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Pumping optimization in coastal aquifers: Comparison of sharp interface and density dependent models

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Abstract: Seawater intrusion in coastal aquifers can be simulated using models of different accuracies, depending on the application and the required approximation level. In the present work, two seawater intrusion models of different complexities are employed to calculate the optimal pumping rates in coastal aquifer management problems. The first model simulates variable-density flow and salt transport processes and utilizes SEAWAT code. It is considered a time-intensive numerical model which hinders the implementation of simulation-optimization routines in coastal aquifer management. The second model coarsely approximates seawater intrusion by considering the sharp interface approach. The sharp interface model is faster compared to the variable density models, yet, it may introduce errors in the prediction of seawater intrusion since it neglects dispersion mechanisms. In this study, we investigate the potential of three sharp interface model variations to produce satisfactory approximations of the variable density based optimization. A pumping optimization problem is solved for an unconfined coastal aquifer with multiple pumping wells. The efficiency and effectiveness of the sharp interface models are compared to the optimal solutions and the computational time from the SEAWAT based optimization, which is used as benchmark. Results are further analysed based on the capability of the sharp interface models to produce feasible solutions for the SEAWAT based optimization.

Key words: Sharp interface models, SEAWAT, pumping optimization, coastal aquifer, seawater intrusion

1. INTRODUCTION

Seawater intrusion simulation is mainly based on two modelling approaches, the sharp interface models and the variable density and salt transport models. The latter emulate the dispersion zone between freshwater and saltwater and are considered more realistic than the sharp interface assumption, however, at increased computational cost (Werner et al., 2013). As a result, the coupling of variable density models with optimization algorithms for coastal aquifer management may lead to impractical computational times. On the contrary, the sharp interface models have been widely used in problems of pumping optimization of coastal aquifers due to their simple formulation and their fast runtimes (e.g. Mantoglou et al., 2004; Mantoglou and Papantoniou, 2008; Christelis et al., 2012; Karatzas and Dokou, 2015).

However, sharp interface models tend to overestimate seawater intrusion and thus may lead to a significant underestimation of the maximum allowable pumped groundwater. In this work, we perform a comparison between sharp interface and variable density models based on the optimal solutions obtained for a single-objective pumping optimization problem of coastal aquifers. First, optimization is performed based on the variable density model to obtain a benchmark solution and computational time. Then, we utilize the corresponding sharp interface model which is based on the single potential formulation of Strack (1976), to solve the same optimization problem. The sharp interface model is also employed using the density correction approach proposed by Pool and Carrera (2011) and that of Lu and Werner (2013). The objective is to identify if the corrected sharp interface models could provide reasonable approximations of the variable density optimal solutions while offering a much cheaper-to-run approach for coastal aquifer management.

2. MATERIAL AND METHODS

2.1 Variable Density Model

Variable density models consider that freshwater and seawater are mixed due to the hydrodynamic dispersion mechanism. In the simplified approach adopted in the current study, viscosity and thermal effects are neglected and density depends only on concentration. SEAWAT numerical code solves the coupled flow and solute-transport equations, which are expressed as follows (Guo and Langevin, 2002):

$$-\nabla\cdot\left(\rho\mathbf{q}\right)+\rho_s q_s=\rho S_f\frac{\partial h_f}{\partial t}+n\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} \tag{1}$$

where ρ is the fluid density $\mathbf{q}$ is the specific discharge vector, ρ_s is the density of water entering from a source or leaving through a sink, q_s is the volumetric flow rate per unit volume of porous medium representing sources and sinks, S_f is the specific storage, h_f is the freshwater head, n is porosity and C is the solute concentration. It should be noted that $\rho = \rho(P,C)$, where P is the fluid pore pressure and

$$\frac{\partial C}{\partial t}=\nabla\cdot\left(\mathbf{D}\cdot\nabla C\right)-\nabla\cdot\left(\mathbf{v}C\right)-\frac{q_s}{n}C_s \tag{2}$$

in which $\mathbf{D}$ is the hydrodynamic dispersion tensor, $\mathbf{v}$ is the fluid velocity vector and C_s is the solute concentration of water entering or leaving through sources and sinks respectively. It should be noted that no solute reactions are considered.

