Constraints on the Use of Three-Dimensional Models for the Simulation of Dynamic Freshwater Lenses

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Abstract Freshwater lenses are the major sources of water supply in many atoll islands in the Pacific and Indian oceans, particularly in dry seasons. Presently, numerous two- and three-dimensional mathematical models are available for the simulation of atoll island aquifers. The two-dimensional models such as the powerful SUTRA are unable to represent the three dimensional distribution of various parameters, the boundary conditions of the problem, and adequately simulate pumping wells. These limitations may be overcome by using a three-dimensional model, however, this will be a very challenging task. To demonstrate the related problems, an attempt was made to simulate the case of Home Island in the Indian Ocean. This exercise demonstrated that such modelling required a very fine three-dimensional discretisation of the island and short time steps of a few hours, in order to overcome the numerical instability. This required a very significantly large CPU time, even on the most sophisticated workstations. Obviously, this problem can be overcome by running the model on a super computer. However, the main problem is due to the paucity of knowledge of various parameters involved (e.g.: hydraulic conductivity, porosity, longitudinal, transverse and vertical dispersivity values, spatial and temporal variations of the recharge and extraction rates). While the Home Island dataset is comprehensive, the quality and quantity of the available data proved inadequate to meet calibration needs. The Home Island modelling clearly demonstrates the practical limitations of three-dimensional models.

1. INTRODUCTION

Freshwater lenses are the major sources of water supply in many atoll islands in the Pacific and Indian oceans, particularly in dry seasons. In most atolls a transition zone of variable density separates the freshwater lens from the saline seawater, while in the others, transition from freshwater to saline seawater can be represented by a sharp interface. Development of the atolls' limited freshwater resources is seriously constrained by the presence of brackish and saline seawater at shallow depths. Therefore, groundwater extraction by pumping methods will cause upconing of the brackish and saline seawater and will reduce the quality of the pumped water. To prevent this problem, extraction via horizontal galleries laid at shallow depths are recommended. However, an accurate estimation of the sustainable extraction rate of the lens and its sensitivity to reduced recharge during the drought periods requires application of advanced modelling techniques.

This paper describes relevant studies of the Home Island freshwater lens in the Indian Ocean as a case study. Alam and Falkland [1997 & 1998] used the two-dimensional model SUTRA [Voss, 1984] to revise the sustainable yield estimate for the Home Island freshwater lens. Simultaneously, an attempt was made to develop a three-dimensional numerical model of the Island in order to: consider the three dimensional boundary conditions of the problem; simulate adequately the extraction galleries; gain insight into the major processes affecting the freshwater lens; and to estimate its sustainable yield. Ghassemi et al. [1999] describe preliminary results of this modelling.

Subsequent to its preliminary steady state calibration, numerous difficulties were encountered during calibration of the model under transient conditions, mainly due to: numerical instability; very large CPU time; and paucity of knowledge of three-dimensional distribution of various parameters involved (e.g. hydraulic conductivity, porosity, dispersivities, spatial and temporal variations of recharge and extraction rates). These problems prevented adequate calibration of the model and its parameterisation.

2. NUMERICAL MODELLING OF FRESHWATER LENSE

2.1 Introduction

During the past few decades, a large volume of literature has been published dealing with various aspects of hydrogeology and salinity in atoll island aquifer systems and its numerical modelling. Reilly and Goodman [1985 and 1987] give a historical perspective of quantitative analysis of the relationship between saltwater and freshwater in groundwater systems. Huyakorn et al. [1987] provide a literature review of models developed for the simulation of seawater intrusion. Underwood et al. [1992] present an overview of models that have been applied to the study of atoll island groundwater systems.

Currently, several density dependent solute transport models suitable for the simulation of atoll island aquifer systems are commercially available. These include SUTRA [Voss, 1984], which is a two-dimensional model, while HST3D [Kipp, 1987 and 1997], VTT [Jacob, 1993] and SALTFLOW [Molson and Frind, 1994] are examples of three-dimensional models. These models provide solutions of two simultaneous, non-linear partial differential equations that describe the conservation of mass of fluid and conservation of mass of solute in porous media.

