática y
Computacional

Special section

Mathematical and Computational
Geophysics



Assimilating chemical observations in the Mexico City Metropolitan Area using WRFDA-Chem

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Abstract

Air pollution exceedances are important air quality events for its associated effects on public health. Chemical transport models are frequently used for estimating pollution concentrations, especially in areas with limited monitoring capacity. Even though their performance may be improved by combining observations from different platforms through data assimilation, in Mexico these applications are limited, especially those aiming to assimilate chemical composition observations. In this study, surface observations of O₃, CO and NO₂ from the local monitoring network (RAMA) together with conventional global meteorological observations, were assimilated over the Mexico City Metropolitan Area (MCMA) using the WRFDA-Chem v4.5.2 assimilation system and the 3DVAR algorithm. The global observations were obtained in PREPBUFR format, and consisted of upper-air and surface weather reports collected worldwide. The observations included pressure, temperature, dew point, wind speed and direction, from several platforms including surface, radiosondes, and aircraft reports. Two sets of experiments focusing on the impact of the chemical initial and boundary conditions were conducted. One experiment used default chemical initial and boundary conditions provided. In the experiment denoted by "default", the WRF-Chem model was initialized through predetermined NALROM (NOAA Aeronomy Lab Regional Oxidant Model) ideal profiles that are included in the model. These profiles represent a northern-hemispheric, mid-latitude, relatively clean atmospheric composition and provide values for species such as O₃, CO, NO_x (WRF-Chem user guide). The other experiment, denoted by "global", the NALROM ideal profile was replaced with external chemical fields obtained from the global chemical transport model WACCM (Whole Atmosphere Community Climate Model). These fields provide spatially and temporally varying initial and boundary conditions that reflect realistic large-scale chemical distributions rather than a static climatology. Results showed that chemical data assimilation corrected pollutants concentrations. Regarding CO and NO₂, differences between model results and observations were rather small, suggesting the need of tuning the background error covariance matrix parameters for these pollutants. However, for ozone, using global model outputs to initialize the model, tended to better represent regional maximum concentration, whilst using default conditions tended to better represent regional average concentration. However, both setups estimated similar daily ozone peaks. This suggests that using default chemical conditions cycled over a long period may optimize storage and computing resources.

Key words: WRFDA-Chem, data assimilation, air quality modeling, ozone.

Resumen

Las excedencias de contaminación atmosférica son eventos importantes de calidad del aire por sus efectos asociados en la salud pública. Los modelos de transporte químico se utilizan con frecuencia para estimar las concentraciones de contaminantes, especialmente en zonas con capacidad de monitoreo limitada. Si bien su rendimiento puede mejorarse combinando observaciones de diferentes plataformas mediante la asimilación de datos, en México estas aplicaciones son limitadas, especialmente aquellas que buscan asimilar observaciones de composición química. En este estudio, se asimilaron las observaciones en superficie de O₃, CO y NO₂ reportadas por red de monitoreo local (RAMA), junto con observaciones meteorológicas globales convencionales, en la Zona Metropolitana de la Ciudad de México (ZMCM) mediante el sistema de asimilación WRFDA-Chem v4.5.2 y el algoritmo 3DVAR. Las observaciones globales se obtuvieron en formato PREPBUFR y consistieron en informes meteorológicos de altitud y superficie recopilados a nivel mundial. Las observaciones incluyeron presión, temperatura, punto de rocío, velocidad y dirección del viento, provenientes de diversas plataformas, incluyendo informes de superficie, radiosondas y aeronaves. Se realizaron dos conjuntos de experimentos centrados en el impacto de las condiciones químicas iniciales y de frontera. Un experimento utilizó las condiciones químicas iniciales y de frontera predeterminadas. En el experimento "default", el modelo WRF-Chem se inicializó mediante perfiles ideales NALROM (NOAA Aeronomy Lab Regional Oxidant Model) predeterminados, incluidos en el modelo. Estos perfiles representan una composición atmosférica relativamente limpia en el hemisferio norte, en latitudes medias, y proporcionan valores para especies como O₃, CO y NO_x (Guía del usuario de WRF-Chem). En el otro experimento, "global", el perfil ideal NALROM fue reemplazado por campos químicos externos obtenidos del modelo global de transporte químico WACCM (Whole Atmosphere Community Climate Model). Estos campos proporcionan condiciones iniciales y de contorno que varían espacial y temporalmente, reflejando distribuciones químicas realistas a gran escala, en lugar de una climatología estática. Los resultados mostraron que la asimilación de datos químicos corrigió las concentraciones de contaminantes. En cuanto al CO y el NO₂, las diferencias entre los resultados del modelo y las observaciones fueron relativamente pequeñas, lo que sugiere la necesidad de ajustar los parámetros de la matriz de covarianza del error de fondo para estos contaminantes. Sin embargo, en el caso del ozono, el uso de las salidas del modelo global para inicializar el modelo tendió a representar mejor la concentración máxima regional, mientras que el uso de las condiciones predeterminadas tendió a representar mejor la concentración media regional. No obstante, ambas configuraciones estimaron picos diarios de ozono similares. Esto sugiere que el uso de condiciones químicas predeterminadas cicladas durante un período prolongado puede optimizar los recursos de almacenamiento y cómputo.

Palabras clave: WRFDA-Chem, asimilación de datos, modelación de la calidad del aire, ozono.

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1. Introduction

Air pollution is a problem that has intensified in recent years due to urban expansion, resulting in an increase in pollutant emissions. Pollution episodes (periods with high concentrations of pollutants) may last for several days and can impact public health, especially sensitive groups (INECC, 2024; WHO, 2024). These episodes coincide with low dispersion conditions, biomass burning activities, and high solar radiation, which altogether favor ground-level ozone production. In Mexico, they typically occur between February and May, during the so-called ozone season, and mainly affect Mexico City Metropolitan Area (MCMA) (INECC, 2020). However, the lack of surface observations in other metropolitan areas within the Megalopolis of Central Mexico, complicates monitoring these episodes at the regional level (Molina *et al.*, 2023). For this reason, analyzing these events could help identify their causes and contribute to developing control measures aimed at reducing pollution levels during episodes.

The complexity of atmospheric chemical reactions is influenced by emissions, transport, deposition, and chemical transformation. All these processes and their associated uncertainties impact model performance when estimating pollutants concentrations using chemical transport models (CTM) (Mallet & Sportisse, 2006; Aleksankina *et al.*, 2019). One approach to improve model performance consists in using observational data to constrain the model through data assimilation (DA). This technique aims to obtain a more accurate representation of the atmospheric state at a particular time. Traditionally, data assimilation has been mostly applied to meteorological forecasting in numerical weather prediction (Lee & Barker, 2005; Huang *et al.*, 2009). However, assimilation of chemical composition observations is a relatively more recent field and it has been used more frequently for air quality applications, including reactive gases and aerosol forecasting (Saide *et al.*, 2014; Bocquet *et al.*, 2015; Ha *et al.*, 2024).

Currently, there are several operational forecasting systems based on data assimilation worldwide. For example, the ECMWF/Copernicus Integrated Forecast system (IFS) developed in Europe, the Met Office UKV hourly 4D-Var system that has been operational since 2017 in the United Kingdom (Milan *et al.*, 2020), the DWD COSMO-KENDA and ICON-D2 global and regional numerical prediction systems, which have been operational since 2015 focusing on the European continent (Zängl *et al.*, 2015), and the NASA's GEOS-5 (Baklanov & Zhang, 2020) for global applications. Besides, a few examples of operational forecasting systems based on chemical data assimilation are CAMS (Copernicus Atmosphere Monitoring Service) system developed by ECMWF for global applications of both gas and aerosols (Peuch *et al.*, 2022), MERRA-2 (Modern-Era Retrospective analysis for Research and Applications Version 2) developed by NASA for global application focusing on aerosols

(Gelaro *et al.*, 2017) and the WRF-Chem/DART regional system (Mizzi *et al.*, 2016).

In Mexico, the number of published studies related to data assimilation is limited and mostly have focused on the assimilation of meteorological variables (Yang *et al.*, 2017; Risanto *et al.*, 2021). In addition, previous studies related to air quality applications have applied only meteorological data assimilation with the objective of improving modeled pollutant concentrations. For example, between 2008 and 2012, studies applied different techniques to assimilate meteorological variables (Bei *et al.*, 2008; 2010; 2012) with the aim of enhancing chemical simulations, particularly ozone and secondary organic aerosol (SOA) concentrations in Mexico City. Later, Bei *et al.*, (2014) analyzed the impact of using the Ensemble Kalman Filter in air quality simulations in the California-Mexico border area during the Cal-Mex field campaign to improve ozone concentration. More recently, Martínez-Sabari & García-Reynoso (2021) evaluated the impact of assimilating meteorological variables on ozone concentration in the MCMA using the 3DVAR assimilation technique. Chemical data assimilation (CDA) has not yet been implemented in Mexico and could become a key tool to enhance air quality model performance. To the best of our understanding this is the first application in Mexico of online chemical data assimilation using variational methods with WRFDA-chem.

The objective of this study is to present a sensitivity analysis of the WRFDA-Chem system for the MCMA under different initial and boundary conditions when assimilating ozone (O_3), carbon monoxide (CO) and nitrogen oxide (NO_2) surface observations. In this sense, this work may contribute to the ongoing effort of enhancing the forecasting capability of CTM in Mexico through data assimilation of reported criteria pollutants.

This work is organized as follows. Section 2 presents a description of the WRFDA-Chem assimilation system, including the WRF-Chem configuration and WRFDA assimilation requirements. Section 3 presents the numerical experiments conducted for sensitivity analysis. Modeling results and model evaluation are also discussed. Finally, conclusions are summarized in Section 4.

2. Data and Methods

2.1. WRFDA-Chem system

In this study WRFDA-chem is employed to conduct chemical data assimilation (CDA) over the Mexico City Metropolitan Area (MCMA). This system was developed recently with the aim of ingesting surface observations from monitoring networks and couples the WRFDA assimilation system with the WRF-Chem air quality model (Sun *et al.*, 2020; Ha, 2022). The main components are briefly described as follows.

2.1.1. WRF-Chem

The Weather Research Forecast Model coupled with Chemistry (WRF-Chem) model (Grell *et al.*, 2005) is a mesoscale regional online chemistry transport model that was developed as a collaborative effort of different research centers led by the Global Systems Laboratory (GSL, NOAA) and the National Center for Atmospheric Research (NCAR). It is capable of jointly simulating meteorological fields, emissions from anthropogenic sources, biomass burning activities and chemical species concentrations using an available set of chemical mechanisms.

In this study, WRF-Chem v4.5.2 with the RACM/MADE-VBS chemical mechanism was used to simulate ozone (O₃), carbon monoxide (CO) and nitrogen dioxide (NO₂) concentrations.

2.1.2. WRFDA

The Weather Research and Forecast Data Assimilation (WRFDA) is an assimilation system that combines observations, modeled data and their associated errors to improve model estimations (Barker *et al.*, 2012). Different DA algorithms have been implemented in this assimilation system such as the Three-dimensional variational assimilation (3DVAR), the Four-dimensional variational assimilation (4DVAR), and their respective hybrid options (3DEnVAR and 4DEnVAR) that make use of ensemble background errors within a variational framework (Vendrasco *et al.*, 2016; Ban *et al.*, 2017; Davis *et al.*, 2021; Yang & Wang, 2024).

In this study we used WRFDA-Chem v4.5.2 to assimilate meteorological and chemical observations with the 3DVAR variational algorithm that estimates the optimal combination with the modeled variables (analysis) through a minimization process of a cost function represented by $J(x)$ (equation 1):

$$J(x) = \frac{1}{2}(x - x_b)^T B^{-1}(x - x_b) + \frac{1}{2}(H(x) - y)^T R^{-1}(H(x) - y) \quad (1)$$

where x_b is the background field vector, y is the observation vector, H is the observation operator that converts the model state to the observed quantities, and B and R represent the background error and observation error covariance matrices respectively.

This system has the capability of assimilating meteorological variables from surface networks, radars, buoys, ships, and other observational platforms. On the other hand, WRFDA-chem was developed based on WRFDA to ingest chemical compo-

sition observations at ground level. Currently this chemical data assimilation system has the capability to process surface observations of 6 chemical species, 4 in gas phase (SO₂, NO₂, O₃ and CO) and 2 in particulate phase (PM_{2.5}, PM₁₀) (Sun *et al.*, 2020; Ha, 2022). In addition, it only supports GOCART (Chin *et al.*, 2000), MOSAIC (Zaveri *et al.*, 2008) and RACM/MADE-VBS (Stockwell *et al.*, 1997; Ahmadv *et al.*, 2012) chemical mechanisms (Ha, 2022).

One of the main reasons for using the 3DVAR algorithm is that although its limitations such as using a static background error covariance and a linearized forecast model, its computational time is feasible for operational settings related to air quality (Ha, 2022). The expensive computations required for solving stiff chemical mechanisms with hundreds of prognostic variables is a parameter to be accounted for when considering the implementation of an operational forecasting with limited resources. Using 3DVAR lets us optimize computational resources compared to 4DVAR due to the extra computational cost required to solve the adjoint and tangent-linear models in the four-dimensional variational assimilation technique.

2.1.2.1. Background error

The background error covariance matrix (**B**) was estimated using the GEN_BE 2.0 software (Descombes *et al.*, 2015), which modifies the original GEN_BE (included in the WRFDA system) to process chemical observations. This tool allows the estimation of several statistics for meteorological variables as well as chemical species; such as the standard deviation, vertical and horizontal length scales, and vertical correlations. Currently, it supports different aerosols mechanisms such as MADE-VBS, GOCART and MOSAIC.

In this study, **B** was calculated for each domain using the National Meteorological Center (NMC) method (Parrish & Derber, 1992) with 12h and 24h WRF-Chem forecasts valid at the same time from March 22 to 29, 2023.

2.2. Emissions

Emissions data from the 2016 Mexican National Emissions Inventory (SEMARNAT, 2019) was processed for modeling by using the Spatial, Temporal and Speciation Distribution Model (DiETE) (García-Reynoso *et al.*, 2018) in order to prepare model-ready files with the RACM chemical mechanism speciation.

Emissions of volatile organic compounds (VOCs) and nitrogen oxides (NO_x) were scaled for the modeling period with the objective to better represent O₃, NO₂ and CO concentrations to surface observations due to the uncertainty associated with the estimation of emissions (West *et al.*, 2004; Lei *et al.*, 2007).

2.3. Observations

Global observations were obtained in PREPBUFR format, which are generated operationally by NCEP and consisted of upper-air and surface weather reports collected worldwide. The observations included pressure, temperature, dew point, wind speed and direction, from several platforms including surface, radiosondes, and aircraft reports (NCEP, 2025b). Important to highlight is the scarce number of available data over Central Mexico, which is about 1 station close to the MCMA on March 31st at 18:00 UTC (Figure 1).

In addition, O₃, CO and NO₂ surface measurements reported by the Mexico City local monitoring network (RAMA) (SEDEMA, 2025) were employed to assimilate pollutants concentrations (Figure 2). This monitoring network covers Mexico City and part of State of Mexico and is hosted by the Environmental Secretariat. It reports hourly observations of criteria pollutants (ozone, carbon monoxide, nitrogen oxides, sulfur dioxide and particulate matter) and meteorological variables (temperature, relative humidity, wind speed and wind direction). It began operations in 1986 and currently operates with more than 30 stations and are publicly available as 1-h averages after being validated following the US Environmental Protection Agency standards (SEDEMA, 2025).

2.4. WRF-Chem model configuration

In this study, the WRF-Chem model was forced with the meteorological Global Forecast System at 0.25° resolution from NCEP (NCEP, 2025a) and configured with two nested

domains. The outer domain consisted of a 215 by 150 cells with 15 km resolution, while the inner domain comprised a 96 by 63 cells grid with 5 km resolution (Figure 3). Additionally, an updated 30" resolution urban coverage dataset for the MCMA (López-Espinoza *et al.*, 2012) was employed.

The following parameterizations were used to simulate physical processes occurring in the atmosphere: 1) the YSU scheme for the boundary layer (Hong *et al.*, 2006); 2) the WSM6 (WRF Single-Moment 6-class) option for microphysical processes (Hong & Lim, 2006); 3) the Rapid Radiative Transfer Model (RRTM) for processes related to shortwave and longwave radiation (Iacono *et al.*, 2008); and 4) the Grell-3D ensemble scheme for the convection (cumulus) option (Grell, 1993; Grell & Dévényi, 2002).

The modeling period spans from March 31st to April 3rd, 2023, with 1 day of spin-up. The criteria to select this period were: 1) meteorological conditions without much influence of synoptic-scale phenomena (cold fronts) (CONAGUA, 2024); 2) negligible fire emissions from biomass burning activities (CONAFOR, 2024); 3) no additional emissions adjustment. The mobility restrictions associated with the COVID-19 lockdown ended in Mexico in late 2022, so that a modeling period in 2023 was preferred.

2.5. Experiment design

In this study, WRF-Chem and WRFDA cycling experiments were conducted from March 31st to April 3rd, 2023, every 6 hours for forecast and assimilation cycles, with one day of spin-up in a WRF-Chem one-way nesting configuration (Table 1). Since one of the aims of data assimilation is to improve the initial state of

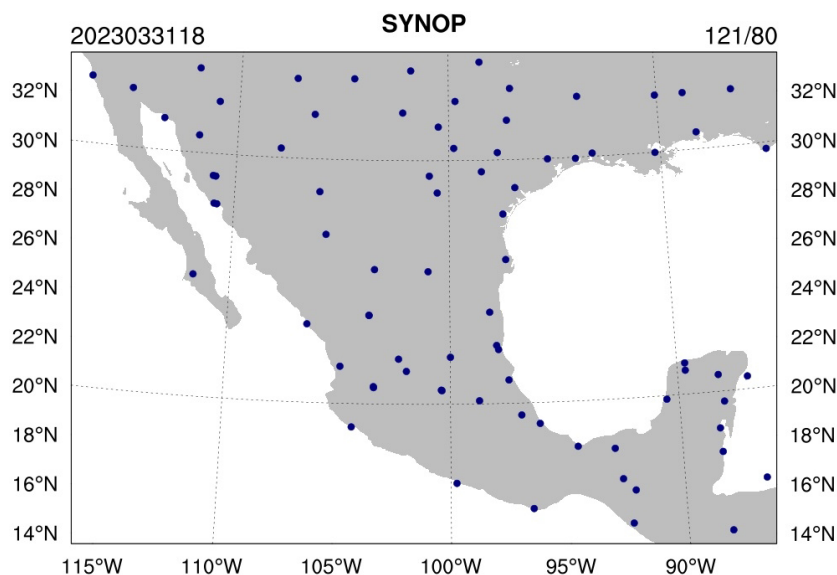


Figure 1. Available synoptic stations on March 31st at 18:00 UTC in NCEP PREPBUFR dataset.

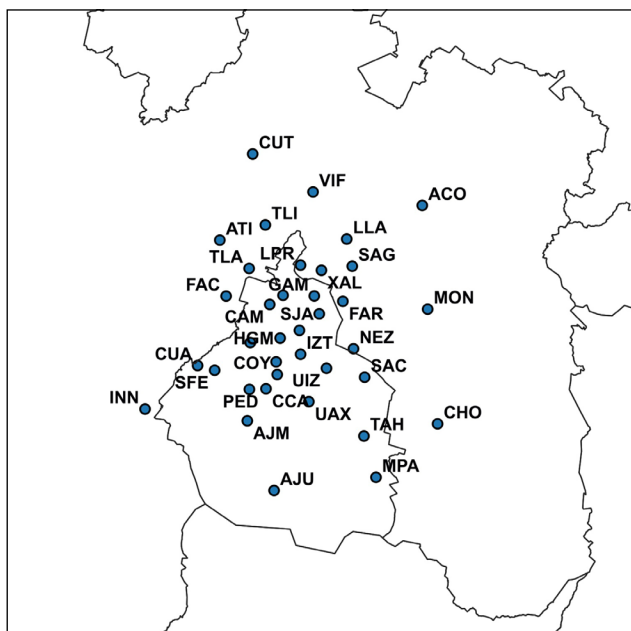


Figure 2. RAMA surface monitoring network in MCMA.



Figure 3. Modeling domains at 15 km (black) and 5 km (blue) resolution.

a model, a total of two numerical experiments focusing on the impact of the chemical initial and boundary conditions were considered. One experiment used the default (DFLT) chemical conditions provided by the WRF-Chem model through the NALROM (NOAA Aeronomy Lab Regional Oxidant Model) ideal profile (McKeen *et al.*, 2002). The other experiment used chemical conditions provided by a separate global chemical transport model (GLOB). For this case, outputs from the Whole Atmosphere Community Climate Model (National Center

for Atmospheric Research, 2026.) (WACCM) was used. The meteorological initial conditions were kept the same in all experiments because analyzing the coupled impact of chemistry and meteorology is beyond the scope of this study.

These numerical experiments were designed considering a limited computational resources framework. For this reason, choosing how to solve the stiff chemical mechanism was very important. Two approaches were considered. One approach consisted on solving the chemistry only in the innermost

domain, which implies to firstly run the outer domain and then run separately the innermost domain. The advantage of this approach is that there is no need to solve the chemistry at the national level, which is computationally intensive. The second approach consisted of running the chemistry in both domains, which means running the model in a 1-way simultaneous run and solving the chemistry at both the national level (domain one, D01) and the regional level (domain two, D02). The workflow of both approaches is described as follows.

D01_NoDA simulation was carried out for the outer domain without data assimilation and chemistry turned off. Meteorological fields from the first cycle were used to initialize the next cycle and so on. In addition, meteorological initial and boundary conditions from GFS (Global Forecast System) were updated in every 6-hour cycle. Then, the control experiment (NoDA-chem) was carried out without data assimilation and chemistry turned on. Initial and boundary conditions were provided from D01_NoDA experiment through a one-way nesting setup. Besides, similar to meteorological variables, the chemical fields from the first cycle were used to initialize the next cycle and so on.

The D02_DFLT experiment was performed with assimilation of O₃, CO and NO₂ surface observations from RAMA network. As mentioned before, the initial and boundary conditions were carried over from D01_D_ICBC simulation based on the ideal NALROM profile. The difference with respect to the D02_GLOB experiment is that the initial and boundary conditions were generated from D01_G_ICBC simulation using WACCM model outputs. In both D01_D_ICBC and D01_G_ICBC experiments,

meteorological observations (temperature (T), relative humidity (RH), wind components (U, V) and pressure (P)) were assimilated by employing global data in PREPBUFR format (NCEP, 2025b).

Subsequently, the quality of the assimilation was evaluated using metrics such as the observation minus background (OMB), observations minus analysis (OMA), and increments (difference between analysis and background). OMB is calculated using prior information (i.e. before assimilation) and OMA is estimated *a posteriori* (i.e. employing the DA outcome). Therefore, the magnitude of OMA should be smaller than OMB if the assimilation is working properly (Ha, 2022).

Model evaluation was estimated using traditional statistical metrics, like the index of agreement (d) (Willmott *et al.*, 1985), the root mean square error (RMSE) and the Pearson correlation coefficient.

3. Results and Discussion

The results presented in this section will consider two aspects. First, evaluating the quality of the assimilation using the observation minus background (OMB), observation minus analysis (OMA) and the increments. Second, evaluating the impact of the assimilation on model performance employing both the regional hourly average and regional hourly maximum concentrations of O₃, CO and NO₂ based on 34 RAMA monitoring stations. All the presented results in this section correspond to the inner domain (D02).

Table 1. Simulation experiments and their main settings.

Domain	Experiment	Meteorological or chemical variables assimilated	Assimilated time (UTC)	Simulation features
Outer domain (D01)	D01_NoDA	None	-	Default chemical initial and boundary conditions. Chemistry turned off.
	D01_D_ICBC	T, U, V, RH, P	00:00, 06:00, 12:00, 18:00	Default chemical initial and boundary conditions. Chemistry turned off.
	D01_G_ICBC	T, U, V, RH, P	00:00, 06:00, 12:00, 18:00	Chemical Initial and boundary conditions from WACCM model. Chemistry turned on.
	NoDA-chem	None	-	Control experiment. Chemistry turned on
Inner domain (D02)	D02_DFLT	O ₃ , CO, NO ₂	00:00, 06:00, 12:00, 18:00	Default chemical initial and boundary conditions from outer domain (D01_D_ICBC)
	D02_GLOB	O ₃ , CO, NO ₂	00:00, 06:00, 12:00, 18:00	Global chemical initial and boundary conditions from outer domain (D01_G_ICBC)

3.1. Assimilation quality

Figure 4 shows time series of the observation minus background (OMB) and the observation minus analysis (OMA) in terms of the RMSE for O_3 , CO and NO_2 for the simulation period. With respect to O_3 the OMA tended to be smaller than the OMB for both DA experiments (D02_DFLT and D02_GLOB) which means that data assimilation tended to correct the model concentration. On the other hand, for both CO and NO_2 the OMA was lower than the OMB in some assimilation cycles for both DA experiments, but no significant changes were found associated with the use of different initial and boundary conditions. On the contrary, in other assimilation cycles (for example on 2023-03-31 06:00 UTC, 2023-04-01 12:00 UTC or 2023-04-02 12:00 UTC) both RMSE magnitudes of OMB and OMA were very similar to each other. This indicates that the assimilation had a small impact on modeled concentrations at these hours.

Figures 5 and 6 show the horizontal distribution of average analysis increments (obtained as the difference between the

analysis minus the background) in the assimilated variables (O_3 , CO, and NO_2) for both DA experiments. D02_DFLT (upper row) and D02_GLOB (bottom row). These increments correspond to the lowest model level, averaged at 00:00 UTC and 18:00 UTC assimilation cycles for the simulation period.

The 00:00 UTC hour was selected because it is important for representing fresh emissions linked to early-morning mobile emissions in the MCMA. Conversely, the 18:00 UTC period was selected because it represents the increase in ozone concentration, reflecting photochemical processes that occur during daylight hours.