An additional set of equations is required, to describe the relation between the fluid density and velocity and solute transport. Darcy equations serve this purpose, which could be expressed as:

$$q_x=-K_{fx}\left(\frac{\partial h_f}{\partial x}\right),\quad q_y=-K_{fy}\left(\frac{\partial h_f}{\partial y}\right),\quad q_z=-K_{fz}\left(\frac{\partial h_f}{\partial z}+\frac{\rho-\rho_f}{\rho}\right) \tag{3}$$

in which q_x, q_y, q_z are the specific discharge components in the principal directions, K_{fx}, K_{fy}, K_{fz} are the freshwater hydraulic conductivity components in the same directions, and ρ_f is the freshwater density.

For incompressible fluids, water density is related to solute concentration through the following equation:

$$\rho=\rho_o\left(1+\frac{\alpha}{(C_s-C_o)}\left(C-C_o\right)\right) \tag{4}$$

where ρ_o is the freshwater density, α is the density difference ratio and C_o, C_s are reference and maximum concentration respectively. In the current paper we consider $C_o = 0$ kg/m^3 and $C_s = 35$ kg/m^3.

The density ration has the following form:

$$\alpha=\frac{\rho_s-\rho_o}{\rho_o} \tag{5}$$

where ρ_s is the maximum seawater density.

2.2 Sharp interface model

Sharp interface models are simplified a approximation of the coastal aquifer physical processes, since they neglect density variability in space, due to mixing between freshwater and saltwater. In the current study a steady state sharp interface model is employed, which assumes that horizontally-flowing freshwater floats above static saltwater (Essaid, 1999). The position of the interface is estimated using Ghyben-Herzberg approximation. Figure 1 presents vertical cross-sections for an unconfined coastal aquifer, where a sharp interface separates freshwater from saltwater.

As shown in the figure, there are two distinct zones in the aquifer. In zone 1 the aquifer behaves as an unconfined while in zone 2 a freshwater lens floats above the static saltwater layer. In zone 1 fresh groundwater is pumped by *M* fully penetrating pumping wells. Variable d [L] represents the depth from sea level to the aquifer base and variable ξ(x,y) [L] is the freshwater depth from sea level to the interface. Variable τ represents the point in the cross-section where the interface intersects the base of the coastal aquifers. Point τ is usually called "toe" of seawater wedge and comprises a typical measure of the extent of seawater intrusion.

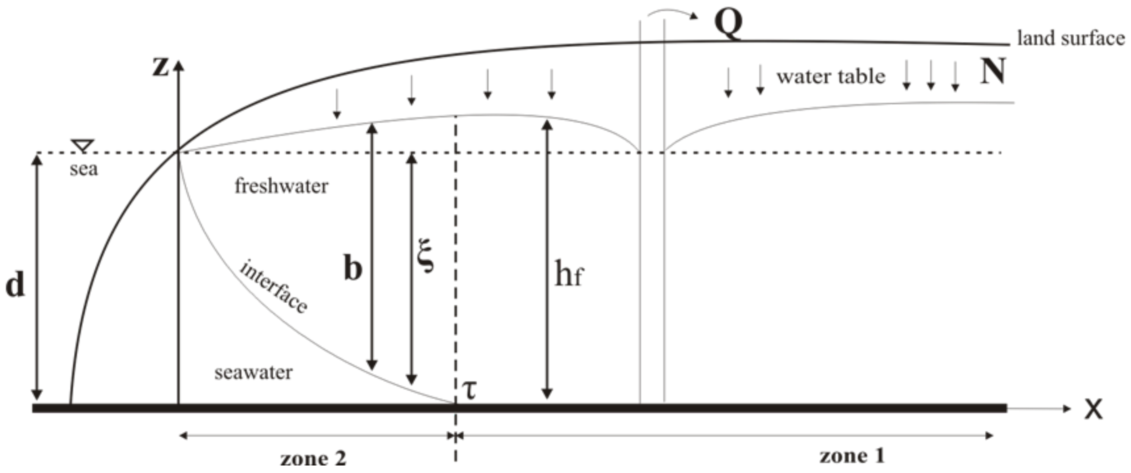

Figure 1. Schematic vertical cross-sections of an unconfined coastal aquifer based on the sharp interface approximation.

