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Schematization of Converging Groundwater Flow Systems Based on 3D Geostatistics

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Abstract: Groundwater is the main source of freshwater available for human beings and is generally extracted through wells. The objective of this work was to schematize the groundwater flow systems within the Calera Aquifer through 3D geostatistical estimations of hydraulic head and physico-chemical parameters and the integration of hydrogeological features. The evolution of groundwater during its circulation in the subsoil can be done by identifying different types of flow (local, intermediate, regional, or mixed). Two main approaches have been proposed for the identification of flow systems: explaining the evolution of physico-chemical parameters of water through its interaction with the geologic medium, and using cluster analysis; however, these approaches usually do not consider simultaneously the 3D distribution of hydraulic head, water quality parameters, and the geological media that can be useful to delineate converging flow systems with a differentiated origin. In this paper, the determination of groundwater flow systems within the Calera aquifer in Mexico is supported with 3D representations of these hydrogeological variables besides constructive data of the sampled well. For the case study, the convergence of different flow systems that are not identified through a single cluster analysis was actually noticed by the proposal done in this paper.

Keywords: groundwater; flow systems; 3D geostatistical estimates

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1. Introduction

Groundwater is an important part of the hydrological cycle. Aquifers are fed with rainwater that infiltrates the soil that reaches impermeable strata that prevent the passage of water.

For decades, groundwater has served as a very important source of water in the world for domestic use, agricultural production, mining, and industrial activities. This fact has produced in some regions a rapid lowering of water levels and extensive contaminated volumes [1,2].

The availability of groundwater within a region is usually determined through the water budget, which consists of estimating the difference between the total sum of inputs (recharge) and the total sum of outputs (discharge). The result represents the volume of water lost or gained by the aquifer storage for an established period of time, and the availability of water resources is varied in the different regions of the planet [3,4].

The way in which aquifers in Mexico are delimited and administrated does not allow for a comprehensive understanding of groundwater dynamics, which precludes an adequate planning and control of this resource. An alternative to achieve this goal is the implementation of the flow systems theory [5], which establishes that groundwater has three main types of flow: local, intermediate, and regional.

This theory states that groundwater is controlled by geological and hydrogeological factors, showing a physicochemical evolution in the water while flowing [6,7].

A groundwater flow system is a coherent natural and spatiotemporal unit with specific physicochemical properties. The definition of flow systems is possible because water has a "route memory in its molecule", and it includes the inputs from water precipitation (in mountains or plains), changes in temperature (T), pH, electric conductivity (EC, alkalinity, major Cations: Calsium $\left(Ca^{2+}\right)$, Magnesium $\left(Mg^{2+}\right)$ y Sodium $\left(Na^{+}\right)$ and anions: Chlorite $\left(Cl^{-}\right)$, Sulfate $\left(SO_4^{2-}\right)$ and Hydrogen carbonate $\left(HCO_3^{-}\right)$, and other elements in the routing of each system and area [8,9].

Laboratory and field analyses have been used to determine changes in groundwater composition along its flow path, in addition to recognizing groundwater as a geological agent causing a wide variety of processes and manifestations from the recharge to the transit and discharge zones. The integration of hydrogeochemical analyses of water within a geological framework is useful to identify the different types of flow regimes in a specific area [10,11].

When water comes into contact with the atmosphere, vegetation, and geology, it acquires chemical characteristics that provide valuable information to determine the origin, transit time, flow patterns, and water regimes. The chemical composition of groundwater is controlled by several factors, and the relative importance of these factors varies with the scale of the flow and the size of the geological environment [12,13].

By establishing the functioning of water through flow systems and its relationship with the components of the environment, integrating elements of the geological environment, soil and human factors, it is possible to identify the areas with the best conditions for the extraction of groundwater [14,15].

Several methods have been implemented to determine the flow systems within an aquifer, and most of them consider the physicochemical characteristics of the water extracted through wells [16]. The use of cluster analysis to group wells with similar characteristics and consequently define flow systems has been a very common option [17–20]. Another approach is to obtain hydrogeochemical patterns and mathematical relationships between ionic composition and electrical conductivity [21,22]. The characterization of the flow systems has been routinely done based on three elements: temperature, major ions, and the depth of wells [23–25].

To understand the environmental phenomena that surround groundwater, flow systems are usually characterized based on the distribution of hydrogeochemical parameters, without considering the hydraulic head and drainage systems, as well as converging flows [26,27].

The general objective of this manuscript is to outline the mechanisms of groundwater within the study area, which allows for obtaining a systematic vision of groundwater functioning by integrating various elements from the perspective of flow systems theory. To that end, cross sections of groundwater flow were constructed through the integration of 3D geostatistical estimates of hydraulic head and physicochemical parameters, the depth of the wells, as well as the geology of the study area.

This approach allowed for identifying the convergence of different flow systems within the Calera aquifer in Mexico. According to the knowledge of the authors of this work, these 3D representations have not been addressed by previous works, however, they could be useful for a better identification of water quality and quantity problems, environmental impacts, ecosystem conservation, and landscape schemes.

2. Materials and Methods

2.1. Description of the Study Zone

The Calera administrative aquifer is located in the highlands of the central part of Mexico and covers an approximate area of 2226 km^2 (Figure 1). It is administrated by the Local Direction of the state of Zacatecas. The climate of the region is semi-dry, and it presents an average annual rainfall of 425 mm, with an average temperature of 16.3 °C and average annual evaporation of 2263 mm [28].

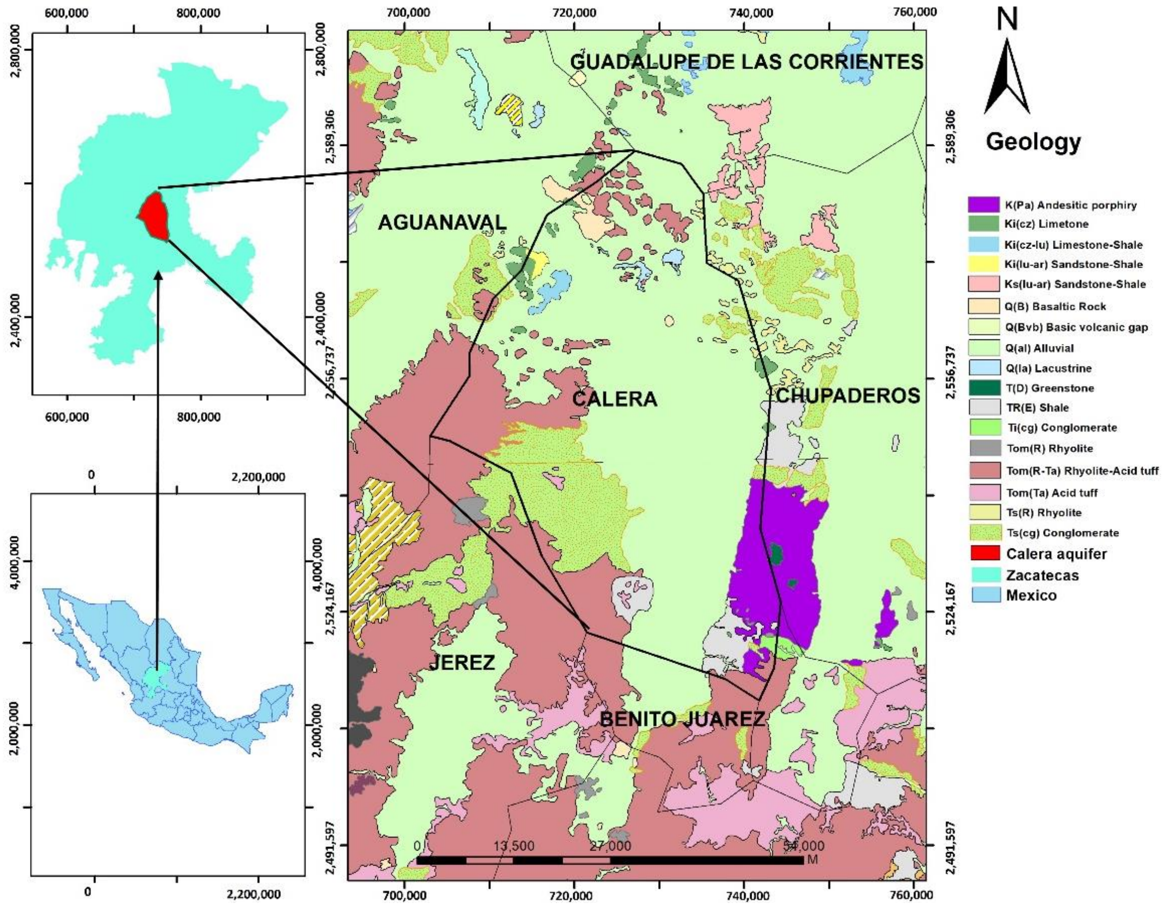

Figure 1. Geological map and location of the Calera administrative aquifer.