At 00:00 UTC, average ozone concentration was increased to southeast of MCMA using the default initial and boundary conditions, indicating that it was underestimated in the background forecasts (upper row). On the contrary, it was reduced to the northwest of MCMA suggesting that the O_3 concentration was overestimated in the background concentration. However, when using the global chemical conditions, ozone concentration was reduced in all the MCMA (bottom row). This suggests that the

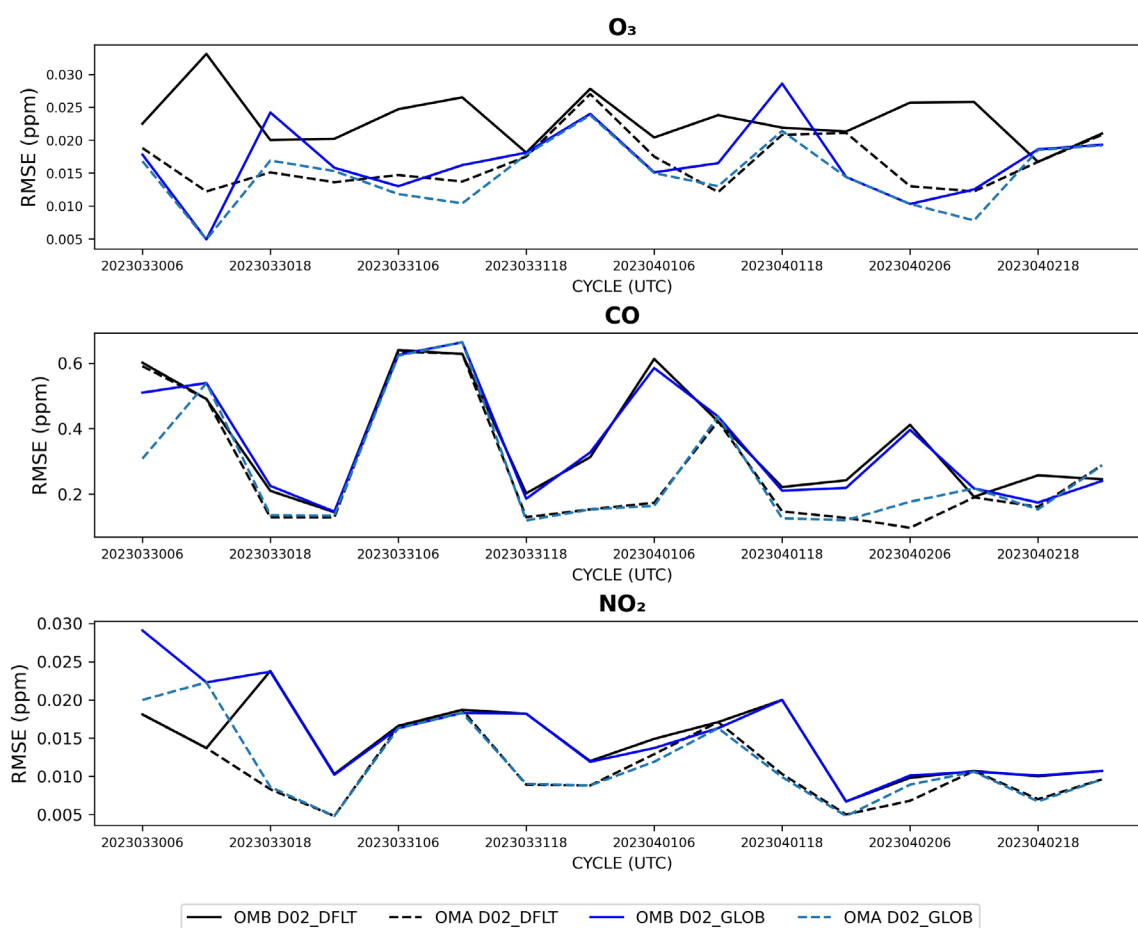


Figure 4. Time series of observation minus background (OMB, solid lines) and observation minus analysis (OMA, dashed lines) at each assimilation cycle in terms of root-mean-square error. Black line denotes D02_DFLT experiment and blue line denotes D02_GLOB experiment.

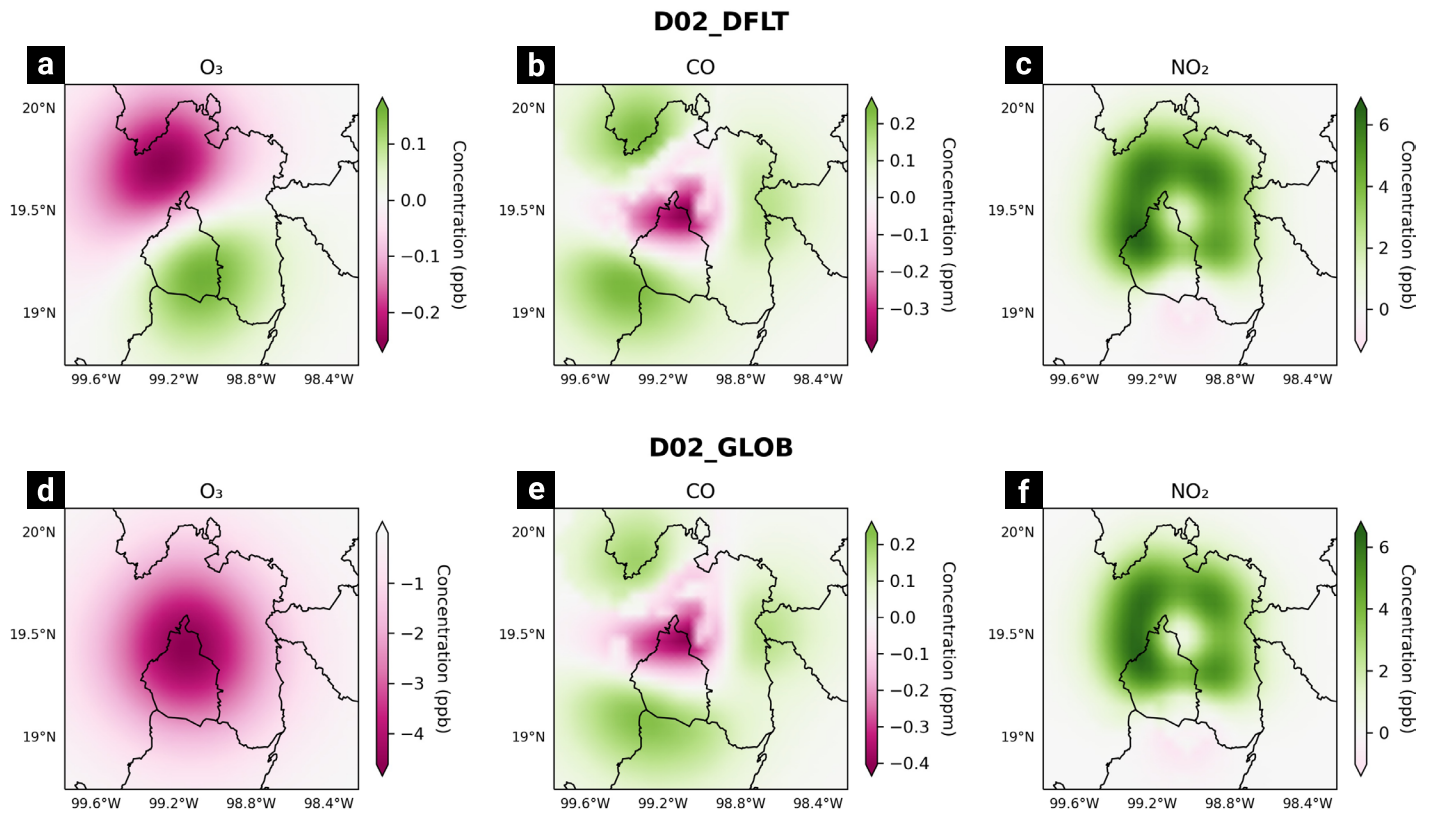


Figure 5. Horizontal distribution of the analysis increments for O_3 , CO and NO_2 averaged at 00:00 UTC assimilation cycles.

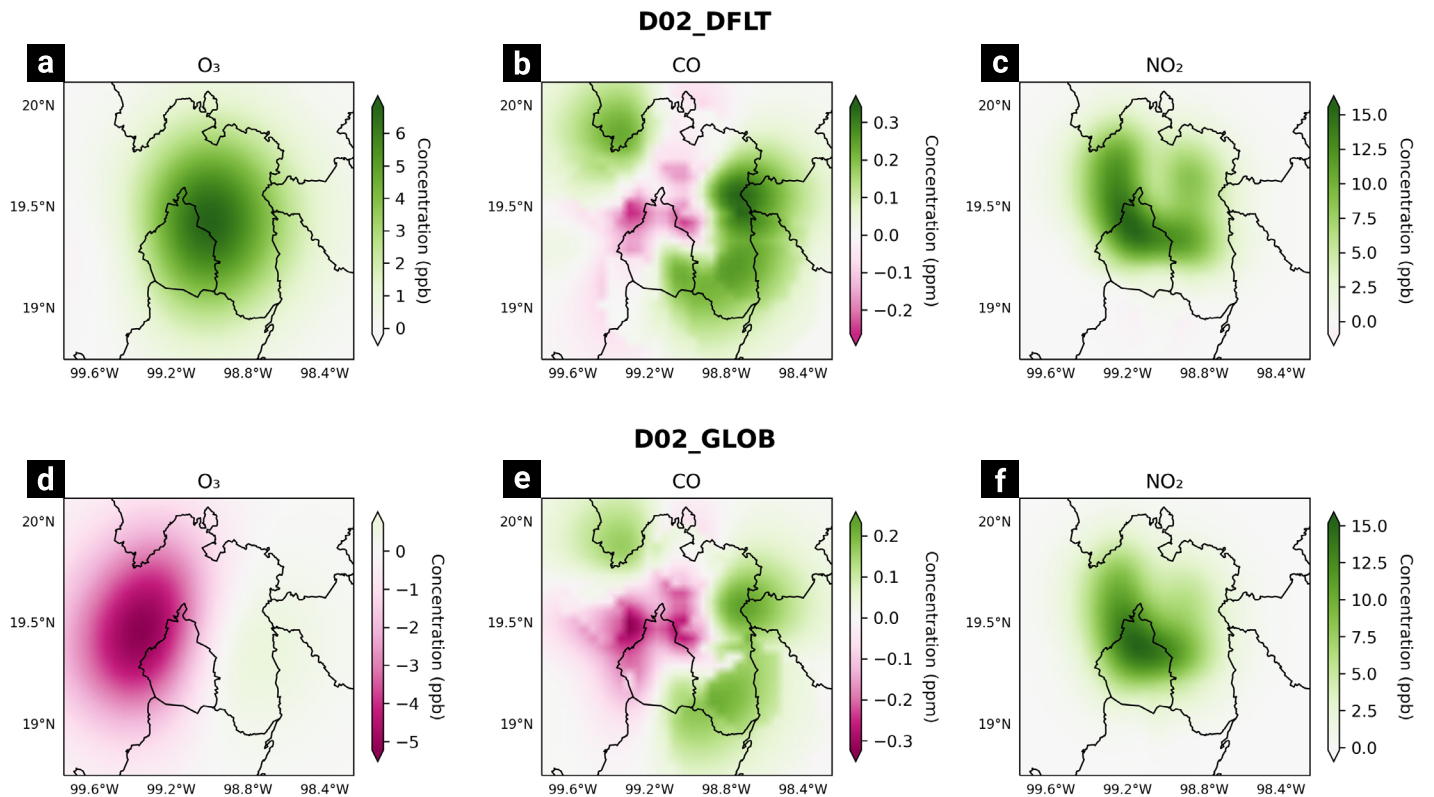


Figure 6. Horizontal distribution of the analysis increments for O_3 , CO and NO_2 averaged at 18:00 UTC assimilation cycles.

background ozone level in the global model is higher than the default chemical conditions. In addition, CO concentrations increased in the periphery of MCMA but decreased in the center area in both DA experiments. This implies that CO background concentration was underestimated around the MCMA center whereas it was overestimated on the outskirts of this metropolitan region. Finally, NO₂ concentrations augmented in most of MCMA in both DA experiments. This means that the background concentration was increased in order to approximate model results to observations.

These results illustrate that integrating chemical surface observations into the model may help diminish differences between modeled and observed concentrations data likely driven by the uncertainty in the emission inventory. Likewise, it is shown that for O₃ and CO concentrations, their concentrations increased in some areas but in contiguous regions they decreased. This may be related to the uncertainty in the estimation of ozone precursors (VOCs and NO_x) and CO emissions in the emission inventory. Furthermore, the magnitudes of the increments and the impacted area are similar using default and global chemical conditions (D02_DFLT and D02_GLOB experiments, respectively) for CO and NO₂ which indicate that the use of different initial and boundary conditions did not have an impact on their concentrations at 00:00 UTC. However, it is worth investigating for an extended period.

At 18:00 UTC, average ozone concentration was primarily enhanced all over the MCMA when using default chemical conditions (D02_DFLT experiment). However, similar to the 00 UTC, the concentration was reduced mostly over the northern

and western areas of the MCMA when using global chemical conditions (D02_GLOB case). These results may be related to the underestimation in D02_DFLT and an overestimation in D02_GLOB in the model background concentration possibly because its precursors emissions are likely not well represented in the emission inventory.

Regarding CO, the magnitudes of the increments were significantly different in both experiments probably as a result of different background concentrations (corrected by assimilation in previous cycles) and distinct initial and boundary conditions.

With respect to NO₂, an increase in its concentration was suggested in both DA experiments, most likely related to underestimated emissions in the emissions inventory; therefore, its concentration was underestimated in the model background concentration and a correction was needed through the assimilation process. Furthermore, no significant difference was observed when using default and global initial and boundary conditions. This means that background concentrations were similar for both DA experiments suggesting that the magnitude of the assimilation correction was comparable in both DA experiments.

Figure 7 illustrates the vertical profiles of the average increments O₃, CO and NO₂ estimated at a point within MCMA (lat=19.1, lon -99). These profiles characterize the magnitude and vertical distribution of the adjustments performed by the assimilation system for both DA experiments (D_ICBC and G_ICBC) at two key synoptic hours (00z and 18z).

The O₃ profiles showed different sensitivity patterns depending on times of day and experiments configurations

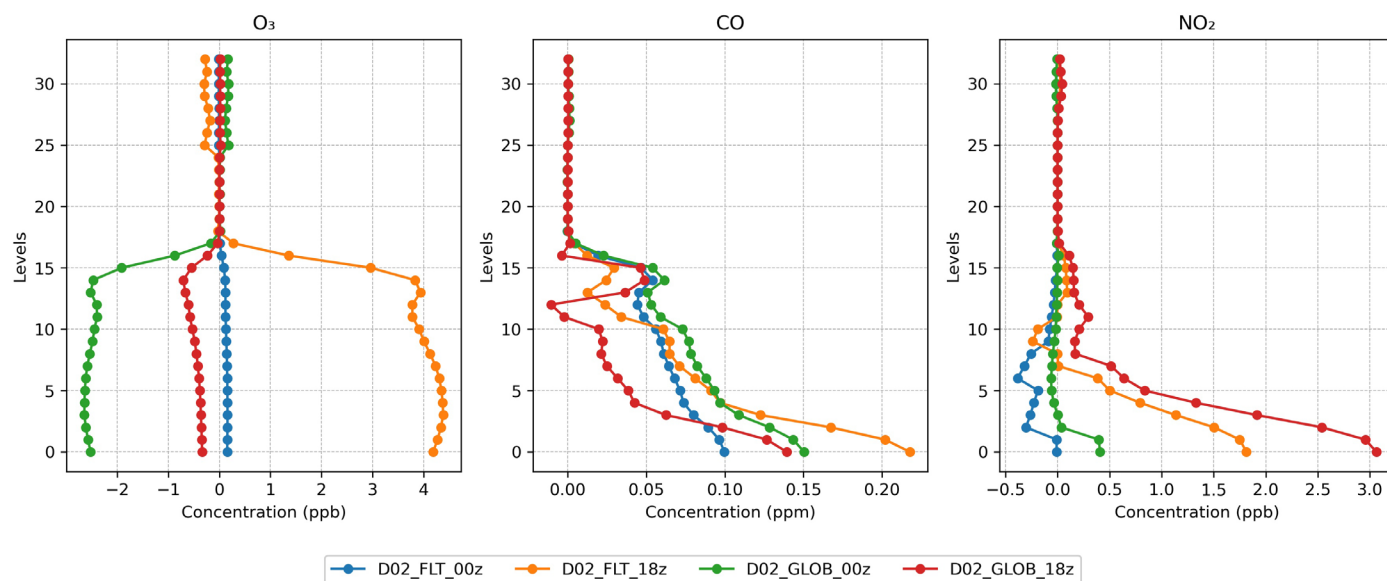


Figure 7. Average vertical profiles of the assimilation increments (analysis minus first guess) at a point located within the ZMVM (lat=19.1, lon -99) for O₃ (ppb), CO (ppm), and NO₂ (ppb) obtained from WRFDA-Chem. The profiles compare the D_ICBC and G_ICBC configurations at 00z (blue and green) and 18z (orange and red) over the study period.

within the lower troposphere (levels 0 to 17). In this sense, the D02_FLT_18z configuration (orange) shows significant positive increments, peaking at approximately 4 ppb near surface. Considering that the increment is equal to the difference between analysis and background, this result indicates that the first guess underestimated the O_3 concentrations compared to the assimilated observations. Conversely, the D02_GLOB_00z profile (green) exhibits a substantial negative reduction of about 2.5 ppb suggesting that the DA system reduced the O_3 concentrations to correct the bias in the first guess. Above level 20, the increments for all experiments converge toward zero, indicating that the impact of the assimilated surface data is primarily confined to the planetary boundary layer (PBL).

The CO profiles exhibit positive corrections across all DA experiments in the lowest 10 levels, but the largest adjustment occurs in the D02_FLT_18z experiment, with an increment exceeding 0.20 ppm at surface. This suggests an underestimation of CO concentration in the first guess, potentially due to low CO emissions or insufficient vertical transport near the surface. Moreover, all increments decrease monotonically with height, reaching near-zero values at level 17. This vertical structure suggests that the DA system corrected CO concentration mostly within the PBL.

NO_2 corrections are localized to the lowest levels (0-10), consistent with the short atmospheric lifetime of this species. Besides, significant adjustments are observed at 18z (orange and red lines), with the D02_GLOB_18z experiment showing the highest positive increment (approximately 3 ppb) at surface which implies a first guess underestimation of NO_2 observations. At 00z, the increments for both D02_FLT and D02_GLOB are close to zero or slightly negative, suggesting that the first guess is more accurately aligned with observations.

Figures 8 and 9 illustrate the analysis statistics of O_3 averaged at 00:00 UTC and 18:00 UTC assimilation cycles for D02_DFLT and D02_GLOB experiments. Ozone was chosen for this discussion because pollution episodes frequently occur due to high concentrations of this pollutant.

At 00:00 hours the model performance was better in the D02_DFLT experiment. However, the spread of the data suggests that the background concentration had a small correction in both DA experiments since RMS and standard deviation slightly decreased (Figure 8). Consequently, further investigation is required to improve model performance. For example, the assimilation of meteorological and chemical variables simultaneously in the inner domain, since in this study meteorological data assimilation was considered just for the outer domain.

At 18:00 UTC the magnitude of the correction through data assimilation was greater than at 00:00 UTC. It is observed that the model performance was best for the D02_GLOB experiment

on account of the lower magnitudes of statistical metrics (RMS around 19 and 15 respectively) (Figure 9). However, tuning the assimilation parameters in WRFA-Chem system will likely improve model performance. This will be explored in a future study.

These results also imply that additional research about the impact of the background and observation error covariance matrices in the analysis estimation is needed given that the solution of the minimization of the cost function (equation 1) depends on these terms. Excessively small values of B (background error covariance matrix) could lead to J being predominantly dependent on the term associated with model estimations, and vice versa.

3.2. Model evaluation

Figure 10 shows time series comparing the hourly regional average of all monitoring stations within the MCMA for the two DA experiments in the inner domain and the control (NoDA_chem) experiment. Compared to NoDA_chem experiment (blue line), the chemical data assimilation (red and green lines) improves hourly average estimations for O_3 with closer values to observed peaks for the D02_GLOB (red line). However, using default chemical conditions tended to better approximate evening and early morning ozone concentrations. As for CO, we found that during the first two days the three experiments showed similar concentrations at peaks values, but their magnitudes were lower than the observations. Besides, the minimum values were overestimated in the DA experiments. With respect to NO_2 , the assimilation improved the model performance during the first 12 hours of March 31st but in the following assimilation cycles estimations were lower than the measurements and closer to the control experiment. This implies that the assimilation system is discarding observations that even though they might correct the model concentration estimation, they are instead being considered as outliers based on strict thresholds.

Furthermore, despite that the average increments were greater than 4 ppb for O_3 , 6 ppb for NO_2 and 0.4 ppm for CO at 00:00 UTC (Figure 5), these changes were not directly reflected in the concentrations, particularly for CO and NO_2 . This could be explained by a degraded model performance in terms of meteorology, requiring improvements in the estimation of temperature, wind direction, wind speed or relative humidity through the assimilation of meteorological data within the study domain. As previously mentioned, there is just one synoptic station over the MCMA area (Figure 1) and most of the time there is only one radiosonde data available during the day. Thus, it is likely that the impact of a single observation is impacting a wide region. Since the MCMA is located in complex terrain, this impact might not be representative for an entire region, neither in the horizontal extent nor in the vertical extent, because it may also be

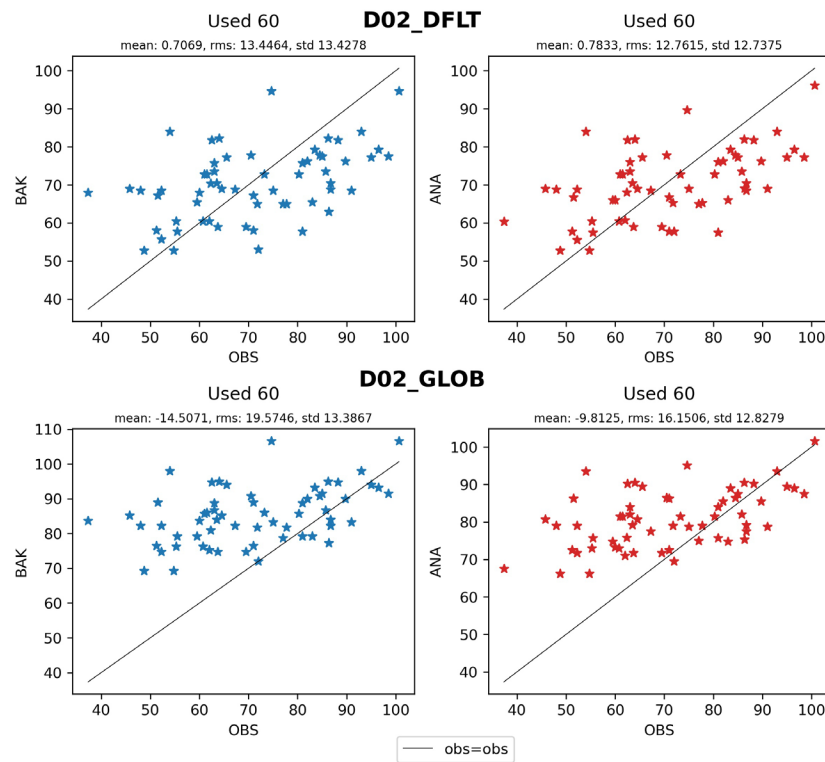


Figure 8. Averaged scatterplot of observation versus background (BAK, left column) and observation versus analysis (ANA, right column) for O_3 at 00:00 UTC. The top plots show results for D02_DFLT and bottom plots for D02_GLOB. The numbers above each panel denote numbers of the observations used in the assimilation process.

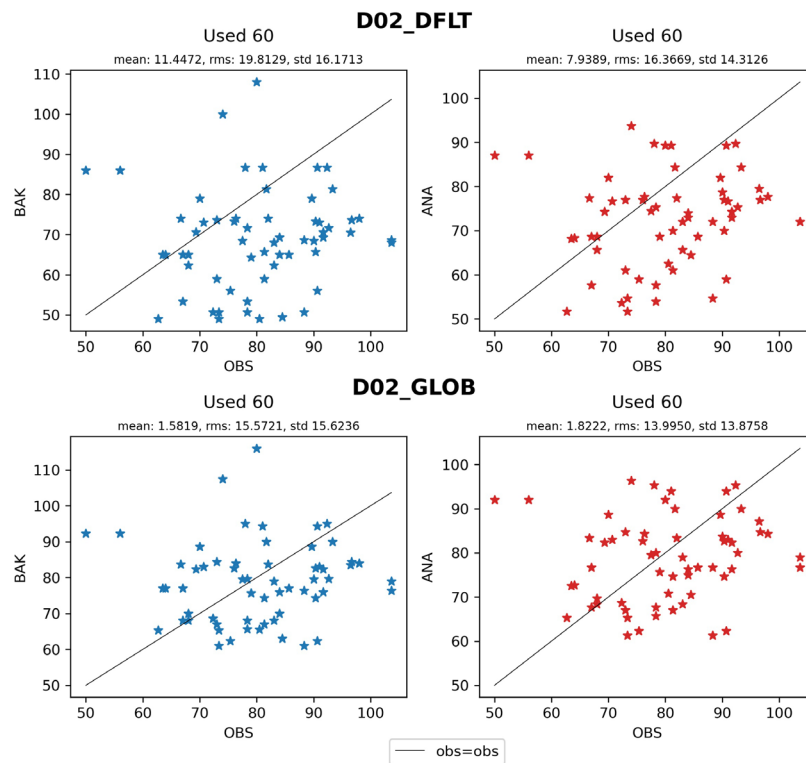


Figure 9. Averaged scatterplot of observation versus background (BAK, left column) and observation versus analysis (ANA, right column) for O_3 at 18:00 UTC. The top plots show results for D02_DFLT and bottom plots for D02_GLOB. The numbers above each panel denote numbers of the observations used in the assimilation process.

