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A FINITE DIFFERENCE-RANDOM WALK PARTICLE TRACKING MODEL FOR SIMULATING SEAWATER INTRUSION PROBLEM

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ملخص البحث:

يتم انشاء نموذج ثنائى الابعاد لمحاكاة مشكلة تسرب مياه البحر الى المياه الجوفية الساحلية باستخدام طريقة الفروق المحددة و طريقة تتبع الحركة العشوائية للجسيمات تحت ظروف التدفق المتغير. يستند النموذج المقدم على حل معادلات تدفق المياه الجوفية متغيرة الكثافة مع حركة الملوثات في وقت واحد متبعا طريقة الفروق المحددة و وتقنية تتبع الحركة العشوائية للجسيمات على التوالي. المعادلات التي استخدمت لتمثيل تدفق المياه الجوفية متغيرة الكثافة هي معادلة التدفق ، معادلة حركة الملوثات ، معادلة Darcy والمعادلة التجريبية التي تربط بين تركيز الملح وكثافة السائل. يتم حل معادلة التدفق ومعادلة حركة الملوث فى ان واحد حيث انه لا يمكن الفصل بينها. جميع المعادلات هي بدلالة منسوب المياة العذبة المكافىء. يتم التحقق من صلاحية النموذج بمقارنة النتائج مع الحل التحليلي لمشكلة Henry و التى تعد من المشاكل المعروفة ذات المرجعية الجيدة فى اختبار هذا النوع من النماذج. وجد ان نتائج المقارنة مرضية حيث انها متوافقة الى حد كبير مع الحل التحليلي.

Abstract:

A two-dimensional Finite Difference-Random Walk Particle Tracking (FD-RWPT) model is developed to simulate the seawater intrusion problem in the coastal aquifer under unsteady state conditions. The developed model is based on solving Variable Density Groundwater Flow (VDGWF) with solute transport simultaneously considering FD approach and RWPT technique, respectively. The governing equations that describe the VDGWF are the flow equation, advection-dispersion equation (ADE) considering advection and hydrodynamic dispersion processes, Darcy's equation and an empirical equation that relates the salt concentration and the fluid density assuming isothermal conditions. Since flow and transport equations are two coupled equations, they are jointly solved with each other. All equations are in terms of equivalent fresh water head. The model is verified by comparing its results with the analytical solution of the well-established benchmark problem (Henry problem). The comparison results are quite similar and satisfied.

Keywords: Finite Difference; Random walk particle tracking; Seawater intrusion; Coastal aquifers; Variable Density Groundwater Flow; Solute Transport

1. Introduction:

Seawater intrusion is a natural phenomenon which occurs in coastal aquifers due to the different densities between the saltwater and freshwater. These different densities allow the saltwater to intrude into the freshwater aquifer. The intruding saltwater creates an area known as the dispersion zone, where the freshwater and saltwater mix and form an interface. This interface moves naturally due to the variations in the recharge rate of freshwater into these coastal aquifers. The main factor that affects the saltwater intrusion in coastal aquifers is the excessive pumping in these areas. These areas are usually associated with large populations and accordingly the abstraction of groundwater may exceed the recharge rate. Many other factors contribute in affecting saltwater intrusion such as precipitation, surface runoff, temperature, and increasing carbon dioxide emissions in the atmosphere.

Several authors modeled the saltwater intrusion considering a sharp interface between fresh and saline water based on the Ghyben-Herzberg relationship (Bear, 1979), for example the work of (Reilly and Goodman, 1985) and (Huyakorn et al., 1996). On the other hand, several investigators reported that the freshwater and saltwater are miscible fluids and can be mixed. This leads to consider the zone of dispersion in solutions at the interface between fresh and saline water. (Henry, 1964) was one of the first authors who solve the coupled flow and transport equations considering this mixing. Henry presented an analytical solution for the saltwater intrusion in confined coastal aquifer under steady state conditions considering the dispersion zone. (Pinder and Cooper, 1970) determined the movement of saltwater front in confined coastal aquifers including the effect of dispersion. (Pinder and Frind, 1972) used Galerkin's procedure in conjunction with the finite element technique to simulate seawater intrusion into confined coastal aquifers. (Panigrahi et al., 1980) developed a finite difference numerical model to analyze and solve the saltwater intrusion problem in the unconfined coastal aquifer under normal flow conditions. (Sherif et al., 1988) developed a two-dimensional finite element model to simulate the saltwater intrusion problem in confined and leaky aquifers under steady state conditions.