The aquifer is located in the volcanic terrain of the Sierra Madre Occidental, south of a regional graven structure that gives rise to the Calera endorheic basin. Two geological formations are located in the southeastern part, the Zacatecas Formation (maximum elevation 2700 masl) and Chilitos Formation in the southwest. These mountainous areas are linked to a flat area (average elevation of 2010 masl) in the center-south part and another flat area (of an average elevation of 2100 masl) in the north [29].

There is an important area with small intermittent streams that descends from the west towards the center of the study area and continues to the north. The area covers an important part of the state of Zacatecas, where the main social activities are established.

The Calera aquifer represents the main water supplier for the development of agriculture, industry, and mining in the region. On the other hand, approximately 50% of the total drinking water supplied to Calera, Morelos, and the Zacatecas-Guadalupe metropolitan area is extracted from the central and western part of the Calera aquifer, whereas mining and other industrial activities have gained influence in the evolution of groundwater availability during the last 30 years [30].

2.1.1. Geology

The regional geological framework of the study area is represented by the events related to the establishment of the Sierra Madre Occidental and the evolution of the Guerrero Territory [31]. The lithostratigraphy in the Guerrero terrain is composed of metamorphosed units of Cretaceous age, whereas the western Sierra Madre comprises units of Tertiary volcanic origin as well as units from the Quaternary age.

The Calera aquifer overlays an alluvium unit that extends between the tectonic pillars, which consists mainly of rocks from the Chilitos and Zacatecas formations. The Zacatecas Formation is composed of igneous (acid and basic) and sedimentary rocks, and metalimestone in thin laminated strata. The Chilitos Formation presents sandstone-siltstone, shale, volcanic rocks, and tertiary sediments of dioritic composition. Among the volcanic rocks are included: limestone, sandstone, and fissure basalt, whereas rhyolites, tuffs, and ignimbrites are related to igneous activity [32].

2.1.2. Hydrography

The area corresponds to a closed basin with an irregular shape, slightly elongated, with a north-south orientation, and delimited by the watershed formed by the Zacatecas Formation in its eastern portion, the Sierra de Fresnillo in its northwestern part, the Chilitos Formation in its western part, as well as some low elevation hills and ridges.

There are no significant surface currents in the aquifer, only small intermittent streams that flow into the Santa Ana and Sedano lagoons to the north.

2.1.3. Hydrogeology

The Calera aquifer is mainly unconfined with local leaky conditions, heterogeneous and anisotropic. The lower part is constituted by alluvial and fluvial sediments, of varied granulometry, conglomerates, and lacustrine deposits, whose thickness can be greater than 400 m in the center of the alluvial plain (Figure 2). The lower portion is housed in a sequence of volcanic rocks with a rhyolitic composition, among which acid tuffs, rhyolites, and ignimbrites predominate, and sedimentary rocks (limestone, shale and sandstone) that present secondary permeability due to fracturing [17]. At greater depths, limestones and sandstones represent a potential aquifer that may have leaky conditions.

The limits of the hydrogeological zone coincide with the watershed that delimits a closed surface and subterranean basin. The recharge of the aquifer comes from the pluvial precipitation that takes place on the formations, mountains and hills, which infiltrates and feeds the aquifer horizontally.

Another important aspect is the infiltration of water in the same valley and through stream beds where some water flows torrentially. An important recharge volume is related to irrigation excess.

Under natural conditions, the discharge should have been carried out through springs, by evapotranspiration in areas with shallow levels, and by horizontal flow towards the lagoons. Nowadays, the discharge is carried out artificially by pumping wells, and naturally a small volume is being drained by underground flow towards the Santa Ana and Sedano lagoons.

The preferential direction of the groundwater flow is from south to north, within the limits of the Mountains and hills, and the equipotential lines of elevation of the static level, appear slightly parallel to these, converging in the center of the valley to continue north.

2.2. Databases

Geological and hydrogeological factors essentially control the groundwater flow. When the water enters into contact with rocks, it presents hydrogeochemical characteristics that allow for identifying three general types of flow: local, intermediate, and regional [33,34]. Therefore, a multivariate model can be useful to understand the relationships between the groundwater variables and their relevance to the problem under study.

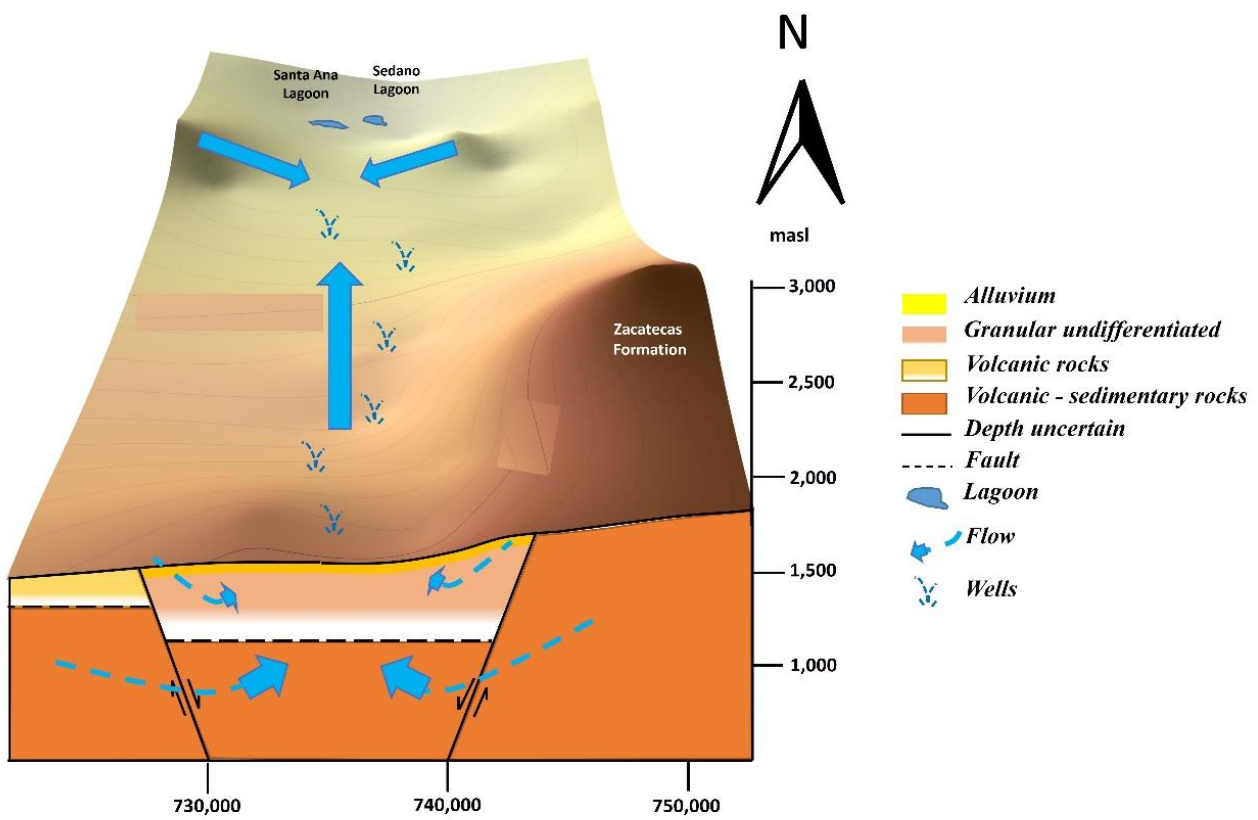

Figure 2. Schematic illustration of the Calera aquifer.