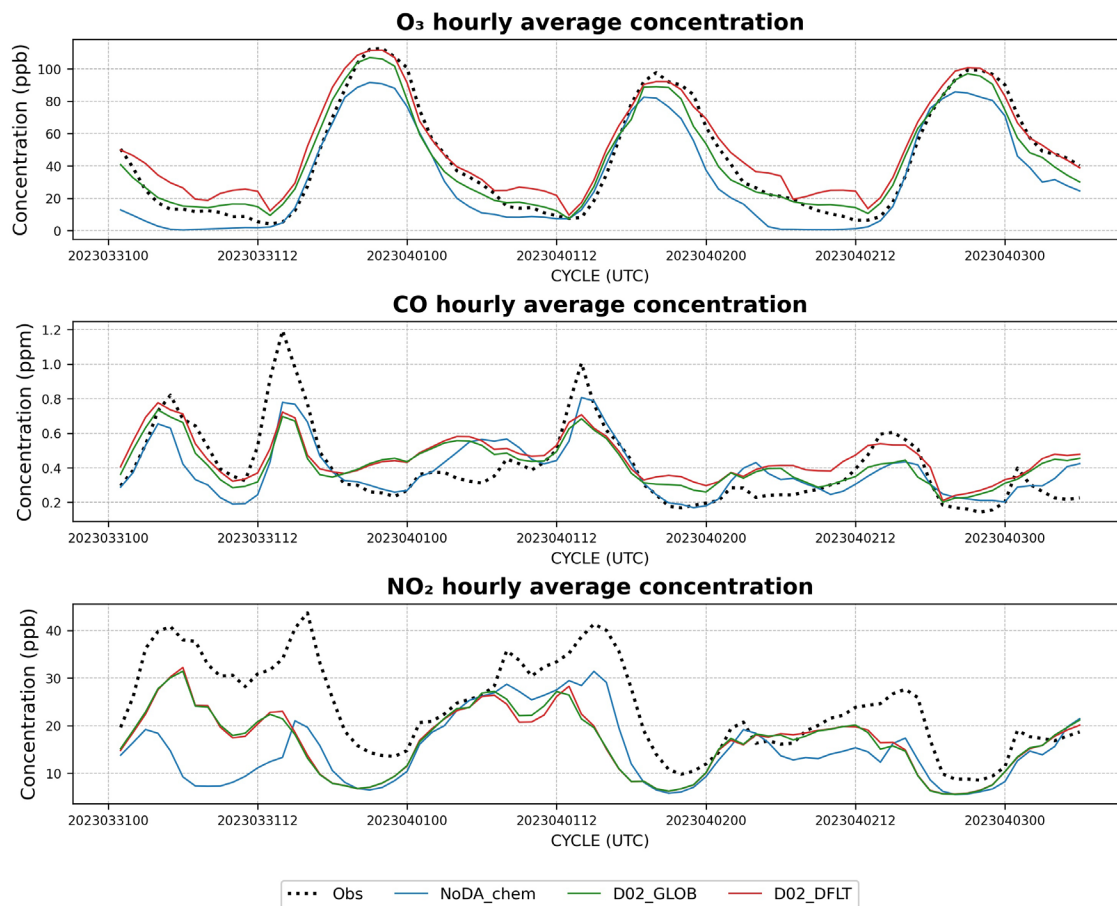


Figure 10. Time series of O_3 , CO and NO_2 comparing observed (dots) and modeled hourly regional average concentrations for the NoDA_chem (blue), D02_GLOB (green) and D02_DFLT (red) experiments.

impacting the boundary layer as resolved by the model. Thus, in a future study, meteorological surface data from RAMA and the National Weather Service will be considered in the assimilation. Additionally, adjusting assimilation parameters in the background error covariance matrix (variance, length scale, among others) could enhance model performance for both chemical and meteorological variables.

Table 2 shows the model evaluation for the control case and D02_DFLT and D02_GLOB experiments using the hourly average concentration for O_3 , CO and NO_2 concentrations. In addition, even though the main objective of this study is to evaluate the model performance for chemical species, statistical metrics for temperature (T), relative humidity (RH), zonal wind component (U) and meridional wind component (V) are presented just for completeness, with the aim of having a complete overview of all aspects that affect the concentration of pollutants.

It is observed that the DA experiment improved the average modeled concentrations of O_3 and NO_2 , finding the best performance for the D02_DFLT experiment. Conversely, the model performance slightly decreased for CO in the DA experiments. Important to mention, is that statistical metrics for meteorological

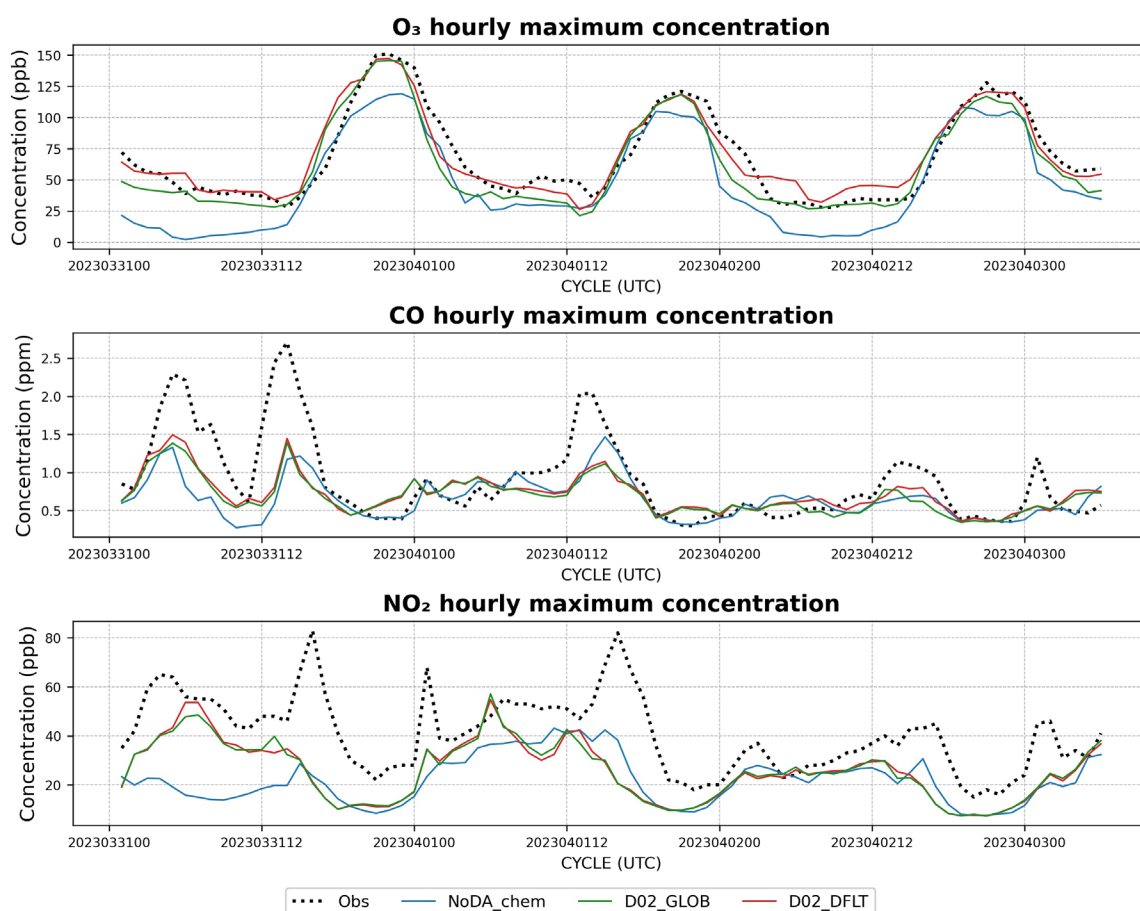
variables did not change in both DA experiments, because WRFDA-chem does not allow that meteorological state variables impact the chemical state variables in the assimilation step. In addition, there were few meteorological observations available for assimilation in the modeling domain (Figure 1).

Time series using hourly maximum concentrations are also presented due to the importance that maximum ozone concentrations have on pollution episodes in MCMA. In this sense, Figure 11 depicts time series comparing the hourly regional maximum of all monitoring stations within the MCMA for the NoDA_chem (blue), D02_DFLT (green) and D02_GLOB (red) experiments.

With respect to O_3 , hourly maximum estimations for both D02_GLOB and D02_DFLT were closer to the peak observed values compared to the control experiment without data assimilation. Similar to the hourly average concentration time series, assimilating chemical observations improved the modeled ozone during the late evening and early morning hours. Regarding CO , these results showed a slight improvement in early hours and also at the estimation of the lowest maximum values, but modeled concentrations didn't reach the peak value on April 1st 12:00 UTC, April 2nd 12:00 UTC and April 3rd 00:00 UTC cycles. As

Table 2. Statistical metrics using hourly regional average concentrations for NoDA_chem, D02_DFLT and D02_GLOB experiments.

		NoDA_chem	D02_DFLT	D02_GLOB
O ₃	d	0.83	0.92	0.85
	RMSE	10.72	5.92	10.35
	Pearson	0.99	0.99	0.98
CO	d	0.71	0.58	0.55
	RMSE	0.13	0.14	0.14
	Pearson	0.74	0.64	0.73
NO ₂	d	0.28	0.38	0.38
	RMSE	9.00	8.25	8.21
	Pearson	0.96	0.85	0.87
T	d	0.90	0.89	0.89
	RMSE	1.09	1.18	1.18
	Pearson	0.99	0.99	0.99
RH	d	0.92	0.87	0.87
	RMSE	2.71	4.52	4.54
	Pearson	0.99	0.99	0.99
U	d	-0.18	-0.33	-0.33
	RMSE	1.36	1.60	1.61
	Pearson	-0.66	-0.89	-0.89
V	d	-0.09	-0.21	-0.21
	RMSE	1.58	1.63	1.63
	Pearson	-0.27	0.23	0.22

**Figure 11.** Time series of O₃, CO and NO₂ comparing observed (dots) and modeled hourly regional maximum concentrations for the NoDA_chem (blue), D02_GLOB (green) and D02_DFLT (red) experiments.

for NO₂, even though the assimilation process improved model concentrations during the first 14 hours of March 31st and during the April 1st 06:00 UTC cycle, the model showed a tendency to underestimate the concentrations of this pollutant after several cycles. As previously mentioned, the assimilation of more meteorological variables could help improve model performance because of the impact that meteorology has on the transport of pollutants.

Table 3 illustrates the statistical metrics estimated using the hourly regional maximum values. It shows that the model performance improves significantly when estimating ozone maximum concentration, particularly in the D02_GLOB experiment. For CO and NO₂, however, no improvements were observed in pollutant concentrations estimation. Regarding meteorology, the model's performance shows significant enhancement compared to the statistical metrics calculated using the regional hourly average (Table 2).

These results suggest that using the initial and boundary conditions from a global model was more effective for estimating regional maximum ozone concentrations during the day. However, the modeled peak ozone concentrations were very similar when using global and default initial conditions.

Furthermore, additional research on the impact of using different tuning parameters (horizontal and vertical scaling) for the background error covariance matrix (**B**) is required. In this sense, future investigations will discuss the impact of estimating

B using 24-48 hours forecasts valid at the same time instead of 12-24 hours and the effect of employing a longer period for its calculation (for example, several months). This will allow us to increase our understanding about the specific conditions under which a static background error covariance matrix could lead to an improved assimilation quality and therefore model performance.

4. Conclusions

This work presents one of the first efforts to improve the estimation of pollutant concentrations using chemical data assimilation in México. We analyzed the sensitivity of the WRF-DA-Chem assimilation system to different initial and boundary conditions when surface observations were assimilated.

The observation minus analysis (OMA) and observation minus background (OMB) statistics showed differences between the data assimilation (DA) experiments. For example, root mean square error (RMSE) decreased for ozone in both DA experiments and was slightly higher for the global chemical conditions (D02_GLOB case). For carbon monoxide (CO) and nitrogen dioxide (NO₂), OMB RMSE decreased in some cycles when the observations were assimilated in both DA experiments but remained similar in others. This may be related to an insufficiently accurate representation of meteorological variables during these

Table 3. Statistical metrics using hourly regional maximum concentrations for NoDA_chem, D02_DFLT and D02_GLOB experiments.

		NoDA_chem	D02_DFLT	D02_GLOB
O ₃	d	0.73	0.84	0.90
	RMSE	20.24	12.32	8.20
	Pearson	0.96	0.98	0.98
CO	d	0.60	0.60	0.66
	RMSE	0.53	0.50	0.46
	Pearson	0.70	0.70	0.71
NO ₂	d	0.13	0.13	0.15
	RMSE	23.97	24.99	24.76
	Pearson	0.70	0.56	0.57
T	d	0.80	0.81	0.81
	RMSE	2.40	2.13	2.12
	Pearson	0.98	0.98	0.98
RH	d	0.88	0.72	0.72
	RMSE	6.78	15.18	15.19
	Pearson	0.97	0.97	0.97
U	d	0.42	0.48	0.47
	RMSE	1.62	1.36	1.36
	Pearson	0.17	0.59	0.59
V	d	0.56	0.79	0.78
	RMSE	1.21	0.61	0.62
	Pearson	0.64	0.91	0.91

cycles, since the reduced impact observed in these experiments may be related to an insufficiently accurate representation of meteorological variables during the assimilation cycles, because no clear sensitivity to boundary conditions was identified. Although meteorological initial conditions can be improved with data assimilation, uncertainties in key processes, in particular wind fields and planetary boundary layer height, might determine the improvement of chemical forecasts, and systematic errors that affect chemical transport and reactive processes might not be fully reduced (Cho *et al.*, 2025; Zhang *et al.*, 2012).

Regarding the average increments, their magnitudes exceeded 5 ppb for O₃, 15 ppb for NO₂ and over 0.3 ppm for CO. However, the absence of a clear reflection of the analysis increments in modeled concentrations at 00:00 UTC is consistent with known limitations of data assimilation in coupled meteorology–chemistry models based on 3DVAR, where the analysis increments are applied only at the initial assimilation time and are heavily dependent on the prescribed background error covariance matrix, since if the length scales are not adequately representing the true error structures of meteorological variables relevant for chemical transport, the resulting increments might be not enough to modify the large-scale flow patterns that impact pollutants transport and their spatial distribution (Descombes *et al.*, 2015). Therefore, at 00:00 UTC (immediately after the analysis), the model might need an additional integration time for the meteorological increments to have an effect on chemical composition. This has been reported in previous studies using this data assimilation system, where the impact of data assimilation on chemical fields is more evident at short forecast lead times rather than at the initial assimilation time (Ha, 2022).

With respect to model evaluation, the performance in estimating ozone concentration improved in both assimilation experiments compared to the case without data assimilation in terms of the statistical metrics. For CO and NO₂, assimilation experiments generally missed observed values during peak concentration hours, though improvements were seen in early assimilation cycles compared to the control case. Differences between D02_DFLT and D02_GLOB experiments for these pollutants were minor, likely due to the need of additional tuning of the background error covariance matrix assimilation parameters (variance, length scale, among others). Furthermore, the assimilation of meteorological variables in the inner domain could enhance model performance for chemical species by improving meteorological fields in MCMA.

The results also suggested that using global model outputs as initial and boundary conditions for the larger domain led to a small increase in hourly regional average ozone concentrations and tended to perform best for estimating hourly regional maximum concentrations. However, in terms of daily peak

ozone values, there was no clear difference of using a global model over using a default profile for boundary conditions. This is important, because computational resources costs for both storage and processing may be reduced and optimized if solving the chemistry only at the regional level. Thus, a workflow of solving first the meteorology at the synoptic scale and then solving the chemistry at the regional level might be better for optimizing limited resources. In this regard, a longer cycled experiment using the default chemical conditions can result in more frequent initializations and thus in an improved and spun up chemical conditions.

Statistical metrics for meteorological fields show minor changes between the DA experiments and the control case. This indicates that the control run is already providing a reasonable representation of the atmospheric state, and that data assimilation is resulting more in fine adjustments to the initial conditions rather than large corrections, which may not be captured by aggregated metrics such as RMSE or correlation (Zou, 2025). Thus, these small changes in meteorological metrics are suggesting a more localized correction to the atmospheric state by the assimilation process.

Future work will address surface-level meteorological data assimilation using observations that are not included in the global meteorological data set, as well as the tuning of the assimilations system parameters associated with background error with the aim of constructing tools to support stakeholders during pollution episodes in the MCMA.

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Euler-Poincaré Characteristic and Invasion Percolation for Critical Radius Determination: A Systematic Comparison in Synthetic Porous Structures

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Abstract

Critical radius (R_c) determination in porous media is essential for permeability estimation through analytical models. This study presents the first systematic comparison of the Euler-Poincaré Characteristic (EPC) method and queue-based Invasion Percolation (QBIP) algorithm using four synthetic porous structures (SPS) with controlled geometry and topology to determine R_c . QBIP demonstrated universal applicability, determining $R_c = 0.09–0.15 \mu\text{m}$ across all SPS. EPC required negative initial connectivity for its application; positive values prevented zero-crossing identification, and while the derivative criterion detected pore size distribution (PSD) transitions, these do not correspond to percolation thresholds in disconnected structures. Deviations from design modal radii ranged from 0–70% for EPC and 6.7–50% for QBIP; no single criterion was uniformly superior. Despite morphological operations altering the initial PSD to accomplish the target porosity in SPS generation, both methods identified R_c within the same order of magnitude as the design modes (0.10–0.15 μm). These findings demonstrate that EPC and QBIP provide complementary insights: EPC reveals topological transitions while QBIP captures invasion physics, enabling geometric, topological, and capillary characterization of porous media. This dual-method approach provides quantitative criteria for the selection of the method based on sample connectivity and enables cross-validation to reduce uncertainty in R_c determination for use in analytical permeability models.

Key words: Permeability, Critical radius, Invasion Percolation, Euler-Poincaré Characteristic, Digital Rock Physics.

Resumen

La determinación del radio crítico (R_c) en medios porosos es esencial para la estimación de permeabilidad mediante modelos analíticos. Este estudio presenta la primera comparación sistemática del método de la Característica de Euler-Poincaré (EPC) y el algoritmo de Percolación por Invasión basado en cola de prioridad (QBIP) utilizando cuatro estructuras porosas sintéticas (SPS) con geometría y topología controladas para determinar R_c . QBIP demostró aplicabilidad universal, determinando $R_c = 0.09–0.15 \mu\text{m}$ en todas las SPS. EPC requirió conectividad inicial negativa para su aplicación; valores positivos impidieron la identificación del cruce por cero, y aunque el criterio de derivada detectó transiciones en la distribución de tamaño de poro (PSD), estas no corresponden a umbrales de percolación en estructuras desconectadas. Las desviaciones respecto a las modas de diseño variaron entre 0–70% para EPC y 6.7–50% para QBIP; ningún criterio fue uniformemente superior. A pesar de que las operaciones morfológicas alteraron la PSD inicial para lograr la porosidad objetivo en la generación de SPS, ambos métodos identificaron R_c dentro del mismo orden de magnitud que las modas de diseño (0.10–0.15 μm). Estos hallazgos demuestran que EPC y QBIP proporcionan perspectivas complementarias: EPC revela transiciones topológicas mientras QBIP captura la física de invasión, permitiendo la caracterización geométrica, topológica y capilar de medios porosos. Este enfoque dual proporciona criterios cuantitativos para la selección del método basados en la conectividad de la muestra y permite la validación cruzada para reducir la incertidumbre en la determinación de R_c para su uso en modelos analíticos de permeabilidad.

Palabras clave: Permeabilidad, Radio crítico, Percolación por Invasión, Característica de Euler-Poincaré, Física de Roca Digital.

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1. Introduction

The study of porous media is relevant for many industrial applications, particularly oil and gas extraction. Reservoir management requires accurate characterization of rock properties for optimal drainage point selection, production rate optimization, completion and perforation design, and enhanced oil recovery strategies (Ahmed *et al.*, 1991). One intrinsic property that controls fluid flow through reservoir rocks is absolute permeability (hereafter referred to as permeability). This property can be expressed through the scaling relation (Bernabé *et al.*, 2010):

$$k = Hl^2, \quad (1)$$

where H is a connectivity factor that depends on the microstructural characteristics of the medium, e.g., porosity, fractal dimensions, tortuosity (Ghanbarian *et al.*, 2013), coordination number (Z), and formulations derived from various theoretical frameworks (Bernabé *et al.*, 2010; Rezaee *et al.*, 2012; Li *et al.*, 2016; Daigle, 2016; Bernabé *et al.*, 2016), and l is a characteristic length. Permeability k has units of m^2 (SI) or millidarcys (md) in petroleum engineering applications. In percolation theory, critical path analysis (Katz & Thompson, 1986, 1987; Hunt, 2001) establishes that pore throats control macroscopic flow, with conductances exceeding a critical threshold. In this context, l corresponds to the critical radius (R_c), defined as the representative pore-throat radius at the percolation threshold—when continuous fluid pathways first connect opposite faces of the porous medium.

When direct permeability measurements such as well tests or permeameter analyses (Spivey & Lee, 2013; McPhee *et al.*, 2015) are not available, Eq. 1 provides an alternative for its estimation. Determining both H and l becomes essential. While establishing H is beyond the scope of this study, multiple studies have successfully used R_c as the characteristic length l in this framework (Bernabé, 1995; Arns *et al.*, 2005; Daigle, 2016; Robins *et al.*, 2016; Nishiyama & Yokoyama, 2017; Zhao, 2019). Experimentally, R_c can be estimated through mercury intrusion capillary porosimetry (MICP) (Katz & Thompson, 1986; Amann-Hildenbrand *et al.*, 2013; Franco-Villegas *et al.*, 2025) or gas breakthrough experiments such as the water expulsion method (WEM) (Hildenbrand *et al.*, 2002; Nishiyama & Yokoyama, 2017). However, experimental methods present limitations, including sample alteration, extended equilibration times, and lack of three-dimensional (3D) spatial information (León y León, 1998; Amann-Hildenbrand *et al.*, 2013; Rashid *et al.*, 2015). These challenges motivate the development of computational approaches for determining R_c from digital images of rocks.

The Digital Rock Physics (DRP) paradigm utilizes rock images to simulate physical processes (Andrä *et al.*, 2013a, 2013b; Blunt *et al.*, 2013; Kelly *et al.*, 2015). Although DRP allows estimation of permeability (Kelly *et al.*, 2015; Aguilar-Madera *et al.*, 2020) using numerical approaches to solve Navier-Stokes equations (Narsilio *et al.*, 2009; Mostaghimi *et al.*, 2013; Guibert *et al.*, 2016; Verri *et al.*, 2017), or Lattice Boltzmann (Kelly *et al.*, 2015; Bultreys *et al.*, 2016; Santos *et al.*, 2022), the use of computational resources is extensive, depending on the porous space computational domain, limiting its applicability (Mostaghimi *et al.*, 2013; Blunt *et al.*, 2013; Bultreys *et al.*, 2016).

Within this paradigm, two computational methods have emerged as alternatives for R_c determination from 3D images. The first approach is rooted in the Minkowski functionals framework, which provides a set of morphological measures to quantify pore structure (Vogel *et al.*, 2010). Among these functionals, the Euler-Poincaré Characteristic (hereafter referred to as EPC) quantifies connectivity changes through topological analysis (Vogel, 1997; Vogel, 2002; Zhao, 2019; Armstrong *et al.*, 2019). Chaniot *et al.* (2022) extended this approach to quantify morphological accessibility on stochastic models using the full set of Minkowski functionals. The second approach employs invasion percolation algorithms that simulate fluid displacement processes (Hilpert & Miller, 2001; Gostick *et al.*, 2022). This study implements the Image-Based Invasion Percolation (IBIP) algorithm using the priority-queue-based variant (QBIP) (Gostick *et al.*, 2024), selected for its computational efficiency and open-source implementation in the PoreSpy package (Gostick *et al.*, 2019). Despite the application of both methods, no systematic comparison has been conducted to establish their relative performance, operational limits, and convergence conditions for R_c estimation.

Part of DRP is the Digital Rock Modeling (DRM) discipline for generating computational representations of rocks (Roth *et al.*, 2011). Methods include process-based approaches simulating geological processes (Zhu *et al.*, 2012; Luo *et al.*, 2020), multiple-point statistics (Okabe & Blunt, 2005), and machine learning techniques (Mosser *et al.*, 2017). However, for method validation, realistic reconstruction introduces complexity and uncertainty. When evaluating EPC and QBIP capabilities, the requirement is not geological realism but precise control of microstructure (Zhu *et al.*, 2012). Synthetic Porous Structures (SPS) provide this control, serving as phantoms with deliberately designed geometries and known properties (Kaczmarek *et al.*, 2017; Goral & Deo, 2020). This established validation approach (Jiang *et al.*, 2013; Jivkov *et al.*, 2013; Raeini *et al.*, 2017; Armstrong *et al.*, 2019) enables systematic parameter variation while maintaining ground truth. To allow comparison between EPC and QBIP, four SPS were designed from a bundle of parallel capillaries to

degree-constrained networks, preserving full 3D morphological complexity at voxel resolution for direct image-based analysis. Figure 1 summarizes the relationships between these approaches.

This study provides a controlled comparison between topological (EPC) and invasion-based (QBIP) approaches for R_c determination, identifying the conditions under which each method is applicable. The specific objectives are: (i) to quantify the agreement between EPC and QBIP methods across four SPS with varying topology, and (ii) to evaluate whether one EPC criterion (zero-crossing or derivative) shows consistently better agreement with invasion percolation results.

This article is organized as follows: Section 2 presents the theoretical foundations of percolation theory and the mathematical basis for both computational methods. Section 3 describes the SPS generation and the implementation details of EPC and QBIP algorithms. Section 4 presents the comparative results and discussion. Section 5 summarizes the conclusions and future research directions.

2. Theoretical framework

2.1. Geometric and topological measures of porous media

Porous media structure can be characterized through two complementary perspectives: geometric measures that quantify size and shape, and topological measures that characterize connectivity.

One of the representations of an interconnected porous medium consists of pore bodies connected by pore throats. Pore

bodies (hereafter pores) provide storage capacity, while pore throats control fluid flow. Characterization of the pore network requires both geometric and topological measures.

2.1.1. Geometric characterization: size distributions

The irregular morphology of pores and pore-throats in porous materials can be quantitatively described through size distributions that provide statistical descriptors of their characteristic dimensions. The pore size distribution (PSD) is defined as the probability density of the pore radii within a given volume of porous medium, capturing the spatial variability of the void space responsible for fluid storage (Patmonoaji *et al.*, 2020). In contrast, the pore-throat size distribution (PTSD) represents the statistical distribution of the narrow constrictions that connect adjacent pores, which governs pore connectivity and fluid flow across the network (Nelson, 2009; Xu *et al.*, 2019). These constrictions typically act as flow-limiting elements, exerting control on percolation thresholds and the continuity of fluid pathways. Together, PSD and PTSD provide a geometric framework that links pore-scale morphology to permeability (Vogel, 2002). Figure 2 illustrates the distinction and complementarity between PSD and PTSD.