Moreover, many computer codes have been developed to simulate saltwater intrusion problem for example: (Voss, 1984) developed a two-dimensional hybrid finite element method and integrated finite difference method to simulate the fluid density dependent saturated-unsaturated groundwater flow and transport of solute in groundwater (SUTRA), (Lin et al., 1997) presented the finite element FEMWATER code, (Diersch, 2005) constructed the finite element FEFLOW code and (Langevin and Guo, 2006) presented an approach for coupling MODFLOW and MT3DMS into a single computer program (SEAWAT) for the simulation of variable density groundwater flow. Since then SEAWAT has been used in modeling the seawater intrusion problem in different regions all over the world by many researchers as (Lin et al., 2009; Abdullah et al., 2010; Webb and Howard, 2011).

Recently, (Thomas et al., 2016) developed a numerical model based on a Meshfree method to study the seawater intrusion problem. Meshfree Point Collocation method based on the Radial Basis Function was used for the simulation. The model verified with Henry's problem and gave satisfactory results. The model also applied to another benchmark problem and the influence of pumping and recharges rates on the saltwater intrusion were examined.

The objective of this study is to develop a two-dimensional FD-RWPT model to simulate the seawater intrusion problem in coastal aquifers. The simulation is developed where the simultaneous solution of the flow problem and the transport problem is carried out using finite differences for the flow problem (e.g., MODFLOW) and the RWPT method for the transport equation. The novel in this study is using RWPT technique in solving DDF instead of the traditional numerical methods as finite difference and finite element. RWPT in contrary with traditional methods is free from the numerical dispersion and artificial oscillations (Kinzelbach, 1988; LaBolle et al., 1996; Salamon et al., 2006). Moreover, it can be implemented on top of any flow model and the mass conservation that is automatically satisfied because the particles cannot secretly disappear. Furthermore, the RWPT method does not require solving large systems of equations and it does not require any space discretization if velocities are known everywhere.

The developed model is then verified by comparing its result and the SEAWAT computer program (Guo and Langevin, 2002) results for solving Henry problem. It is worth to mention that Henry problem is one of the most popular benchmark problems for testing the DDF and that SEAWAT was already verified using four well-known benchmark problems (Box, Henry, Elder and Hydrocoin). A full description of these problems can be found in (Voss, 1987) and Konikow et al., 1997).

2. Methodology:

Since the flow and transport equations in VDGWF are two coupled equations so they are simultaneously solved with each other. The equivalent freshwater head (h_f) concept will be used in all VDGWF equations. Conversion between h and h_f is, therefore, necessary in converting model results or field data and in model calibration or in the interpretation of calculated results. These conversions can be made using the following relation:

$$h_f = \frac{\rho}{\rho_f} h - \frac{\rho - \rho_f}{\rho_f} Z \tag{1}$$

where h_f is the equivalent freshwater head [L], h is the aquifer saline-water head [L], ρ is the fluid density (e.g., 1025 kg/m^3 for seawater) [ML^{-3}], ρ_f is the freshwater density (1000 kg/m^3) [ML^{-3}] and Z is the elevation [L].

2.1. Governing equations:

There are four equations govern and describe the VDGWF in porous media:

1) The mass balance equation for the fluid (Fetter, 1988) which can be written as:

$$-\nabla.(\rho\vec{q}) + \overline{\rho}\, q_s = \frac{\partial(\rho\theta)}{\partial t} \tag{2}$$

where ∇ is the gradient operator, ρ is the fluid (saline-water) density [LT^{-1}], $\vec{q}$ is the specific discharge vector [LT^{-1}], ρ is the density [ML^{-3}], q_s is the sources/sinks flow rate per unit volume [T^{-1}], θ is the porosity and t is the time [T].