The sampling was carried out in the period between July and August of 2020, following the methodology described in Apha-SMWW (2006), and the Mexican regulations stablished in 2020 for the parameters analyzed. The sampling campaign consisted in visiting 31 wells. Laboratory determinations were done at the Universidad Autónoma de Zacatecas facilities.

The sampling campaign consisted in visiting 31 well within the period between July and August of 2020, following the methodology described in Apha-SMWW (2006) and the Mexican regulations stablished in 2020 for the analyzed parameters.

The field measurements were executed in the following manner: volumetric alkalinity with an AL-DT Model Titulator with H2SO4 to 0.16 N, electrical conductivity (EC) and temperature (T) with Orion 4 STARTM Series Enter and dissolved oxygen (DO) with Lutron Oxygen Meter Model: DO-5510ha with isolation to avoid alterations in the contact of water with the atmospheric conditions during sampling [35]. Laboratory determinations were done at the Universidad Autónoma de Zacatecas facilities.

Additionally, for each visited well, it was obtained the elevation at surface, the depth to the water level and the well depth. The data obtained for all the visited wells are presented in (Table 1).

2.3. Determination of Groundwater Flow Systems Using Cluster Analysis

To find the factors, linear combinations of all the variables included in the analysis are created, observing the correlation coefficient presented in the correlation matrix.

Cluster analysis is a statistical technique designed to group elements, trying to achieve maximum homogeneity in each group [17–20].

Finally, some elementary statistical functions are defined, such as: minimum value, maximum value, mean, median, and standard deviation for each determined group. The values obtained for these statistical functions allow for identifying the flow systems.

Next, the theory corresponding to the Analysis of Conglomerates is approached.

Table 1. Data from the wells sampled in the Calera aquifer for the year 2020 (ES = Elevation at surface, SWLE = Static water level elevation, WDE = Well depth elevation, WD = Well depth).

ID	ES (masl)	SWLE (masl)	WDE (m)	WD (m)	T (°C)	EC (μs/cm)	DO (mg/L)	TDS (mg/L)	Ca^{2+} (mg/L)	Mg^{2+} (mg/L)	Na^{+} (mg/L)	K^{-} (mg/L)	Cl^{-} (mg/L)	HCO_3^- (mg/L)	SO_4^{2-} (mg/L)
P-2	2086	2071.8	14.2	120	22.8	1090	6.7	534.1	77.13	37.83	97.99	22.05	193.6	236.68	90
P-3	2095	2078.4	16.5	110	20.4	3390	5.7	1661.1	374.37	197.59	168.5	30.92	620.4	259.86	1040
P-5	2075	2016.6	58.3	300	24.5	440	5.8	215.6	33.52	3.46	45.81	12.34	11.9	208.62	28
P-6	2078	2043.1	34.9	100	25.3	660	4.3	323.4	47.24	24.02	55.71	12.85	25.3	334.28	38
P-7	2105	2062.9	42.0	190	22.6	500	6	245	23.12	7.36	69.14	11.65	13.9	259.86	26
P-8	2144	2047.0	96.9	179	33.7	426	5.3	208.7	25.19	3.99	61.46	9.76	16.9	234.24	6
P-9	2084	2036.4	47.6	150	23.6	513	5.9	251.4	28.71	20.43	43.3	11	13.9	234.24	32
P-10	2105	2022.2	82.8	110	23	454	6.3	222.5	71.21	6.18	41.8	14	13.4	292.80	6
P-12	2100	2017.6	82.3	100	27.3	520	6.7	254.8	25.47	16	60.66	6.65	10.4	256.2	58
P-14	2116	2049.1	66.8	100	27.9	404	6.1	198	25.28	8.73	51.02	13.37	36.7	191.54	24
P-15	2137	2060.8	76.1	100	26	476	5.4	233.2	28.58	4.87	62.12	12.35	13.9	235.46	45
P-16	2135	2037.2	97.7	130	23	470	6	230.3	20.48	14.49	21.36	5.16	13.9	152.26	28
P-17	2184	2100.6	83.3	150	27	390	5.7	191.1	31.11	7.24	18.94	8.68	14.9	141.52	10
P-18	2171	2105.0	65.9	120	26.4	470	4.6	230.3	17.82	2.79	70.43	11.02	20.3	235.22	26
P-19	2251	2185.8	65.1	160	27.3	630	6.3	308.7	49.98	22.14	30.67	12.21	37.2	155.18	110
P-22	2250	2151.1	98.8	200	27.3	467	5.9	228.8	39.4	6.37	52.97	10.44	19.8	287.92	20
P-23	2250	2142.0	108.0	200	25.7	707	5.8	346.4	49.9	27.76	31.59	11.01	33.3	284.26	22
P-24	2196	2094.1	101.8	180	25.5	624	6.2	305.8	19.53	40.76	35.08	12.06	31.8	219.6	72
P-25	2102	2015.2	86.8	190	25.5	437	7	214.1	19.41	11.39	47.74	13.25	11.4	204.96	28
P-26	2183	2084.7	98.2	175	26	499	6.8	244.5	14.94	13.06	62.17	13.38	16.9	214.72	32
P-27	2115	2041.4	73.6	300	26.1	487	5.9	238.6	16.84	26.71	37.31	10.39	14.4	258.64	20
P-28	2100	2046.9	53.1	300	23.6	553	6	271	42.01	30.93	15.63	5.76	10.4	239.12	32
P-29	2105	2040.5	64.4	277	24	560	5.3	274.4	29.35	27.57	48.35	10.98	11.4	259.62	70
P-31	2055	2031.8	23.1	120	27.8	501	5.7	245.5	33.67	4.78	92.63	7.49	37.2	244	34
P-32	2124	2065.3	58.7	190	37	570	6.6	279.3	1.85	0.1	106.73	4.93	10.4	225.7	15
P-33	2271	2132.3	138.6	260	27	601	6.6	294.5	52.48	10.32	53.31	16.76	31.7	268.4	56
P-34	2186	2082.4	103.6	200	21.7	500	5.4	245	43.25	28.03	15.46	5.03	22.8	214.72	45
P-35	2224	2161.9	62.1	120	28.8	400	5.2	196	36.63	26.73	20.61	5.73	19.9	176.66	56
P-36	2113	2031.0	81.9	200	25	390	3.7	191.1	24.73	2.88	34.54	8.18	11.9	151.8	24
P-38	2079	2008.6	70.3	120	26.4	441	6	216.1	56.17	4.52	53.64	17.91	14.9	331.84	12
P-39	2064	2010.0	53.9	100	26.4	441	6	216.1	56.17	4.52	53.64	17.91	14.9	331.84	12
P-40	2071	2030.9	40.1	120	24.4	1441	6.8	706.1	148.92	17.33	121.3	19.18	183.6	151.28	275

2.3.1. Correlation Matrix

Pearson's correlation coefficient measures the statistical relationship between two continuous variables.

The correlation coefficient can take a range of values from +1 to −1. A value of 0 indicates that there is no association between the two variables. A value greater than 0 indicates a positive association. That is, as the value of one variable increases, so does the value of the other. A value less than 0 indicates a negative association; that is, as the value of one variable increases, the value of the other decreases [18–36].

The Pearson correlation coefficient formula is as follows:

$$r_{xy} = \frac{\sum z_x z_y}{n} \tag{1}$$

where x is equal to the first variable, y belongs to second variable, z_x is the standard deviation of first variable, z_y is the standard deviation of second variable, and n is the number of data elements. [37,38].

2.3.2. Cluster Analysis

Cluster analysis is a set of multivariate techniques used to classify a set of individuals into homogeneous groups. Therefore, it is essential to define a measure of similarity or divergence to classify individuals into one group or another.

To join chemical samples in a cluster, it is necessary to know the measures of similarity or distance between them. Thus, a great similarity between the groups means a small value of distance [39,40].

Fundamentally, it consists of solving the following problem: given a set of individuals (N elements) characterized by the information of n variables X_i, $(i = 1,\ 2, \ldots, n)$, classify them so that the individuals belonging to a group (cluster) are as similar to each other as possible, with the different groups being as dissimilar to each other as possible [24,40].

