Chapter 4

Theoretical Background

Several forward model simulations would be performed during the second phase of this study. A stochastic approach will be adopted to investigate multiple equally likely scenarios for parameter distribution in the heterogeneous shelf environment.The simulations will be performed using SHEMAT-Suite which is capable of solving the set of coupled transient partial differential equations describing the pressure- and density-driven flow of a fluid in a porous rock matrix in three dimensions Clauser (2012). The finite difference code is also able to correctly handle diffusive and bouyancy-driven salt transport. The 3D model would take into consideration saline flow associated with seawater circulation and thermal convection as indicated by Wilson (2005) as contributors to fluid flow across the continental shelf. This approach seeks to realistically represent the driving forces in the New Jersey shelf environment as well as the distribution of physical properties in three dimensions. The integrated approach provides the necessary detail to understand the observed complex distribution of fresh and saline groundwater and give new insight into the associated processes.

4.1 Density Dependent Flow Modeling

Governing equations and principles.

4.1.1 Benchmarking - The Henry problem

Verifying numerical codes against a standard analytical solution is a key step to ensuring the validity of numerical simulations. The verification of density dependent flow models is challenging due to the limited availability of analytical solutions and standard test cases (Simmons et al. 1999). The Henry saltwater intrusion problem has been widely used to benchmark numerical codes that are capable of simulating density driven fluid flow (Simpson and Clement 2003; Voss and Souza 1987). The problem considers a vertical slice through a confined coastal aquifer with homogeneous and isotropic properties. A constant influx of fresh water was applied to the landward boundary of the aquifer, with higher density seawater resting at the seaward boundary. The upper and lower boundaries of the domain were assigned constant Neumann boundary conditions representing a confined system. The domain and boundary conditions are summarized in figure 4.1.

Henry (1964) introduces dimensionless quantities to the governing equations for the dispersion of salt and fresh water in a porous medium. The general vector form of Darcy's equation and the

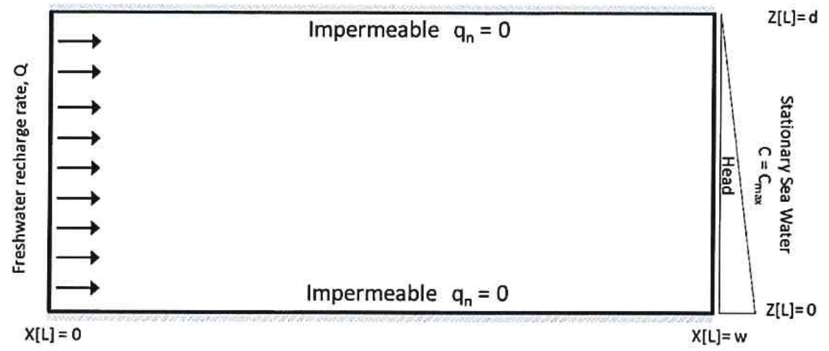


Figure 4.1: Boundary conditions and domain dimensions for modified Henry problem

equation of continuity were simplified by a combination of assumptions and empirical relationships which revealed three significant parameters that characterise the problem, $a = \frac{Q}{k_1 d}$, $b = \frac{D}{Q}$ and $\xi = \frac{w}{d}$. Note that Q $[L^2T^{-1}]$ is the freshwater recharge rate, w[L] and d[L] represent the width and depth of the domain respectively. $k_1 = K\left(\frac{\rho_s - \rho_o}{\rho_o}\right)$, where $K[LT^{-1}]$ is the saturated hydraulic conductivity of the medium, $\rho_s[ML^{-3}]$ the salt water density and $\rho_o[ML^{-3}]$ the fresh water density. It is important to note that the parameter, a, mathematically represents the balance between advective and density driven flow. When $a \gg 1$, the flow regime is dominated by advection, conversely, a value of $a \ll 1$ represents a regime where density driven flow is dominant (Simpson and Clement 2004). The selection of these parameters were governed by two main considerations, the desire to correspond closely to field data as well the numerical stability of the computation.