2) Darcy's law for groundwater flow and can be expressed by:

$$\vec{q} = -\frac{k}{\mu}[\nabla P + \rho g \nabla z] \tag{3}$$

where $\vec{q}$ is the specific discharge vector [LT^{-1}], k is the intrinsic permeability[L^2], μ is the dynamic viscosity[$ML^{-1}T^{-1}$], P is the pressure [$ML^{-1}T^{-2}$], ρ is the density [ML^{-3}], g is the gravitational acceleration [ML^{-3}] and z is a space coordinate [L].

3) An empirical equation relating the density of saltwater (ρ) and concentration (C) assuming constant temperature which can be used as developed by (Baxter and Wallace, 1916):

$$\rho = \rho_f + EC \tag{4}$$

where E is a dimensionless constant having an approximate value of 0.7143 for salt concentration (C) [ML^{-3}] ranging from zero to that of seawater. This equation is applied only for typical seawaters for which the relation between ρ and C can be expressed as a linear function as in Eq. 4. If the fluid has a different composition from typical seawater or if the salt concentration in the fluid is much higher than normal seawater concentration, then this equation is invalid and in that case a different empirical relation between C and ρ should be used for that application.

4) The advection-dispersion equation that describes the solute transport given by the following equation:

$$\frac{\partial C}{\partial t} = -\nabla.(\vec{u}\, C) + \nabla.\ (D\, \nabla C) \tag{5}$$

where ∇ is the gradient operator, $\frac{\partial C}{\partial t}$ is the Concentration derivative with respect to time [$ML^{-3}T^{-1}$], C is the solute concentration (salt), $\vec{u}$ is the velocity vector [LT^{-1}] and D is the hydrodynamic dispersion coefficient [L^2T^{-1}].

This equation (Eq. 5) can be used as the fluid densities are in the seawater range (1000-1025) (De Marsily, 1986) otherwise the concentration gradient, ∇C, should be formulated as $\rho\nabla(C/\rho)$ at which the fluid is of high density as in brine transport.

2.2. Model construction:

A vertical two-dimensional *x-z* domain is used for solving the VDGWF problem under unsteady state flow condition. Thus, the governing equation for two dimension and unsteady flow using the h_f concept can be written as:

$$\frac{\partial}{\partial \mathrm{x}}\left(\rho K_{fx}\left[\frac{\partial h_f}{\partial x}\right]\right) + \frac{\partial}{\partial \mathrm{z}}\left(\rho K_{fz}\left[\frac{\partial h_f}{\partial z} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial z}{\partial z}\right]\right) = \rho S_f \frac{\partial h_f}{\partial t} + \theta E \frac{\partial C}{\partial t} \tag{6}$$

where S_f is the specific storage in terms of freshwater head [L^{-1}], θ is the porosity, K_{fx} and K_{fz} are the freshwater hydraulic conductivities in x and z directions [LT^{-1}], respectively, $\frac{\partial C}{\partial t}$ is the concentration derivative with respect to time [$ML^{-3}T^{-1}$] and it will be obtained from solving the transport equation using RWPT technique as will be discussed later. The left-hand side represents the difference between the inflow and outflow of fluid per unit volume and the right-hand side indicates to the rate of change of fluid mass per unit volume due to pressure change (first term) and concentration change (second term). The equation is solved using the FD approximation to get the head values.

This equation demonstrates that the flow and transport equations are coupled equations and they should be solved jointly or simultaneously. The solution criterion depends on solving the flow needs the density values and getting the density values needs the concentration values and calculating the concentration values needs the head values and so on. Due to the complexity of the problem, no analytical solutions for these coupled equations are available and these equations are solved numerically.

In addition to the flow equation, a second partial differential equation Eq. 5 is required to describe solute transport (salt in case of seawater) in the aquifer at which solute mass is transported in porous media by the flow of groundwater (advection), molecular diffusion, and mechanical dispersion. This equation is going to be solved using the RWPT technique to obtain the concentration values.