2.2 Calibration of a Freshwater Lens Model

Numerical models of freshwater lenses should be adequately calibrated in the following cases in order to be reliable for simulation of various management options:

- Calibration of the model in steady state in order to provide a reasonable initial condition for transient calibration.
- Calibration of tidal transmission in order to compare the measured and computed tidal efficiencies and lags.
- Transient calibration over a relatively long period of time in order to compare the measured and the computed time series of salinity at various locations and depths.

It should be noted that the above calibrations could not be achieved in a step-by-step process. Instead, it requires frequent forward and backward runs in order to obtain a set of parameters that could provide reasonable calibrated results in all three cases. In particular, the last two calibrations are much more important than the first one. Because the system is dynamic, in many cases it may not be possible to achieve a very good steady state calibration. However, the final assessment of the model calibration remains with the results of transient simulation, which reflects truly the dynamic response of the modelled system.

3. HOME ISLAND

Home Island is in the Kocos (Keeling) Islands situated in the Indian Ocean, approximately 2800 km northwest of Perth, Western Australia. It is a low-lying island with elevation of 1 to 3 m above mean sea level. It has an average annual rainfall of 1950 mm and annual potential evaporation of 2000 mm.

The island consists of a dual aquifer system. The upper unconsolidated coral sediments of Holocene age overlay unconformably the Pleistocene hard coral limestone. The depth to unconformity ranges from 9.6 m to more than 17 m below ground surface.

The measured values of hydraulic conductivity at the depths of 3 to 12 m ranged from 1.6 to 26 m day $^{-1}$, while below 12 m, they ranged between 20 and 650 m day^{-1}.

In order to explore the hydrogeology of the Island, 9 boreholes (HI1 to HI9) were drilled in 1987 to depths ranging from about 12 m to 21 m and a multi-level water sampling system was installed in each borehole (Figure 1). These systems comprised up to 8 nylon tubes, each terminated at pre-determined sampling levels. Gravel was placed around each sample intake and bentonite was used to provide a seal between the sampling levels. In 1990, four boreholes (HI9 to HI12 with HI9 relocated) and in 1996 two additional boreholes (HI13 and HI14) were drilled and equipped with multi-level water sampling systems. Although the monitoring system was designed to provide reliable point measurements of groundwater electrical conductivity (EC), values indicate some anomalies. For example, Figure 2 shows that the measured EC values at the depths of about 4.9 and 7.9 m below mean sea level (BMSL) are almost identical. Another type of anomaly (not shown on Figure 2) is the sharp rise and fall of the measured values. While the anomalies could be due to inadequate well seals or measurement errors, they may also be a natural artefact of the highly karstic behaviour of the coral limestone.

The Home Island water supply is based on groundwater extracted from the freshwater lens (Figure 3) with supplementary rainwater collected from roofs. In 1983 water was pumped from three shallow wells (PS1 to PS3). In 1984 and 1987 a fourth (PS4) and a fifth (PS5) well of similar construction were commissioned. From March to October 1991, five infiltration galleries (1 to 5) were constructed at the sites of former pump wells. Two additional galleries of similar constructions were commissioned in mid 1992 (Gallery 6) and May 1997 (Gallery 7). Total average pumping from the freshwater lens increased from about 100-115 m^3 day^{-1} in the period 1983-1988 to higher values of 223 and 194 m^3 day^{-1} in 1996 and 1997. The volumes of water pumped are measured at each gallery as well as by the main meter connected to the storage tank. However, the inflows measured on the main meter are about 20 percent greater than the combined flow measured by the individual gallery meters. Therefore it was necessary to correct the flow rates by a discrepancy factor. It is also important to note that because gallery meters were not installed until late 1992, flow measurements for the period 1988-1991 were only available at the main meter. Finally, because flow rates for 1992 are missing, estimated pumping rates for 1991 were substituted for 1992.