The similarity calculation is based on the squared Euclidean distance presenting high values in case of a large distance or small similarity. The distance is calculated by the sum of the differences of the variable values. For the two cases of $\boldsymbol{X}$ and $\boldsymbol{Y}$, the Euclidean distance D results in:

$$D^2 = \sum_{i=1}^{n} (\boldsymbol{X}_i - \boldsymbol{Y}_i)^2 \tag{2}$$

From the matrix of the distances, the cluster analysis is carried out based on a classification of the distance where cases with a small distance are joined to a cluster, whereas cases with large distances are joined in different clusters [30–38].

2.4. Determination of Groundwater Flow Systems Based on 3D Multivariate Data

To understand groundwater evolution, it is necessary to analyze the relationships between the dynamics of groundwater and the hydrogeological elements that are present in the study area. To characterize the flow systems, it is necessary to analyze simultaneously, from a 3D perspective, the distribution of the chemical parameters present in water, the geological framework, and the hydraulic head distribution [41,42].

Knowledge of the hydraulic head *(h)* distribution throughout the aquifer, that is, a 3D representation of this variable, is essential to understand the dynamics of the flow. In this study, a 3D geostatistical estimation of h is performed [43].

The knowledge of the distribution of the hydraulic head as well as the hydrogeochemical parameters of the water throughout the aquifer, that is, a 3D representation of these variables, is essential to understand the dynamics of the flow. In this study, a 3D geostatistical estimation is performed [44].

The 3D estimation of the hydraulic head and of the hydrogeochemical parameters within the aquifer allowed for determining the various directions of groundwater flow and the behavior of the hydrogeochemical parameters. The results obtained from the analysis of h in conjunction with the hydrogeochemical evolution of the water, as well as the characteristics of the wells within the geological framework, allowed for a scheme to be carried out in order to identify the existence of converging flow systems with different origins. In the next subsections, we define the hydraulic head and the geostatistical theory for its 3D estimation.

2.4.1. Hydraulic Head

The hydraulic head is defined as a specific measure of liquid pressure above a datum, whose properties are such that flow always occurs from regions where this quantity has high values to regions where the quantity has lower values [45,46]. Figure 3 shows a representation of the hydraulic head (h) measured in the point P of a well drilled in an aquifer with an essentially horizontal flow.

The hydraulic head (h) at point P can be calculated with the following expression:

$$h = z + \frac{p}{\gamma} \tag{3}$$

where z is the elevation head (it is the elevation of the point where the hydraulic head is measured with respect to a datum) and $\frac{p}{\gamma}$ is the pressure head (it corresponds to the height of the water column above z).

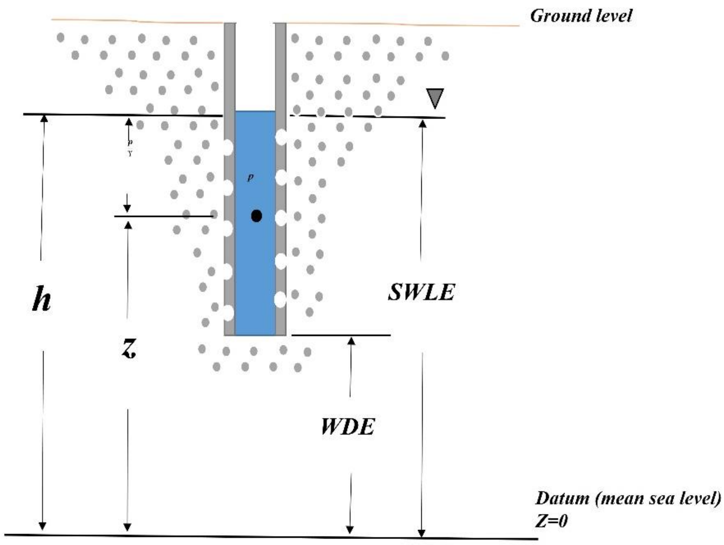

Figure 3. Representation of the hydraulic head h measured at point P within a well.

The static water level elevation (*SWLE*) represents the value of the hydraulic head at the intake point of a borehole. For a piezometer, the intake point is well known. However, the *SWLE* measured in screened wells is a weighted value of the hydraulic head variations through the screen length. In the case study, we assume that the *SWLE* is a measure of the hydraulic head at the central point (P) of the water column inside the well. The elevation of this measurement point (z) is obtained with the following expression:

$$z = \frac{SWLE - WDE}{2} + WDE \tag{4}$$

where *WDE* is the well depth elevation.

2.4.2. 3D Geostatistical Analysis

The methodology to perform the geostatistical analysis consists of three steps: exploratory analysis, structural analysis, and spatial estimation [47].

Exploratory Analysis

The first step is to carry out an exploratory analysis which is based on descriptive statistical techniques that allow characterizing the data according to its behavior, trying to obtain a normal distribution [48].

Structural Analysis

Structural analysis is the estimation and modeling process that describes the spatial correlation by means of a variogram. A variogram is a function that describes the degree of spatial correlation that allows for analyzing the behavior of a variable over a defined area [27,36].

The experimental variogram $\overline{\gamma}(\mathbf{h})$ is based on the data and the structure of the phenomenon:

$$\overline{\gamma}(\mathbf{h}) = \frac{1}{2N(\mathbf{h})} \sum_{i=1}^{N(\mathbf{h})} [\mathbf{Z}(\mathbf{x}_i + \mathbf{h}) - \mathbf{Z}(\mathbf{x}_i)]^2 \tag{5}$$

where: $\overline{\gamma}(\mathbf{h})$ is the sample variogram, $\boldsymbol{N}(\mathbf{h})$ is the number of pairs $\mathbf{Z}(\mathbf{x}_i)$, and $\mathbf{Z}(\mathbf{x}_i + \mathbf{h})$, which are separated by a distance $\mathbf{h} = |\mathbf{h}|$, are known as "lag."

The structural analysis consists of plotting the sample variogram and fitting an authorized model. Some models to choose from are: Circular, Spherical, Exponential, Gaussian, Linear, among others. The selected model influences the prediction of unknown values; each model is designed to fit different types of phenomena more precisely [36,41].

Spatial Estimation

The kriging technique uses the characteristics of variability and spatial correlation (variogram) in the estimation and implies a previous analysis of the information in order to define or extract from this initial information a model that represents its spatial continuity. The best possible estimated value is obtained at each location from the measured data, accompanied by the kriging variance as a measure of the estimation error [39–48].

3. Results and Discussion

For a preliminary analysis, the flow systems in the Calera aquifer are determined by means of cluster analysis, and these results are compared with 3D multivariate data that includes the hydraulic head 3D estimation, geology, and hydrogeochemical parameters.

3.1. Groundwater Flow Systems Using a Cluster Analysis

For the 2020 data, a correlation matrix was generated to represent the statistical relationship between two or more variables. Pearson's correlation is a tool that can help analyze the relationships identified in the water quality analysis (Table 2).

Table 2. Correlation matrix for physicochemical parameters in water sampled in 2020.

Correlation	T	DO	TDS	SO_4^{2-}	HCO_3^-	Ca^{2+}	Mg^{2+}	Na^+	Cl^-
T	1.000								
OD	−0.008	1.000							
SDT	−0.359	0.100	1.000						
SO_4^{2-}	−0.340	0.024	**0.976**	1.000					
HCO_3^-	−0.075	0.034	0.046	−0.013	1.000				
Ca^{2+}	−0.409	0.067	**0.967**	**0.960**	0.102	1.000			
Mg^{2+}	−0.397	−0.044	**0.910**	**0.934**	0.053	**0.873**	1.000		
Na^+	0.013	0.244	**0.744**	0.677	0.172	0.675	0.479	1.000	
Cl^-	−0.363	0.094	**0.987**	**0.966**	0.019	**0.962**	**0.900**	**0.745**	1.000

The percentages of anions and cations were analyzed for each well in order to group them into different families (Figure 4).