To translate these geometric concepts into measurable quantities, various experimental and computational techniques have been developed. Among them, MICP remains one of the most widely used methods for estimating PTSD (Hou *et al.*, 2025; Quan *et al.*, 2025; Zhang *et al.*, 2025). MICP produces PTSD through the relationship between invasion pressure and pore-throat radius (Giesche, 2006), providing valuable information

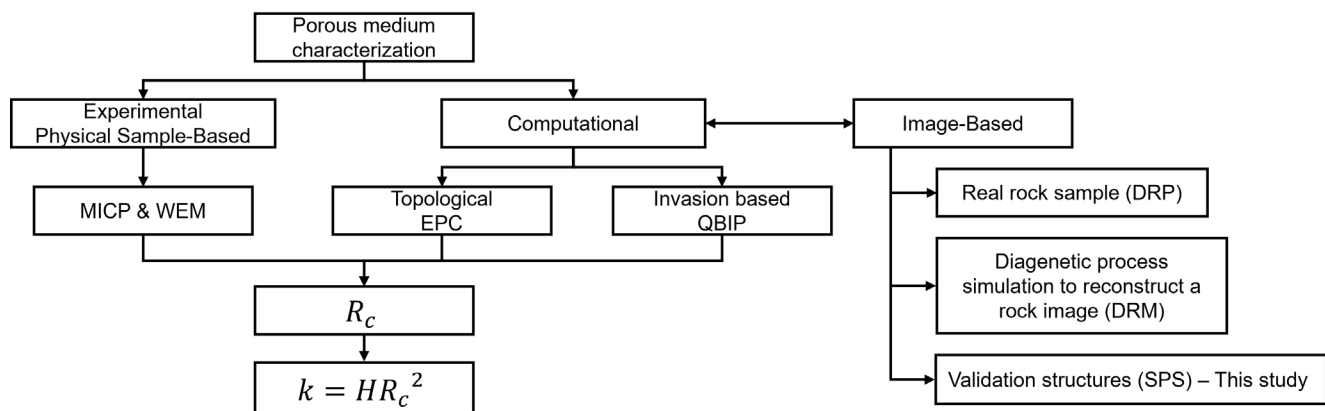


Figure 1. Conceptual framework for R_c determination in porous media. Two characterization approaches: experimental methods (MICP, WEM) operating on physical samples, and computational methods (EPC, QBIP) operating on 3D binary images. Within the Digital Rock Physics (DRP) paradigm, these images are obtained from real rocks or generated through Digital Rock Modeling (DRM). Synthetic Porous Structures (SPS), used in this study, provide controlled geometry for method validation. The characteristic length l in the permeability model $k = Hl^2$ corresponds to the critical radius R_c .

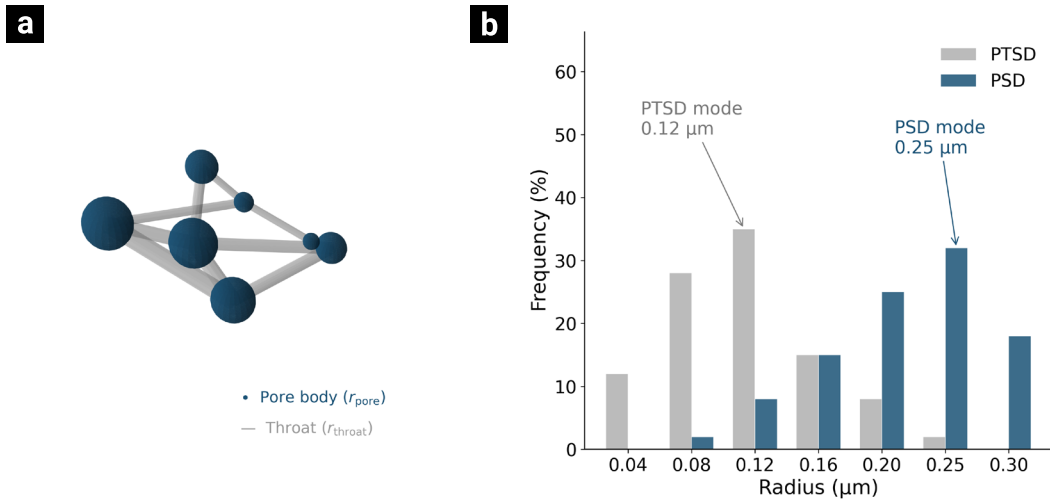


Figure 2. Schematic representation of PSD and PTSD in an interconnected porous medium. Pore radii define the PSD, while the narrow constrictions connecting adjacent pores define the PTSD.

on the pore-throat size distribution, entry pressure threshold, and cumulative porosity. PTSD is particularly relevant for determining the characteristic length scale l in permeability models, where pore-throat radii constrain permeability.

Alternatively, nuclear magnetic resonance (NMR) provides non-invasive estimations of pore size distribution (PSD) based on the relaxation times of hydrogen nuclei within saturated pore spaces, which correlate with pore radii (Arns, 2004; Zhang *et al.*, 2016; Morales-Chávez *et al.*, 2025). While NMR does not directly image pore-throat geometry, advanced interpretation of relaxation data can provide indirect insight into pore-throat connectivity, particularly in systems with complex pore structures (Ghomeshi *et al.*, 2018; Zheng *et al.*, 2018; Huang *et al.*, 2020).

Conversely, X-ray micro-computed tomography (micro-CT), with spatial resolution typically in the micrometer range, when combined with segmentation algorithms (e.g., watershed or deep learning), enables direct 3D reconstruction of porous networks. This allows extraction of both PSD and PTSD by identifying individual pores and their connecting pore-throats (Patmonoaji *et al.*, 2020; Guo *et al.*, 2024; Hou *et al.*, 2025). These image-derived pore networks can subsequently be used in pore network models to simulate flow, thereby linking microscopic geometry to macroscopic permeability (Raeini *et al.*, 2017; Ma *et al.*, 2025).

2.1.2. Topological characterization

The topology quantifies the way the pores and the pore throats are connected (Sahimi, 2011). For this study, two topological descriptors are particularly relevant, the Z and the Betti numbers.

Z quantifies the average number of pore throats connected to each pore (Rabbani *et al.*, 2016). Higher Z values indicate greater

connectivity and enhanced permeability (Bernabé *et al.*, 2010). This parameter is relevant for generating SPS.

The Betti numbers quantify topological features in different dimensions on the global scale. For 3D porous media, the first three Betti numbers suffice to characterize connectivity (Sahimi, 2011; Robins *et al.*, 2016). These combine to form the Euler-Poincaré Characteristic (χ), which quantifies overall network connectivity through:

$$\chi = \beta_0 - \beta_1 + \beta_2, \quad (2)$$

where β_0 is the number of connected components, β_1 is the number of independent loops, and β_2 is the number of enclosed cavities (Vogel *et al.*, 2010). For porous media, $\chi < 0$ indicates multiply-connected structures with redundant pathways, $\chi = 0$ represents marginal connectivity, and $\chi > 0$ means disconnected or simply-connected structures.

2.2. Invasion percolation

Invasion percolation describes a dynamic process fundamentally different from ordinary percolation (Wilkinson & Willemsen, 1983). While ordinary percolation theory considers static accessibility, where all pores with radius $r > r_{threshold}$ become simultaneously available (pressure or size-controlled process)—invasion percolation models a sequential displacement process between defending and invading fluids (volume or rate-controlled invasion) (Gostick *et al.*, 2022).

In this representation, pores and pore throats initially contain defending fluid (Knackstedt & Paterson, 2009). When injection occurs at infinitesimal flow rates where capillary forces dominate

viscous effects, the dynamics follow local pore-throat dimensions. During drainage—the displacement of wetting by non-wetting phases—capillary resistance concentrates at the narrowest constrictions: the pore throats. The displacement therefore proceeds through discrete jumps across the pore throats, with the non-wetting phase advancing through the largest available opening that offers the least resistance (Knackstedt & Paterson, 2009).

This mechanism produces self-organized invasion patterns distinct from random percolation (Wilkinson & Willemsen, 1983), naturally identifying the flow pathways that control network connectivity.

Invasion percolation and image-based porosimetry via morphological opening both approximate quasi-static drainage, representing volume-controlled and pressure-controlled protocols, respectively (Hilpert & Miller, 2001; Gostick *et al.*, 2024). The relationship between capillary pressure P_c (Pa) and pore-throat radius r (m) follows the Young-Laplace equation (Washburn, 1921):

$$P_c = \frac{2\gamma \cos \theta}{r}, \quad (3)$$

where γ is the interfacial tension (N/m) and θ is the contact angle (degrees). For practical reporting, capillary pressures were converted to psi (1 psi = 6,895 Pa) and pore-throat radii are expressed in micrometers (μm) throughout this study.

2.3. Critical radius determination

Experimentally, R_c can be determined by multiple approaches. In MICP tests, R_c corresponds to the inflection point of the invasion curve, identified as the maximum of $dS/d\log(r)$, which represents the modal radius of the PTSD (Katz & Thompson, 1986; Comisky *et al.*, 2007; Amann-Hildenbrand *et al.*, 2013; Franco-Villegas *et al.*, 2025). This modal radius indicates the pore-throat radius class that contributes most significantly to mercury saturation when percolation occurs. Similarly, the WEM provides direct observation of the percolation threshold: R_c is

determined when the first gas bubble emerges at the opposite face of the sample, with the corresponding pressure converted to radius via Eq. 3 (Nishiyama & Yokoyama, 2017).

These experimental observations reveal fundamental characteristics of R_c . First, its correspondence with the PTSD mode indicates that R_c represents the most abundant pore-throat radius in the PTSD capable of forming continuous pathways, not simply the largest throats, but those numerous enough to establish connectivity across the sample. If the PTSD differs from a nominal or design distribution (e.g., due to morphological modifications; see Section 3.1), the measured mode—and therefore R_c —shifts accordingly. Second, this modal behavior explains why R_c controls percolation: these throats offer minimal capillary resistance while being sufficiently abundant to connect two external and opposite faces. Once this critical pressure is exceeded, progressively smaller throats ($r < R_c$) become accessible, expanding the flowing fraction of the pore network and increasing permeability beyond the threshold value (Hildenbrand *et al.*, 2002).

3. Materials and methods

3.1. Synthetic porous structures

SPS with known properties are required to quantify and compare the performance of EPC and QBIP methodologies. Four 3D SPS were designed to evaluate both methods across different topological complexities, following the principle that these structures can serve as validation models for real rocks (Kaczmarek *et al.*, 2017).

All SPS were generated within cubic domains of $7.5 \times 7.5 \times 7.5 \mu\text{m}^3$ with voxel resolution of $0.05 \mu\text{m}$. Two pore size distributions were employed. MDC, HTN, and DCN share a trimodal PSD with diameters of $0.8 \mu\text{m}$ (10%), $0.4 \mu\text{m}$ (30%), and $0.2 \mu\text{m}$ (60%), yielding a design modal radius of $0.10 \mu\text{m}$. BPC uses a trimodal PSD with diameters of $0.5 \mu\text{m}$ (20%), $0.3 \mu\text{m}$ (50%), and $0.15 \mu\text{m}$ (30%), yielding a design modal radius of $0.15 \mu\text{m}$. Design radii in Table 1 reflect voxel discretization ($0.05 \mu\text{m}$

Table 1. Structural properties of each SPS.

SPS	Graph type	Design radii (μm)	Fractions (%)	Modal r (μm)	χ_0	$\frac{\phi_{\text{pre}} \phi_{\text{pos}}}{(\%)}$	Operation	
BPC	Forest (disconnected)	0.25/0.15/0.08	20/50/30	0.15	40	5.7	5.7	None
MDC	Connected grid	0.40/0.20/0.10	10/30/60	0.10	-15	3.4	5.9	1D (1 iter.)
HTN	MST with branches	0.40/0.20/0.10	10/30/60	0.10	-127	2.7	4.4	1D (1 iter.)
DCN	Degree-constrained	0.40/0.20/0.10	10/30/60	0.10	-216	3.7	6.7	1D (1 iter.)

resolution) μm . The term "pore size" encompasses both pores and pore throats, as generation algorithms typically do not discriminate between these features (Roth *et al.*, 2011).

After placement of pores and connecting structures, porosity fell below the target in MDC, HTN, and DCN (3.4%, 2.7%, and 3.7%, respectively). A single binary dilation (face-connected structuring element, 1 iteration) was applied to each, increasing porosity to 5.9%, 4.4%, and 6.7%. BPC required no morphological adjustment (final porosity 5.7%). The dilation added voxels at the periphery of existing pores without creating new pores or connections. The resulting porosities (4.4–6.7%) were selected as a representation of tight rock microstructures. Figure 3 shows the 3D pore structure before and after adjustment.

The four SPS represent a systematic progression in network connectivity (Figure 3): (a) Bundle of Parallel Capillaries (BPC)—non-intersecting cylindrical channels traversing the domain independently; (b) Multidirectional Channels (MDC)—orthogonal channels intersecting at the domain center with diagonal connections; (c) Hierarchical Tree Network (HTN)—network constructed via Prim's minimum spanning tree algorithm with branching; (d) Degree-Constrained Network (DCN)—network where each pore has a target coordination number (large: 4–6, medium: 3–4, small: 2–3). For graph-theoretic details, the reader is referred to Saha Ray, 2013. This progression from disconnected parallel structures ($\chi_0 = 40$) to highly connected networks ($\chi_0 = -216$) enables evaluation of how topology affects R_c determination.

3.2. Euclidean Distance Transform

The Euclidean Distance Transform (EDT) assigns to each pore voxel the minimum distance to the nearest solid boundary:

$$d(p) = \min_{s \in S} \|p - s\|, \quad (4)$$

where p represents a pore voxel position, S is the set of all solid voxels, and $\|\cdot\|$ denotes the Euclidean norm. This transform provides the inscribed sphere radius at each voxel (Hilpert & Miller, 2001) defining the range of pore radii used by both the EPC morphological opening loop (Section 3.3) and the QBIP invasion algorithm (Section 3.4).

3.3. EPC implementation

In 3D digital images, the EPC is computed using the Euler formula (Vogel *et al.*, 2010):

$$\chi = n_{\text{vertices}} - n_{\text{edges}} + n_{\text{faces}} - n_{\text{volumes}}, \quad (5)$$

where the n symbol denotes 'number of'. For binary pore space images, each $2 \times 2 \times 2$ voxel neighborhood contributes to the global χ value based on its specific configuration of pore and solid voxels. Eq. 5 provides the computational form of Eq. 2 for voxelized images.

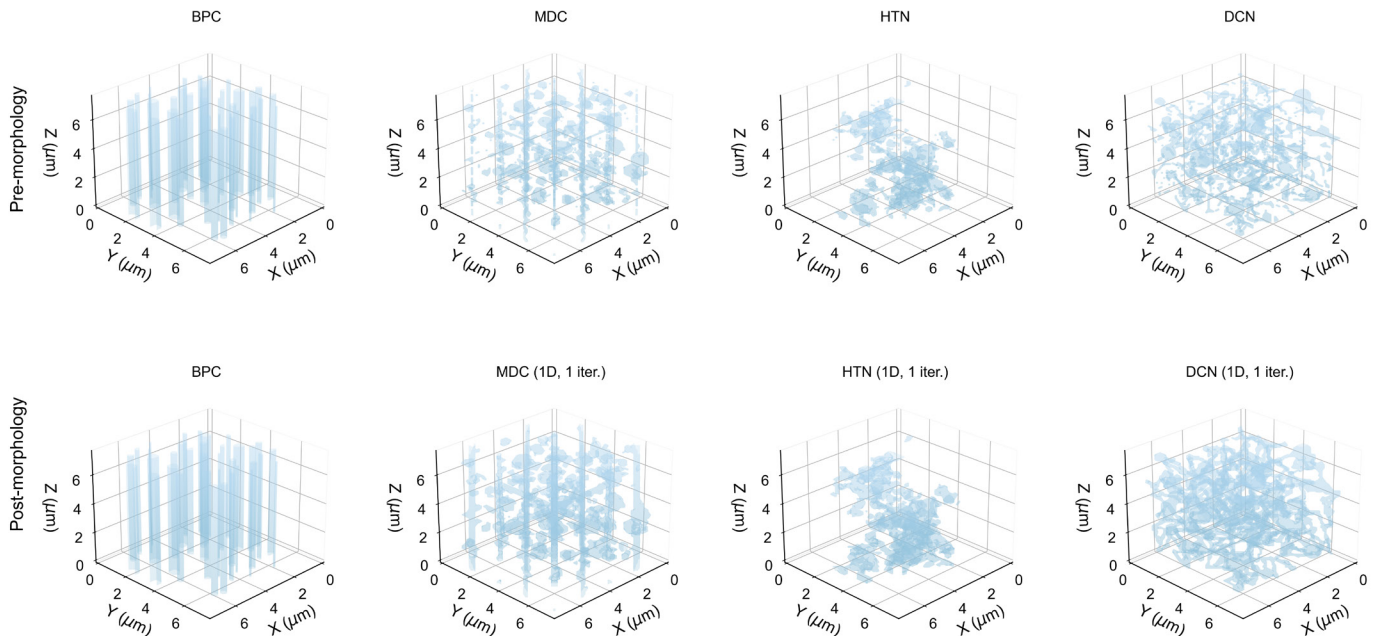


Figure 3. 3D visualization of the four SPS before (top) and after (bottom) morphological adjustment. (a) BPC, (b) MDC, (c) HTN, (d) DCN.

The implementation used in this study computes χ using the scikit-image library (van der Walt *et al.*, 2014). This topological measure proves particularly valuable when tracked as a function of pore radius, as discussed in the following section.

3.3.1. Connectivity function

The connectivity function $\chi(r)$ measures the Euler-Poincaré Characteristic as a function of pore radius. The approach was originally proposed by Vogel (1997) for serial sections of soils and formalized in Vogel (2002): a morphological opening with a spherical structuring element of radius r is applied to the pore space, and Eq. 5 is evaluated on the resulting opened domain $P(r)$ at each radius, yielding $\chi(r)$.

The implementation employs morphological opening, defined as erosion followed by dilation with a spherical structuring element $B(r)$ of radius r :

$$P(r) = (P \ominus B(r)) \oplus B(r), \quad (6)$$

where $\ominus$ denotes erosion and $\oplus$ denotes dilation. This operation removes all pore regions narrower than $2r$ —constrictions that cannot accommodate a sphere of radius r —while restoring the original dimensions of wider regions (Vogel, 1997; Vogel *et al.*, 2010).

The $\chi(r)$ curve is computed by applying Eq. 6 at n radii uniformly distributed between 0 and r_{max} , evaluating χ (Eq. 5) on each opened domain $P(r)$. Figure 4 summarizes this workflow.

3.3.2. Critical radius identification criteria

The determination of R_c from connectivity functions requires robust criteria that can handle diverse structures. This section presents two complementary criteria applied to SPS.

Zero-crossing criterion: The primary criterion defines R_c as the point where the connectivity function crosses zero (Vogel *et al.*, 2010; Zhao, 2019):

$$R_c^{zero} = \{r : \chi(r) = 0\} \quad (7)$$

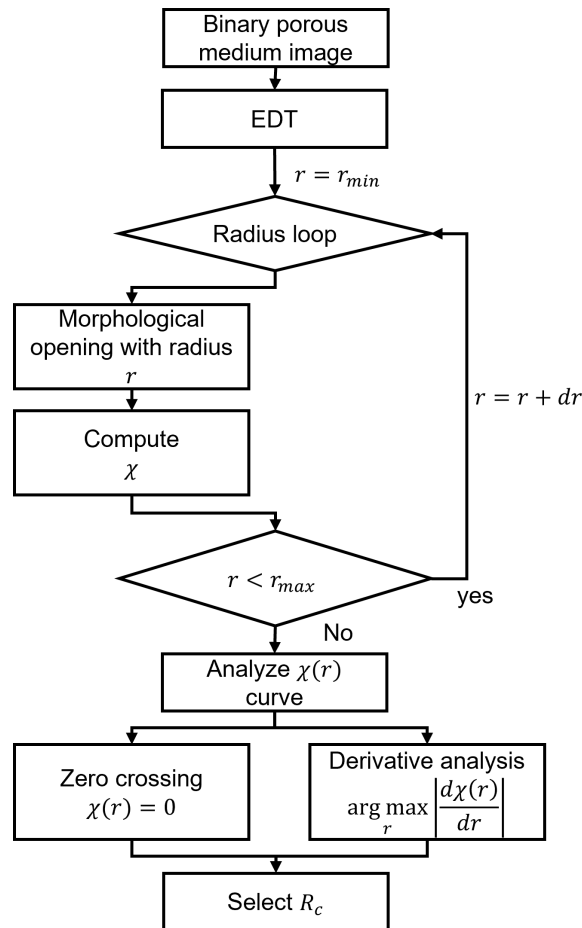


Figure 4. Workflow for R_c determination using the EPC. The algorithm iteratively applies morphological opening operations at increasing radii to compute the connectivity function $\chi(r)$. Two complementary criteria—zero-crossing and derivative criterion—are evaluated to identify the R_c .

This zero-crossing point is invariant under volume normalization, yielding identical R_c values for both $\chi(r)$ and $\chi_v(r) = \chi(r)/V_{sample}$.

However, this criterion has a limitation: in low-porosity media ($\phi < 10\%$), the pore network may become fragmented, causing χ_v to remain positive throughout the entire radius range. This behavior was observed in Eagle Ford shale samples where $\chi \approx 9400$, indicating poor connectivity even at the smallest radii (Davudov *et al.*, 2020).

Derivative criterion: Analogous to the inflection point analysis in MICP (Amann-Hildenbrand *et al.*, 2013; Franco-Villegas *et al.*, 2025), the derivative of the connectivity function identifies the radius of most rapid topological transition. R_c is determined as:

$$R_c^{\text{deriv}} = \arg \max_r \left| \frac{d\chi(r)}{dr} \right|, \quad (8)$$

where the maximum absolute value captures the steepest transition regardless of sign.

3.4. QBIP algorithm implementation

QBIP simulates quasi-static drainage by computationally replicating capillary-controlled displacement in segmented 3D porous media. The algorithm leverages EDT to characterize pore

space morphology (Hilpert & Miller, 2001), advancing the invasion interface through the pore-throat with minimum capillary entry pressure at each step. Implementation was performed in Python using the PoreSpy package (Gostick *et al.*, 2019).

The algorithm implements volume-controlled invasion by incrementally filling fixed volumes (Gostick *et al.*, 2022). Figure 5 illustrates the core invasion loop. This study adopts water-air interface properties: interfacial tension $\gamma = 0.078$ N/m and contact angle $\theta = 180^\circ$ (non-wetting), enabling direct comparison with experimental drainage curves.

3.4.1. Capillary pressure curve reconstruction

The non-wetting phase saturation (S) is defined as the fraction of connected pore volume (V_{pore}) occupied by the invading fluid. For each invasion step i , the saturation increment is:

$$\Delta S_i = \frac{(V_i - V_{i-1})}{V_{pore}} * 100\% \quad (9)$$

where V_i is the cumulative invaded volume (in voxels) at step i . The pore-throat radius r_i at each step is obtained from the EDT value at the newly invaded voxels.

The invasion sequence yields two representations. The volume-controlled curve (Figure 6a) plots S versus r in invasion

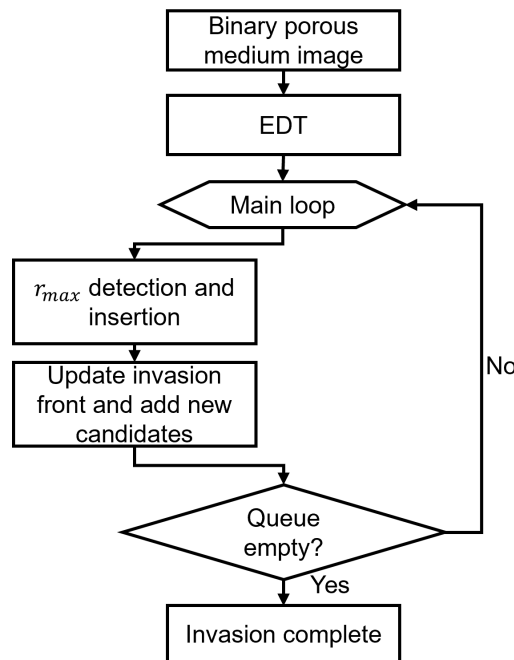


Figure 5. Core invasion loop of the QBIP algorithm. Starting from a binary image and its EDT, the algorithm iteratively selects r_{max} at the invasion front and inserts spheres at these locations. The candidate queue is updated through morphological dilation until it is empty, generating the complete invasion sequence.

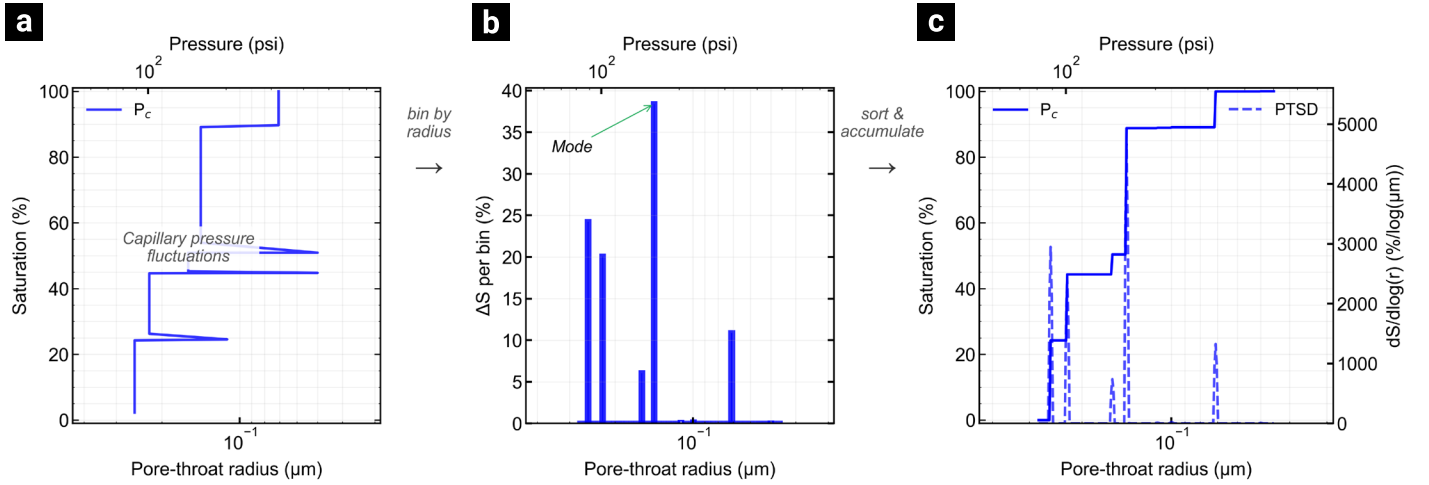


Figure 6. QBIP post-processing pipeline illustrated with BPC data. (a) Volume-controlled invasion curve showing capillary pressure fluctuations at pore-throat breakthroughs. (b) Invasion events grouped into logarithmic bins by EDT-based radius. (c) Pressure-controlled reconstruction: cumulative saturation $S(r)$ with PTSD.

order, displaying capillary pressure fluctuations as the fluid traverses pore-throat constrictions and fills pores. The pressure-controlled reconstruction proceeds in two stages: first, invasion events are grouped into logarithmic bins by EDT-based radius, yielding the saturation contribution per radius class (Figure 6b); then, the bins are sorted from largest to smallest radius and their contributions are accumulated via:

$$S(r) = \sum_{r_i \geq r} \Delta S_i \times 100\%, \quad (10)$$

producing the stepped $S(r)$ curve and its derivative $dS/d\log(r)$, analogous to pressure-based intrusion experiments (Figure 6c).