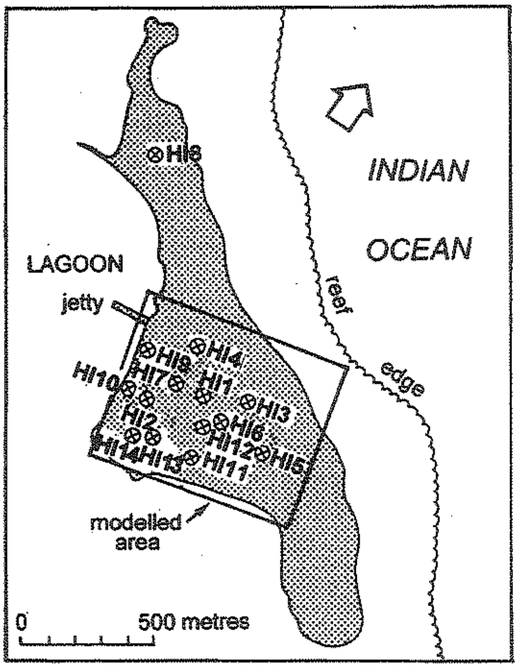

Figure 1. Location of monitoring boreholes in Home Island.

Further detailed information regarding geography, climate, hydrogeology, salinity monitoring systems, recharge estimate, water supply and estimation of the sustainable yield of the Home Island freshwater lens is available in Ghassemi et al., [1999].

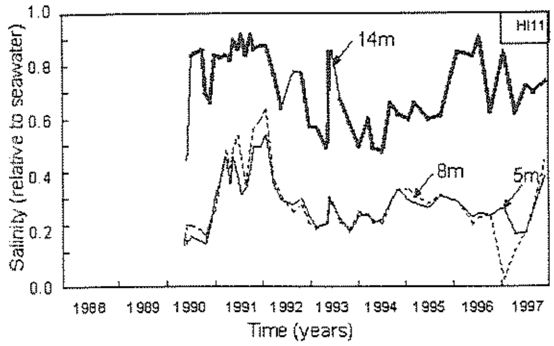

Figure 2. Plots of the measured electrical conductivity (EC) at the monitoring borehole HI11.

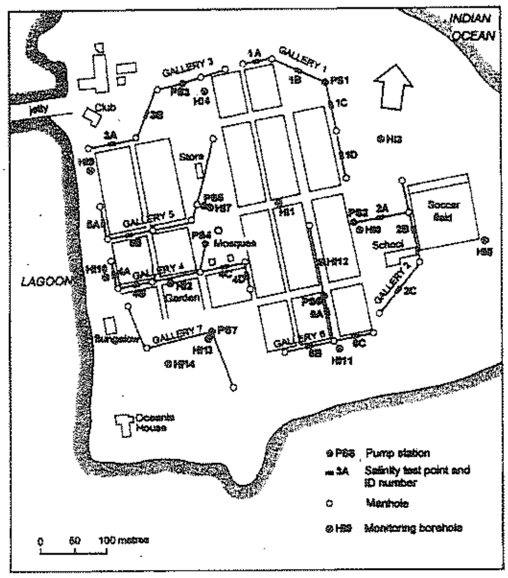

Figure 3. Home Island infiltration gallery and observation boreholes.

4. NUMERICAL SIMULATION OF THE HOME ISLAND AQUIFER

4.1 Model Description

The three dimensional simulation of the Home Island aquifer system described in this paper is based on the application of the SALTFLOW model [Molson and Frind, 1994]. A brief description of the model is provided in the Appendix.

4.2 Discretisation

In the previous 3D-modelling of the Home Island [Ghassemi et al., 1999], the central part of the Island with dimensions of 800 m long, 650 m wide and 30 m deep was simulated for the steady state conditions. In that simulation, following testing of various uniform and variable grids, the aquifer was discretised with a variable spacing