To numerically implement the RWPT methods in two dimensions, the following equations are used (Kinzelbach, 1988; LaBolle et al., 1996; Tompson and Gelhar, 1990):

$$\begin{aligned} x_{t+\Delta t} &= x_t + [V_x(x_t, y_t, t) + (\frac{\partial D_{xx}}{\partial x} + \frac{\partial D_{xy}}{\partial y})]\ \Delta t + \sqrt{2D_{xx}\Delta t}\, Z_1 + \sqrt{2D_{xy}\,\Delta t}\, Z_2 \\ y_{t+\Delta t} &= y_t + [V_y(x_t, y_t, t) + (\frac{\partial D_{yx}}{\partial x} + \frac{\partial D_{yy}}{\partial y})]\ \Delta t + \sqrt{2D_{yx}\Delta t}\, Z_1 + \sqrt{2D_{yy}\Delta t}\, Z_2 \end{aligned} \qquad (7)$$

where x and y are the coordinates of the particle location, V is the velocity, D_{ij} is the ij component of the dispersion tensor, Δt is the time step, and Z is a normally distributed random number with zero mean and unit variance. The second term that is multiplied by Δt on the right-hand side of equation (8) is an effective velocity that combines the local velocity at location (x_t, y_t) and time t plus the gradient of the dispersion tensor at location (x_t, y_t), and the last two terms account for the local-scale dispersion and Brownian diffusion. Implementation details of this method can be found in (LaBolle et al., 1996; Tompson and Gelhar, 1990; Hassan et al., 1997), just to name a few.

2.3. Numerical model:

In this study, the two-dimensional partial differential equation of VDGWF (Eq. 6) is solved using FD approximation with a central FD scheme in space and a backward FD scheme in time. The flow equation will be discretized to the following after applying some handling to the equation terms:

$$\begin{aligned} &-\left[\frac{HK_l H\rho_l}{\Delta x^2} + \frac{HK_r H\rho_r}{\Delta x^2} + \frac{HK_u H\rho_u}{\Delta y^2} + \frac{hK_d hd_d}{\Delta z^2} + \frac{HK_d H\rho_d}{\Delta y^2} + \frac{\rho(i,j)S_f}{dt}\right] h_f^{n+1}(i,j) \\ &+ \left[\frac{HK_l H\rho_l}{\Delta x^2}\right] h_f^{n+1}(i,j-1) + \left[\frac{HK_r H\rho_r}{\Delta x^2}\right] h_f^{n+1}(i,j+1) \\ &+ \left[\frac{HK_u H\rho_u}{\Delta z^2}\right] h_f^{n+1}(i+1,j) + \left[\frac{HK_d H\rho_d}{\Delta z^2}\right] h_f^{n+1}(i-1,j) \end{aligned}$$

$$= -\frac{\rho(i,j) * S_f * h_f^n(i,j)}{dt} + \theta E\left(C^{t+\Delta t}(i,j) - C^t(i,j)\right) - DD_{i,j} \quad (8)$$

where i and j are the column and row layer indices, HK_l, HK_r, HK_u and HK_d are the harmonic mean for hydraulic conductivity between two neighboring cells. $H\rho_l$, $H\rho_r$, $H\rho_u$ and $H\rho_d$ are the harmonic mean for density between two neighboring cells. Δx and Δz are the grid cell size. $Z_{i,j}$ is the cell center elevation [L]. Δt is the time step C^t and h_f^t are the concentration and head at the current time step. The subscript f means that the proposed parameter is based on the equivalent freshwater concept. $C_f^{t+\Delta t}$ is the cell concentration at the new time step. The unknown parameter in this equation is the equivalent freshwater head at the new time step ($h_f^{t+\Delta t}$). $DD_{i,j}$ is the term that count for the relative density difference and can be calculated as:

$$DD_{i,j} = \frac{HK_u H\rho_u}{dz^2}\left(\frac{\rho_{i+1,j} - \rho_f}{\rho_f}(Z_{i+1,j} - Z_{i,j})\right) + \frac{HK_d H\rho_d}{dz^2}\left(\frac{\rho_{i-1,j} - \rho_f}{\rho_f}(Z_{i-1,j} - Z_{i,j})\right) \quad (9)$$

The C values can be obtained from solving another partial differential equation which is the ADE using the RWPT technique considering advection and hydrodynamic dispersion.

