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Impact of Interface Soil Layer on Groundwater Aquifer Behaviour

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***Abstract*—**The geological environment where the groundwater is collected represents the most important element that affects the behaviour of groundwater aquifer. As groundwater is a worldwide vital resource, it requires knowing the parameters that affect this source accurately so that the conceptualized mathematical models would be acceptable to the broadest ranges. Therefore, groundwater models have recently become an effective and efficient tool to investigate groundwater aquifer behaviours. Groundwater aquifer may contain aquitards, aquicludes, or interfaces within its geological formations. Aquitards and aquicludes have geological formations that forced the modellers to include those formations within the conceptualized groundwater models, while interfaces are commonly neglected from the conceptualization process because the modellers believe that the interface has no effect on aquifer behaviour. The current research highlights the impact of an interface existing in a real unconfined groundwater aquifer called Dibdibba, located in Al-Najaf City, Iraq where it has a river called the Euphrates River that passes through the eastern part of this city. Dibdibba groundwater aquifer consists of two types of soil layers separated by an interface soil layer. A groundwater model is built for Al-Najaf City to explore the impact of this interface. Calibration process is done using PEST 'Parameter ESTimation' approach and the best Dibdibba groundwater model is obtained. When the soil interface is conceptualized, results show that the groundwater tables are significantly affected by that interface through appearing dry areas of 56.24 km² and 6.16 km² in the upper and lower layers of the aquifer, respectively. The Euphrates River will also leak water into the groundwater aquifer of 7359 m³/day. While these results are changed when the soil interface is neglected where the dry area became 0.16 km², the Euphrates River leakage became 6334 m³/day. In addition, the conceptualized models (with and without interface) reveal different responses for the change in the recharge rates applied on the aquifer through the uncertainty analysis test. The aquifer of Dibdibba in Al-Najaf City shows a slight deficit in the amount of water supplied by the current pumping scheme and also notices that the Euphrates River suffers from stresses applied to the aquifer. Ultimately, this study shows a crucial need to represent the interface soil layer in model conceptualization to be the intended and future predicted behaviours more reliable for consideration purposes.

***Keywords*—**Al-Najaf City, groundwater aquifer behaviour, groundwater modelling, interface soil layer, Visual MODFLOW.

I. Introduction

In recent decades, in many countries of the world, evidently groundwater has become one of the most crucial natural resources. As this source has the ability to supply water, a number of essential advantages have been provided by groundwater source as compared with surface water source such as higher quality to use it for various life's aspects, better protection from contaminants which may infect this source, less prone to seasonal and long-term fluctuations, and uniformly spread over large areas as compared with surface water where it is very often available in regions which devoid of surface water [20]. Therefore, for domestic uses, industry, and especially agriculture, the freshwater supplied by groundwater source will ultimately become very important, particularly when surface water sources have exposed for depletion problem [32]. For modelling and managing groundwater resources, and accurately predicting groundwater future responses, numerical conceptualization models have recently emerged as an effective and efficient tool that can deal with complex groundwater aquifer systems and heterogeneous formations [36]. Groundwater modelling represents an efficient tool for groundwater forecasting and management and remediation. In general, models are a simplification of the reality in nature that intends to investigate certain phenomena or to predict future behaviour. The challenge in groundwater models is to simplify reality in a way that does not adversely affect either the accuracy or the ability of model outputs to achieve the intended objectives [19]. In the other words, it can be considered the groundwater model that is more powerful if it is quantitatively representing the groundwater heads and time by a simplified way for the complex hydrogeological conditions [7]. A good conceptualization of a groundwater model is the most important step that is needed to represent the real-modelled field and in turn will result in good predictions [33]. As a result of accurate modelling and models of groundwater, decision makers will be able to manage groundwater resource, assess the impacts on aquifers, issue the appropriate plan to negotiate local and regional groundwater supply, evaluate dewatering due to ecological systems, design and control pumping schedules needed, assess drought impact during dry seasons, predict the effects of climate changes and issue the scenarios to control those effects in advance, and many more advantages will be available under consideration for decision makers through these developed groundwater models [22].