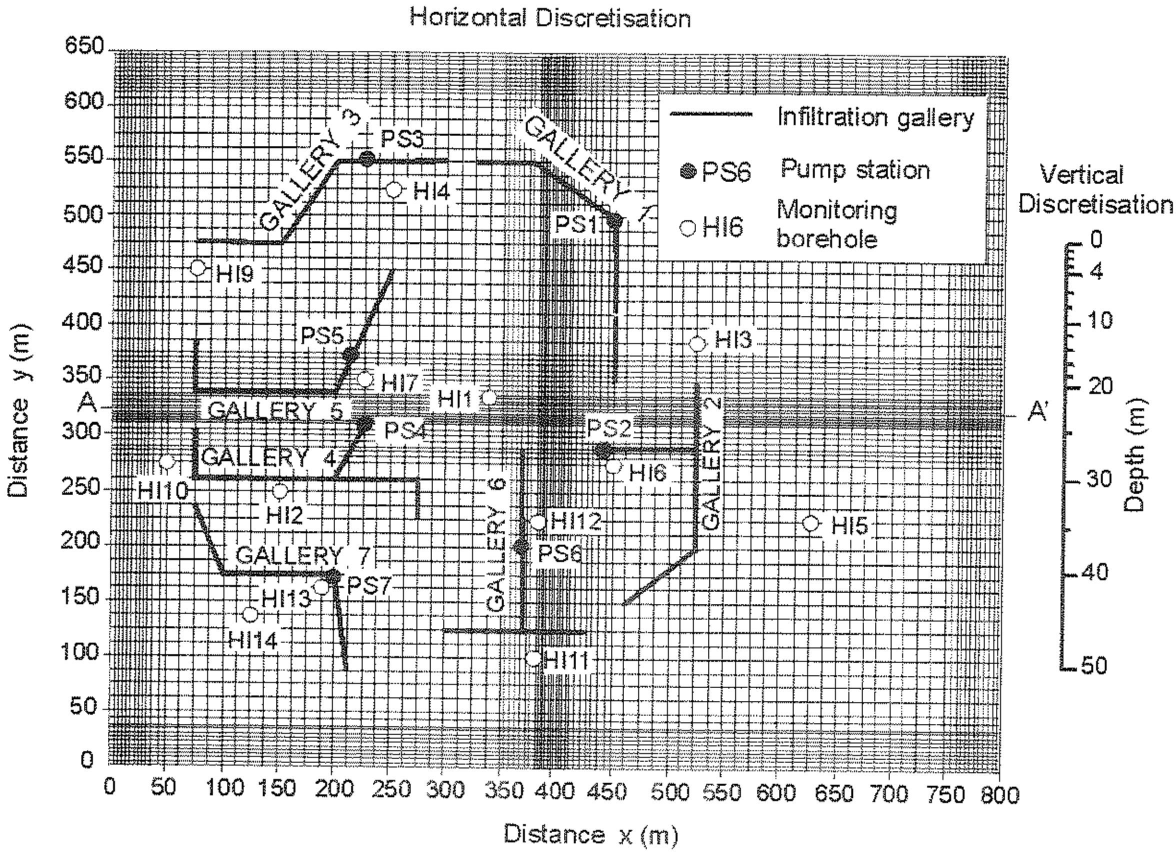

Figure 4. Horizontal and vertical discretisation of the Home Island

grid ranging from 5 m to 12.5 m in the horizontal and from 1 m to 2 m in the vertical direction. This discretisation generated 90,090 (77 x 65 x 18) nodes and 82,688 (76 x 64 x 17) elements. In the current modelling, the aquifer was simulated to the depth of 50 m for the same area. In order to reduce the numerical errors, a finer grid with variable spacing ranging from 2.5 m to 12.5 m in the horizontal and from 1 m to 10 m in the vertical direction was used (Figure 4). This discretisation increased the number of nodes to 148,410 (97 x 85 x 18) and the number of elements to 137,088 (96 x 84 x 17), about 65 percent more than the previous case. It should be noted that in both cases, unconformity between the unconsolidated Holocene sediments and the Pleistocene coral limestone was simulated at the depth of 12 m below MSL.

4.3 Boundary Conditions

Flow boundary conditions consist of: a flux boundary due to recharge from rainfall at the top surface; a no-flow boundary at the bottom surface (at the depth of 50 m); and fixed heads of 0 m along the four lateral sides. SALTFLOW converts these heads to their equivalent freshwater heads in depth, considering a density of 1.0245 kg per litre for seawater. Solute boundary conditions consist of: zero concentration for the rainwater recharging the aquifer from the top; zero concentration gradient at the bottom; and fixed concentration of 1.0 (relative to seawater) on the four lateral sides from MSL to the depth of 50 m, except for the nodes at MSL where a relative concentration of 0.3 was considered.