2.4. Solution Algorithm:

The solution algorithm has been developed to implicitly solve the VDGWF equation as shown in Figure 1. The figure illustrates a flow chart that describes the solution steps from start to end. Initially we start with t=0 at which initial C value of salt concentration and freshwater concentration are set for the areal source and the remaining domain respectively. As time proceed a Δt is added to the current time at which $t=t+\Delta t$. When time equals Δt, $\partial C/\partial t$ is assumed to be equal zero. This is only an initial hypothesis as the value of $C_{t+\Delta t}$ is unknown.

The VDGWF equation is then solved to get the head values ($h_{t+\Delta t}$) all over the domain. It should be noted that these h values are not the desired ones and need to be improved through iteration process. Darcy's law is used to calculate velocities then the code will solve the transport equation using RWPT method to get $C_{t+\Delta t}$ values. These C values also are not the desired ones, as they are computed from h values that still need some improvement. As such, iterations are performed till achieving the right values. Afterward, updated values of $\partial C/\partial t$ and ρ are obtained, VDGWF equation is solved again, and velocities are calculated to solve the transport equation to get new C values.

$\partial C/\partial t$ and ρ values are then updated to check whether ρ values converged or not? If not, the previous steps are repeated until the ρ value converge as shown in Figure 1. If yes, then the initial time step is finished and the algorithm moves to the next time step as long as the total time of simulation (t_{final}) is not reached. At the next time step $\partial C/\partial t$ is assumed to be equal C_t-$C_{t-\Delta t}/\Delta t$. Then the algorithm starts solving the VDGWF equation and calculates velocities to solve the transport equation and get $C_{t+\Delta t}$ then update $\partial C/\partial t$ and ρ values as previous.

These steps are repeated until the ρ converge and finish the time step. Finally, it is checked if the total time of simulation has been reached or not. If not, then go to start new time step and if yes, then stop as the simulation time is finished.