3.4.2. Characteristic radii

The reconstructed capillary pressure curve and the binned saturation data enable R_c identification through two approaches: direct modal analysis of binned saturation data and derivative analysis of the reconstructed capillary pressure curve. Unlike EPC's topological analysis, QBIP tracks the evolution of fluid distribution during invasion.

Critical Radius: The percolation threshold corresponds to the PTSD maximum (Amann-Hildenbrand *et al.*, 2013):

$$R_c = \arg \max_r \left(\frac{dS}{d\log(r)} \right), \quad (11)$$

Modal contribution method: The modal method identifies

R_c as the radius class with maximum saturation contribution:

$$R_c^{modal} = \arg \max_r \sum_{i \in \text{bin}(r)} \Delta S_i, \quad (12)$$

Apex Radius: Following Pittman's graphical method, the apex radius (R_{apex}) represents the threshold for continuous flow path formation (Pittman, 1992).

Weighted Geometric Mean Radius: This radius (R_{WGM}) captures the contribution of the entire pore-throat spectrum, particularly relevant for tight lithologies where pore-throat radii are dimensionally similar (Dastidar *et al.*, 2007). Figure 7 represents the workflow for QBIP implementation used in this study.

4. Results and discussion

The four SPS were analyzed using both EPC analysis and QBIP invasion simulation to determine R_c values and method convergence conditions.

4.1. Bundle of parallel capillaries

The BPC structure contained parallel capillaries without lateral connections.

Figure 8 shows the opening process and the connectivity function $\chi(r)$, which decreased from 40 to 8 in discrete steps. Transitions at $r = 0.08$ and $0.16 \mu\text{m}$ corresponded to removal of small and medium capillaries. The derivative criterion yielded $R_c = 0.17 \mu\text{m}$, corresponding to the PSD mode; however,

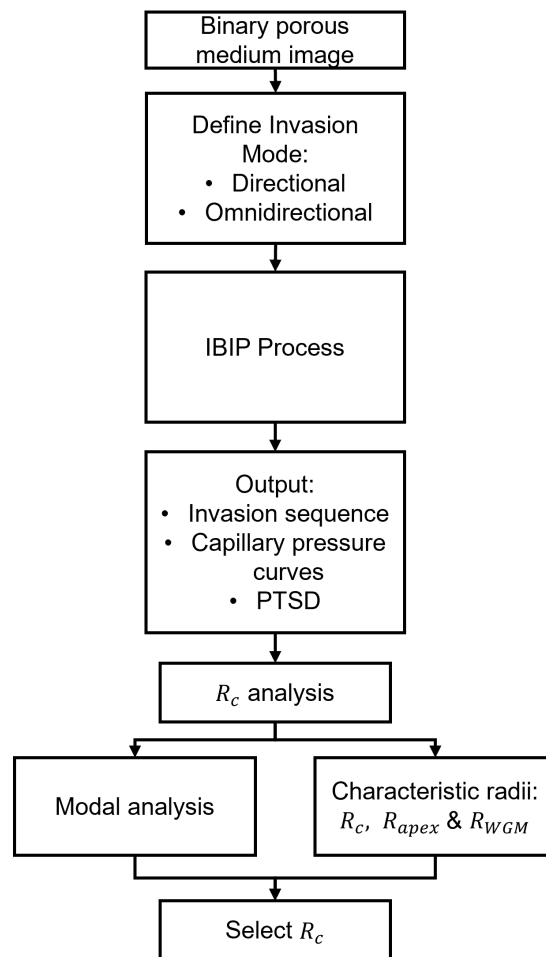


Figure 7. Methodological framework for critical radius determination using QBIP. The algorithm operates in directional mode (invasion from a specified boundary), generating the invasion sequence and enabling reconstruction of the capillary pressure curve. Analysis proceeds through two paths: direct modal analysis of binned data and derivative analysis of the reconstructed curve, both converging to R_c while the latter additionally yields R_{apex} and R_{WGM} .

without lateral connections and with all remaining capillaries providing independent flow paths, no unique percolation threshold exists.

QBIP analysis determined R_c despite the disconnected structure (Figure 9). Invasion proceeded by capillary radius (Figure 9a). Volume-controlled invasion (Figure 9c) showed three plateaus corresponding to the three capillary radius classes. Pressure-controlled analysis (Figure 9d) showed entry events at radii of 0.08, 0.15, and 0.25 μm . Both modal and apex methods yielded $R_c = 0.14 \mu\text{m}$; $R_{WGM} = 0.17 \mu\text{m}$.

Method comparison for BPC is asymmetric: EPC cannot determine a percolation threshold because $\chi_0 = 40$ (positive) prevents zero-crossing identification. The derivative criterion returned 0.17 μm , which exceeded the design modal radius (0.15 μm) by 13.3%. QBIP determined $R_c = 0.14 \mu\text{m}$, 6.7% below it (0.15 μm).

The 0.03 μm difference between the EPC derivative and QBIP does not represent disagreement on the percolation threshold:

BPC percolates by design, but the EPC derivative identifies the PSD mode, and the zero-crossing value (0.21 μm) corresponds to the radius at which $\chi(r)$ reaches zero—the disappearance of the largest capillary—not a topological transition.

4.2. Multidirectional channels

The MDC structure consisted of orthogonal channels with diagonal connections.

Figure 10 shows the connectivity function, which transitioned from $\chi_0 = -15$ to positive values. The zero-crossing occurred at $R_c = 0.10 \mu\text{m}$. The derivative criterion yielded $R_c = 0.14 \mu\text{m}$. The 0.04 μm difference between the criteria indicated that the topological transition and the maximum rate of change occur at distinct radii in this structure.

QBIP analysis of MDC (Figure 11) showed channel invasion (Figure 11a). The maximum invaded saturation reached 90.9%

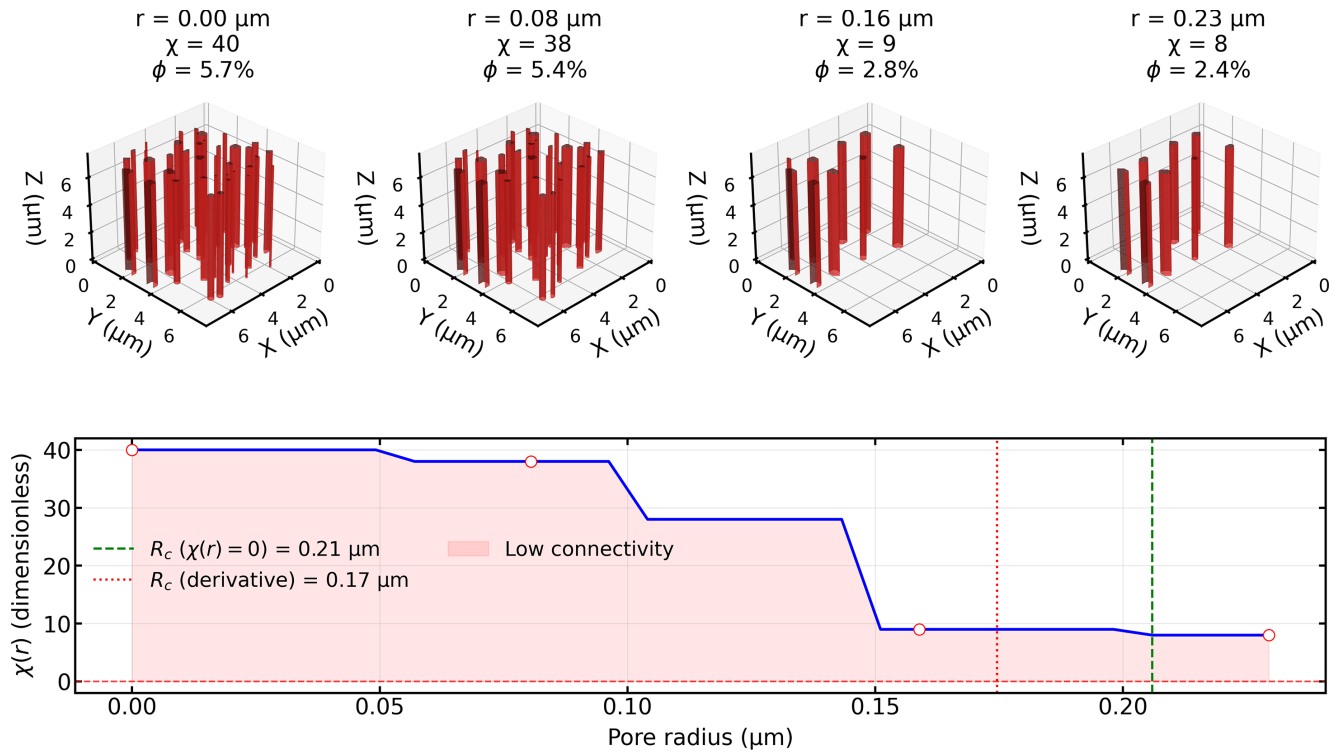


Figure 8. EPC analysis for BPC. Top panels: evolution of the 3D pore structure during morphological opening at increasing radii. Bottom panel: connectivity function $\chi(r)$ remaining positive throughout until it reaches zero. Zero-crossing criterion corresponds with the largest capillary.

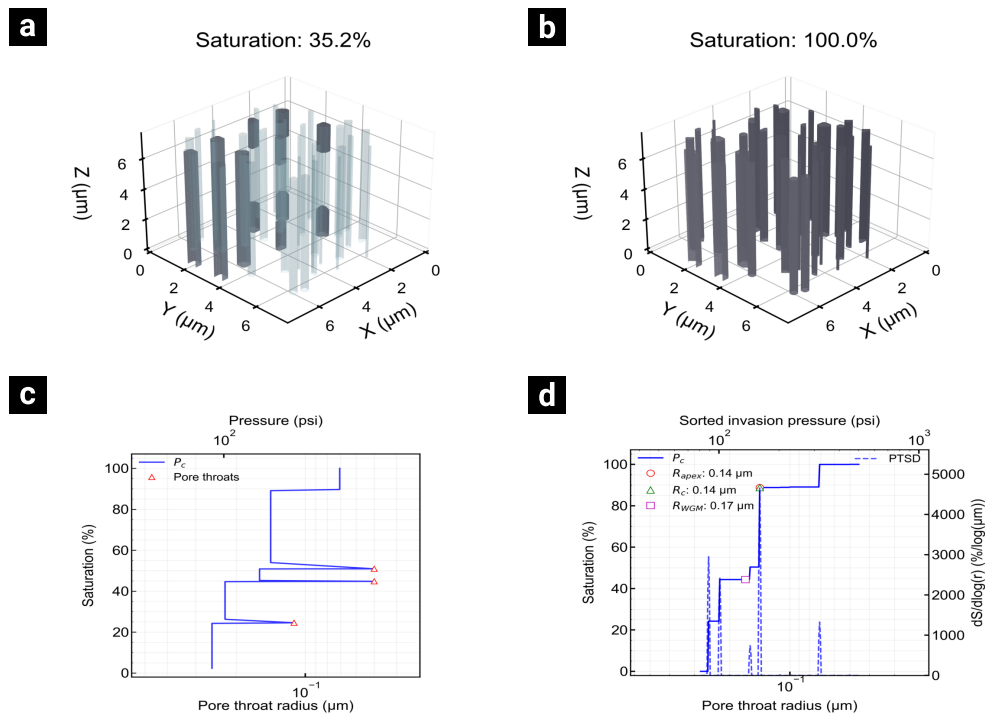


Figure 9. QBIP invasion characterization for BPC. (a–b) 3D visualization of volume-controlled invasion at two saturation states. (c) Volume-controlled invasion curve. (d) Pressure-controlled reconstruction: invasion events sorted by decreasing radius, with PTSD overlay (dashed): $R_{apex} = 0.14 \mu\text{m}$, $R_c = 0.14 \mu\text{m}$, and $R_{WGM} = 0.17 \mu\text{m}$.

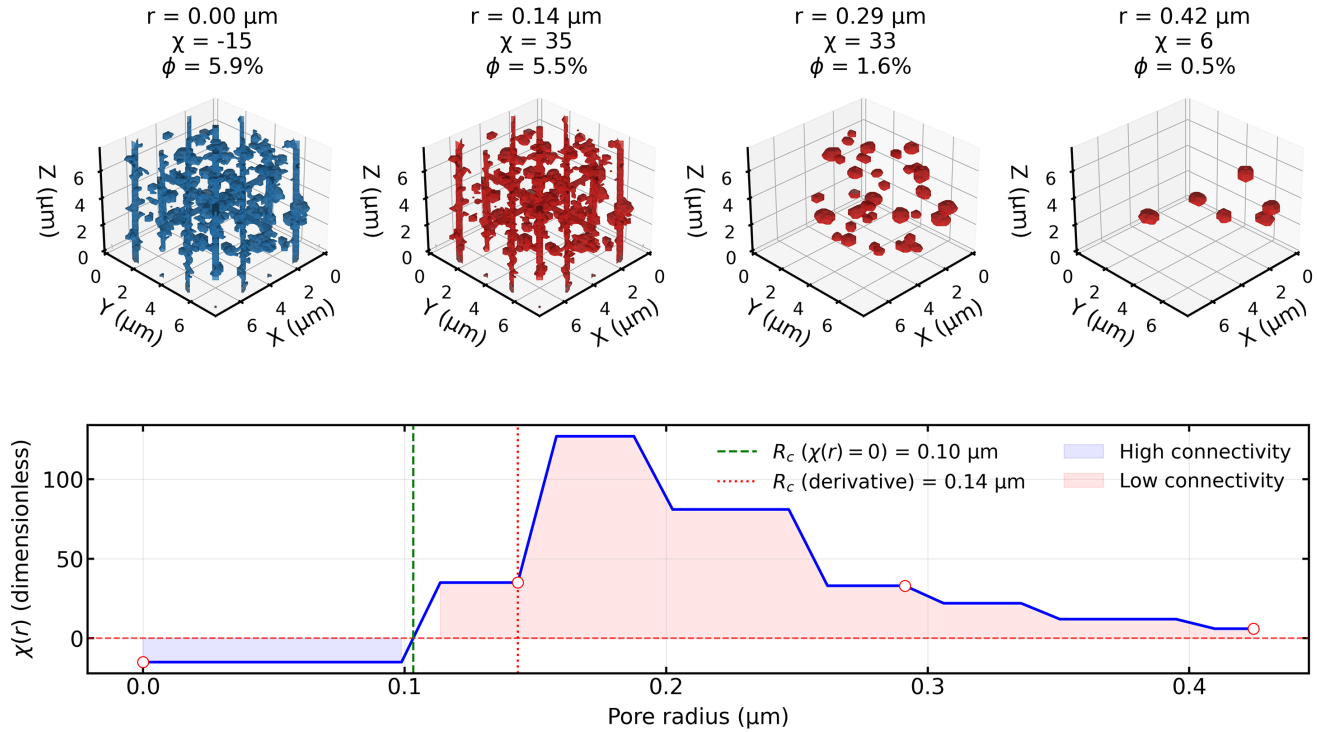


Figure 10. EPC analysis for MDC. Top panels: pore structure at opening radii of 0.00, 0.14, 0.29, and 0.42 μm . Bottom panel: connectivity function $\chi(r)$ starting at $\chi_0 = -15$, with zero-crossing at $R_c = 0.10 \mu\text{m}$ and derivative criterion at $R_c = 0.14 \mu\text{m}$.

(Figure 11b); the remaining porosity corresponds to isolated pores inaccessible to the invading phase. Volume-controlled invasion (Figure 11c) displayed step-wise saturation increases. Pressure-controlled analysis (Figure 11d) yielded $R_c = 0.15 \mu\text{m}$ from modal analysis; $R_{\text{apex}} = 0.14 \mu\text{m}$ and $R_{\text{WGM}} = 0.15 \mu\text{m}$.

Method comparison for MDC showed 0.04 μm internal EPC divergence between zero-crossing ($R_c = 0.10 \mu\text{m}$) and derivative ($R_c = 0.14 \mu\text{m}$) criteria. QBIP yielded $R_c = 0.15 \mu\text{m}$. Relative to the design modal radius, the zero-crossing deviated by 0%, the derivative by 40%, and QBIP by 50%. The zero-crossing coincided with the design modal radius; QBIP yielded a larger value, consistent with the dilation applied in Section 3.1.

4.3. Hierarchical tree network

The HTN structure consisted of branching paths generated via a minimum spanning tree algorithm.

Figure 12 shows the connectivity function, which transitioned from $\chi_0 = -127$ to positive values, with the zero-crossing between $r = 0.15$ and $0.17 \mu\text{m}$. The zero-crossing occurred at $R_c = 0.16 \mu\text{m}$; the derivative criterion yielded $R_c = 0.17 \mu\text{m}$ (0.01 μm internal divergence).

QBIP analysis of HTN (Figure 13) showed hierarchical

invasion through the primary branches (Figure 13a). Volume-controlled invasion (Figure 13c) displayed irregular saturation jumps at branch connections. Pressure-controlled analysis (Figure 13d) yielded $R_c = 0.14 \mu\text{m}$ from modal analysis; $R_{\text{apex}} = 0.14 \mu\text{m}$ and $R_{\text{WGM}} = 0.19 \mu\text{m}$.

Method comparison for HTN showed 0.01 μm internal EPC divergence between zero-crossing ($R_c = 0.16 \mu\text{m}$) and derivative ($R_c = 0.17 \mu\text{m}$) criteria. Relative to the design modal radius (0.10 μm), the zero-crossing deviated by 60%, the derivative by 70%, and QBIP by 40%. Both EPC criteria exceeded QBIP ($R_c = 0.14 \mu\text{m}$) by 0.02 μm and 0.03 μm , respectively. The pore-throat radii at branch junctions are distributed across a range that morphological opening and invasion percolation sample differently; in this structure, the topological transition detected by EPC does not coincide with the percolation threshold.

4.4. Degree-constrained network

The DCN structure assigned size-dependent coordination numbers ($Z = 2-6$) to each pore.

Figure 14 shows the connectivity function, which transitioned from $\chi_0 = -216$ to positive values, reaching $\chi = 130$ within the 0.10–0.15 μm range. The zero-crossing occurred at $R_c =$

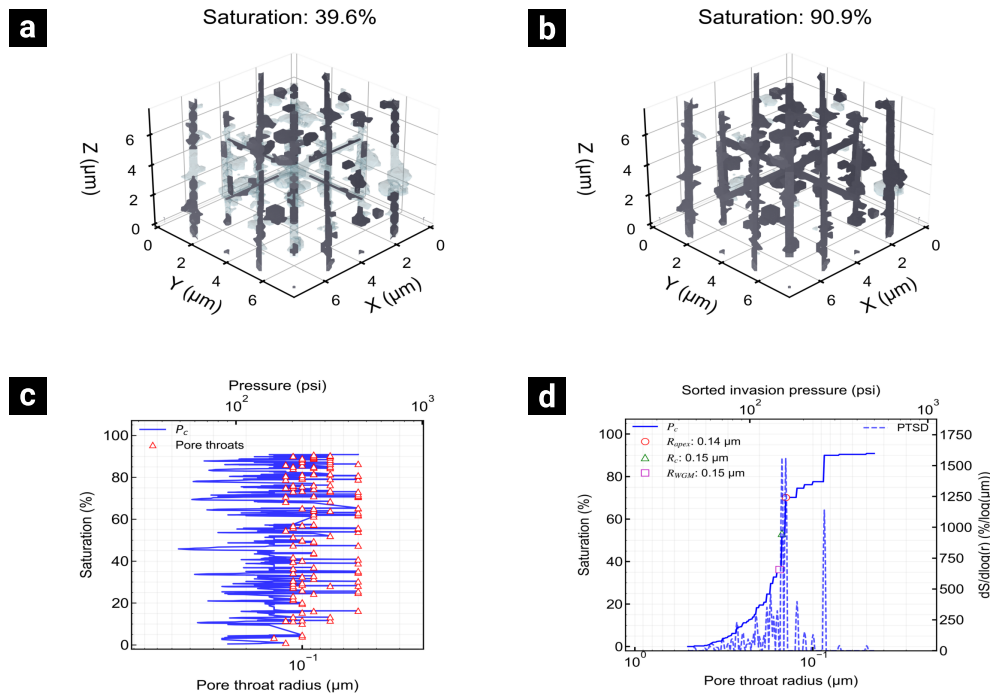


Figure 11. QBIP invasion characterization for MDC. (a–b) 3D visualization of volume-controlled invasion at two saturation states. (c) Volume-controlled invasion curve. (d) Pressure-controlled reconstruction: invasion events sorted by decreasing radius, with PTSD overlay (dashed): $R_{apex} = 0.14 \mu\text{m}$, $R_c = 0.15 \mu\text{m}$, and $R_{WGM} = 0.15 \mu\text{m}$.

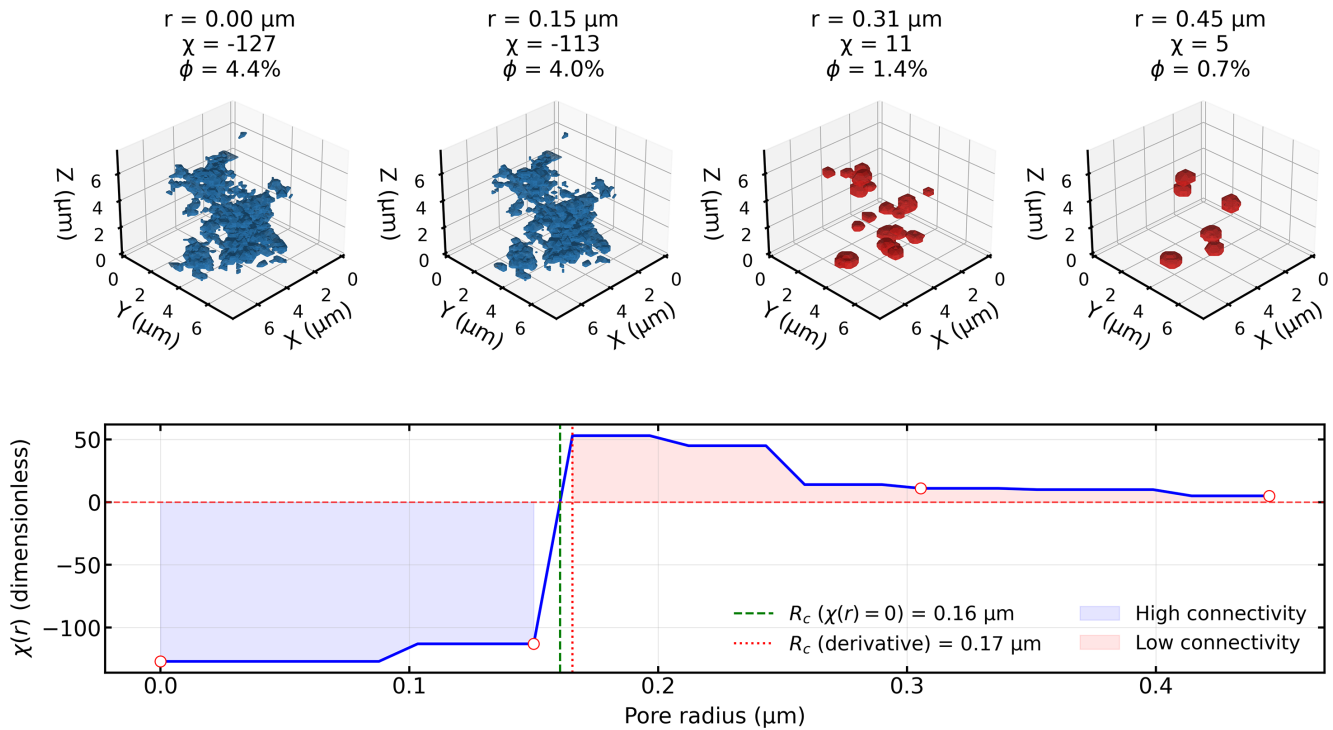


Figure 12. EPC analysis for HTN. Top panels: pore structure at opening radii of 0.00, 0.15, 0.31, and 0.45 μm. Bottom panel: connectivity function starting at $\chi_0 = -127$. Zero-crossing at $R_c = 0.16 \mu\text{m}$; derivative criterion at $R_c = 0.17 \mu\text{m}$.