4.4 Stresses

The aquifer system is affected by various natural and human-induced stresses. Major natural stresses are tidal forces and variable recharge due to climatic variations, while human-induced stresses are due to extractions from wells or infiltration galleries installed at a depth of less than 1 m below MSL.

4.5 Steady State Calibration

The year 1987 was considered for the steady state calibration of the model and for preparation of the initial condition for transient calibration. For this year (1987) extraction rates from 5 shallow wells were: 27.4 m^3 day^{-1} (PS1); 21.6 m^3 day^{-1} (PS2); 27.4 m^3 day^{-1} (PS3); 23.0 m^3 day^{-1} (PS4); and 17.3 m^3 day^{-1} (PS5). Therefore, the total extraction rate was about 117 m^3 day^{-1}. In terms of recharge, an average annual value of 855 mm was used.

The computations were performed on a *Sun UltraSPARC Workstation Model 170E*. In terms of computation time, each run of the model required approximately 50 hours CPU time to simulate a period of 1500 days with time steps of half a day. The SALTFLOW code was compiled with the Fujitsu FORTRAN 90 compiler that accelerated the computations by a factor of 2.5 compared with the FORTRAN 77 compiler.

Model parameters were estimated by trial and error using limited measurements taken on the island and values adopted by Underwood et al. [1992, Table 4] for their generalised atoll island model simulated with SUTRA [Voss, 1984]. The parameter values resulting from model calibration are listed in Table 1. The calibrated values are close to the measured values on the island and compare favourably with values used by Alam and Falkland [1998] and Underwood et al.[1992]. The major exceptions are the horizontal and vertical hydraulic conductivity of the Pleistocene sediments which are significantly lower in the study by Underwood et al. [1992].

In order to check the degree of match between the computed and the measured salinities, their values have been compared at all monitoring boreholes operating in 1987. Figure 5 compares the measured and computed salinities within a longitudinal vertical cross-section of the aquifer system. This figure indicates that the computed salinities are not free from numerical instability represented by unsmooth contours. Discrepancies between the measured and computed salinities are due to: lack of knowledge about model parameters and their three dimensional distributions; differences between the real and simulated boundaries of the aquifer; and the fact that the aquifer system is not in a steady state equilibrium.

4.6 Simulation of Tidal Wave Transmission

The model was set-up for simulation of tidal wave transmission in the aquifer system by using the parameters provided in Table 1 and a sinusoidal tidal wave with amplitude of 0.8 m consisting of two high peaks and two throughs in every 24 hours. The model was run with time steps of about 36 minutes. Results of simulations indicated that tidal efficiencies were approximately 24 percent, which are close to the measured values for sites PS1 to PS4. It should be noted that simulation of tidal waves with lower hydraulic conductivity values of Underwood et al., (1992) produced low tidal efficiencies of about 10 percent.

Table 1. Parameter values used to describe the Home Island aquifer system and their comparison with Alam and Falkland [1998] and Underwood et al. [1992] values.

Parameters and their units	Calibrated values	Alam values	Underwood values
Porosity	0.25	0.20	0.25
Holocene sediments thickness (m)	12	12	15
Holocene sediments horizontal hydraulic conductivity (m day^{-1})	15	10	50
Holocene sediments vertical hydraulic conductivity (m day^{-1})	15	5	10
Pleistocene sediments horizontal hydraulic conductivity (m day^{-1})	1500	1000	500
Pleistocene sediments vertical hydraulic conductivity (m day^{-1})	300	200	100
Longitudinal dispersivity (m)	4	10	6-12
Transverse dispersivity (m)	1	0.5	0.01
Vertical dispersivity (m)	0.05	0.05	0.01-0.05
Average annual recharge (mm)	855	855	500-2000