In most populated areas of the world, groundwater collected in the geological formations constitutes an important component of water supply for agriculture, industry, and domestic use. Withdrawal waters from pumps are supplied by those geological environments capable for yielding large amounts of water where these geological formations exist underneath the ground surface and called aquifers. An aquifer

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is defined as that geological environment, saturated and permeable enough to provide an economic quantity of water for extraction process as it is commonly composed of unconsolidated sand or gravels and sometimes from permeable limestone and sandstone which represents rocky sediments [24]. These aquifers may be confined or unconfined, depending upon the geological and lithological characteristics of the subsurface layers. There may also be more than one aquifer carrying water as this will be called by layered aquifer systems or multi-layered aquifer systems [18]. Layered aquifer system consists of either two or more aquifers separated by aquitards or aquicludes. Typically, aquitard geological unit has limited ability to transmit water vertically where this will make the aquitard capable of assembling very little amounts of water, but these quantities will not be sufficient to meet even very small pumping demands; therefore, as it consists of loams or clays, often aquitard can be considered as an impermeable layer. Aquiclude is classified as a completely impermeable geological unit, consisting of unfractured dense metamorphic or igneous layers [24]. Whilst, sometimes, layered aquifer system consists of two or more aquifers or layers, each has its own geological and hydrogeological characteristics and separated by interfaces which allow completely for crossflow. The interface between layers is considered as an open boundary for transmitting water and continuous potentials [24]. Most studies are either dealing with a layered aquifer system, which contained in its geology on aquitards or aquicludes [3], [36], [1], [8], or dealing with a single aquifer-single soil layer (confined/unconfined) [31], [5], [4], whereas sometimes it may have single aquifer with layered soils separated by interfaces.

The aim of this study is to examine the impact of an interface soil layer separating the single unconfined groundwater Dibdibba-aquifer into two heterogeneous layers and compare the results of this model with those resulted from the groundwater model when the aquifer is treated as a heterogeneous with a single soil layer for a real case study located in Al-Najaf City, Iraq by using the latest state-of-the-art Visual MODFLOW (version 4.6). An additional overall assessment for Al-Najaf City Dibdibba groundwater aquifer behaviour will be under investigation.

II. Site Description

The region of study is located at Al-Najaf City, Iraq and covering an area of 978 km^2 (25.25 km in the longitudinal direction and 38.7 km in the latitudinal direction). It lies between 440 07′ 36.082″E and 440 32′ 5.285″E in the longitude and 310 57′ 36.26″N and 320 11′ 22.899″N in the latitude (the geographical coordinates are between 417474 m and 456150 m easting, and 3536343 m and 3561577 m northing). On the eastern part passes the Euphrates River after bifurcating into two branches (Al-Kufa and Al-Abbasiyah) before entering into the study site. The Western Sahara (Desert) is located on the western side of Al-Najaf City where part of this desert is within the boundaries of the region under study. Dibdibba aquifer is found to be the geological formation collected groundwater in the study site as suggested by the stratigraphic features derived from the longest boreholes in the region. Dibdibba aquifer consists of two types of soil layers, top (upper) made of coarse sand and bottom (lower) made of fine pebbles, and classified as an unconfined aquifer. The hydraulic conductivities of the top and bottom layers are of 14.43 m/day and 17.1 m/day, respectively. The total extraction schedule is 52454 m^3/day pumped from 69 pumping wells available in the study site where these wells provide the important and necessary information for this study. Groundwater withdrawals range from 435 m^3/day to 3256 m^3/day as minimum and maximum extractions respectively over the 69 wells-field. The movement of groundwater over the region is observed flowing from west to east as the wells-field showed. The Iraqi Ministry of Industry and Minerals-General Commission for Geological Survey and Mining department [16] and the Ministry of Transportation [27] have provided the geological and hydrogeological data needed, where these data showed that there exists a cliff on the south-west end of the study site called Tar Al-Najaf, and at the foot of this cliff there is a transversal fault named Abu Jir fault. The groundwater on both sides of Abu Jir fault does not have any connection with each other; therefore, the area on the western side of Abu Jir fault will be excluded from the site conceptualization modelling and considered as inactive area (IA). The "Digital Elevation Model" (DEM) of the Global Land Cover Facility (GLCF) is used to download the topography of the study site, and GIS software is used to extract ground surface elevations. The average calculated gradient of the study site is 0.0018. All details mentioned are shown in Fig. 1.

III. Flow Governing Equation

The simulation process of a groundwater modelling has been already well documented by many codes which are written to solve the flow governing equations for various geological, hydrogeological, and spatial conditions, such as MODFLOW [25], FEFLOW [13], and many more. The three-dimensional Visual MODFLOW (version 4.6) program which is supplied by Waterloo Hydro-geologic Company is chosen as the modelling tool in this study due to its accuracy and efficiency [9]. Visual MODFLOW computer program represents a set of algebraic equations generated to approximate the partial differential equations of flow through solving those equations by using the finite difference technique which is changing the mathematical model into a form that can be solved by a computer [30].