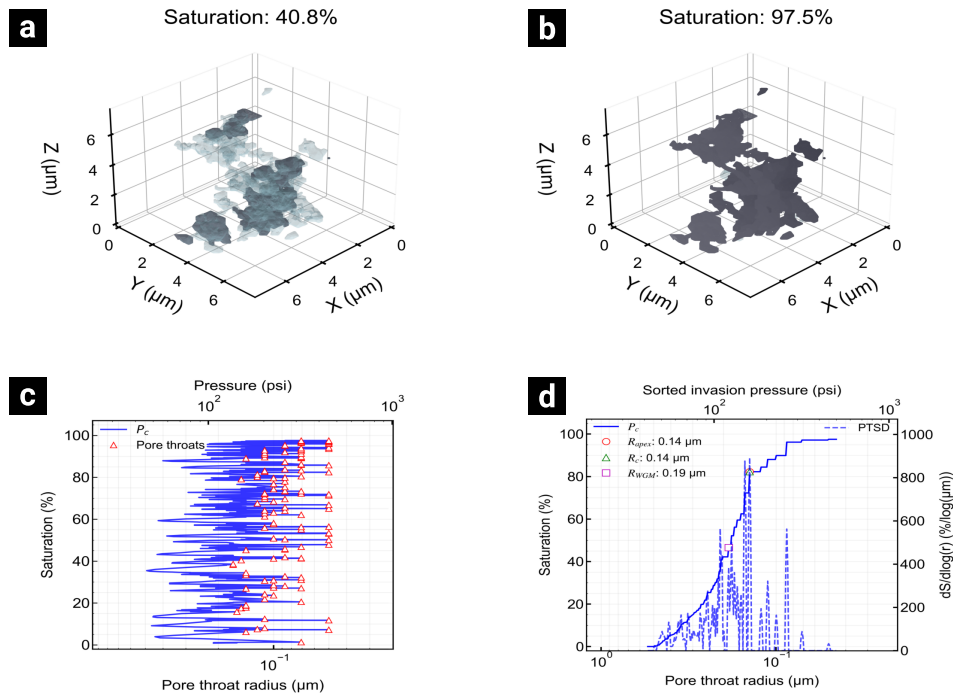


Figure 13. QBIP invasion characterization for HTN. (a–b) 3D visualization of volume-controlled invasion at two saturation states. (c) Volume-controlled invasion curve. (d) Pressure-controlled reconstruction: invasion events sorted by decreasing radius, with PTSD overlay (dashed): $R_c = 0.14 \mu\text{m}$ (modal), $R_{apex} = 0.14 \mu\text{m}$, $R_{WGM} = 0.19 \mu\text{m}$.

0.10 μm ; the derivative criterion yielded $R_c = 0.10 \mu\text{m}$ (0% internal divergence).

QBIP analysis of DCN (Figure 15) showed invasion through the coordinated network (Figure 15a). Volume-controlled invasion (Figure 15c) displayed irregular saturation jumps. Pressure-controlled analysis (Figure 15d) yielded $R_c = R_{apex} = 0.09 \mu\text{m}$; $R_{WGM} = 0.14 \mu\text{m}$.

Method comparison for DCN showed 0% internal EPC divergence: both criteria yielded $R_c = 0.10 \mu\text{m}$. QBIP yielded $R_c = 0.09 \mu\text{m}$, resulting in 0.01 μm difference for both criteria. Relative to the design modal radius (0.10 μm), both EPC criteria deviated by 0% and QBIP by 10%. This is the smallest deviation among all SPS. The controlled coordination numbers ($Z = 2-6$) produce a narrow pore-throat distribution around the design modal radius; under these conditions, the topological transition detected by EPC and the percolation threshold identified by QBIP converge toward the same radius. The 0.01 μm residual difference may reflect the discrete nature of voxelized opening radii in EPC versus the continuous invasion front in QBIP.

4.5. Summary of results

Table 2 compiles R_c determinations, R_{WGM} , and percentage

deviations (%dev) across all SPS. The percentage deviation relative to the design modal radius is defined as:

$$\% \text{ dev} = \frac{|R_c - r_{\text{design}}|}{r_{\text{design}}} * 100. \quad (13)$$

†BPC: EPC does not detect a percolation threshold ($\chi_0 > 0$). Zero-crossing corresponds to disappearance of the largest capillary; derivative identifies PSD mode. Differences are nominal. All percentages use the design modal radius as denominator. *EPC zero-crossing / derivative criteria.

The percentage deviations in Table 2 show that method performance varies across topologies. Three patterns emerge. First, QBIP determined R_c in all four structures (deviations of 6.7–50% from design modal radii), whereas EPC zero-crossing is restricted to structures with negative initial connectivity; in BPC, the zero-crossing and derivative values are nominal because no percolation threshold exists. Second, no single EPC criterion was uniformly closer to either the design modal radius or the QBIP value: the EPC derivative was within 0.01 μm of QBIP in MDC and DCN but diverged by 0.03 μm in HTN, while the zero-crossing was within 0.02 μm in HTN but diverged by 0.05 μm in MDC. Third, internal EPC divergence

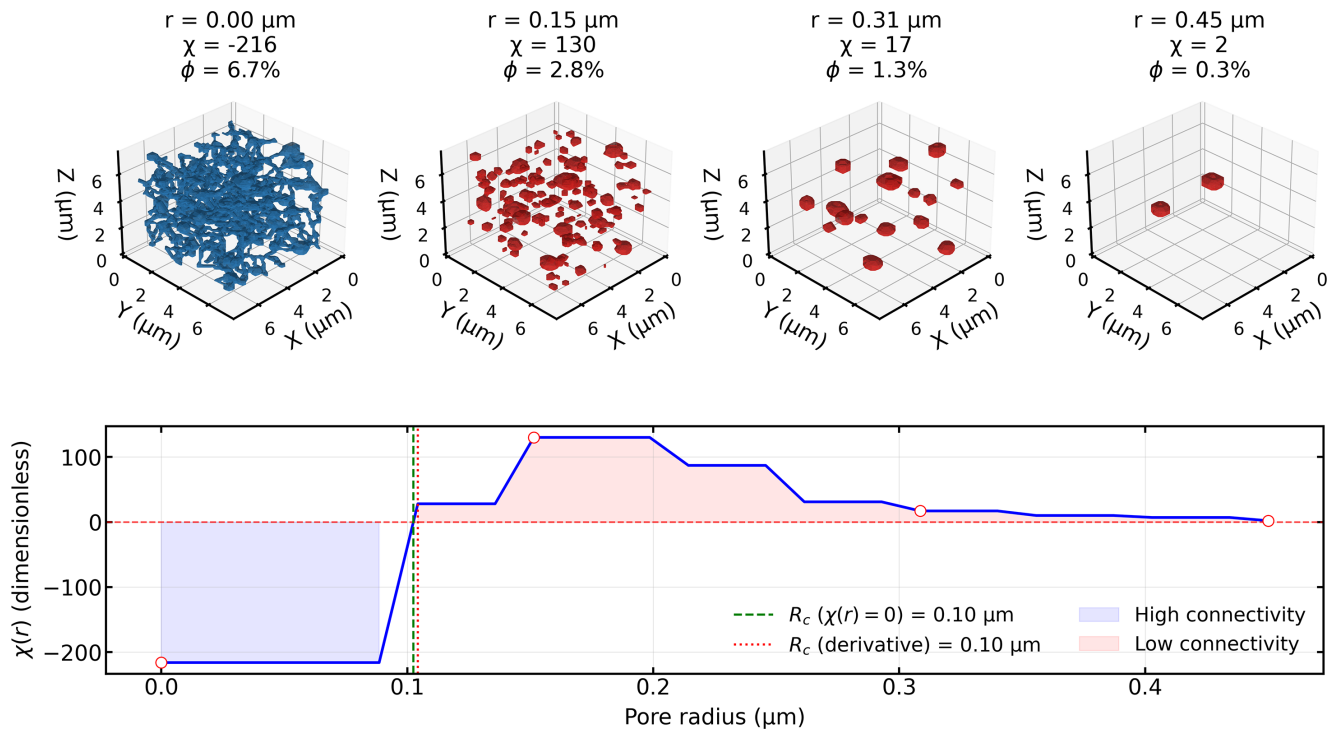


Figure 14. EPC analysis for DCN. Top panels: 3D pore structure at opening radii of 0.00, 0.15, 0.31, and 0.45 μm . Bottom panel: connectivity function with $\chi_0 = -216$, zero-crossing at $R_c = 0.10 \mu\text{m}$ and derivative criterion at $R_c = 0.10 \mu\text{m}$. Transition from $\chi = -216$ to $\chi = 130$ occurs within 0.05 μm range.

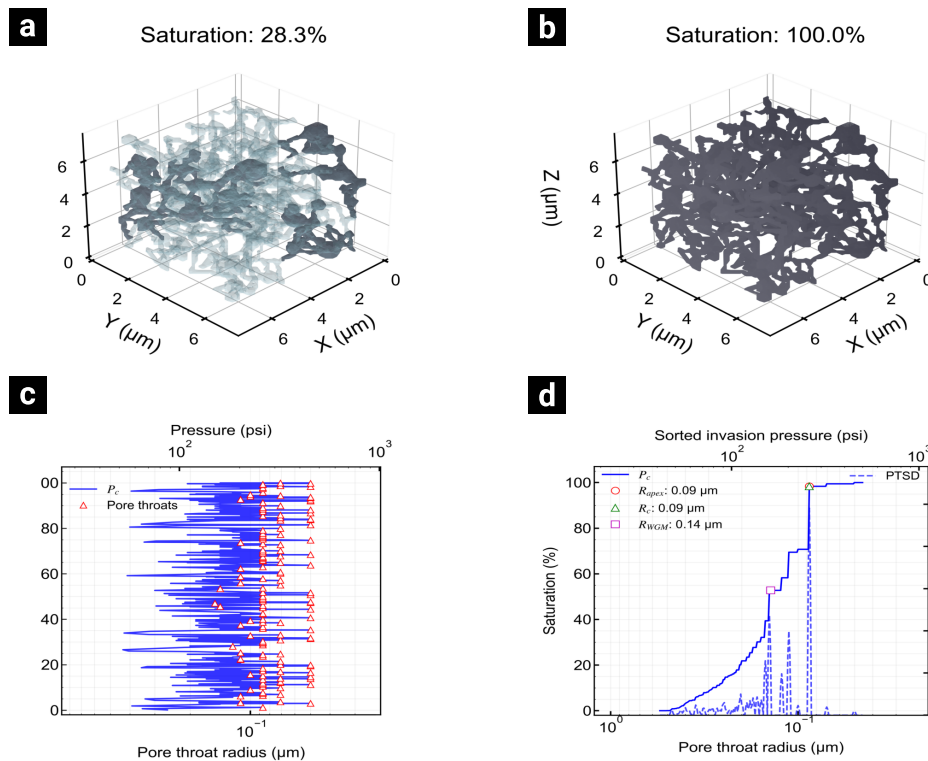


Figure 15. QBIP invasion characterization for DCN. (a–b) 3D visualization of volume-controlled invasion at two saturation states. (c) Volume-controlled invasion curve. (d) Pressure-controlled reconstruction: invasion events sorted by decreasing radius, with PTSD overlay (dashed): $R_c = R_{\text{apex}} = 0.09 \mu\text{m}$, $R_{\text{WGM}} = 0.14 \mu\text{m}$.

Table 2. Critical radius determination across synthetic porous structures. Percentage deviations calculated relative to the design modal radius.

SPS	χ_0	R_c EPC* (μm)	R_c QBIP (μm)	R_{WGM} (μm)	%dev EPC*	%dev QBIP
BPC	40	0.21†/0.17†	0.14	0.17	40†/13.3†	6.7
MDC	−15	0.10/0.14	0.15	0.15	0/40	50
HTN	−127	0.16/0.17	0.14	0.19	60/70	40
DCN	−216	0.10/0.10	0.09	0.14	0/0	10

†BPC: EPC does not detect a percolation threshold ($\chi_0 > 0$). Zero-crossing corresponds to disappearance of the largest capillary; derivative identifies PSD mode. Differences are nominal. All percentages use the design modal radius as denominator. *EPC zero-crossing / derivative.

(difference between zero-crossing and derivative criteria) decreases with increasing connectivity: 0.04 μm (MDC, $\chi_0 = -15$), 0.01 μm (HTN, $\chi_0 = -127$), and 0 μm (DCN, $\chi_0 = -216$); in highly connected structures, the two EPC criteria converge, and the EPC–QBIP gap narrows. Both methods identified R_c within the same order of magnitude as the design modal radii (0.10–0.15 μm); the binary dilation applied during SPS generation accounts for the larger deviations in MDC and HTN. R_{WGM} exceeded R_c in all four SPS (0.14–0.19 μm), consistent with its definition as the weighted mean of the invaded pore-throat spectrum.

5. Conclusions

This study presents the first comparison of EPC and QBIP methods for R_c determination across four SPS with topologies ranging from disconnected to highly connected. The results yield the following conclusions:

1. QBIP determined R_c in all four structures regardless of connectivity. EPC zero-crossing is restricted to $\chi_0 < 0$; in disconnected structures, even when individual flow paths connect opposite faces, the zero-crossing criterion cannot be applied. The derivative criterion returns a value in all cases, but in disconnected structures it identifies the PSD mode, not a percolation threshold.
2. No single EPC criterion was uniformly closer to either the design modal radius or the QBIP value across all topologies. The relative ranking between zero-crossing and derivative criteria depends on network topology.
3. Internal EPC divergence (difference between zero-crossing and derivative criteria) decreases with increasing connectivity. In highly connected structures, the two EPC criteria converge, and the EPC–QBIP gap narrows.
4. Both methods identified R_c values within the same

order of magnitude as the design modal radii, despite morphological operations during SPS generation. R_{WGM} consistently exceeded R_c in all SPS, consistent with its definition as the weighted mean of the invaded pore-throat spectrum.

Based on these results, method selection depends on the initial EPC value of the medium: if $\chi_0 < 0$ is confirmed, EPC provides R_c without invasion simulation, with deviations that depend on network topology; if χ_0 is unknown or positive, QBIP is required. When both methods are applicable, their agreement serves as a consistency check on R_c determination.

The comparison is limited to four SPS with fixed voxel resolution and a single dilation iteration; sensitivity to resolution and binning parameters remains to be evaluated.

Future work should extend this comparison to natural rocks imaged by micro-CT and to stochastic pore models—such as Boolean, Cox, and Gaussian random field models—which provide intermediate topological complexity between the controlled structures studied here and natural pore networks. Gaussian models are of particular interest because the EPC can be computed analytically rather than estimated from voxelized images. Experimental validation against pressure-based experiments-derived R_c values in natural rocks and the evaluation of how uncertainty in R_c propagates to permeability estimation through Eq. 1 remain open directions.

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7. Code Availability

The source codes are available at the link: <https://github.com/MFV-PS/EPC-QBIP-Rc> under the MIT License. The repository includes both EPC and QBIP implementations as Jupyter notebooks with example synthetic porous structures.

8. Nomenclature

k , Permeability, (md)
 Z , Coordination number
 l , Characteristic length
 H , Connectivity factor
 χ , Euler-Poincaré Characteristic number
 χ_0 , Initial EPC value (at $r = 0$)
 β_0 , Number of connected components
 β_1 , Number of independent loops
 β_2 , Number of enclosed cavities
 ϕ , Porosity (fraction)
 r , Pore-throat radius (μm)
 r_{max} , Largest available pore-throat (μm)
 P_c , Capillary pressure (Pa)
 γ , Interfacial tension (N/m)
 θ , Contact angle (degrees)
 R_c , Critical radius (μm)
 R_{WGM} , Weighted geometric mean radius (μm)
 R_{apex} , Apex radius (μm)
 S , Saturation (fraction)
 n , Number of evaluation radii
 $P(r)$, Pore space after morphological opening at radius r
 $B(r)$, Spherical structuring element of radius r
 $d(p)$, EDT value at pore voxel p (μm)
 r_{design} , Design modal radius (μm)
 $\%dev$, Percentage deviation from design modal radius (%)

9. Glossary

EPC, Euler-Poincaré Characteristic method
 QBIP, Queue-Based Invasion Percolation algorithm
 IBIP, Image-Based Invasion Percolation algorithm
 SPS, Synthetic Porous Structures
 PSD, Pore Size Distribution
 PTSD, Pore-Throat Size Distribution
 DRP, Digital Rock Physics
 DRM, Digital Rock Modeling
 MICP, Mercury Intrusion Capillary Porosimetry
 NMR, Nuclear Magnetic Resonance

BPC, Bundle of Parallel Capillaries
 MDC, Multidirectional Channels
 HTN, Hierarchical Tree Network
 DCN, Degree-Constrained Network
 EDT, Euclidean Distance Transform
 WEM, Water Expulsion Method
 micro-CT, X-ray micro-computed tomography

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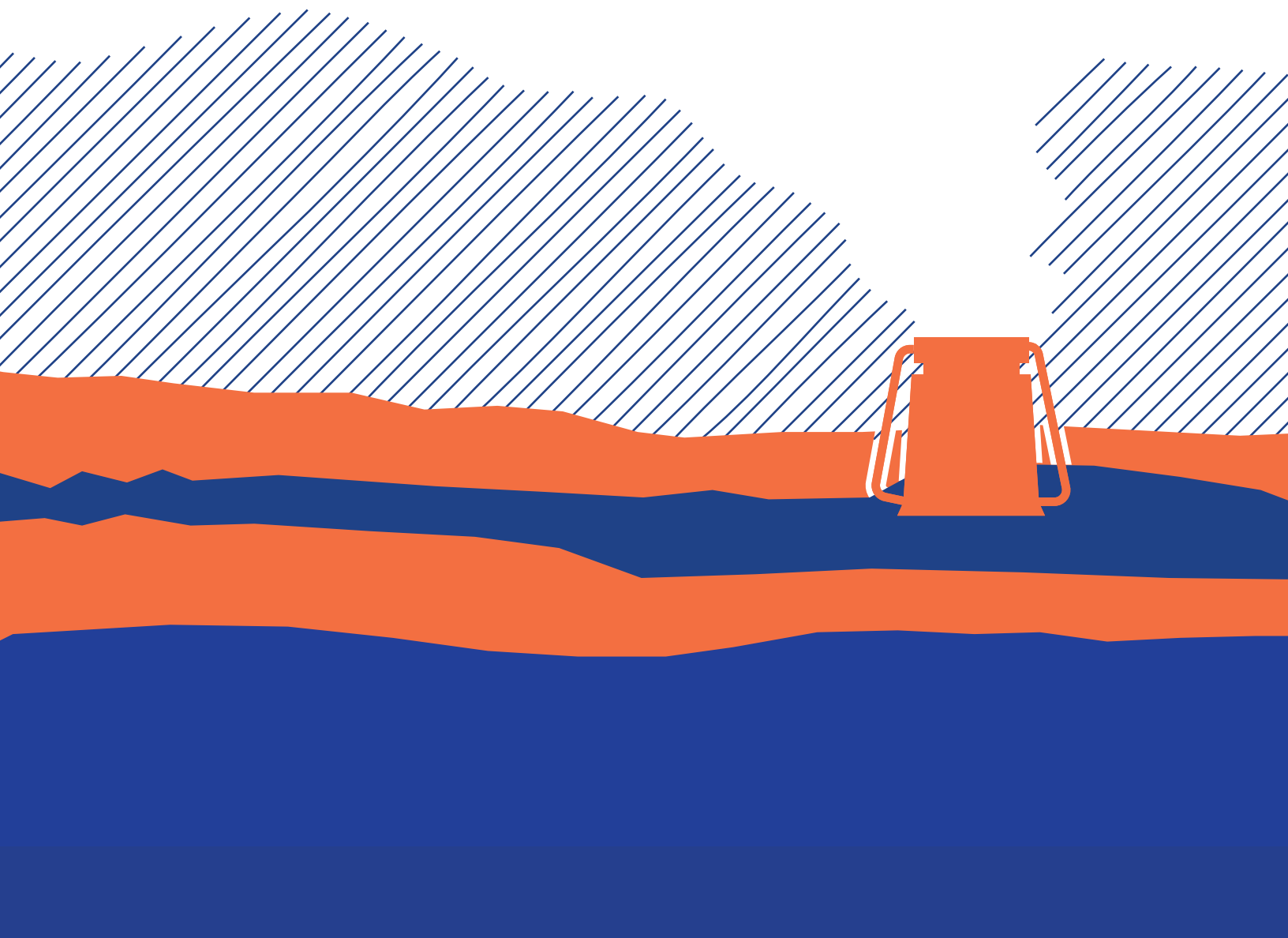
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Sección especial

Vulcanismo y Geotermia

Special section

Volcanism and
Geothermal Energy



Modelo de favorabilidad geotérmica mediante *Play Fairway Analysis* de la zona geotérmica dentro del Complejo Caldera de Acoculco (Puebla, México)

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Abstract

This article presents the results of a Play Fairway Analysis conducted in the geothermal area located within the Acoculco Volcanic Caldera Complex. In this study, considering the proven existence of a geothermal anomaly in the subsurface (identified by deep exploratory wells of >1.5 km depth), geoscientific data from previous studies were considered as proxies for permeability and used to generate a geothermal favorability model. This Play Fairway Analysis has an expert-driven approach, as there are no wells with proven geothermal resources to perform a data-driven Play Fairway Analysis. The data used in this analysis included the location of faults, CO₂ efflux, springs, soil temperature, opal deposits, and hydrothermal eruption craters. The datasets were managed and integrated using QGIS® software. The results highlight two areas with higher geothermal favorability, located approximately 200 m northwest of the exploration well EAC-1, and in the area known as Alcaparrosa. In this article, thanks to data compilation, it is also discussed why the Acoculco geothermal area could be a convective geothermal system and how the resulting areas of higher geothermal favorability are those with the greatest potential for hosting geothermal fluids.

Key words: Geothermal exploration, geoscientific data, proxies, geothermal fluids.

Resumen

En este trabajo se presentan los resultados de un *Play Fairway Analysis* realizado en la zona geotérmica localizada dentro del Complejo Caldera de Acoculco. En este estudio, considerando la existencia probada de una anomalía geotérmica en el subsuelo (identificada con pozos de >1.5 km de profundidad), se han utilizado datos geocientíficos de estudios previos considerados como indicadores o *proxies* de permeabilidad para generar el modelo de favorabilidad geotérmica. Este *Play Fairway Analysis* tiene un enfoque de expertos (*expert-driven*), debido a que no existen pozos con recursos geotérmicos probados para realizar un *Play Fairway Analysis* basado en datos (*data-driven*). Los datos empleados en este análisis fueron la ubicación de las fallas, del flujo de CO₂, de los manantiales, de la temperatura del suelo, de los depósitos de ópalo y de los cráteres de erupciones hidrotermales. Las capas de los datos (*evidence layers*) fueron manejadas e integradas usando el *software* QGIS®. Los resultados muestran dos zonas con mayor favorabilidad geotérmica, ubicadas a aproximadamente 200 m al noroeste del pozo exploratorio EAC-1 y en la zona conocida como Alcaparrosa. En este trabajo, gracias a la recopilación de datos, también se discute por qué la zona geotérmica de Acoculco podría ser un sistema geotérmico convectivo y cómo las zonas con mayor favorabilidad geotérmica resultantes son las que tienen mayor potencial para alojar fluidos geotérmicos.

Palabras clave: Exploración geotérmica, datos geocientíficos, *proxies*, fluidos geotérmicos.

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1. Introducción

El Complejo Caldera de Acoculco (CCA) se localiza en el sector oriental del Arco Volcánico Trans-Mexicano. El CCA, desde el Plioceno tardío hasta el Pleistoceno tardío (2.7 – 0.016 Ma), ha presentado un vulcanismo con una composición que varía desde basáltico a predominantemente félsico (Avellán *et al.*, 2019, 2020). Dentro de este complejo volcánico, se ha presentado actividad hidrotermal a lo largo de su evolución (González-Partida *et al.*, 2024), de la cual la actividad superficial actual es limitada en extensión y temperatura. Dicha actividad hidrotermal se encuentra representada por la presencia de algunos manantiales termales, manantiales ácidos, cráteres de erupciones hidrotermales, emisiones de gas y alteración hidrotermal (Canet *et al.*, 2015a; López-Hernández *et al.*, 2009; Peiffer *et al.*, 2014; Santos-Raga *et al.*, 2021).

La actividad hidrotermal en el CCA ha llamado la atención de geocientíficos y la industria por su potencial geotérmico, particularmente por su relación con un sistema magmático y las altas temperaturas estimadas con geotermómetros (Peiffer *et al.*, 2014; Sanjuan *et al.*, 2020; Santos-Raga *et al.*, 2021). En el área se han realizado actividades de exploración, incluyendo dos pozos exploratorios con profundidades de 1810 y 1900 m, realizados por la Comisión Federal de Electricidad (Figura 1). Las temperaturas de fondo de los pozos son de 307 y 267 °C, respectivamente (López-Hernández *et al.*, 2009), lo cual representa un gradiente geotérmico anómalo de ~150 °C/km.

A pesar de las altas temperaturas identificadas en los pozos, no se encontraron fluidos geotérmicos en el subsuelo (López-Hernández *et al.*, 2009). Esta falta de fluidos geotérmicos ha sido asociada a la reducción de permeabilidad por la mineralización secundaria. De hecho, algunos investigadores interpretan esta zona geotérmica como un potencial sistema de roca seca caliente (*hot dry rock*) (p.ej., Pulido *et al.*, 2011) y candidato a desarrollarse como un Sistema Geotérmico Mejorado (Peiffer *et al.*, 2014; Pulido *et al.*, 2011).

El *Play Fairway Analysis* (PFA) es una metodología creada para la exploración de hidrocarburos y que ha sido utilizada recientemente (ca. 2014) en la exploración geotérmica (p.ej., Faulds *et al.*, 2016; Forson *et al.*, 2015). El PFA aplicado a la geotermia se basa en: i) identificar los elementos necesarios para que se forme un sistema geotérmico (p.ej., anomalía de calor, permeabilidad), ii) seleccionar los datos geocientíficos que sirvan como indicadores o *proxies* de estos elementos necesarios, e iii) integrar los datos (*proxies*) según su importancia (Faulds *et al.*, 2016; Lautze *et al.*, 2017; Siler *et al.*, 2017; Shervais *et al.*, 2020; Lindsey *et al.*, 2021; Pauling *et al.*, 2023; Olvera-García *et al.*, 2024, 2025a, 2025b).

El modo de integrar los datos geocientíficos en los PFA puede separarse en *expert-driven* o *data-driven*. En el *expert-driven* se

basa en el juicio de los expertos y conocimiento actual sobre los sistemas geotérmicos para determinar la importancia de cada tipología de dato y determinar la potencial área de influencia de estos (p.ej., Lindsey *et al.*, 2021; Olvera-García *et al.*, 2023, 2024). En el *data-driven* se realizan análisis estadístico-espaciales entre la ocurrencia de los recursos probados y los datos utilizados, esto para determinar la importancia de cada tipo de dato (Faulds *et al.*, 2016; Olvera-García *et al.*, 2025a).