4.7 Steady State Simulation with Tidal Waves

An attempt was made to simulate the aquifer in steady state mode with inclusion of tidal waves and aquifer parameters reported in Table 1 with the exception of dispersivity values. This simulation required short time steps of 6 hours over less than 1000 days to reach equilibrium and to produce results close to those obtained without considering the tidal waves. Short time steps were required to simulate the tidal waves and to prevent numerical errors. It is important to note that this simulation required very low values of 0.01 m, 0.001 m and 0.0001 m for the longitudinal, transverse and vertical dispersivity respectively. Using higher values such as those indicated in Table 1 resulted in complete invasion of the aquifer by saline water. The results clearly suggest that the real dispersivity values of the aquifer are very low. This is in contradiction to the steady

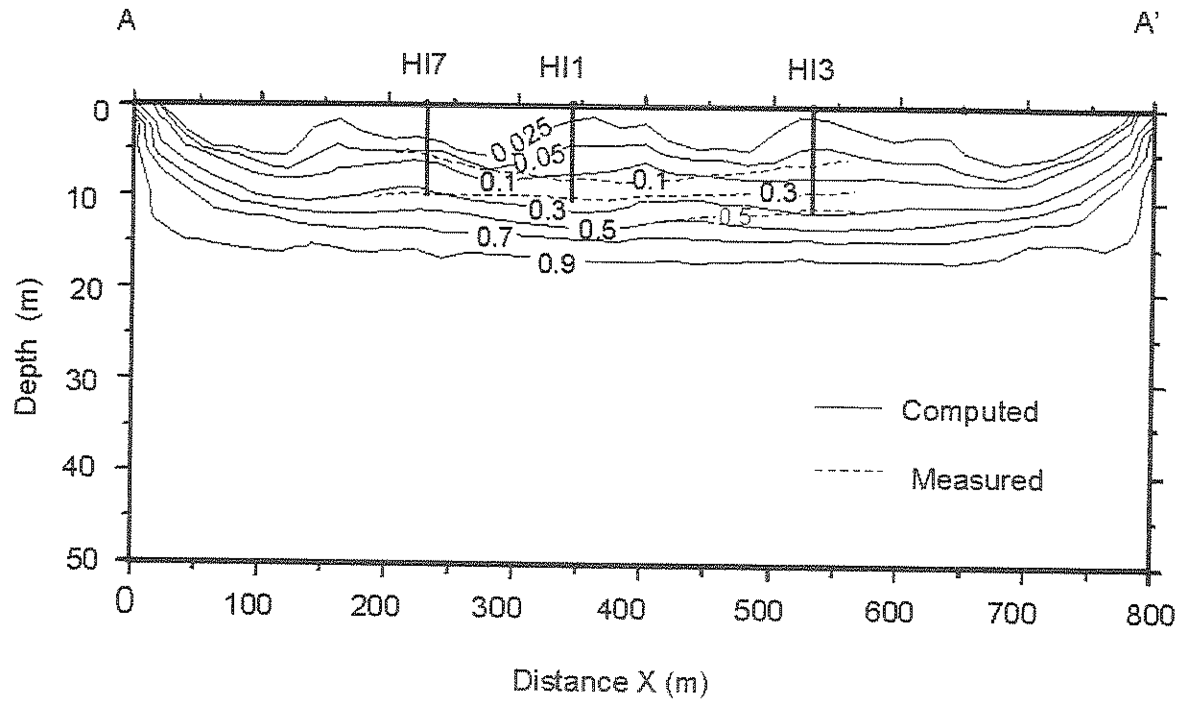

Figure 5. Computed and measured longitudinal groundwater salinity contours (relative to seawater) at profile A-A' (Figure 4).

state simulation without tidal waves where higher dispersivity values were required to produce the mixing effects of tidal movements on the salinity distribution