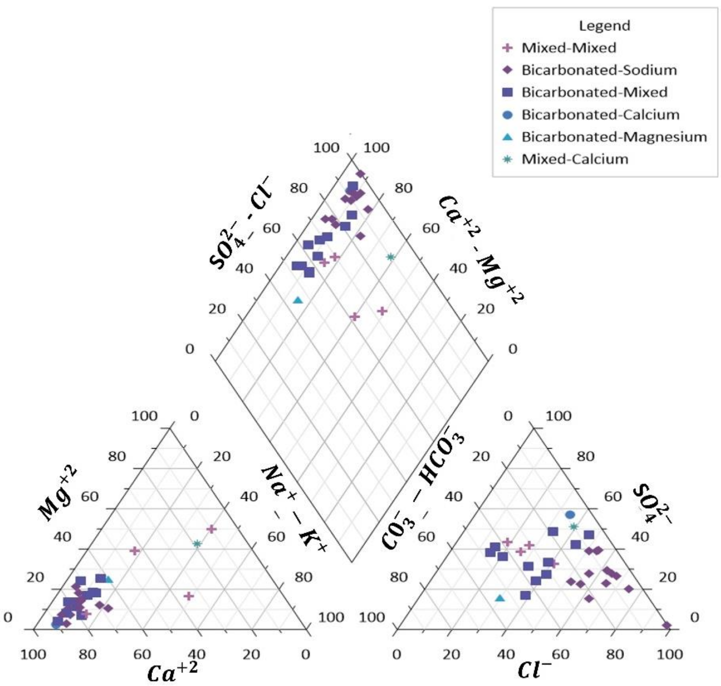

Figure 4. Water families from the Calera aquifer.

To determine if the well captures water from local, intermediate, regional flow or if it is a combination, parameters such as hydraulic head, temperature, TDS, DO, depth of the well and location, and percentage of anions and cations were observed, making a comparison with wells close to the one being analyzed, looking for an evolution in its parameters, and thus determining if they coincide with the same flow system or belong to some other flow with which it is being analyzed or observing the existence of a mixture.

Values greater than 0.7 are highlighted in bold to indicate the close relationship between the variables involved, so the TDS are closely related to the major ions Ca^{2+}, Mg^{2+}, and Na^{+}; this is due to the constant accumulation of these ions in the groundwater flow. The correlation coefficients between Cl^{-} and Ca^{2+} as well as Cl^{-} and Mg^{2+} could be explained as a cationic change. The relationship between Na^{+} and Cl^{-} is mainly due to the existence of waters to which appreciable amounts of salts have been added. SO_4^{2-} shows that a correlation with elements such as Ca^{2+}, Mg^{2+} could be interpreted as possible dissolution of gypsum and dolomite. $HCO_3{}^{-}$ has correlation coefficients less than 0.5 with Ca^{2+} and Mg^{2+}, which suggests low dissolution and/or precipitation of calcite and dolomite.

3.2. Determination of Flow Systems

The flow systems were determined by performing a cluster analysis that allowed the samples to be grouped for the year 2020.

Table 3 shows the groups that resulted from the cluster analysis. Through the analysis of chemical parameters, a flow system was assigned to each of the identified groups.

Table 3. Clustering of flows as a result of the cluster analysis for the year 2020.

Groundwater Flow Systems	Statistics	T (°C)	EC (µs/cm)	DO (mg/L)	TDS (mg/L)	Cl^{-} (mg/L)	SO_4^{2-} (mg/L)	$HCO_3{}^{-}$ (mg/L)	Ca^{2+} (mg/L)	Mg^{2+} (mg/L)	Na^{+} (mg/L)
Intermediate	Min	21.70	400.00	4.30	196.00	15.40	22.00	155.18	19.53	10.32	15.46
	Max	29.00	707.00	6.60	346.40	37.20	110.00	284.26	52.48	41.47	53.31
	Mean	26.25	561.50	5.68	275.14	26.55	63.38	216.77	39.76	28.67	29.58
	Median	26.35	565.50	5.70	277.10	27.25	56.00	217.16	39.94	27.90	29.00
	S. Desv	2.36	97.08	0.73	47.57	7.88	29.94	44.30	11.27	10.05	11.54
Regional	Min	22.60	390.00	3.70	191.10	10.40	6.00	141.52	1.85	0.10	15.63
	Max	37.00	1441.00	7.00	706.10	183.60	275.00	334.28	148.92	30.93	121.30
	Mean	26.24	521.25	5.83	255.41	23.44	37.54	236.57	35.88	11.24	55.35
	Median	26.00	473.00	5.95	231.75	14.15	27.00	235.34	28.65	7.30	53.31
	S. Desv	3.25	205.50	0.79	100.70	34.87	52.79	55.38	28.46	8.98	24.96
Apparently regional	Min	20.40	1090.00	5.70	534.10	193.60	90.00	236.68	77.13	37.83	97.99
	Max	22.80	3390.00	6.70	1661.10	620.40	1040.00	259.86	374.37	197.59	168.50
	Mean	21.60	2240.00	6.20	1097.60	407.00	565.00	248.27	225.75	117.71	133.25
	Median	21.60	2240.00	6.20	1097.60	407.00	565.00	248.27	225.75	117.71	133.25
	S. Desv	1.70	1626.35	0.71	796.91	301.79	671.75	16.39	210.18	112.97	49.86

The distribution of the samples in the groups is presented for the group of intermediate flow (8 samples) and regional (24 samples). In the case of group 3, an apparently regional flow is presented (2 samples). This distribution indicates a low presence of mixed waters within the aquifer.

The intermediate flow has an average temperature of 26.6 °C, and analyzing the trace elements and the average values for TDS (275.14 mg/L), DO (5.68 mg/L), and Cl^{-} (26.55 mg/L) suggest a relatively short travel of groundwater and residence time. The average values for the major ions are: Na^{+} (29.58 mg/L), Ca^{2+} (39.76 mg/L), and Mg^{2+} (28.67 mg/L). The wells associated with the regional flow capture water between 2124–2308 masl, with an average depth of wells of 181 m. Recharge and discharge areas for this flow system are located outside the administrative aquifer.

The regional flow presents average values in trace elements with TDS (255.41 mg/L), DO (5.38 mg/L), Cl^{-} (23.44 mg/L), whereas the average values for the major ions are: Na^{+} (55.35 mg/L), Ca^{2+} (35.88 mg/L), and Mg^{2+} and (11.24 mg/L), which indicates that the water has a long travel and interaction time with the granular material. The wells that apparently capture water from the intermediate flow present an elevation at the surface that ranges from 2055–2250 masl, having an average depth of 112 m. The recharge zone for these wells is located at the Chilitos formation until it reaches a discharge in the area of Calera located between Gral. Enrique Estrada, Pánuco, and Villa de Cos.

An apparently regional flow was also observed with average values in TDS (1097.60 mg/L), DO (6.20 mg/L), and Cl^- (407 mg/L). The average values for the major ions are Na^+ (133.25 mg/L), Ca^{2+} (35.88 mg/L), and Mg^{2+} (117.71 mg/L). The extraction of groundwater in wells for agricultural activities, the supply of drinking water, and mining activities generate a mixture of water from regional and intermediate flows, having an elevation at the surface between 2086 and 2095 masl and an average depth of wells of 112 m.

Figure 5 shows the location of the wells in the Calera aquifer corresponding to each flow system that was determined through cluster analysis using the selected physicochemical parameters.