Mainly, based on Darcy's law [12] (1) and energy conservation (2), the mathematical equations that describe the groundwater flow through a porous medium are established [9]. Equation (1) represents the one dimensional Darcy equation where, V is the velocity of groundwater (L/T), K is the hydraulic conductivity of the soil (L/T), h is the water table of the groundwater (L), and L is the length of flow of the soil particle through the soil media (L):

$$V = -K \frac{dh}{dL} \tag{1}$$

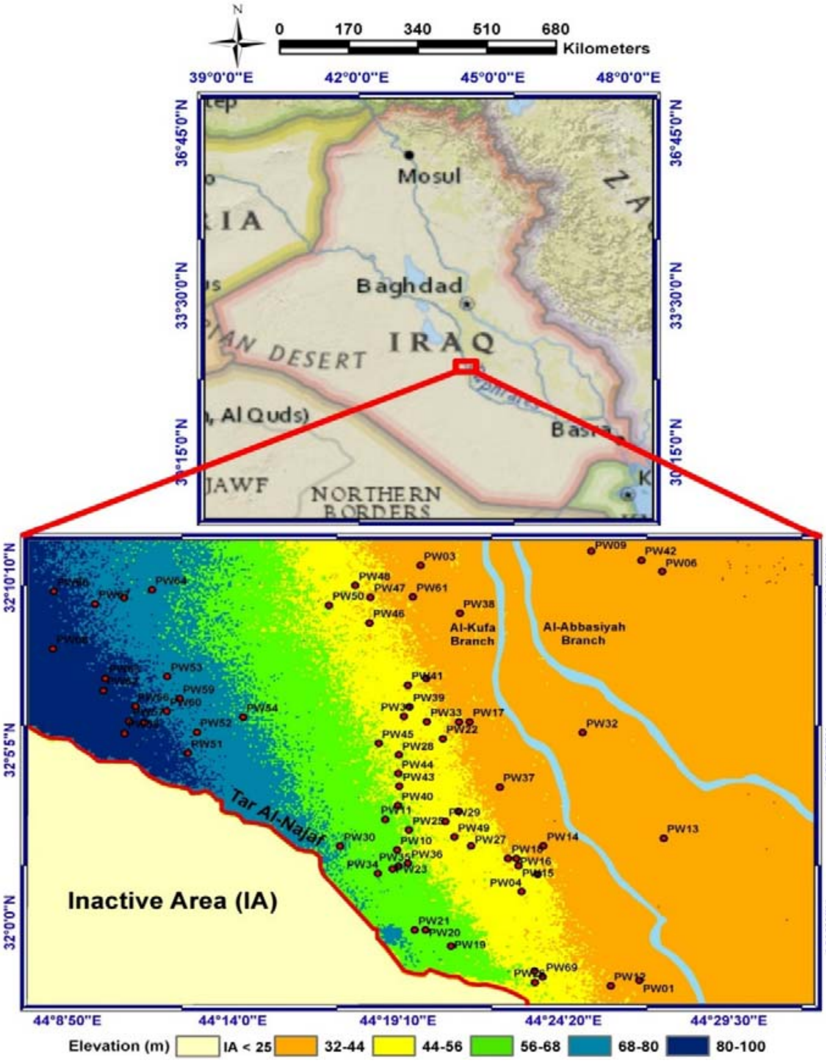


Fig. 1 Geological and hydrogeological details of the study site

The general representation of the conservation of fluid mass equation (Continuity Equation) can be expressed in (2). Equation (2) represents the flow discharge which represented by, Q is the discharge (L^3/T), i is the hydraulic gradient (dh/dL) (dimensionless), and a is the area of flow (L^2).

$$Q = -kiA \qquad (2)$$

Negative signs in both (1) and (2) refer to the convention for the relation between the flow direction and head gradient.

The general form of the equation describing the non-equilibrium, heterogeneous and anisotropic groundwater flow conditions is derived from the combination of the Darcy equation and Continuity equation [23]. The combination of these equations will result in the three-dimensional partial-differential equation of the groundwater movement through porous medium, as expressed by (3):

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)+W=S_S\frac{\partial h}{\partial t} \qquad (3)$$

where, Kxx, Kyy and Kzz are the hydraulic conductivities along x, y, and z coordinates respectively, W is the volumetric flux per unit volume which represents sinks and/or sources of water (T^{-1}) where its value is less than (zero) when flow out of the groundwater system, and it will be greater than (zero) when flow is into the system, S_S is the specific storage of the porous media (L^{-1}), and t is the time (T).

Equation (3) together with the specification of boundary and initial flow and/or head conditions will constitute a groundwater flow mathematical representation of an aquifer system [17].