In the case of the unconfined aquifer, a groundwater recharge rate N [LT^{-1}] replenishes the aquifer. Variable $b = b(x, y)$ [L] is the total freshwater depth where in zone 1 $b = h_f$ and in zone 2 $b(x, y) = h_f - d + \xi(x, y)$, where $h_f(x, y)$ [L] is the freshwater head with reference to the impermeable aquifer base. The Ghyben-Herzberg relation links the hydraulic head h_f with depth ξ through the density ratio ε as $(1/\varepsilon)(h_f - d) = \xi(x, y)$. The following differential equations govern the steady state flow, based on the single potential formulation, which are applicable in both zones of the aquifer (Strack 1976; Mantoglou 2004):

$$\frac{\partial}{\partial x}\left(K\frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(K\frac{\partial \phi}{\partial y}\right) + N - Q\left(x, y\right) = 0, \quad \text{unconfined interface flow} \tag{6}$$

where ϕ [L^2] is the flow potential and K [LT^{-1}] is the aquifer's hydraulic conductivity. The distributed pumping rate $Q(x, y)$ [L^{3}T^{-1}] is expressed as: $Q\left(x, y\right) = \sum_{j=1}^{M} Q_j\, \delta\left(x - x_{wj}, y - y_{wj}\right)$ where (x_{wj}, y_{wj}) are the coordinates of a pumping well *j* with rate Q_j and $\delta\left(x - x_{wj}, y - y_{wj}\right)$ is the Dirac delta function. In the case of unconfined aquifers, the flow potential of Strack (1976) is defined as (Cheng and Ouazar, 1999):

$$\left.\begin{aligned} \phi &= \frac{1}{2}\ \left[h_f^2 - (1+\varepsilon)\varepsilon^2\right], \text{ zone 1} \\ \phi &= \frac{(1+\varepsilon)}{2\varepsilon}\left(h_f - \varepsilon\right)^2, \qquad \text{zone 2} \end{aligned}\right\} \tag{7}$$

At the location of the toe, the potentials have the following values for each coastal aquifer type (Cheng and Ouazar, 1999; Mantoglou, 2004):

$$\phi_\tau = \left[\frac{\varepsilon(\varepsilon+1)}{2}\right]d^2 \tag{8}$$

Depending on the complexity of the problem, equation (6) may be solved analytically or numerically (Mantoglou, 2003). Here, a numerical solution is employed following Mantoglou et al. (2004). In the present paper the academic version of HydroGeoSphere code (HGS) (Therrien and Sudicky, 1996; Graf and Therrien, 2005; Therrien et al., 2006) is used to simulate sweater intrusion for the sharp interface model.

2.3 Sharp interface model modifications

Two additional modifications of the sharp interface model, described in the previous section, are employed in the current study, to test their applicability and usefulness within a pumping optimization framework.

The first modification is an empirical correction for this sharp interface model to better match the corresponding results of the variable density model, proposed by Pool and Carrera (2011). Practically, a specific modified density ratio for the sharp interface model is calculated based on the aquifer depth B and the transverse dispersivity value α_T defined in the variable density model as follows:

$$\varepsilon^* = \varepsilon\left[1 - \left(\frac{a_T}{B}\right)^{1/6}\right] \tag{9}$$

where ε is the saltwater-freshwater density ratio defined as $\varepsilon = \left(\rho_s - \rho_f\right)/\rho_f$, with ρ_s being the saltwater density and ρ_f the freshwater density.

The second modification was introduced by Lu and Werner (2013), who proposed that the exponent 1/6 in equation (9) should be changed to 1/4.