The study by Henry (1964) presents a semi-analytical solution for the steady-state distribution of salt concentration in the confined, saturated porous medium. The Henry problem has been widely discussed in literature (Segol 1994; Lee and Cheng 1974; Pinder and Cooper 1970) and a number of modifications suggested in the decades since its proposal. In this section, the modified version of Henry's problem presented by Simpson and Clement (2004) is reproduced using SHEMAT-Suite, and the results compared to verify the capability of the numerical code to model density driven flow in a porous medium. A quantitative comparison of the density-coupled solution to the standard coupled solution was used by Simpson and Clement (2004) to investigate the relative importance of density-driven effects and boundary forcing in the solution of Henry's problem. It was observed that the due to similarity between the two solutions, it may be possible for a faulty code to reproduce the steady state solution without accurately accounting for density driven effects. The suggested modification was to halve the rate of freshwater recharge used in the original Henry problem from 6.6×10^{-5} ms^{-1} to 3.3×10^{-5} ms^{-1}. This change had the piecewise effect of maintaining the original aspect ratio and boundary effects as well as increasing the relative importance of the density effects. The semi-analtyical solution for the modified Henry's problem was thus obtained using dimensionless parameters $\xi = 2.0$, $a = 0.1315$ and $b = 0.2$. The authors provide the value of dimensionless concentration at 10 m intervals from the top to base of the domain. This salt concentration profile was provided for horizontal positions in the aquifer from 75 cm to 195 cm, again in 10 m intervals, allowing for a spatial quantitative comparison of the SHEMAT-Suite generated salt concentration.

The modified Henry problem as presented by Simpson and Clement (2004) was implemented using SHEMAT-Suite using the medium parameters summarized in table 4.1. The steady-state

Table 4.1: Aquifer Properties

Symbol	Quantity	Value	Unit
D_m	Coefficient of molecular diffusion	1.886×10^{-5}	$m^2\ s^{-1}$
Q	Freshwater recharge rate	3.3×10^{-5}	$m^2\ s^{-1}$
κ	Permeability	1.02×10^{-9}	m^2
η	Fluid viscosity	1.002×10^{-3} (at 20°C)	m^2
θ	Porosity	0.35	–
S_s	Specific Storage	0	–
ρ_s	Salt water density	1025	$kg\ m^{-3}$
ρ_o	Reference density	1000	$kg\ m^{-3}$

salt distribution from the SHEMAT-Suite implementation of the problem is shown in figure 4.2. The position of the 50 % isochlor's intersection point with the base of the aquifer can be used as a comparative metric to estimate the similarity between the SHEMAT-Suite solution and other implementations. Simpson and Clement (2004) give the position of this intersection at 1.073 m. The position in SHEMAT-Suite obtained solution is 1.091 m. The very small discrepancy of less than 2 % shows that the SHEMAT code sufficiently replicates the result and simulates compositionally caused density driven flow correctly.