IV. Setup MODFLOW Model

The preparation of the conceptual model needs to prepare the geological and hydrogeological properties of the study area, including identifying the boundaries of the study site which in turn will specify the appropriate boundary conditions and estimating of sources and sinks, then a three-dimensional model will usually be created from the hydrogeological system [35]. The conceptual model of the study site is performed using Visual MODFLOW with a computational mesh consists of 194 columns and 127 rows with two layers of constant hydraulic conductivity (14.43 m/day-Top layer and 17.1 m/day-Bottom layer) to represent Dibdibba unconfined aquifer model (Initial Forward Model) as shown in the 3D view illustrated in Fig. 2. The size of the cells is approximately 200 m by 200 m and covers the whole 38.7 km by 25.25 km computational domain with 19499 active and 5139 inactive cells, respectively. The Iraqi hydrogeological map provided by [16] enhanced by field observations showed that the movement of groundwater is eastward in general. In addition, the Iraqi hydrogeological map as in [16] revealed that the constant heads along the western and eastern boundaries are 50 m and 20 m, respectively; therefore, the study site boundary conditions are set up accordingly. The Euphrates River with both branches Al-Kufa and Al-Abbasiyah are considered in the conceptualization process. The boundary conditions of these branches are supplied by the Iraqi Ministry of Water Resources [28], as detailed in Table I. According to [26] formula, the study site is generally classified as an arid area with no active vegetation cover, thus no transpiration is applied over the study area in modelling process. By using [34] formula and the calculations for the collected data over the period from 1980 to 2014, it has been specified that Al-Najaf region is exposed for a 16.5 mm/year recharge rate.

TABLE I
CONDITIONS FOR EUPHRATES RIVER USED IN THE MODEL [28]

Branch	Water Elevation		Bed Elevation (m)	Bed layer Thickness (m)	Width (m)	Hydraulic Conductivity (m/d)
	Northern end (m)	Southern end (m)				
Western	24.65	21.05	19.2	0.6	174	0.364
Eastern	24.55	21.35	19.2	0.6	99	0.300

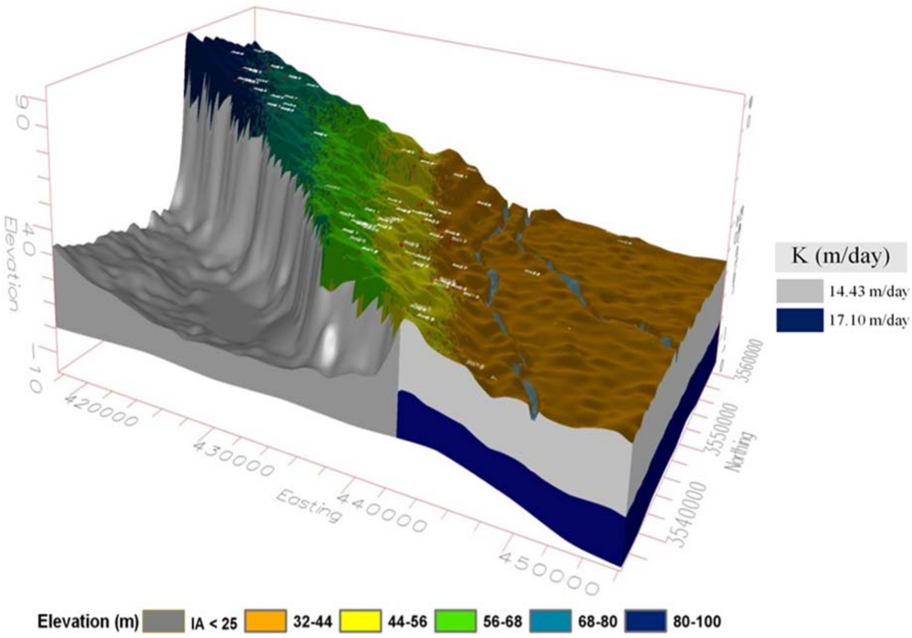


Fig. 2 3D-view of the constructed Forward Model of the study site with two homogenous layers

V. METHODOLOGY

Generally, hydraulic conductivity represents the key role that affects the environmental and water regimes protection. In addition, to analyse, explain, and describe the surface and subsurface flows in various unban, rural, and even landscape regions, it is really needed to understand accurately the process used to identify or estimate the hydraulic conductivity value (K). Several of laboratory and field methods have been used to estimate K-value [21], where, in reality, due to the internal or external environmental impacts, K-value has the ability to change from place to place horizontally and vertically [29]. Generally, two types of groundwater flow models are available at the present time, the Forward and Inverse (PEST) models. Basically, Forward model is used for the solution of the hydraulic head of an aquifer at any time and any point within the aquifer. Where Forward solution will be easily obtained when the transmissivity, storativity, stresses on the aquifer, hydraulic conductivity, and the initial and boundary conditions of the aquifer are known [30]. Fig. 2