3. PUMPING OPTIMIZATION FRAMEWORK

The main objective of pumping optimization in coastal aquifers is to maximize the well pumping rate, while protecting the aquifer from extended seawater intrusion. The extend of seawater intrusion is expressed as the distance between the well location and a specific critical iso-surface. In the case of variable density models the 0.5 kg/m^3 isochlore is selected, while in the case of the sharp interface models the interface between freshwater and saltwater is used as a critical iso-surface. In both cases a constraint is set to prevent the critical iso-surface from reaching or overrunning the wells at the base of the aquifer. This is a nonlinear constraint, which is expressed as follows:

$$\left.\begin{aligned} &\text{maximize: } \sum_{i=1}^{M} Q_i \\ &\text{subject to: } x_{\tau i} \le x_{wi}, \forall i \in (1,2,...,M) \end{aligned}\right\} \qquad (10)$$

where Q_i is the pumping rate of the i well, M is the total number of wells, $x_{\tau i} = x_{\tau i}(Q_1, Q_2,..., Q_M)$ and x_{wi} is the distance of the critical surface and the well from the coast respectively. In this formulation the pumping rates are the decision variables of the optimization. Although the objective function in (10) is linear, the overall optimization problem is nonlinear due to the nonlinear dependence of the constraints on the decision variables (Kourakos and Mantoglou, 2009).

4. APPLICATION AND RESULTS

A rectangular shaped hypothetical unconfined aquifer is used to apply the optimization framework using both the variable density model and the sharp interface model (Figure 2). The hypothetical aquifer is an abstraction of a real unconfined coastal aquifer located at the Greek Island Kalymnos. The size of the aquifer is 7000 m×3000 m×25 m. The inland boundary is a specified flux boundary, while the remaining boundaries and the aquifer bottom are considered impermeable. The aquifer is anisotropic and recharge is distributed uniformly. Table 1 outlines the basic model parameters. The aquifer is pumped by ten wells, which are also depicted in Figure 2.

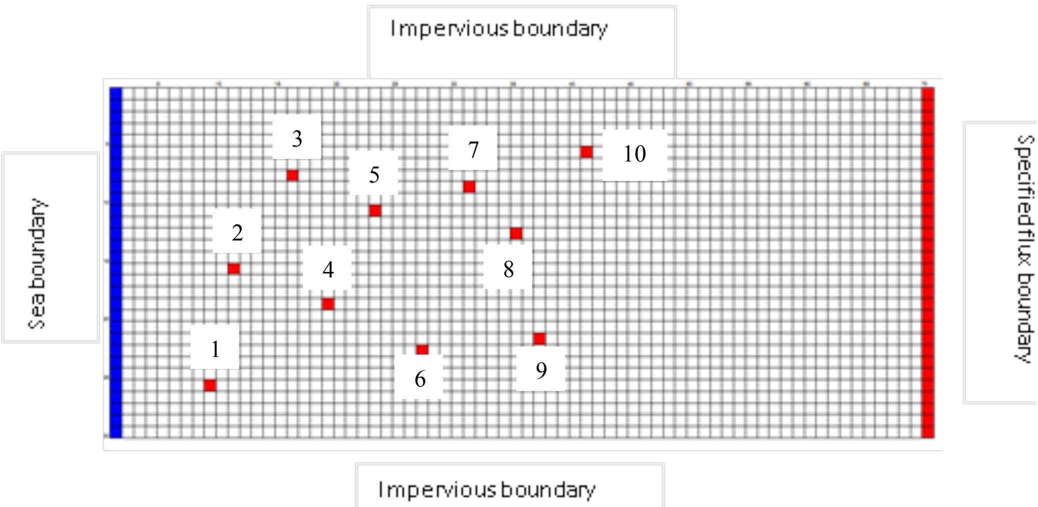

Figure 2. The rectangular shaped unconfined aquifer with the boundary conditions and the well locations.