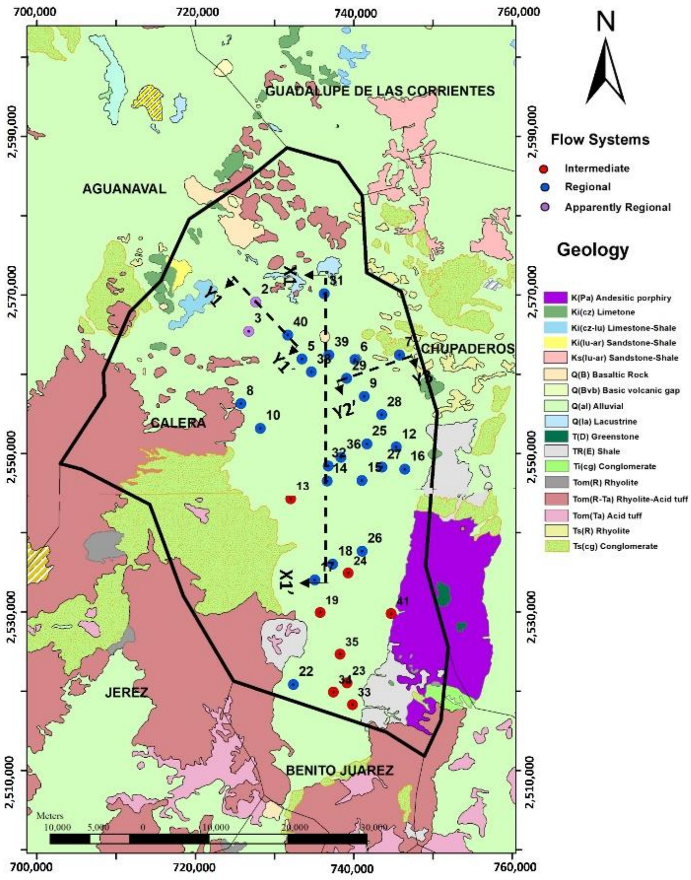

Figure 5. Groundwater flow systems identified at each well using cluster analysis (2020).

To understand the functioning of groundwater, its properties and its manifestations, it is important to know that groundwater is the natural cause of a great variety of processes and phenomena and, therefore, it is a general geological agent [21–40].

Temperature, DO, TDS, and Cl^- were used as trace elements that help to identify flow characteristics; these elements interact inside and outside the earth's surface with increasing and decreasing values. Outside the earth's surface, the water has contact with atmospheric factors that increase the DO values but entering the earth's surface, these values decrease along their route in the subsoil. The travel or contact of water with granular materials increases TDS and Cl^- values.

3.3. Groundwater Flow Systems Determined with 3D Multivariate Data

The initial step consists in obtaining a 3D estimation of the hydraulic head using the kriging method. To that end, it was necessary to determine a z coordinate (using Equation (4)) where the hydraulic head value is assigned. The parameters of the selected spherical variogram model are nugget effect of 50 m and a sill of 5150 m^2 with a range of 23,500 m.

The 3D mesh estimate is made up of 24 cells in x, 52 cells in y, as well as 33 cells in z, resulting in a series of hydraulic head values at each node of the 3D mesh as shown in Figure 6 to identify groundwater flow directions.

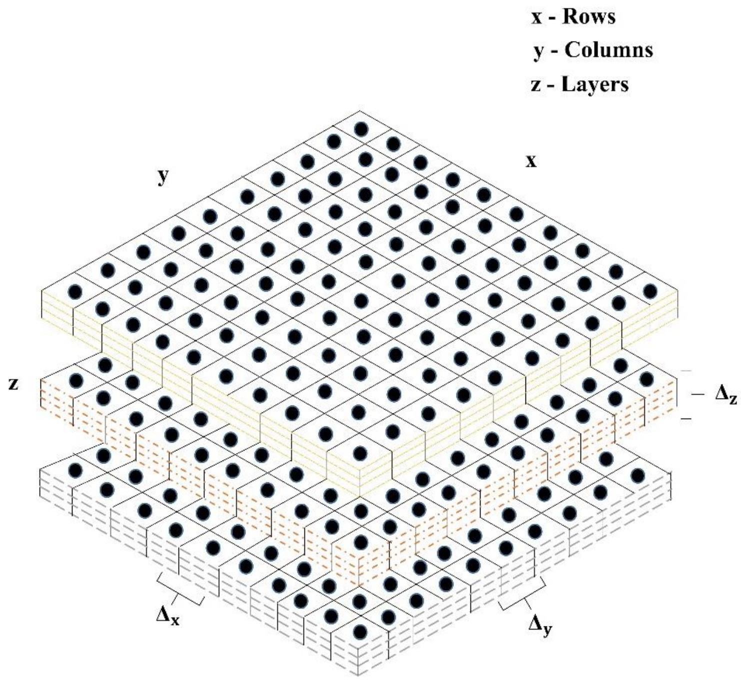

Figure 6. Example of a 3D grid for the geostatistical estimation of the hydraulic head.

For the grouping of wells, analyses of different cross sections were carried out including the 3D estimation of the hydraulic head, the characteristics of the wells, and the physicochemical parameters within the geological framework. This type of analysis favors a more complete analysis for the identification of the flow systems within an aquifer [8–48].

An analysis of water evolution for each well was done. It considered the flow directions that emerged from the hydraulic head estimation; the well depth helped to determine the flow system that is captured. An abnormal evolution of the groundwater physicochemical parameters not explained by the geological conditions was associated with the convergence of a different flow system.

Figures 7–9 show a representation of cross sections of Figure 5. Two of them are oriented from west to east and one from north to south. These analyses allow for identifying the convergence of different groundwater flow systems within the study region [36].

In Figure 7 (cross-section X1–X1′), a predominant flow from south to north is shown, with a large zone of converging flows established in the northern part. A special case corresponds to well P-32, which has characteristics that do not correspond to the natural evolution of groundwater in the flow system (contrasting hydraulic head and groundwater quality parameters), which correspond to a deeper flow. Whereas well P-38 is located in a discharge area where several flows converge, wells P-14, P-17, and P-18 receive water from the southwestern part of the aquifer that enters from the Chilitos Formation (the acid rhyolite tuff) and then flows north toward the cone that was formed by the high-water extraction in that zone of the aquifer.

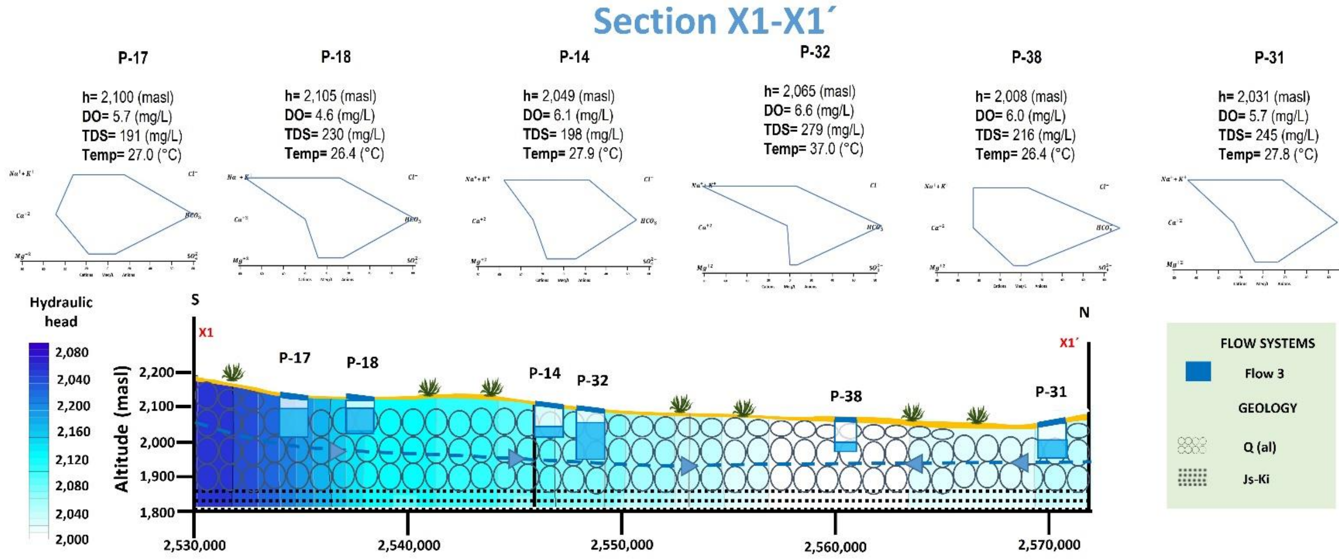

Figure 7. Hydrogeological cross section X1–X1′.

In Figure 8 (cross section Y1–Y1′), water from wells P-2 and P-40 present chemical characteristics and the hydraulic head estimates that suggest an origin from the northwest area of the aquifer. These values suggest a long route of water belonging to this flow, in addition to the fact that in this area there is a good variety of geological elements, such as alluvium sequences (Qal), greywacke, and shale (KIGP), some iterations of limestone (Js-Kj), as well as immature conglomerates formed by limestone clasts, ignimbrites, and shale, resulting in very high TDS values in its water quality.