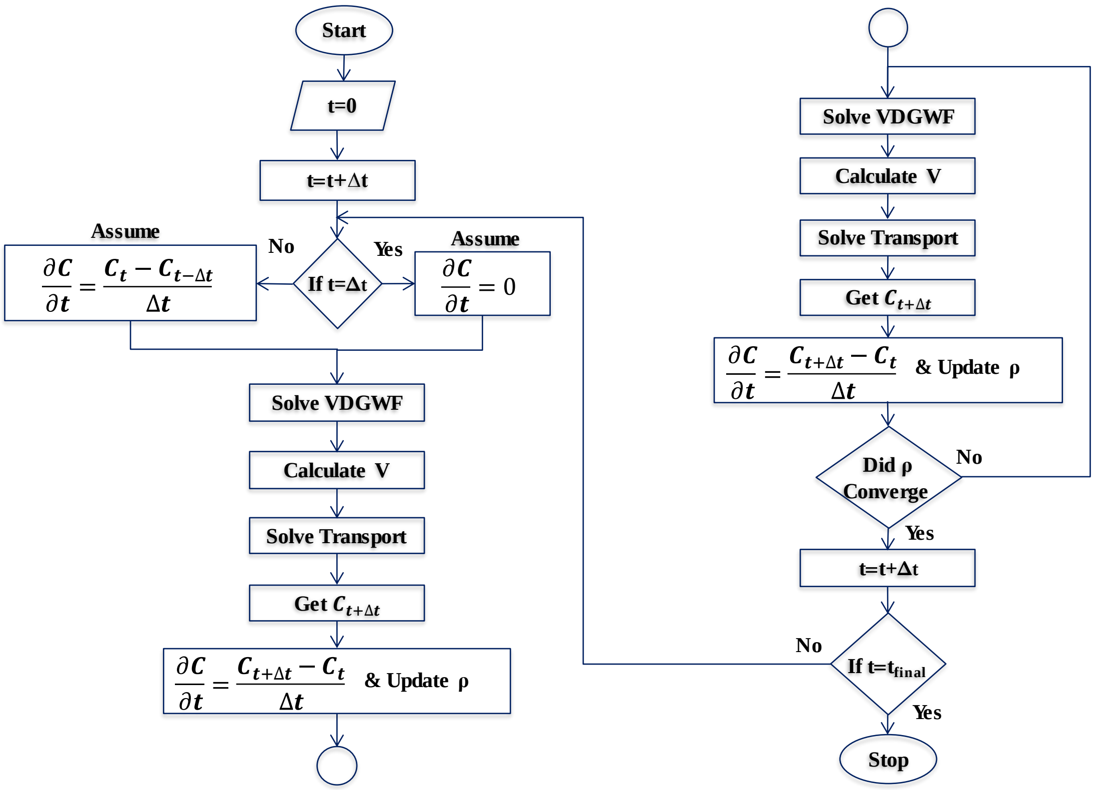

Figure 1: The Solution algorithm of the proposed model to solve VDGWF equation.

It should be noted that for each time step, the cells representing the saline water source at the left boundary lose some particles because of their advective and dispersive steps that take them outside the source. This leads to a decrease in the concentration at the source. As such, additional particles are added to maintain the source concentration at its specified value while the total number of particles in the simulation domain increases with time. To avoid reaching a critical limit for the computer virtual memory capacity, the initial number of particles is set by trial and error depending on the size of the time step and the total simulation time.

The number of particles exists in each grid cell is counted and then multiplied by the single particle's mass to get the total cell mass and the total cell mass is then converted to concentration by dividing it by volume. This is applied to all grid cells to obtain the concentration distribution in all domain.

2.5. Model verification:

The developed model is verified by solving the well-established benchmark problem "Henry problem" (Henry, 1964). Henry problem is a problem that involves the simulation of saltwater intrusion into a confined aquifer under steady state conditions. The higher density of saltwater intrudes the salt to the freshwater side and moves the seawater under the freshwater. The problem has an analytical solution which will be compared to the developed model results.

Henry problem is an x-z domain of 2.0 m × 1.0 m size. Figure 2 shows the problem boundary conditions at which the upper and lower boundaries are no flow boundaries. The left boundary is the seaside which intrudes seawater to the aquifer under a hydrostatic pressure and is considered as a specified head boundary. The right boundary is the fresh side which recharges a freshwater flow and is considered as constant flux boundary. Table 1 summarizes the parametric values used in the problem. Porosity and hydraulic conductivity (K_f) are 0.35 and 864 m/day respectively considering constant porosity and homogenous field aquifer.

Hydrodynamic dispersion is estimated only from the diffusion coefficient (D_m) as the longitudinal and transverse dispersivity (α_L and α_T) are set to be equal zero. Freshwater flux (Q_{in}) of 5.702 m^3/day/m and concentration (C_{in}) equals zero are considered for the fresh side of the problem. Seawater concentration ($C_{seawater}$) of 35 mg/L and seawater head (h) of 1.0 m are set for the seaside taking the density values for seawater (ρ) and freshwater (ρ_f) as 1025 and 1000 Kg/m^3. The total time of the simulation is considered one day.