Table 1. Basic model parameters

Parameters	Values
K_x	100 m/d
K_y	100 m/d
K_z	1 m/d
Longitudinal dispersivity	50 m
Transverse dispersivity	5 m
Vertical dispersivity	0.5 m
Density ratio	0.025
Recharge	$8.22\text{x}10^{-5}$ m/d
Lateral inflow	3696 m^3/d

The evolutionary annealing-simplex algorithm (Efstratiadis and Koutsoyiannis, 2002), which is a probabilistic heuristic global optimization technique, is used to calculate the maximum allowed pumping rates, based on the optimization framework described in Section 3. Table 2 contains the optimized pumping rates for the seawater intrusion models used in the current study.

Table 2. Optimised pumping rates (m^3/d)

Seawater Intrusion Model	Well number 1	2	3	4	5	6	7	8	9	10	Total
Variable Density	1.9	0.7	999.3	134.8	919.6	746.0	377.9	636.0	25.2	675.0	4516.6
Sharp Interface (Strack)	0.0	92.9	1000.0	0.00	999.4	0.0	5.7	480.3	0.7	167.8	2746.8
Sharp Interface (Pool & Carrera)	3.0	0.0	216.6	397.9	249.6	496.8	1000.0	605.6	748.2	999.8	4717.4
Sharp Interface (Lu & Werner)	0.0	0.3	60.7	3.2	777.6	35.2	718.6	985.2	920.2	999.2	4500.2

The results indicate that the Strack sharp interface model, as expected, overestimated the seawater penetration and provided a much lower optimal solution compared to the other seawater intrusion models. Interestingly, the total amount of the allowable pumped water calculated using the Lu and Werner (2013) modification, is similar to the variable density results, however, with a different distribution among the wells. The optimal solutions obtained with the sharp interface models were further evaluated using the more accurate variable density model. Both modified sharp interface models provided an optimal pumping rate distribution which violated the constraints and resulted in a non-feasible optimal solution (Figure 3).

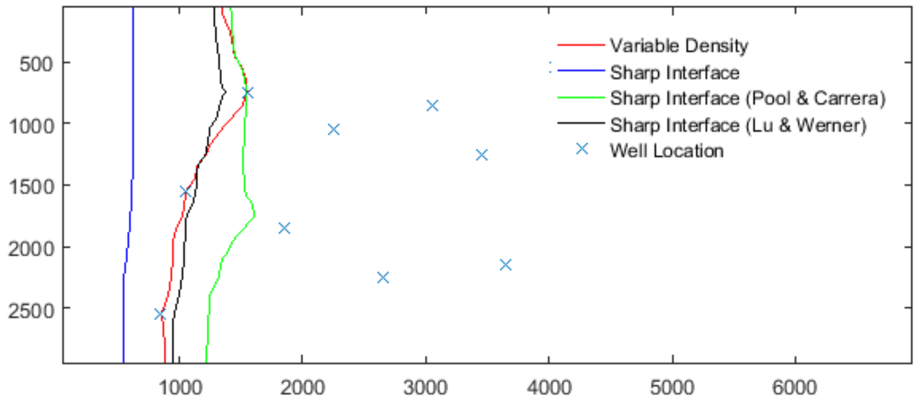

Figure 3. Presentation of the 0.5 kg/m^3 iso-chlore at the aquifer bottom, using the optimal pumping rates from each seawater intrusion model.

5. CONCLUSIONS

In the current paper an effort was made to couple several seawater intrusion models with an optimization module. The objective of the study was to examine if the simplified sharp interface models could replace the time consuming and complex variable density model in the optimization process. The results indicated that the sharp interface model introduced by Strack (1976) significantly underestimates the maximum allowed pumping rates. Regarding the modified sharp interface models, despite the fact that none of them led to a feasible solution, the results are promising and could potentially substitute the variable density model in the optimization procedure. The differences in the model solutions could be attribute to the fact that sharp interface models tend to have abrupt behavior near the critical pumping rates. Further study, could clarify the differences of the models in several levels of the pumping rates, in order to cope with the non-feasible solution problem.

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