illustrated previously is the established Forward model for Al-Najaf City's Dibdibba aquifer which geologically consists of two soil layers with constant hydraulic conductivities separated by an interface soil layer. In fact, in the real field, the entire aquifer domain's parameters are rarely found complete or represent the whole area of interest, as in most cases those parameters are found to be as scattered measurements in the study site. Therefore, to accurately predict the behaviour of an aquifer, the aquifer criteria or parameters should be well interpolated, to be the established groundwater model more reliable [30]. According to [7], typically, to solve or interpolate the groundwater aquifer parameters, there are two common trial-and-error methods, manually and automatically. Although the manual approach helps largely in developing the modeller's hydro-sense, but it still is imperfect process because sometimes the parameters that affect the model are large and thus it is impossible to track each parameter [7]. Therefore, automated trial-and-error rigorous mathematical methodology by using "PEST" "Parameter ESTimation Method" has been used firstly by [37], [11], [10] as an efficient tool to solve the Inverse model through the automatic interpolation of the groundwater parameters. Inverse model is used by depending upon the head or flux observations as a dependent variable in the governing equation of flow (Laplace equation), where usually those field-measured observations are having a higher degree of confidence. In regarding to Al-Najaf City study site, PEST method is applied to the layers of Dibdibba aquifer to interpolate the constant K-values of the top and bottom layers and obtaining PEST model. PEST method has recently simplified by using pilot points at discrete locations to reduce the computational burden. Number and locations of pilot points are specified over the computational domain where the number should be neither extremely large (thousands) nor sparsely, the usual number is fewer than 100 [15], [2], [14]. In this research, K-values are estimated automatically at those pilot points which are distributed throughout the model domain to result the PEST model with one unconfined aquifer-two heterogeneous soil layers.

The procedure that is used to evaluate the model acceptability is called the calibration process. Model calibration is the process of adjusting one or more aquifer's parameters to reach the best matching between the simulated results and the measured data [30]. The dynamic heads of the in-operation's wells are used to calibrate the model dynamically through comparing those heads with the calculated ones when the wells-field is under operation. Fig. 3 shows the relationship between the calculated and observed heads resulted from running Visual MODFLOW model for two models, 1) the Forward model when there are only two soil layers with a constant hydraulic conductivity of each, and 2) the Inverse model after applying the automated parameter estimation approach (PEST) on the Forward model to arrive for the best representation of field domain. The values of the Standard Error of the Estimate (SEE) (m), Root Mean Squared Error (RMSE) (m), Normalized Root Mean Squared Error (NRMSE) (%), and the Correlation Coefficient (CC) of both models shown in Table II are used to assess those models.

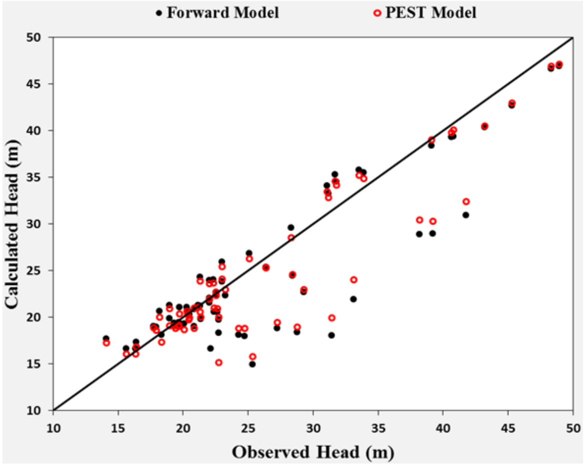


Fig. 3 Comparison of the calculated and observed heads for the Forward and PEST models

TABLE II
THE STATISTICAL PARAMETERS RESULTS FOR THE FORWARD AND PEST MODELS

Calibration Case	SEE m	RMSE m	Normalized RMSE (%)	CC
Forward Model	0.399	3.607	10.358	0.919
PEST Model	0.363	3.152	9.053	0.931

Clearly from Fig. 3 and Table II, it can be noticed that the results of the mathematical model (the calculated heads) after applying the estimation process of the hydraulic conductivity (PEST model) become better than those when the model is consisting of two layers of constant hydraulic conductivity (Forward Model). Therefore, PEST Model with one unconfined aquifer and two heterogeneous soil layers (separated by an interface) will be used to simulate Al-Najaf City Dibdibba-aquifer as it is shown in Fig. 4.

At this point, to assess the impact of the soil interface layer on the behaviour of aquifer, it will remove that interface from the PEST Model which is considered ultimately to conceptualize Al-Najaf region to become comprised of one unconfined aquifer with one heterogeneous soil layer as shown in Fig. 5.