Las limitaciones del *data-driven* se refieren a que se necesita una gran cantidad de recursos probados y son pocas las zonas con estas características (Faulds *et al.*, 2016; Olvera-García *et al.*, 2025a). Un ejemplo donde se aplicó exitosamente un PFA *data-driven* en México fue en el campo geotérmico de Los Hornos (Olvera-García *et al.*, 2025a), debido a la gran cantidad de pozos de explotación, los cuales representan recursos probados y, por ende, *training sites*. Estos últimos podrían definirse como los puntos (sites) con los que se puede hacer un análisis espacial de correlación entre los recursos probados y el área que cubren los datos. Esto sirve como ejercicio de entrenamiento (training) o ilustración para determinar qué datos aportan la información más relevante sobre el sistema geotérmico, además de que permiten validar modelos.

En este trabajo, se presentan los resultados de un PFA de tipo *expert-driven* a escala local, realizado en la zona geotérmica localizada dentro del CCA. En este PFA, considerando la anomalía geotérmica identificada en el subsuelo con la información de los pozos profundos, se utilizaron datos que sugieren la presencia de permeabilidad para obtener el modelo de favorabilidad geotérmica (p.ej., Bólos *et al.*, 2022; Canet *et al.*, 2015a; Liotta *et al.*, 2023; Pérez-Zárate *et al.*, 2024; Santos-Raga *et al.*, 2021). Los datos utilizados se integraron con diferentes pesos usando la calculadora ráster en el *software* QGIS® (versión 3.40 LTR) para crear el modelo final de favorabilidad geotérmica.

2. Contexto geológico

Las rocas más antiguas que afloran en la región de Acoculco están conformadas por una secuencia de rocas calizas de edad Cretácica (Figura 1), que forman parte de la Sierra Madre Oriental, y afloran en la región norte, oriente y sureste del CCA (Avellán *et al.*, 2019, 2020). Sobre estas rocas se encuentra una secuencia de flujos de lavas de composición basáltica conocidas como Zacatlán (Avellán *et al.*, 2020). Según su posición estratigráfica, estas rocas de edad Mioceno inferior cubren una gran región al noreste, oriente y sureste del CCA (Figura 1). Sobre yaciendo estas rocas se encuentra un complejo de domos de lava de composición dacítica (Peñuela) con edades entre 13 y 10 Ma (Avellán *et al.*, 2020). Sobre yaciendo estas rocas se encuentra

el CCA, el cual se construyó cronológicamente en cinco fases eruptivas (Figura 1): pre-caldera, *syn*-caldera, *post*-caldera temprana, *post*-caldera tardía y vulcanismo extra-caldera (Avellán et al., 2019, 2020).

El vulcanismo pre-caldera está conformado por domos de lava de composición dacítica y edades entre 4 y 3 Ma (Avellán et al., 2019; 2020). Posteriormente, la erupción que dio origen a la ignimbrita Acoculco ocurrió hace 2.7 Ma, provocando el colapso del techo de la cámara de magma y la formación de una caldera en superficie de 18×16 km de diámetro (Figura 1). La erupción formadora de caldera es de composición andesítica y la erupción emitió hasta un volumen total de ignimbrita de 127 km^3 (Avellán et al., 2019, 2020). Posterior a esto, la actividad *post*-caldera temprana se caracterizó por un vulcanismo que se centró al interior de la caldera (Figura 1), produciendo erupciones predominantemente efusivas de flujos y domos de lava de composición traquiandesita-basáltica a basáltica con una edad entre 2.6 y 2.1 Ma (Avellán et al., 2019, 2020). Luego, la

actividad *post*-caldera tardía migró a lo largo del anillo de falla de la caldera, emplazando domos, flujos de lava e ignimbritas de composición predominantemente riolítica con edades entre 2 y <0.016 Ma (Avellán et al., 2019, 2020). Finalmente, la actividad volcánica extra-caldera está relacionada a la actividad del vulcanismo distribuido del campo volcánico Apan-Tezontepec (Avellán et al., 2019, 2020). Varias de las erupciones de este campo volcánico se encuentran intercaladas con el vulcanismo asociado a la caldera de Acoculco, y han sucedido desde hace 2.4 Ma hasta <16 ka (Ref?).

En el área de CCA, las rocas están afectadas por dos sistemas de fallas regionales (NO-SE, NE-SO) y otro menor encontrado solo en el interior de la caldera (E-O) (Figura 1). El sistema de fallas de rumbo NO-SE contiene estructuras regionales como los ejes de pliegues y las fallas de cabalgadura de la orogenia Laramide en la Sierra Madre Oriental (Lermo et al., 2009; Rocha et al., 2006; Suter, 1984). Este sistema estuvo activo desde mediados hasta finales del Mioceno, y comprende fallas de tipo

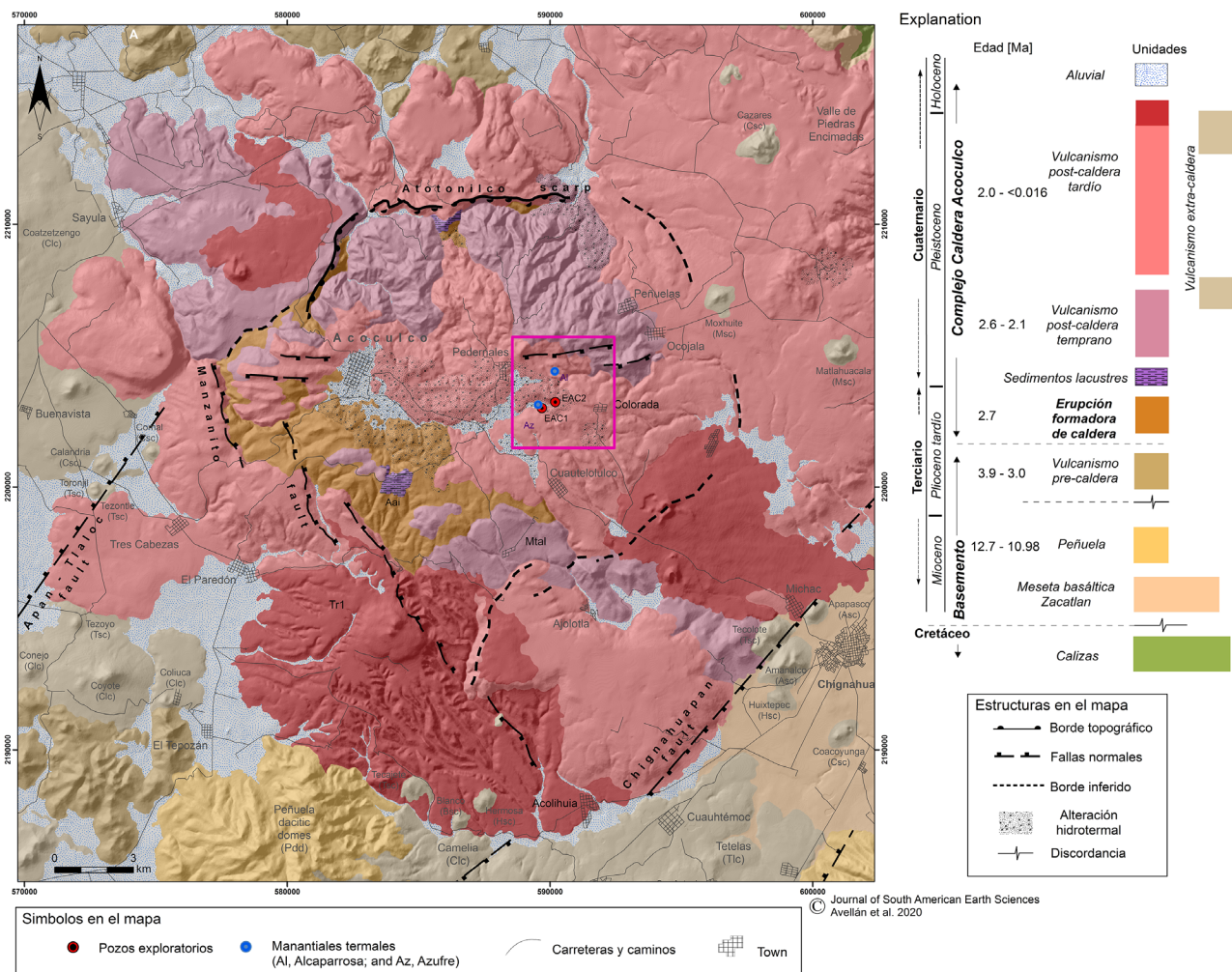


Figura 1. Mapa geológico simplificado del Complejo Caldera de Acoculco, modificado de Avellán et al. (2020). El rectángulo color rojo representa la extensión y ubicación del área de estudio.

normales con rumbo NO-SE y fallas de rumbo lateral derecho que son sincrónicas con el vulcanismo regional (Andreani *et al.*, 2008). Las fallas de rumbo NE-SO pertenecen al sistema de fallas Apan-Tenochtitlan y han estado activas desde el Mioceno hasta la actualidad (García-Palomo y Macías, 2000; García-Palomo *et al.*, 2002, 2018). Este sistema está constituido por fallas normales con componente lateral izquierda, las cuales presentan dos generaciones de estrías (*ca.* 30 y 80°) (García-Palomo *et al.*, 2018; Avellán *et al.*, 2020). En cuanto a los sistemas de fallas con rumbo E-O, están representadas por al menos 10 segmentos de fallas normales con rumbo E-O (*ca.* N085°) y buzamiento hacia el S (Avellán *et al.*, 2020). Solo se observan dentro del CCA, afectando principalmente el vulcanismo *post*-caldera en la parte central (Avellán *et al.*, 2020).

3. Descripción de datos utilizados

Los datos geocientíficos que se utilizaron en este PFA fueron obtenidos de trabajos previos. En esta sección se justifica el uso de cada dato en este trabajo, se describen sus características y se presenta la fuente bibliográfica. Los datos utilizados fueron fallas geológicas, flujo de CO₂, manantiales, temperatura del suelo, depósitos de ópalo y cráteres de erupciones hidrotermales (Tabla 1).

Se han clasificado estos grupos de datos en elementos geotérmicos activos y elementos geotérmicos fósiles. Donde los elementos activos son las fallas geológicas, el flujo de CO₂, manantiales y la temperatura del suelo. Mientras que los elementos fósiles son los depósitos de ópalo y cráteres de erupciones hidrotermales.

3.1. Elementos geotérmicos activos

3.1.1. Fallas

En este estudio, se consideraron las fallas como indicador de

permeabilidad por su estrecha relación con los sistemas geotérmicos convectivos (Barton *et al.*, 1997; Brogi *et al.*, 2005; Curewitz and Karson, 1997; Faulds *et al.*, 2004; Faulkner *et al.*, 2010; Olvera-García *et al.*, 2020a; Rowland y Sibson, 2004). Además, por la presencia de estas en la zona de estudio y la relación que presentan con los elementos hidrotermales activos y fósiles.

En el área se han identificado dos sistemas de fallas principales (Bólos *et al.*, 2022; Liotta *et al.*, 2023), los cuales se consideran contemporáneos y potencialmente activos (Liotta *et al.*, 2023): un sistema de fallas con rumbo NO-SE y otro con rumbo NE-SO (Figura 2a) (Calcagno *et al.*, 2022; Liotta *et al.*, 2023). El sistema NO-SE presenta dos movimientos superpuestos: una primera fase con movimiento de cinemática lateral a oblicuo. Seguido por una segunda fase dominada por una componente normal (Liotta *et al.*, 2023). El sistema NE-SO muestra un movimiento normal dominante.

En la zona también se ha identificado actividad sísmica local a partir de una red local que operó el consorcio GEMex durante un año (Esquivel-Mendiola *et al.*, 2022; Pertón *et al.*, 2022; Maldonado-Hernández, 2025). Particularmente, en la zona de estudio se localizó un sismo que ocurrió el 18 de septiembre del 2018 con una profundidad de 3.2 km (Figura 2a). El mecanismo focal del sismo fue determinado a partir de análisis de polaridades de primeros arribos de la onda P, el cual, presentó soluciones de strike, dip, slip de 120.00°/ 61.00°/ 28.00° para el primer plano auxiliar y de 15.55°/ 65.76°/ 147.8° para el segundo plano (Figura 2a). La primera solución se puede asociar al sistema de fallas lateral (de lateral a oblicuo) de dirección NO-SE.

3.1.2. Flujo de CO₂

Valores elevados de CO₂, relacionados con sistemas geotérmicos y/o magmáticos, se relacionan con canales permeables en la corteza superior que permiten el ascenso de gases profundos hasta la superficie (p.ej., Jentsch *et al.*, 2020; Pérez-Martínez *et al.*, 2021). Por este motivo, los datos de CO₂ se usan en este análisis como *proxies* de permeabilidad.

Tabla 1. Datos utilizados en este análisis (Bólos *et al.*, 2022; Canet *et al.*, 2015a; Liotta *et al.*, 2023; Pérez-Zárate *et al.*, 2024; Santos-Raga *et al.*, 2021). Para cada dato se indica también el búfer y el peso correspondientes, determinados mediante criterio de expertos.

Dato	Tamaño de búfer	Peso utilizado
Fallas	140	1
Flujo de CO ₂	70	1
Manantiales	70	1
Temperatura del suelo	140	1
Depósitos de ópalo	140	0.5
Cráteres de erupciones hidrotermales	140	0.5

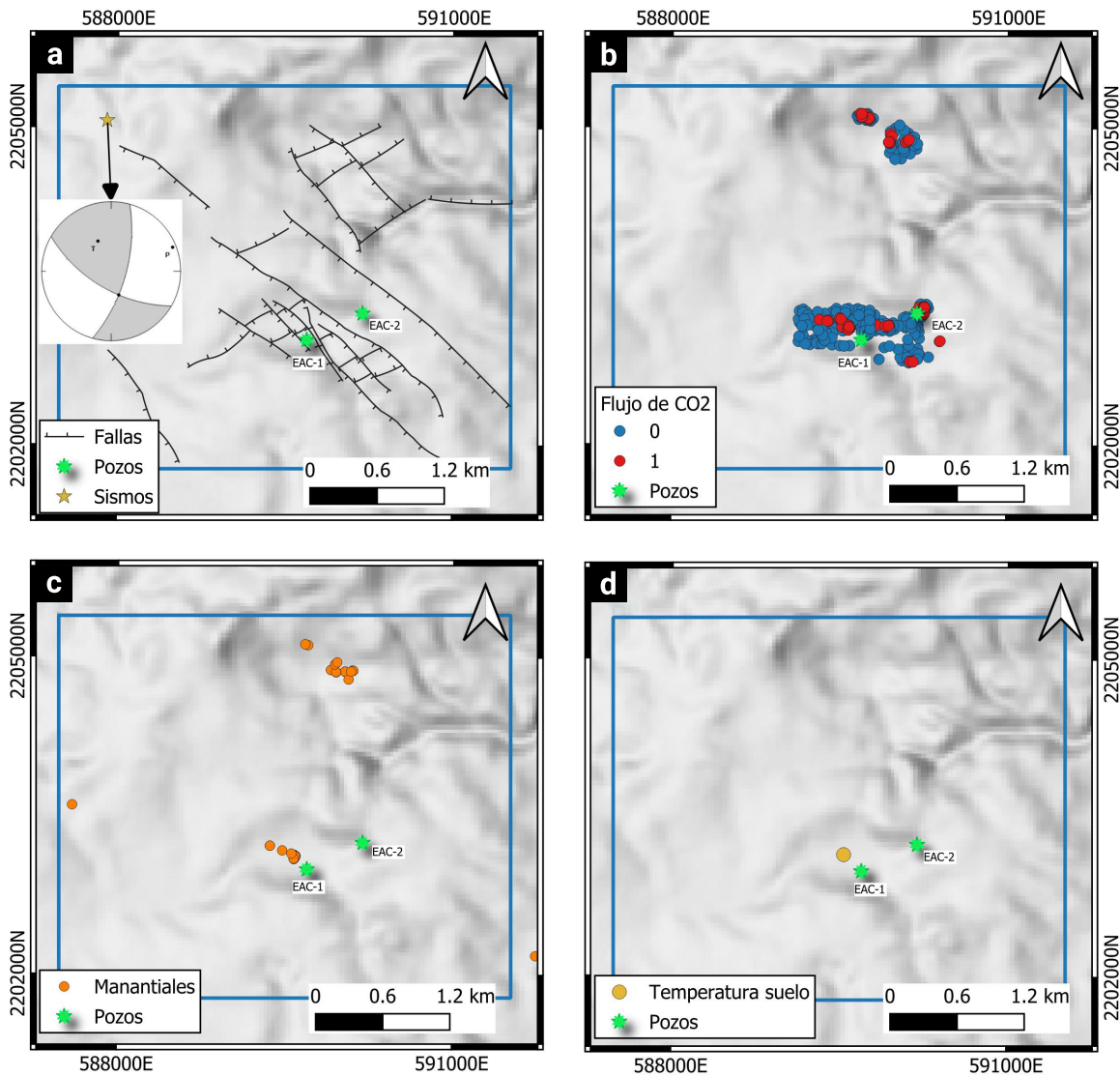


Figura 2. Localización de parte de los datos utilizados en este trabajo. a) Distribución de las fallas y localización de un evento sísmico; b) distribución de los datos de flujo de CO_2 , donde los que se presentan en rojo (1) presentan valores superiores a $29 \text{ g m}^{-2} \text{ d}^{-1}$, mientras que los azules presentan valores inferiores (0). Los valores de 1 y 0 son los pesos que usarán para la creación del modelo de favorabilidad; c) distribución de los manantiales; d) ubicación de la zona con temperaturas anómalas del suelo. El rectángulo azul representa el área de estudio.

Los datos de flujo de CO_2 utilizados en este trabajo fueron obtenidos y publicados por Pérez-Zárate *et al.* (2024). En dicho estudio, se documenta la medición del flujo de CO_2 utilizando el método de cámara de acumulación de gases con detector infrarrojo, los cuales fueron medidos en más de 1,200 puntos en la superficie del suelo en seis diferentes áreas de la CCA. Los valores de flujo de CO_2 variaron desde 1 hasta $26,000 \text{ g m}^{-2} \text{ d}^{-1}$, mientras que los flujos con valores $< 29 \text{ g m}^{-2} \text{ d}^{-1}$ se establecieron como la línea base de desgasificación (Pérez-Zárate *et al.*, 2024). En este trabajo se emplean los datos correspondientes a las áreas donde Pérez-Zárate *et al.* (2024) identificaron valores anómalos, localizadas en la parte central y norte del CCA (Figura 2b).

3.1.3. Manantiales

Los manantiales se forman cuando fluidos del subsuelo encuentran zonas permeables que les permiten ascender a la superficie (p.ej., Keegan-Treloar *et al.*, 2022). Normalmente, estas zonas permeables pueden estar asociadas con estructuras geológicas (p.ej., fallas, fracturas, contactos litológicos). Por este motivo, en este trabajo se utilizan los manantiales como *proxies* de permeabilidad (e.g., Lindsey *et al.*, 2021; Olvera-García *et al.*, 2023).

Dentro de la zona de estudio, Santos-Raga *et al.* (2021) identificaron 54 manantiales (Figura 2c), los cuales se usan en

este análisis. La información sobre estos manantiales como; coordenadas geográficas, altitud, temperatura, pH, entre otras, se encuentra en la Tabla 1 del artículo mencionado. Estos manantiales presentan temperaturas que van desde los 9.8 hasta los 26.1 °C (la temperatura media anual es de 12.7 °C). Por otro lado, el pH de los manantiales va desde muy ácido hasta ligeramente alcalino (p.ej., Botero-Gómez *et al.*, 2025), con valores que van desde 1.62 hasta 8.85.

3.1.4. Temperatura del suelo

Las temperaturas termales anómalas del suelo pueden ser indicadores de canales permeables que permiten que flujos hidrotermales convectivos calienten el mismo. Por este motivo, los datos de temperaturas anómalas del suelo se utilizaron en este trabajo como indicadores de permeabilidad.

Bolós *et al.* (2022) realizaron varias mediciones de temperatura del suelo en diferentes puntos en el área de estudio, utilizando un termómetro digital con una sensibilidad de 0.1 °C. Cada medición se llevó a cabo a una profundidad de 30 cm $\pm$ 1 cm. Las temperaturas anómalas sólo se detectaron en la parte central de la zona de estudio, registrando un máximo de 34 °C (Figura 2d).

3.2. Elementos geotérmicos fósiles

3.2.1. Depósitos de ópalo

En Acoculco existen rocas alteradas hidrotermalmente y depósitos minerales expuestos en la superficie. El ópalo es

un mineraloide amorfo de sílice hidratada ($\text{SiO}_2 \cdot n\text{H}_2\text{O}$) que presenta una estructura parcialmente cristalina (Curtis *et al.*, 2019; Olvera-García *et al.*, 2020b, 2020c). El ópalo presente en zonas alteradas hidrotermalmente es de origen hidrotermal. El ópalo de origen hidrotermal se deposita en conductos permeables o cerca de ellos, y por este motivo se utiliza como un indicador de permeabilidad en este trabajo.

Canet *et al.* (2015b) realizaron estudios de espectroscopía de reflectancia en las rocas alteradas dentro del CCA, identificando que el ópalo es el mineral hidrotermal más abundante en la zona de estudio. En este trabajo se utilizó la localización de 18 puntos dentro de la zona de estudio donde Canet *et al.* (2015b) identificaron los depósitos de ópalo (Figura 3a). La localización de los depósitos de ópalo en algunos casos coincide con la de depósitos de sínter de sílice identificados en la zona por Liotta *et al.* (2023). El sínter de sílice es una roca sedimentaria química compuesta de ópalo y que se forma a partir de manantiales termales. La distinción que se hace en este trabajo entre el ópalo y el sínter se debe a que el sínter se forma exclusivamente en la superficie terrestre, ligada a manantiales termales, mientras que el ópalo puede depositarse en el subsuelo. En el caso de Acoculco, este último se encontró mayormente en rocas exhumadas.

3.2.2. Cráteres de erupciones hidrotermales

Las erupciones hidrotermales son eventos explosivos que eyectan material sólido (al menos en parte) y cuya energía proviene exclusivamente de la pérdida de calor y las transiciones de fase en un sistema convectivo (hidrotermal), dominado por agua caliente o vapor de agua (Browne y Lawless, 2001; Montanaro *et*

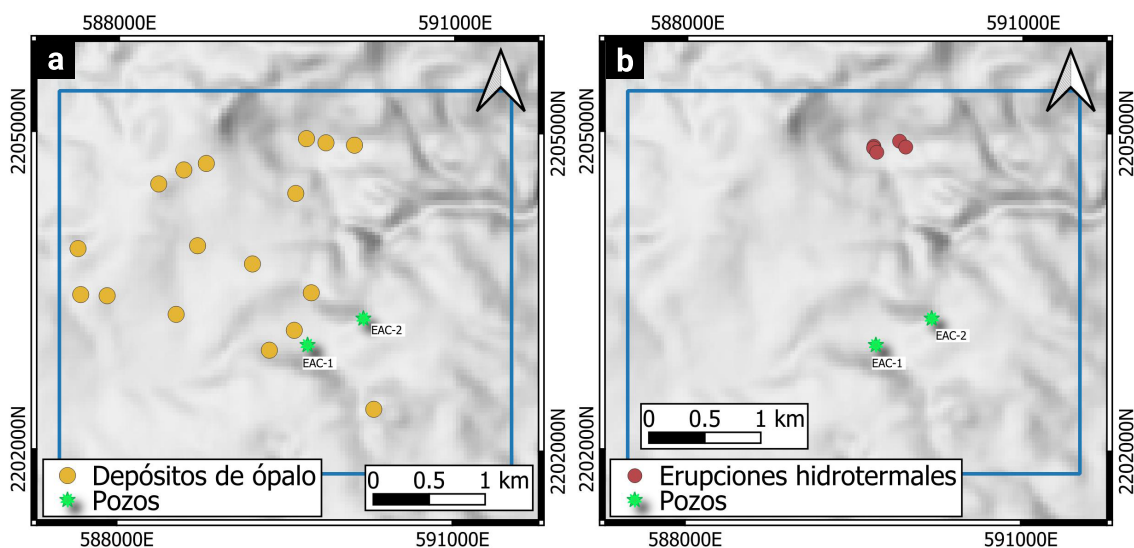


Figura 3. Mapas que muestran la localización de parte de los datos utilizados en este trabajo; a) depósitos de ópalo; b) cráteres de erupciones hidrotermales. El rectángulo azul representa el área de estudio.

al., 2022). Los cráteres de erupciones hidrotermales son comunes en muchos sistemas geotérmicos convectivos y por su relación con los fluidos hidrotermales profundos se consideran un *proxy* de permeabilidad en este trabajo.

Canet *et al.* (2015a) identificaron cráteres de erupciones hidrotermales en Acoculco. Los cráteres identificados en Acoculco son seis y se encuentran exclusivamente en la parte norte de la zona de estudio, muy cercanos entre sí, formando un clúster (Figura 3b). Los cráteres identificados se formaron durante el Holoceno, con edades absolutas determinadas por datación de Carbono 14 que oscilan entre ~5,000 y ~500 años antes del presente (Canet *et al.*, 2015a).

4. Metodología

Este PFA aplicado a la zona geotérmica de Acoculco cubre un área de 200 km² y, debido a la falta de datos de recursos probados (p.ej., pozos de explotación), está basado en el criterio de expertos (*expert-driven*). Este PFA se puede separar en tres etapas: 4.1. recopilación de datos, 4.2. procesamiento individual de datos y 4.3. integración y modelo final. Estas etapas se describen a continuación.

4.1. Recopilación de datos

A partir de información publicada previamente, se seleccionaron datos que pudieran servir como *proxies* para este análisis. Se creó un polígono rectangular para definir el tamaño y los límites del área de estudio basados en la distribución de los elementos hidrotermales activos.