4.8 Transient Simulation

The model was run over a ten-year period (1988-1997) using quarterly recharge and pumping data. Extractions via shallow wells with short galleries were simulated at pumping sites and neighbouring nodes from 1988 to 1991. Pumping was extended to include gallery nodes when they were converted to galleries in 1991. Extraction rates for each gallery were distributed over the nodes representing the gallery, and proportional to the effective area of each node, at the depth of 0 m to 1 m. The quarterly recharge rates were uniformly distributed over the nodes at the top layer of the model. For this simulation the parameters shown in Table 1 were used. The computed salinities were compared with the measured values at all boreholes (except HI8) at 3 different depths to obtain a good assessment of the quality of the computed values. The results showed that the model reflects changes in computed salinity values due to changes in pumping rates and recharge. However, there was a clear discrepancy between the measured and the computed values (compare Figures. 2 and 6). For this simulation, the size of the input file was about 6300 lines, while it was approximately 200 lines in the steady state simulation. Moreover, the computation time was about 150 hours or 6.25 days for 14,600 time steps of 6 hours (10 years x 365 day x 4).

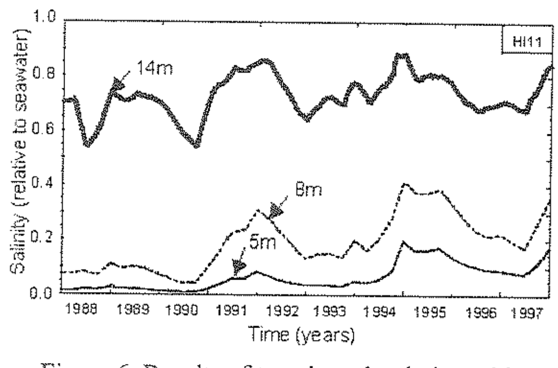

Figure 6. Results of transient simulation with quarterly recharge and pumping data at borehole HI11 for three different depths.

To improve the computed values, the model was run with monthly values of recharge and pumping data. For this simulation run, the size of input file increased to about 19,000 lines, which is three times longer than the previous case. The computation time remained almost the same (150 hours) for the same 10-year period because the number of time steps remained unchanged. The computed values (Figure 7) show some improvement compared to the previous run with quarterly data. However, they failed to match the measured values at similar locations and depths. Despite numerous runs with modified values of the hydraulic conductivity, porosity and other parameters, no further improvement in the overall distribution of the computed salinity values could be achieved.

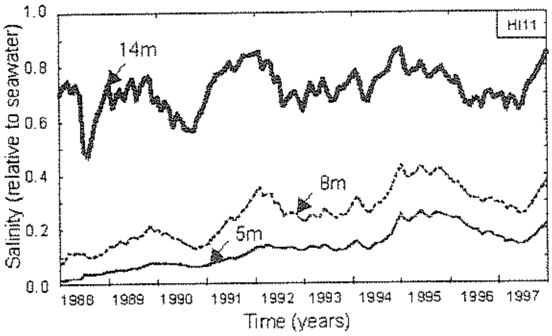

Figure 7. Results of transient simulation with monthly recharge and pumping data at borehole HI11 for three different depths.

4.9 Sensitivity Analysis

A sensitivity analysis indicated the sensitivity of the model outputs with respect to important parameters such as hydraulic conductivity of the Holocene and Pleistocene sediments, recharge and pumping rates, porosity, and dispersivity. Some of the results are as follows:

- Higher values of the Holocene hydraulic conductivity facilitate intrusion of seawater and will increase the computed salinities.
- The hydraulic conductivity of the Pleistocene sediments has no major impact on the steady state salinity distribution in the Holocene aquifer. However, higher values increase the computed tidal efficiencies and salinities in the transient simulation.
- Increased recharge will dilute the saline water in the aquifer and will reduce the computed salinities.
- Increased extraction rates will increase the computed salinities.
- Reduced porosity will increase tidal efficiencies.
- Increased dispersivity values will increase the computed salinities.

5. CONCLUSIONS

Recently, significant progress has been made towards the development and application of three-dimensional density-dependent solute transport models that can accommodate three-dimensional boundaries and adequately represent extraction via shallow wells and galleries of the type commonly used in coastal and island aquifers. While the development of powerful workstations has facilitated this task, the Home Island modelling exercise using SALTFLOW demonstrated that even the most advanced workstations will be challenged by the three-dimensional simulation of a relatively small atoll island aquifer systems with consideration of all parameters and processes affecting the aquifer system including tidal forces. For example, to reduce numerical errors to an acceptable levels, the simulated area on Home Island (800 m x 650 m x 50 m) required discretisation into about 148,400 nodes and 137,000 elements. When this fine discretisation is combined with short time steps of six hours over a 10 year period, 150 hours CPU time is required on an advanced workstation using the model compiled with a Fujitsu FORTRAN 90 compiler. On the same workstation, running the model compiled with a FORTRAN 77 compiler, the required run time was 2.5 times higher.