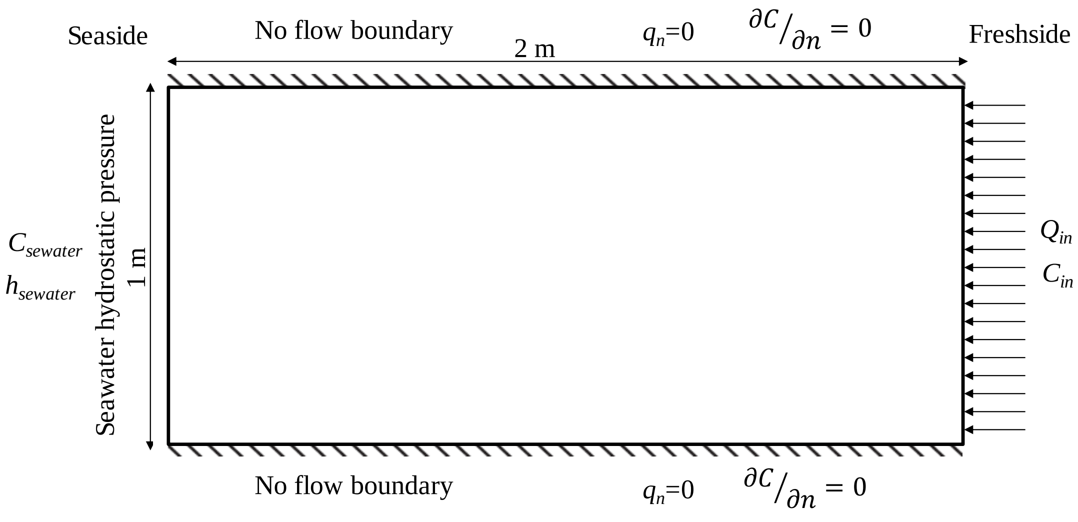

Figure 2: Henry problem domain and boundary conditions.

Table 1: Henry problem parametric values.

Parameter	Value
θ	0.35
K_f	864 m/day
$\alpha_T=\alpha_L$	0
D_m	1.62925 m^2/day
Q_{in}	5.0702 m^3/day/m
C_{in}	0
$C_{seawater}$	35 mg/l
h	1 m
ρ	1025 Kg/m^3
ρ_f	1000 Kg/m^3

Initially the aquifer is full of freshwater then seawater starts to encroach the aquifer. The seawater boundary is considered as a continuous line source. A number of particles of 16000 particles are considered reasonable as they are updated each time step as time proceed. Time step of 0.0001 day is practically considered until reaching the steady state. Particles are free to exit from the left or right boundary if any. For upper and lower boundaries particles are not allowed to exit them as they are no flow boundaries so particles try to exit these no flow boundaries will be reflected into the domain.

3. Results:

Head and concentration results are obtained by solving the equations that govern the VDGWF. The 0.25, 0.5 and 0.75 isochlor lines are illustrated to analyze and assess the obtained results. Figure 3 shows the 0.25, 0.5 and 0.75 isochlor lines results of the developed model compared to SEAWAT solution of Henry problem where a quiet similarity between the two results is found. It can be noticed that the effect of the conjunction of the no flow and specified head boundary in addition to the random nature of RWPT techniques highly influences the results. This conjunction leads to some complication in solution procedures that are related to the numerical methods or the PT technique capabilities. In addition, it is noticed from the figure that the continuous behavior of particles in source location gives some shortening in C values in this location leading to some deviation from the exact solution. However, looking for h distribution there is an acceptable agreement between the results of the developed model and the SEAWAT solution shown in Figure 4. Mostly, the results appear satisfactory taking into consideration the limitations that may exist in capabilities of PT technique and numerical methods.

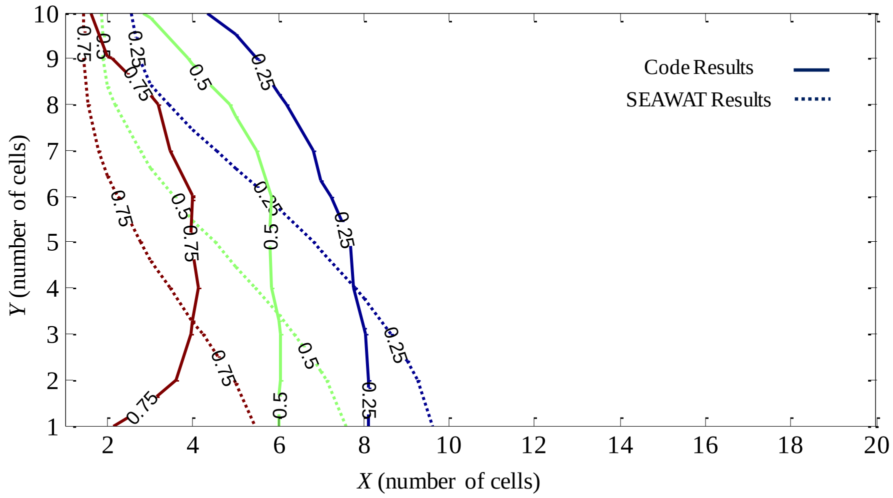

Figure 3: Henry problem verification results compared with SEAWAT (0.25, 0.5 and 0.75 isochlor lines).