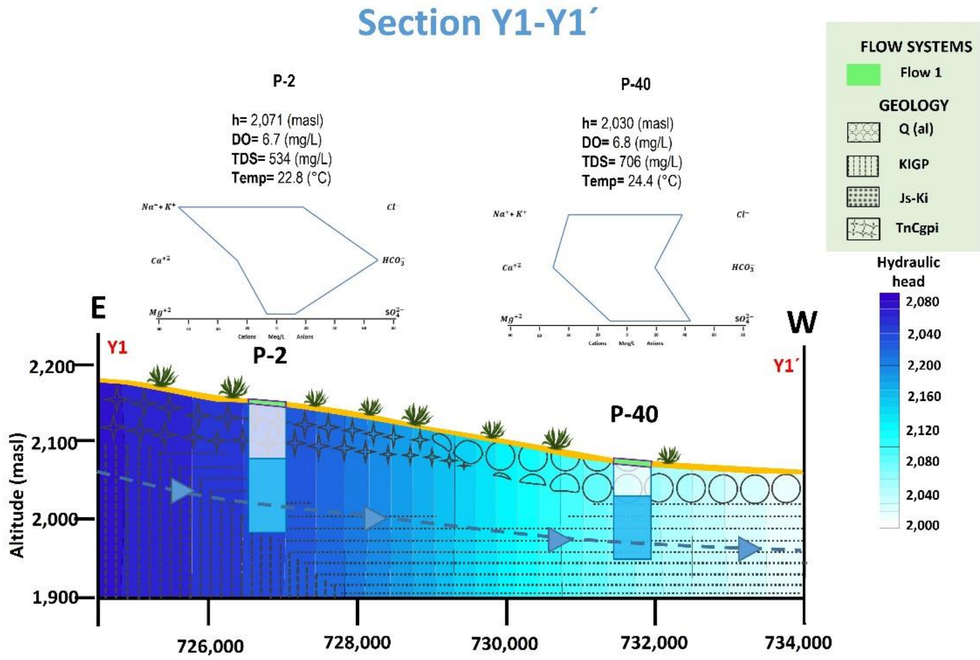

Figure 8. Hydrogeological cross section Y1–Y1′.

In Figure 9 (cross-section Y2–Y2′), well P-7 captures water from the flow that occurs in the northwest part of the aquifer, towards the cone formed to the north of the aquifer where several flows converge. The water quality parameters evolve from the characteristics of well P-7 to those of well P-29.

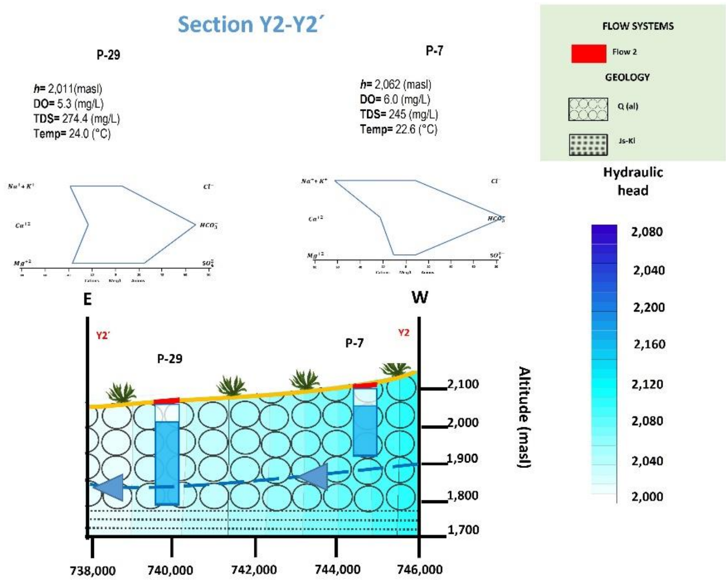

Figure 9. Hydrogeological cross section Y2–Y2′.

The estimation of the hydraulic head in 3D, the characteristics of the wells, the physicochemical parameters of the water, and the geology allowed for identifying the existence of flows that converge. Through this analysis, three flows were identified, in which intermediate converge of flows and regional flows could be observed (Figure 10).

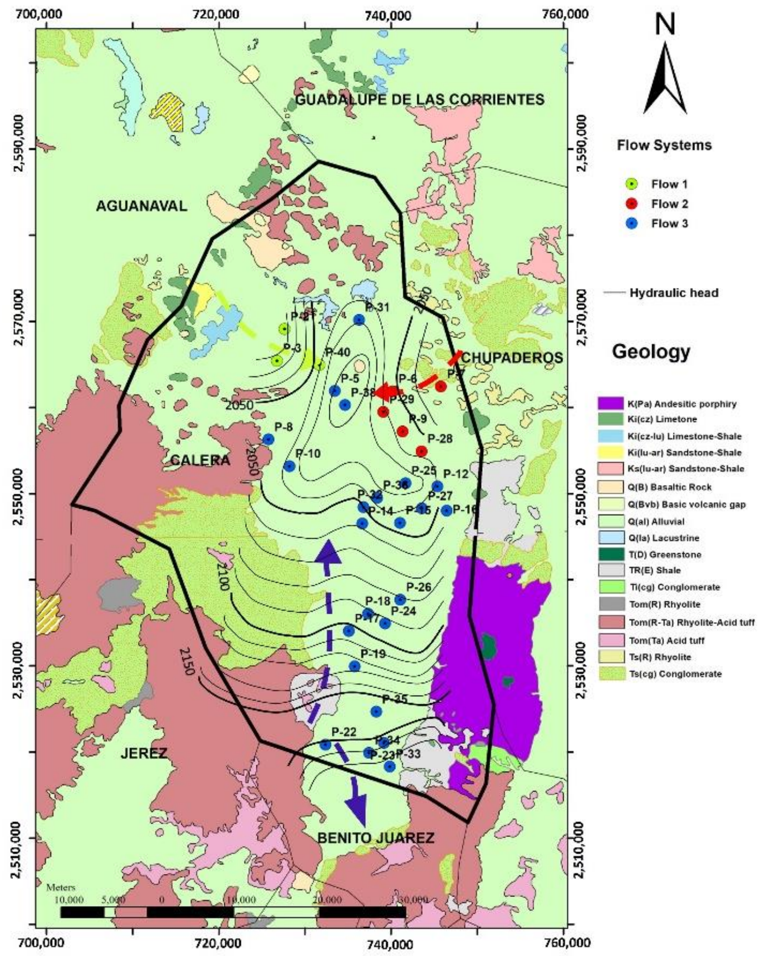

Figure 10. Groundwater flow systems identified within the aquifer using 3D multivariate data (2020).

Using statistical data such as: maximum, minimum, mean, median, and standard deviation values, the characteristics of each identified flow are shown in Table 4.

Table 4. Grouping of flow systems as a result of 3D geostatistical analysis of hydraulic head and physicochemical parameters of water, (*h* = Hydraulic Head, TDS = Total dissolved solids, and DO = Dissolved oxygen).