VI. RESULTS AND DISCUSSIONS

A. Model Uncertainty

Groundwater models' uncertainty is caused by the uncertainty of either the aquifer parameters or the models' boundary conditions. The fundamental concept of the application of uncertainty analysis is to explore the behaviour of the groundwater system under the effects of systematic changing the model parameters and hydrogeological stresses to ultimately identify the parameter that has the greatest impact on the characteristics and consequences of the aquifer system, thus giving those parameters special attention in the intended and future studies [6]. In this study, the uncertainty test shown in Fig. 6 is carried out using a systemic change of the recharge rate values. The results of the SEE values (The Standard Error of the Estimate (m)) of the PEST Model-One Unconfined Aquifer-Two Heterogeneous soil layers are found to be the lowest and highest when the recharge rate equals 10.5 mm/year and 31 mm/year, respectively. In addition, when the recharge rate ranges between 10 and 15 mm/year, the model is less sensitive, whereas the overall trend shows that the model is sensitive for those recharge rates less than 10 mm/year and higher than 15 mm/year. In referring to PEST Model-One Unconfined Aquifer-One Heterogeneous soil layer, it is found that the SEE values are higher than those for the PEST Model of Two Heterogeneous soil layers when the recharge rate is less than 15 mm/year, and lesser than those SEE values for PEST Model-Two Heterogeneous soil layers when the recharge values are greater than 15 mm/year, as an overall trend. Where the PEST Model-One Unconfined Aquifer-One Heterogeneous soil layer has a reversal case around the 15 mm/year recharge rate, where the groundwater model is sensitive to recharge values smaller than 15 mm/year and less sensitive to those recharge rates greater than 15 mm/year. Therefore, the presence of one or more interfaces within an aquifer reveals a great importance of the process of conceptualization of the mathematical model because those interfaces have the capability to affect the aquifers' behaviours and change the results as this will affect the credibility of the models' results, particularly as these models are created for the purpose of predicting the future behaviour of aquifers.

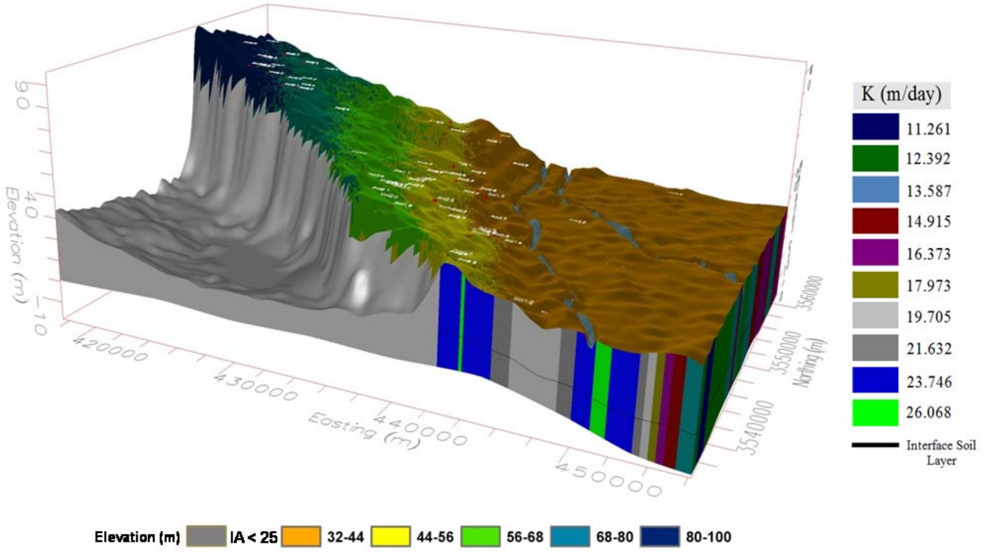


Fig. 4 3D-view of the PEST Model-One Unconfined Aquifer-Two Heterogeneous Soil Layers separated by interface soil layer