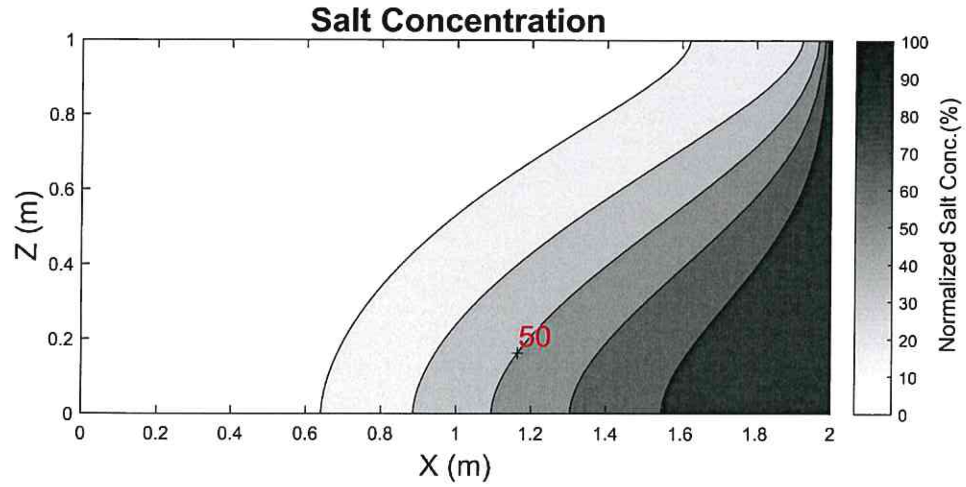
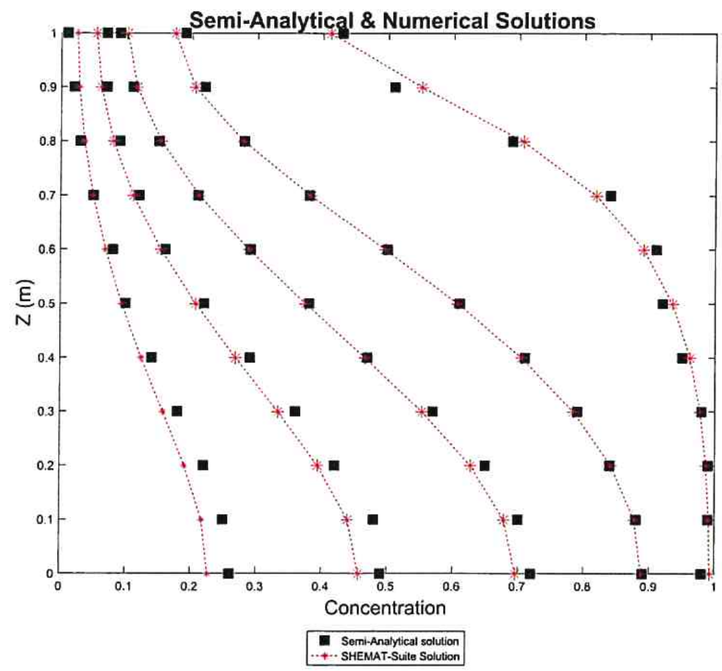
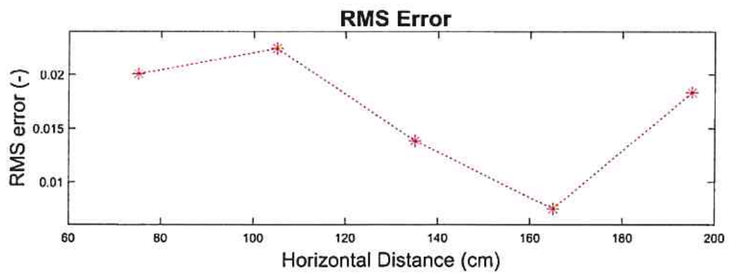


Figure 4.2: Numerical results for SHEMAT-Suite execution of modified Henry's saltwater intrusion problem for dimensionless paramaters $\xi = 2.0, a = 0.1315$ and $b = 0.2$

The dimensionless salt concentration values were extracted from the SHEMAT-Suite result and a graphical comparison between the two sets of results is shown in figure 4.3a. Vertical concentration profiles at 30 cm intervals from 75 cm to 195 cm can be directly compared to corresponding values obtained by Simpson and Clement (2004). The five profiles show very little discrepancy throughout the domain. The root-mean-square (rms) error of each profile, plotted in 4.3b, shows a maximum value of 0.023. This constitutes an acceptable fit between the two data sets.



(a) Comparison of semi-analytical solutions of modified Henry's problem and SHEMAT-Suite simulated results



(b) RMS Error

Figure 4.3: RMS Error between SHEMAT-Suite and semi-analytical solutions