Flows	Staticstics Data	*h* (masl)	T (°C)	DO (mg/L)	SDT (mg/L)	Cl^- (mg/L)	SO_4^{2-} (mg/L)	$HCO_3{}^-$ (mg/L)	Ca^{2+} (mg/L)	Mg^{2+} (mg/L)	Na^+ (mg/L)	K^- (mg/L)
FLOW 1	Min	2030.90	20.40	5.70	534.10	183.60	90.00	151.28	77.13	17.33	97.99	19.18
	Max	2078.45	24.40	6.80	1661.10	620.40	1040.00	259.86	374.37	197.59	168.50	30.92
	Mean	2060.38	22.53	6.40	967.10	332.53	468.33	215.94	200.14	84.25	129.26	24.05
	Median	2071.80	22.80	6.70	706.10	193.60	275.00	236.68	148.92	37.83	121.30	22.05
	S. Desv	25.75	2.01	0.61	607.14	249.35	503.65	57.18	155.10	98.69	35.92	6.12
FLOW 2	Min	2036.40	22.60	4.30	245.00	10.40	26.00	234.24	23.12	7.36	15.63	5.76
	Max	1878.00	25.30	6.00	323.40	25.30	70.00	334.28	47.24	30.93	69.14	12.85
	Mean	1687.60	23.82	5.50	273.04	14.98	39.60	265.42	34.09	22.06	46.43	10.45
	Median	1725.00	23.60	5.90	271.00	13.90	32.00	259.62	29.35	24.02	48.35	11.00
	S. Desv	10.21	0.98	0.73	30.81	5.97	17.52	40.22	10.09	9.11	19.77	2.73
FLOW 3	Min	2035.41	22.57	4.73	196.97	12.40	10.33	167.31	19.38	3.31	26.19	5.82
	Max	2112.64	33.17	6.63	299.23	37.03	72.00	292.80	50.76	24.99	84.22	16.02
	Mean	2072.19	26.79	5.86	239.50	20.66	32.20	231.32	35.58	11.95	48.18	10.76
	Median	2071.11	26.47	5.90	231.43	17.20	28.33	226.11	32.15	12.68	45.11	11.27
	S. Desv	26.85	3.32	0.62	35.60	9.21	21.40	49.33	11.43	7.66	19.67	3.75

Through the estimation of the hydraulic head, it was possible to identify three flows that presented the following average values:

Flow 1 presents an average temperature of 22.53 °C, and when analyzing the trace elements, the average values of TDS (967.10 mg/L), DO (6.40 mg/L), and Cl^- (332.53 mg/L) suggest a long way groundwater and a wide variety of geology. The average values of the main ions are: Na^+ (129.26 mg/L), Ca^{2+} (200.14 mg/L), and Mg^{2+} (84.25 mg/L). The wells associated with the regional flow present a hydraulic head between (2031–2078 masl), and the recharge zone of this flow system is located outside the administrative aquifer, having its origin in the northwestern part until it ends in the central part of the aquifer.

Flow 2 has an average temperature of 23.82 °C, and when analyzing the trace elements, the average values of TDS (273.04 mg/L), DO (5.50 mg/L), and Cl^- (14.98 mg/L), suggest that the water they have a short travel and interaction time with the granular material. The average values of the main ions are: Na^+ (46.43 mg/L), Ca^{2+} (34.09 mg/L), and Mg^{2+} (22.06 mg/L). Presenting a hydraulic head between (2036–2062 masl), this flow comes from the northern part of the aquifer.

Flow 3 shows an average temperature of 26.79 °C, and when analyzing the trace elements, the average values of TDS (239.50 mg/L), DO (5.86 mg/L), and Cl^- (20.66 mg/L), present a relationship between water with very short granular material as well as the travel time of the water. The average values of the main ions are: Na^+ (4818 mg/L), Ca^{2+} (35.58 mg/L), and Mg^{2+} (11.95 mg/L). Presenting a hydraulic head between the values (2008–2185 masl), this flow travels from the northeast part until it reaches the central part of the aquifer.

4. Comparative Discussion

This chapter is made a comparative discussion between cluster analysis and 3Dmultivariate data, and it shows to which flow system each well belongs (Table 5).

The cluster analysis forms groups, which are made up of wells that share similar patterns and, through statistical analysis, make a comparison to determine the flow system to which this group that shares similarities belongs, being that this analysis is carried out in 2D and only includes water quality parameters.

Table 5. Comparison of the identification of flow systems by cluster analysis and 3D multivariate data (3Dmd).

Well	Cluster Analysis	3Dmd
P-2	Apparently regional	Flow 1 (Intermediate)
P-40	Intermediate	Flow 1 (Intermediate)
P-3	Apparently regional	Flow 1 (Intermediate)
P-7	Intermediate	Flow 2 (Intermediate)
P-9	Intermediate	Flow 2 (Intermediate)
P-28	Intermediate	Flow 2 (Intermediate)
P-29	Intermediate	Flow 2 (Intermediate)
P-6	Intermediate	Flow 2 (Intermediate)
P-5	Intermediate	Flow 3 (Intermediate)
P-31	Intermediate	Flow 3 (Intermediate)
P-38	Intermediate	Flow 3 (Intermediate)
P-8	Intermediate	Flow 3 (Intermediate)
P-10	Intermediate	Flow 3 (Intermediate)
P-25	Intermediate	Flow 3 (Converge of flows)
P-32	Intermediate	Flow 3 (Converge of flows)
P-36	Intermediate	Flow 3 (Converge of flows)
P-14	Intermediate	Flow 3 (Converge of flows)
P-15	Intermediate	Flow 3 (Converge of flows)
P-17	Intermediate	Flow 3 (Converge of flows)
P-18	Intermediate	Flow 3 (Converge of flows)
P-19	Regional	Flow 3 (Converge of flows)
P-27	Intermediate	Flow 3 (Converge of flows)
P-22	Intermediate	Flow 3 (Intermediate)
P-23	Regional	Flow 3 (Intermediate)
P-33	Regional	Flow 3 (Intermediate)
P-34	Regional	Flow 3 (Intermediate)
P-35	Regional	Flow 3 (Intermediate)
P-16	Intermediate	Flow 3 (Intermediate)
P-26	Intermediate	Flow 3 (Intermediate)

The 3D multivariate data analysis allows us to observe the direction of the flow within the aquifer, identify where the water comes from, and from there carry out an analysis to observe the chemical and physical evolution of the water to determine which flow system it belongs to, being that in this analysis, a parameter such as hydraulic head is used.

Due to its 2D analysis, the cluster analysis is limited in relation to the interpretation of results, whereas the 3D multivariate data analysis allows for creating diagrams or visualizing in a clearer way the behavior of the water as well as its chemical evolution that the water has within the aquifer.

The proposed analysis offers a robust view of the different flow systems present in the Calera aquifer that can be useful to identify the best areas for water catchment in the region and to identify the movement of water with the help of hydraulic head.

The diagrams shown allow us to describe the trajectory of the water, observe the chemical evolution that the water presents in that area, and thus be able to have a clearer idea of the functioning that the water presents within an aquifer.

5. Conclusions and Future Perspectives

The proposed integrative multivariate approach that includes 3D spatial distribution of hydraulic head, water quality, and well characteristics within a geological framework helped to delineate the convergence of flow systems in the Calera aquifer. It is observed that the aquifer received water from three different origins.

The cluster analysis is limited in its interpretation of results, because it works only with chemical parameters and its results are presented in 2D, whereas the 3D multivariate data analysis considers the hydraulic head, physical and chemical parameters, and geological material present in the aquifer. By analyzing the results that involve all these parameters, it is possible to create schemes that help us to visualize the characteristics and behaviors that groundwater presents, such as its chemical evolution of water and how the geological material can be related to this evolution, the direction of the flow that allows us to identify the origins of the water, and the convergence of flows that can be visualized through 3D analysis.

The proposal allows for integrating the factors that are involved in the circulation of groundwater, interpreting through quantitative and qualitative knowledge the evolution of water and how this is linked to its geological framework, in order to identify flow systems.

The constructed cross-sections contributed to a better understanding of groundwater flows. The identification of the flow systems by means of the proposal allowed for identifying intermediate, regional, and mixture flows by means of the capture elevation, chemical evolution, path, and interaction with the geology. This analysis allowed us to delineate the convergence of flow systems in the northern region of the aquifer.

The determination of flow systems within an aquifer is a process that facilitates the understanding of how complex the behavior of water is within a geological framework, and its application is necessary to manage or substantially improve the productivity of the aquifer, being a solution to problems that may arise.

The importance of identifying the flow systems is essential to adequately manage the resource, and this information will allow for the formulation of the aquifer management plan, identify recharge zones to protect, provide guidelines, grant concessions, and approve explorations and exploitations to secure this valuable resource.

The described methodology can be applied to the study of aquifers by characterizing convergent flow systems. A better understanding and identification of recharge, transit, and discharge areas can provide better comprehension of groundwater functioning. This knowledge could be useful to avoid undesirable concentrations of heavy elements such as arsenic, mercury, and nickel in water extracted from existing wells. Therefore, this approach could be useful in the design of wells and the control of water quantity and quality.

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