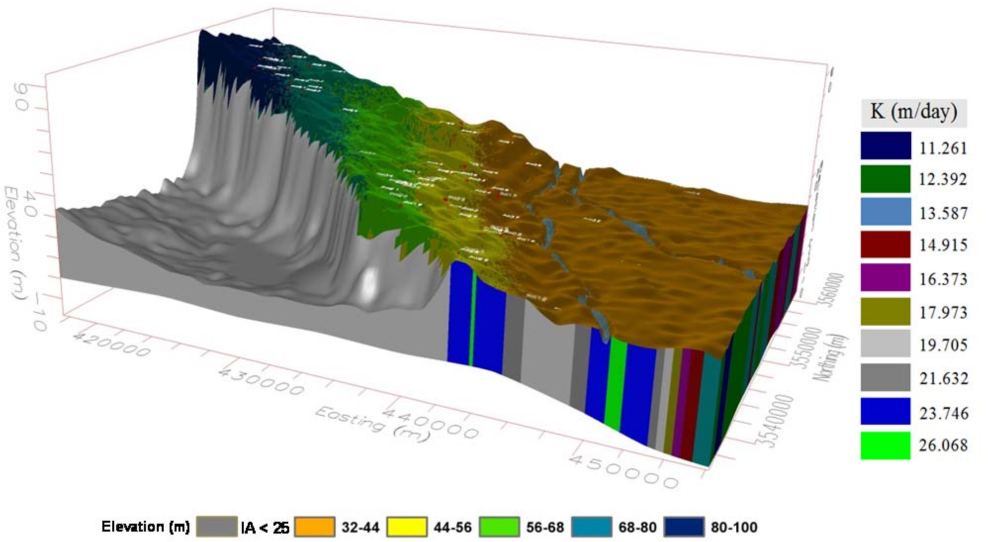


Fig. 5 3D-view of the PEST Model-One Unconfined Aquifer-One Heterogeneous Soil Layer without interface soil layer

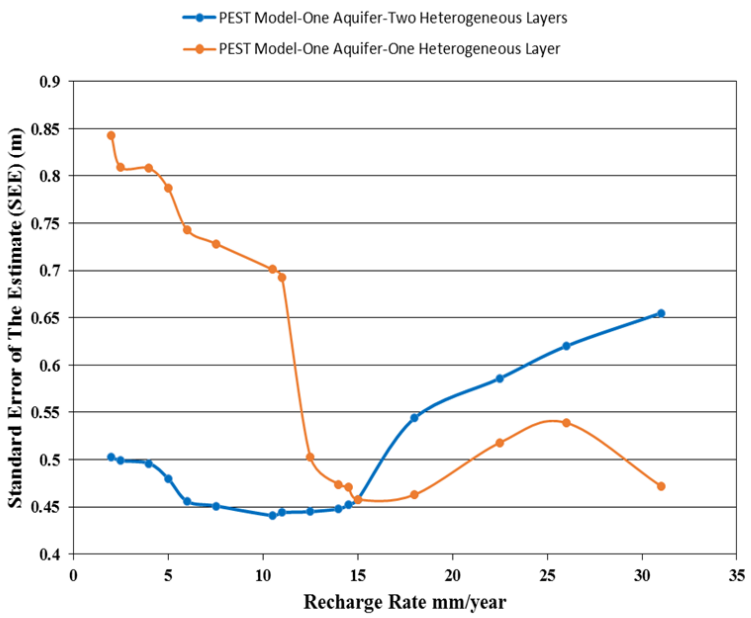


Fig. 6 Uncertainty test of the recharge rate

B. Groundwater Table

The computed groundwater table in the top and bottom layers of the unconfined groundwater PEST Models (with and without soil layer interface) when applying a recharge rate of 16.5 mm/year is shown in Fig. 7. Obviously, the PEST Model with the presence of an interface (PEST Model-One Unconfined Aquifer-Two Heterogeneous soil Layers) (Fig. 7 (a)) has a dry area in the top and bottom layers of Dibdibba aquifer. These dry areas are extending to 56.24 km^2 and 6.16 km^2 in the upper and lower layers respectively. Comparing PEST Model which does not contain an interface (PEST Model-One Unconfined Aquifer-One Heterogeneous soil Layer) (Fig. 7 (b)) to that one with the existence of an interface, the dry area is only 0.24 km^2. Therefore, there is an interface soil layer in the real field domain, but it does not adopted in the model's conceptualization, the behaviour of the aquifer will greatly affect the groundwater table results and this means that the model's future impacts predictions results will not represent the field in the reality.