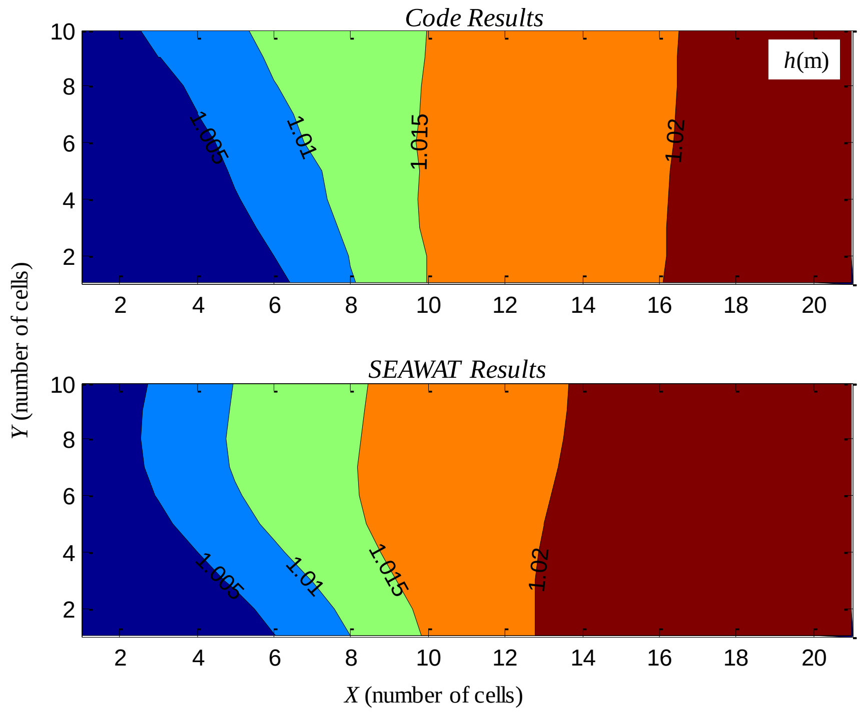

Figure 4: Henry problem verification results compared with SEAWAT (*h* distribution).

4. Summary and Conclusions:

In this study, the two-dimensional FD-RWPT model is developed to simulate the saltwater intrusion problem in coastal aquifers. The model is constructed for the *x*-*z* domain under unsteady state conditions. The two-dimensional partial differential equation that governs the VDGWF is solved using FD approximation with a central FD scheme in space and a backward FD scheme in time. A second partial differential equation which is the ADE is solved using the RWPT technique considering advection and hydrodynamic dispersion processes to get the concentration values. Fluid density depends on concentration only assuming isothermal conditions. The two partial differential equations are coupled equations so they are solved simultaneously and the mathematical and numerical description of the developed model is presented. The solution algorithm followed to solve the VDGWF and obtain the desired results is presented and the developed model is verified using the well-established benchmark problem (Henry problem) through a comparison of the problem outputs that include the head distribution and the isochlor lines. The comparison is between the developed model and SEAWAT software. The results show an accepted agreement which indicates that the model is working efficiently. To the best of the authors' knowledge, the developed tool is the first attempt in the literature that implements the use of RWPT in solving VDGWF. This will add value to the modeling community by taking all the advantages of RWPT in solving VDGWF equation. In addition, the newly developed tool will save the time of simulation, especially for complicated simulations of VDGWF at field sites. The hypothesis that RWPT method could be used in solving VDGWF equation is the first step on a way for software developers to start using this method instead of traditional numerical techniques which suffer from the numerical dispersion and time-intensive computations.

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