4.2. Procesamiento individual de datos

En la segunda etapa, dado que todos los conjuntos de datos consisten en puntos y líneas, se determinó la distancia de los búferes para los datos originales. Los búferes representan las potenciales áreas de influencia de los datos (e.g., Olvera-García *et al.*, 2023). Posteriormente, se transformaron los archivos de forma (*shapefiles*) en archivos ráster, los cuales representan las capas de evidencia. Se generaron los archivos ráster con un tamaño de celda de 10×10 m, asignando un valor de 1 a los elementos del *shapefile* (p.ej., fallas) y 0 a las áreas sin datos. Para el tamaño de celda, se consideró menor que los valores de búfer, con el fin de obtener buena resolución y evitar un aspecto pixelado.

Este procedimiento de la etapa 2 se explica con detalle para cada dato.

4.2.1. Fallas

Para las fallas, inicialmente se creó un búfer de 140 m de radio para las líneas que representan las fallas. Posteriormente, las fallas con el búfer se convirtieron en un archivo ráster (capa de evidencia) asignando un peso de 1 a la zona de las fallas con el búfer y 0 al resto del área (Figura 4a).

Para las fallas, temperatura del suelo, depósitos de ópalo y cráteres de erupciones hidrotermales se usaron 140 m de búfer porque corresponde a la distancia mínima registrada entre un pozo productor y uno no productor en el campo geotérmico de Los Humeros (p.ej., Jentsch *et al.*, 2020). Este valor se optó bajo el razonamiento de que representa la distancia mínima conocida a partir de la cual ya no se tienen recursos explotables (pozo no productor) respecto de un pozo productor. Se usó como referencia para este trabajo el campo geotérmico de Los Humeros, ya que se encuentra en un ambiente tectónico, geológico y estructural similar al de la zona de estudio, además de que Los Humeros dispone de una gran cantidad de datos de pozos.

4.2.2. Flujo de CO₂

Para el flujo de CO₂, se determinaron los valores límite a partir de los cuales los valores superiores se podrían considerar anómalos; para esto se utilizó el valor de 29 g m⁻² d⁻¹ estimado por Pérez-Zárate *et al.* (2024) como valor de fondo. Después, se creó un búfer de 70 m de radio para cada medición de CO₂. Posteriormente, los puntos de CO₂ con el búfer se convirtieron en archivo ráster (capa de evidencia). Consecutivamente, con la calculadora ráster se asignó un peso de 1 a los puntos con el búfer con valores >29 g m⁻² d⁻¹ (porque se consideran anomalía) y 0 a los puntos con valores inferiores al valor de fondo y al resto del área (Figura 4b).

Se utilizó como radio para el búfer el valor de 70 m que representa la mitad de la distancia mínima registrada entre un pozo productor y uno no productor en el campo geotérmico de Los Humeros. Se utilizó solo la mitad de dicho valor debido a la alta densidad de puntos en algunas zonas de esta capa de datos.

4.2.3. Manantiales

Para los manantiales, se creó un búfer de 70 m de radio para los puntos que representan manantiales debido a la gran densidad de datos en algunas zonas. Posteriormente, los manantiales con el búfer se convirtieron en archivo ráster (capa de evidencia) asignando un peso de 1 a cada manantial con el búfer y 0 al resto del área (Figura 4c).

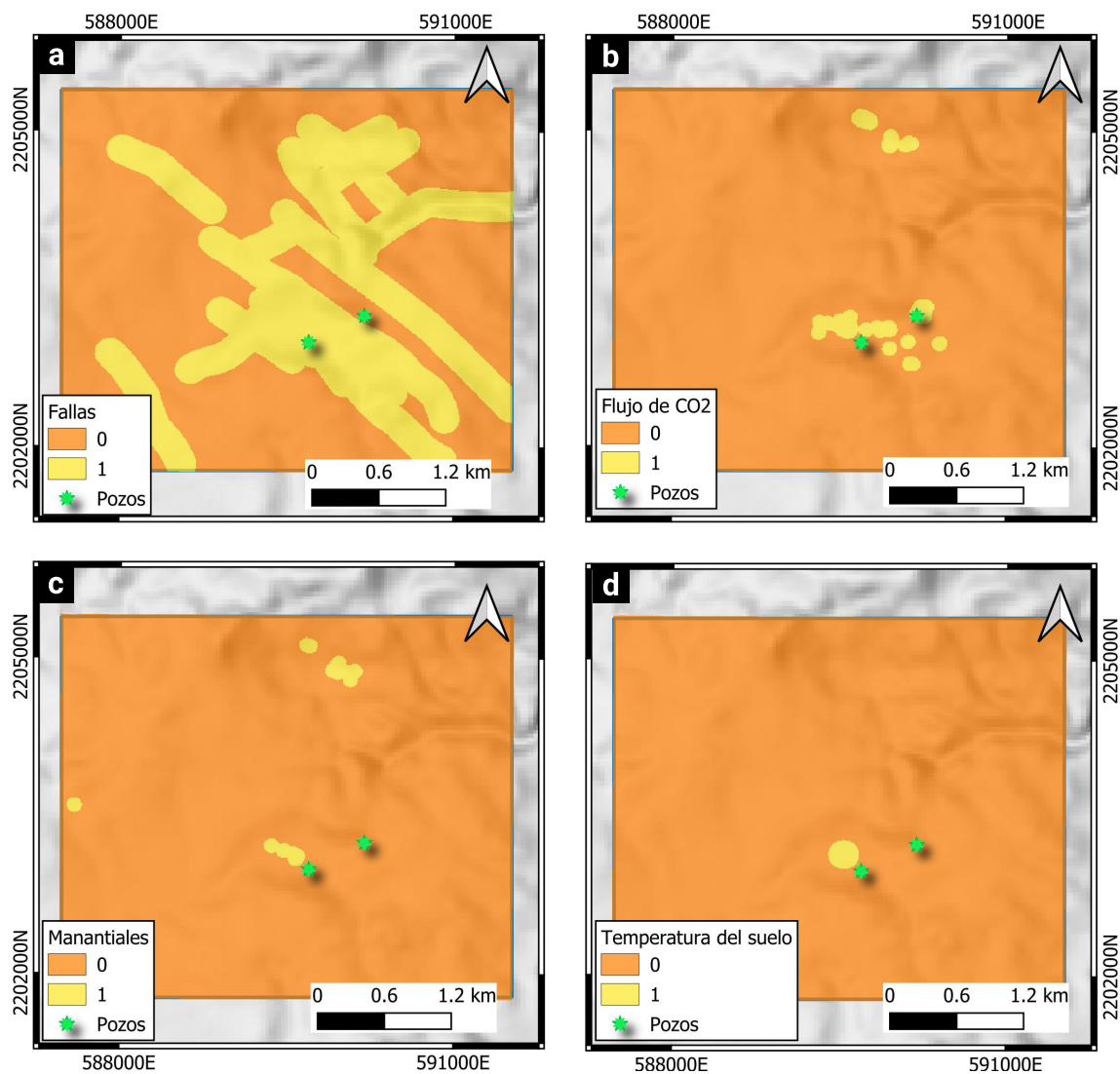


Figura 4. Capas de evidencia de parte de los datos utilizados en este trabajo; a) fallas; b) flujo de CO₂; c) manantiales; d) temperatura del suelo.

4.2.4. Temperatura del suelo

Para la temperatura del suelo, primero se creó el búfer para el punto que representa una anomalía en el área de estudio. Posteriormente, la temperatura con el búfer se convirtió en archivo ráster (capa de evidencia) asignando un peso de 1 a la zona de temperatura con el búfer y 0 al resto del área (Figura 4d).

4.2.5. Depósitos de ópalo

Para los depósitos de ópalo, primero se creó el búfer para cada punto que representa la ubicación de los depósitos de ópalo. Posteriormente, el *shapefile* con los puntos y el búfer se convirtió en archivo ráster (capa de evidencia) asignando un peso de 1 a los puntos con el búfer y 0 al resto del área (Figura 5a).

4.2.6. Cráteres de erupciones hidrotermales

Para los cráteres de erupciones hidrotermales, primero se creó el búfer para cada punto que representa la ubicación de los cráteres de erupciones hidrotermales. Posteriormente, el *shapefile* con los puntos y el búfer se convirtió en un archivo ráster (capa de evidencia) asignando un peso de 1 a los puntos con el búfer y 0 al resto del área (Figura 5b).

4.2.7. Integración y modelo final

Finalmente, en la tercera y última etapa se creó el modelo de favorabilidad geotérmica. Este modelo se creó a través de una suma ponderada de los *proxies* de permeabilidad usados, seguida de la normalización a 1. Para la suma ponderada se asignó un

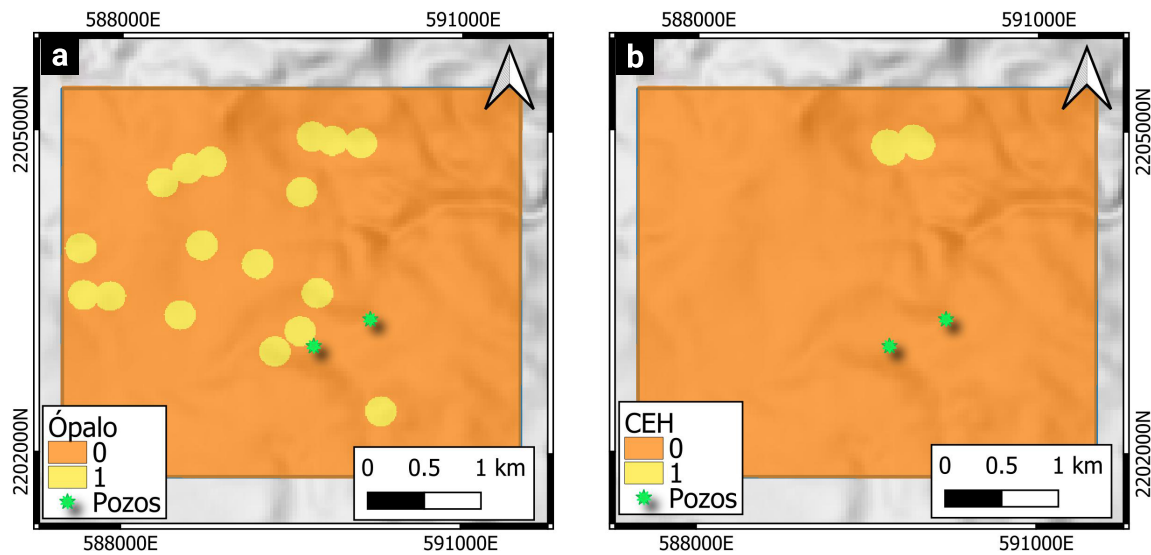


Figura 5. Capas de evidencia de parte de los datos utilizados en este trabajo; a) depósitos de ópalo; b) cráteres de erupciones hidrotermales (CEH).

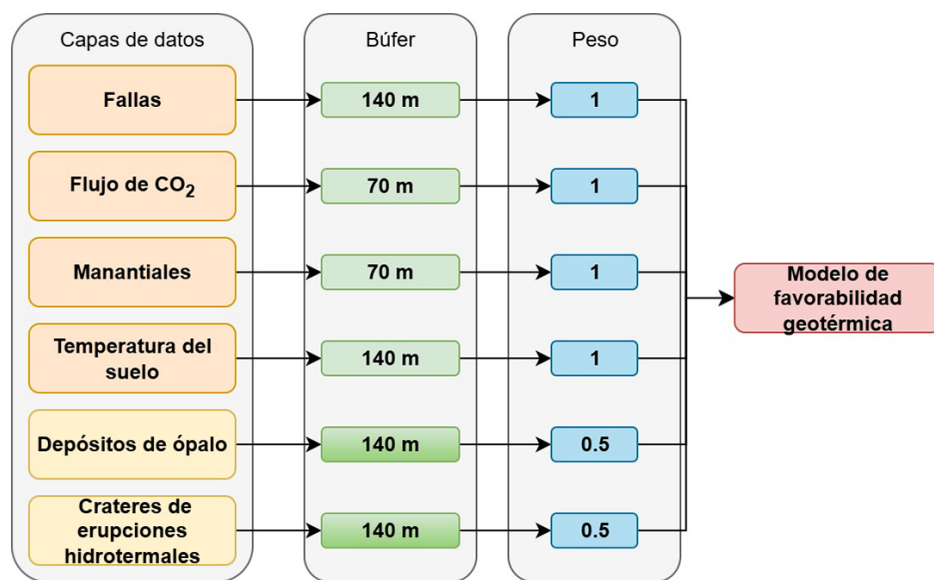


Figura 6. Diagrama de flujo con la metodología de integración de los datos usados.

peso de 1 a los elementos geotérmicos activos, de 0.5 a los elementos geotérmicos fósiles (Figura 6) y de cero a las zonas que se considera que no tienen anomalías, así como para el resto del área sin datos. Para la normalización a 1, se dividieron los resultados de la suma entre el número de elementos sumados. Para dicho procedimiento se utilizó la calculadora ráster en QGIS®.

5. Resultados

Los resultados de este trabajo son las capas de evidencia para

cada dato y el modelo de favorabilidad geotérmica. Las capas de evidencia se crearon a partir de cada dato, determinando anomalías para algunos datos y creando una potencial área de influencia para estos (Figura 4 y 5). El área de influencia para los datos fue basada en expertos y el conocimiento actual sobre los sistemas geotérmicos. Las capas de evidencia muestran las zonas con potenciales efectos positivos en la permeabilidad (Figura 4 y 5) y, por ende, en el modelo final de favorabilidad geotérmica.

Las capas de evidencia se separan en capas de elementos geotérmicos activos y elementos geotérmicos fósiles. Las capas

de elementos activos incluyen datos que evidencian procesos hidrotermales o tectónicos actuales, tales como manantiales, flujo de CO_2 , fallas del Holoceno y temperaturas anómalas del suelo, lo que indica que, si el sistema existe, se encuentra en funcionamiento. Las capas de elementos fósiles incluyen evidencias de actividad geotérmica pasada pero geológicamente reciente (Holoceno), como son cráteres de erupciones hidrotermales y depósitos de ópalo. Esto indica que el sistema estuvo activo en el pasado reciente y podría seguir activo en la actualidad (p.ej., Campbell *et al.*, 2015).

Las capas de evidencia se integraron con diferentes pesos (Figura 6) para crear el modelo de favorabilidad geotérmica. El modelo de favorabilidad geotérmica obtenido para la zona de estudio muestra dos áreas discretas y aisladas entre sí con la mayor favorabilidad geotérmica (Figura 7). Estas zonas con

mayor favorabilidad geotérmica se encuentran ubicadas en la parte central y norte del área de estudio, al noroeste del pozo de exploración EAC-1 y en la zona de Alcaparrosa, y se encuentran representadas por las letras A y B en la Figura 7. Estas zonas representarían las zonas con mayor potencial de alojar fluidos hidrotermales en el subsuelo.

6. Discusión

Los componentes necesarios para la formación de un sistema geotérmico convectivo son una anomalía de calor, la permeabilidad y la presencia de fluidos (Moeck, 2014; Jolie *et al.*, 2021). En Acoculco se sabe de la existencia de una anomalía de calor (López-Hernández *et al.*, 2009). Asimismo, se asume

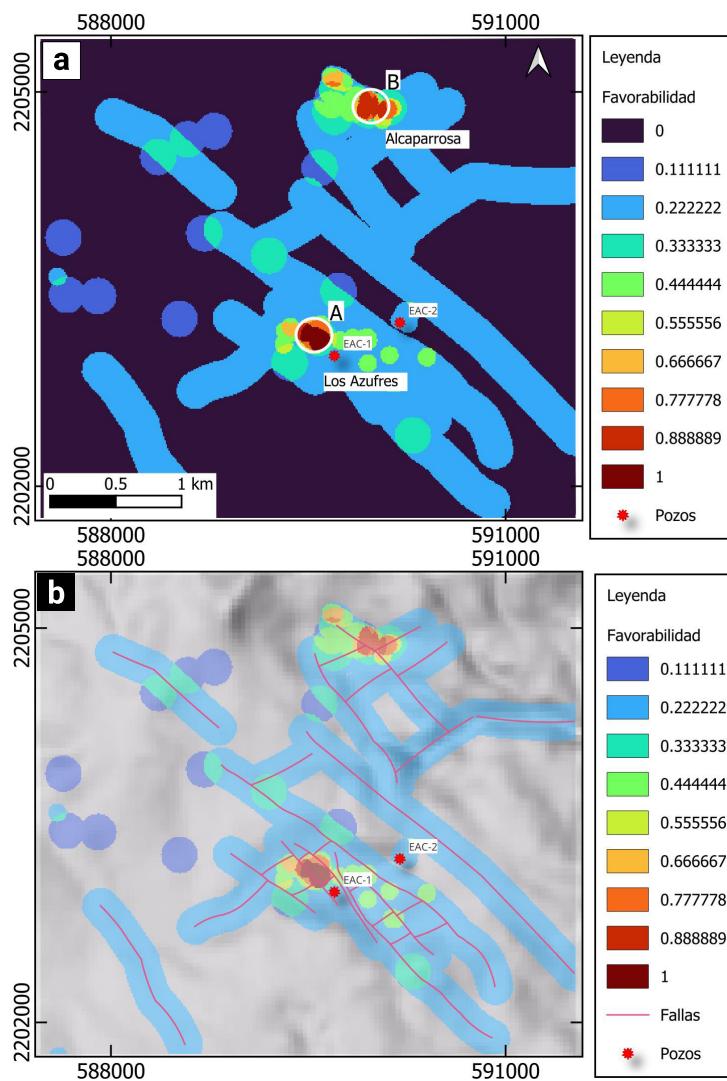


Figura 7. a) Modelo de favorabilidad geotérmica. A y B representan anomalías identificadas. Los colores rojizos representan mayor favorabilidad; b) Modelo de favorabilidad geotérmica de la zona. Se muestran las fallas y pozos para referencia espacial.

que existe disponibilidad de fluidos por la elevada tasa anual de lluvia (entre 1,000 y >2,000 mm); de hecho, la tasa de lluvia en Acoculco es muy superior a la de Los Humeros, el cual tiene más de 35 años en operación. Cabe mencionar que >90% de los fluidos explotados en los campos geotérmicos convencionales son de origen meteórico (Truesdell y Hulston, 1980; Sillitoe y Brogi, 2021). Por último, hasta ahora la permeabilidad en Acoculco se considera inexistente. Sin embargo, en este trabajo se sugiere que podría existir permeabilidad en la zona debido a: 1) la actividad reciente de las fallas (Holoceno), las cuales son consideradas activas por Liotta *et al.* (2023), sugiere que estas presentan potencial para actuar como conductos permeables para la circulación de fluidos. 2) Existe actividad tectónica local en el área representada por sismos (la actividad tectónica es la que mantiene la permeabilidad en las zonas geotérmicas). 3) Se identificaron sismitas del Holoceno en el área de estudio (Liotta *et al.*, 2023). 4) Los cráteres de erupciones hidrotermales y el sínter están asociados a sistemas geotérmicos convectivos (lo implica la presencia de permeabilidad), y los identificados en la zona han ocurrido en el Holoceno (último hace ~500 años). 5) Los manantiales y los elevados valores de flujos de CO₂ se ubican en zonas con permeabilidad. Todo lo anterior apoya la posible existencia de permeabilidad localizada.

En este sentido, este PFA incluye solamente datos geocientíficos que sugieren la presencia de permeabilidad para determinar el modelo de favorabilidad geotérmica. Este enfoque es similar al realizado por Faulds *et al.* (2016), aunque dicho trabajo es a escala regional. En el trabajo de Faulds *et al.* (2016) se utilizaron principalmente *proxies* de permeabilidad para determinar el modelo de favorabilidad geotérmica en el centro de Nevada (EUA), ya que consideran que el calor está ampliamente distribuido en la región y no es una limitante para la formación de sistemas geotérmicos. Por la anomalía geotérmica encontrada en Acoculco mediante los pozos profundos, también se considera que el calor no sería una limitante para la formación de un sistema geotérmico convectivo en Acoculco. Ya que en caso de que existiese permeabilidad, esta permitiría que los fluidos meteóricos se filtren, se calienten y formen el sistema geotérmico.

El modelo de favorabilidad geotérmica evidencia las zonas donde se encuentra la sobreposición de la mayor cantidad de datos considerados como *proxies* para la permeabilidad (Figura 7). Lo que sugiere las zonas, con base en la disponibilidad de datos, con mayor potencial para alojar fluidos geotérmicos en el subsuelo en caso de que existan (p.ej., Lindsey *et al.*, 2021). El modelo de favorabilidad geotérmica de la zona de estudio muestra dos zonas principales de favorabilidad. Dichas zonas con favorabilidad se encuentran localizadas a aproximadamente 200 m al noroeste del pozo EAC-1 y en la zona de Alcaparrosa (Figura 7).

Por otra parte, debido a la anomalía geotérmica, la edad reciente de los elementos hidrotermales fósiles (Holoceno), el origen de los mismos elementos fósiles (convectivo), la actividad geotérmica actual (p.ej., manantiales, flujo de CO₂, temperaturas del suelo), y la actividad tectónica activa, se considera que en la zona podría existir un sistema geotérmico activo de tipo convectivo. Sin embargo, este presenta escasas y tenues manifestaciones hidrotermales en la superficie debido a; 1) el sistema en este momento se encuentra sellado en la parte superior del sistema por la mineralización y alteración intrínseca a los sistemas convectivos (p.ej., ejerciendo de capa sello, pero ligada a mineralización y alteración). Esta alteración y mineralización se observó en los pozos exploratorios (López-Hernández *et al.*, 2009); 2) es un sistema geotérmico ciego (*blind geothermal system*); o 3) es un sistema de tipo *Kaipohan*. Este último se puede definir como sistemas geotérmicos sin manantiales termales pero que se identifica por su alteración hidrotermal intensa y emisiones difusas y frías de gases activos (Bogie *et al.*, 1987). Estos últimos tres puntos se desarrollan con más precisión en los siguientes párrafos.

1) El sellado de las fracturas en la parte superior del sistema es un fenómeno común y se genera debido a que los fluidos geotérmicos son muy salinos y tienden a depositar los minerales en la parte superior del sistema a causa del descenso de la temperatura, sellando los conductos (Cox *et al.*, 2001; Liotta *et al.*, 2010). 2) Los sistemas geotérmicos ciegos se pueden formar debido a que las fallas que controlan los sistemas comúnmente forman cuencas sedimentarias que permiten la acumulación de sedimentos arcillosos en la superficie que sirven de capa sello (p.ej., Craig *et al.*, 2021), lo cual evita que estos tengan una clara y ampliamente distribuida área con manifestaciones hidrotermales (p.ej., Rea-Downing *et al.*, 2026; Zheng *et al.*, 2026). Esto podría estar ocurriendo en Acoculco con los sedimentos lacustres encontrados en los alrededores del pozo EAC-1 (López-Hernández *et al.*, 2009; Liotta *et al.*, 2023).

3) La zona geotérmica de Acoculco presenta características similares a los sistemas de tipo *Kaipohan* (Bogie *et al.*, 1987; Prol-Ledesma *et al.*, 2025), como ha sido previamente propuesto por otros autores (López-Hernández *et al.*, 2009; Peiffer *et al.*, 2014). Estos sistemas se encuentran en zonas de alto relieve, se caracterizan por significativas emisiones frías de gases (dominadas por CO₂) y la presencia de alteración argílica (Bogie *et al.*, 1987). Acoculco cumple con estos criterios de manera notable: i) está situado a una elevación de ~2900 msnm, ii) registra un importante flujo de CO₂ (Bólos *et al.*, 2022; Pérez-Zárate *et al.*, 2024) y iii) exhibe alteración argílica (Canet *et al.*, 2015b).

La migración vertical de fluidos de Acoculco, evidenciada por los elementos hidrotermales en superficie, estaría sujeta al proceso clásico de sellamiento periódico de los conductos

permeables por precipitación de minerales y la alteración hidrotermal (aunado a que los sedimentos lacustres también actúan como capa sello). Dicho sellamiento es contrarrestado ocasionalmente por la actividad tectónica. Adicionalmente, el relieve topográfico favorecería una significativa migración lateral de fluidos a lo largo de estructuras y otros niveles permeables. De hecho, las descargas termales más notables, como los manantiales de Chignahuapan (hasta 49 °C; López-Hernández *et al.*, 2009; Santos-Raga *et al.*, 2021), Agua Salada y Madroño (Prol-Ledesma *et al.*, 2025), se localizan en la periferia de la caldera, a elevaciones menores (ver Figura 1), lo que respalda este modelo de flujo lateral más que vertical. La elevación a la que se encuentra la actividad hidrotermal en el centro de la caldera es de 2840 msnm, la elevación de Agua Salada y Madroño es de aproximadamente 2400 msnm, mientras que la de Chignahuapan es de 2290 msnm.

Finalmente, las zonas con mayor favorabilidad para alojar fluidos geotérmicos en el subsuelo serían las zonas con mayor favorabilidad identificadas en el modelo de este trabajo (Figura 7). De hecho, mediante un pozo exploratorio somero (132 m), donde se midió la temperatura a diferentes profundidades, se determinó que la zona de Alcaparrosa presenta temperaturas anómalas a profundidad con características convectivas (Prol-Ledesma *et al.*, 2025), lo cual da importante sustento a los resultados de este trabajo. El perfil de temperatura en pozos con características convectivas se caracteriza por presentar valores superiores al gradiente geotérmico medio (30 °C/km) y, a partir de cierta profundidad, tiende a estabilizarse, manteniendo la temperatura constante.

7. Conclusiones

El modelo de favorabilidad geotérmica de la zona de Acoculco muestra dos zonas principales, localizadas a aproximadamente 200 m al noroeste del pozo exploratorio EAC-1 y en la zona de Alcaparrosa (Figura 7). Si existiese un sistema hidrotermal activo en Acoculco, las zonas con mayor favorabilidad para alojar fluidos geotérmicos en el subsuelo serían las zonas identificadas en este trabajo con mayor favorabilidad geotérmica. En este sentido, se considera que, debido a la anomalía geotérmica existente, la edad reciente y el origen convectivo de los elementos hidrotermales fósiles, así como por la actividad hidrotermal actual y la actividad tectónica activa, en la zona de Acoculco podría existir un sistema geotérmico activo de tipo convectivo. La zona geotérmica de Acoculco debe continuar siendo explorada como un sistema convencional. Finalmente, para confirmar el potencial de las áreas favorables y continuar la exploración, se recomienda la perforación de pozos exploratorios de tipo TGH (*Temperature*

Gradient Holes) dentro de las zonas con favorabilidad obtenidas en este trabajo.

8. Referencias

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