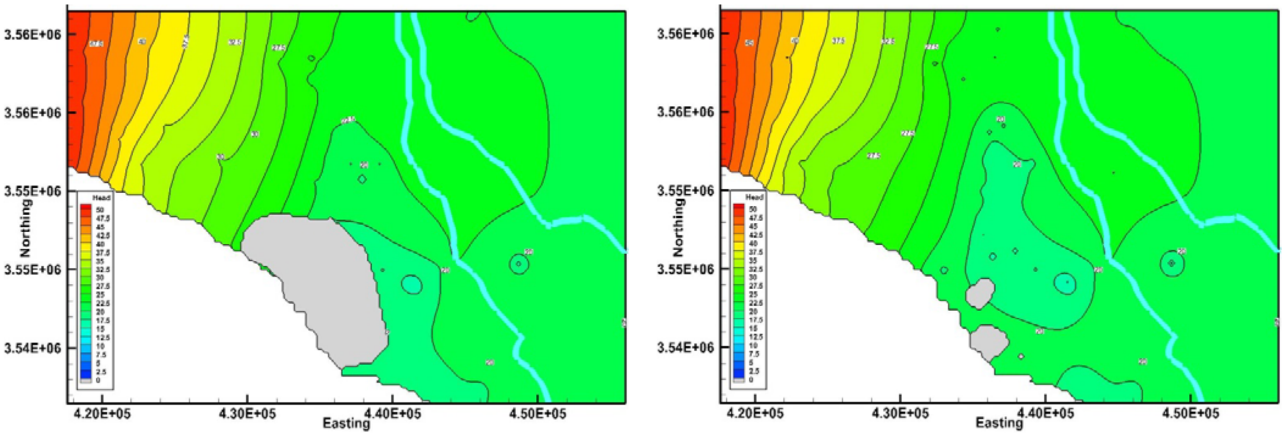
C. Groundwater Balance

To explore and assess the impact of whether there is or not a soil interface between the layers of Dibdibba aquifer, on the exchange between the groundwater and surface water represented by the Euphrates River for the two PEST Models, the groundwater balance is examined. With the presence of the soil layer interface, the PEST Model-One Unconfined Aquifer-Two Heterogeneous Soil Layers shows that the Euphrates River leaks water into the aquifer of 7359 m^3/day (inflow into the river: 1723 m^3/day and outflow from the river: 9082 m^3/day), whereas this quantity was less as the PEST Model-One Unconfined Aquifer-One Heterogeneous Soil Layer revealed when there is no interface implemented in Dibdibba aquifer where the leakage from the Euphrates River was 6334 m^3/day (inflow into the river: 1810 m^3/day and outflow from the river: 8144 m^3/day). Due to the over-pumping from some wells, it is found that four wells are stopped to pump water to be out of the pumping schedule when the interface soil layer is modelled (PEST Model-One Unconfined Aquifer-Two Heterogeneous Soil Layers), where the total extracted water is 48614 m^3/day. Whereas those wells become five with the absence of the interface soil layer as the PEST Model-One Unconfined Aquifer-One Heterogeneous Soil Layer reveals to be the total extracted water equals to 47693 m^3/day. Overall, an important leakage quantity is resulting from the two PEST Models (with and without interface) due to the impact of the pumping schedule. These quantities were different from each other and the reason is due to the interface soil layer, which clearly shows a significant impact on the groundwater model's behavior. Therefore, it requires to represent the interface soil layer in the process of conceptualization of the groundwater mathematical model when the aquifer is comprising of layered soils separated by interfaces, not to ignore these interfaces in the modelling process.

D. Dibdibba Aquifer Behaviour's Assessment

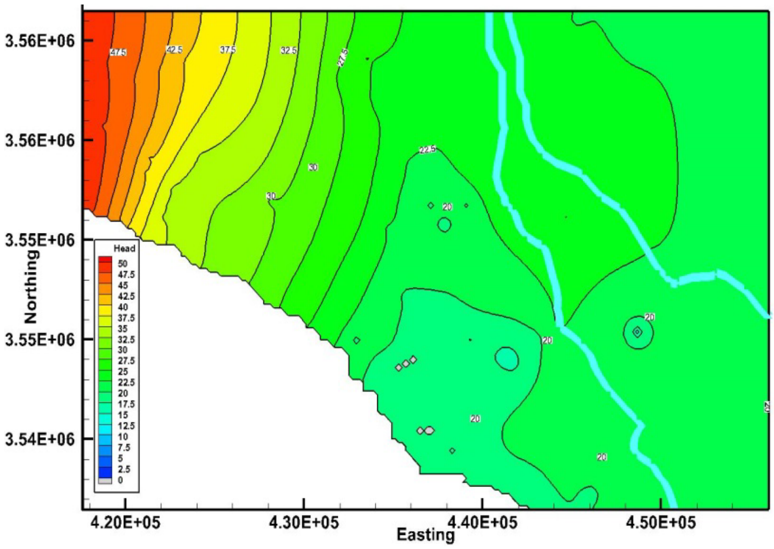
In order for the established mathematical groundwater model to be more reliable by decision makers to give the appropriate possibility and ability to use these models for future forecasting, the modelling process must be fairly accurate to represent the field reality. Through the results of the research, it is noticed that with the existence of the interface soil layer, the Dibdibba aquifer suffers from large dry areas and the same problem is true for the Euphrates River as it loses its water into the aquifer to supply a part of pumping schedule applied. The amount of pumping applied is not fully supplied by the aquifer, as only 84% of it is provided.

However, with the absence of the interface soil layer, although the Dibdibba aquifer is also exposed for the same extractions stresses applied for that model with an interface, its behaviour was different in terms of the results, which indicates the importance of the efficient modelling process which in turns will produce accurate and reliable behaviours reflected by the results.



Top Layer Bottom Layer

(a) PEST Model-One Unconfined Aquifer-Two Heterogeneous Soil Layers



(b) PEST Model-One Unconfined Aquifer-One Heterogeneous Soil Layer

Fig. 7 Computed groundwater table of the PEST Models with and without an interface soil layer

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