Long CPU time and high memory demand (about 0.5 Gb) represented a problem as it reduced the opportunity to test the model with alternative sets of aquifer parameters. Nevertheless, these cannot be considered serious limitations of three-dimensional models, it will simply become less of an impediment as more powerful and cheaper workstations become available.

In the Home Island modelling exercise, high computational demand was an unwelcome difficulty, but it was not the reason why calibration could not be achieved. The Home Island modelling exercise failed because the quantity and quality of the available data were simply inadequate to meet calibration needs. Important lessons can and should be learnt. As an indication of the exhaustive data demands of the model (e.g. three-dimensional distributions of hydraulic conductivity, porosity, dispersivities, spatial and temporal variations of recharge and extraction rates) the input data file for transient simulation with monthly time steps consisted of about 19,000 lines. The high demand for quality data represents an immense challenge for the field hydrogeologists as very few of these data can be reliably generated via the lengthy model calibration procedure. From a practical standpoint this type of modelling exercise should not be contemplated without outstandingly good spatial and temporal datasets and first class computing facilities. It also raises the concern that our ability to develop computer codes capable of simulating complex aquifer systems is beginning to exceed our ability to supply the input data necessary for their reliable calibration.

REFERENCES

Alam, K., and A.C. Falkland, Home Island groundwater modelling and potential future groundwater development. ECOWISE Environmental, ACTEW Corporation, Canberra, 1997.

Alam, K., and A.C. Falkland, Home Island groundwater modelling Stage 2. ECOWISE Environmental, ACTEW Corporation, Canberra, 1998.

Ghassemi. F., J.W. Molson, A. Falkland and K. Alam, Three-dimensional simulation of the Home Island freshwater lens: preliminary results. *Environmental Modelling & Software* 14(2-3), 181-190, 1999.

Huyakorn, P.S., P.F. Andersen, J.W. Mercer, and H.O. Jr White, Salt water intrusion in aquifers - Development and testing of a three dimensional finite element model. *Water Resources Research* 23(2), 293-312, 1987.

Jacob, F., Modélisation tridimensionnelle par la méthode des éléments finis de l'ecoulement et du transport en milieu poreux saturé. Laboratoire de Calcul Scientifique, Université de Franche-Comté, Besançon, France, PhD dissertation, 1993.

Kipp, K.L., HST3D - A computer code for simulation of heat and solute transport in three dimensional ground-water flow systems. Water Resources Investigation Report 86-4095, US Geological Survey, Denver, Colorado, 1987.

Kipp, K.L., Guide to the revised heat and solute transport simulator: HST3D-Version 2. Water-Resources Investigations Report 97-4157, US Geological Survey, Denver, Colorado, 1997.

Molson, J.W., and E.O. Frind, SALTFLOW: Density dependent flow and mass transport model in three dimensions, User Guide. Waterloo Centre for Groundwater Research, University of Waterloo, Waterloo, Ontario, 1994.

Reilly, T.E., and A.S. Goodman, Quantitative analysis of saltwater freshwater relationships in groundwater systems - A historical perspective. *Journal of Hydrology* 80, 125-160, 1985.

Reilly, T.E., and A.S. Goodman, Analysis of saltwater upconing beneath a pumping well. *Journal of Hydrology* 89,169-204, 1987.

Underwood, M.R., F.L. Peterson, and C.I. Voss, Groundwater lens dynamics of atoll islands. *Water Resources Research* 28(11), 2889-2902, 1992.

Voss, C.I., SUTRA (Saturated-Unsaturated TRAnsport), a finite-element simulation model for saturated-unsaturated fluid density-dependent groundwater flow with energy transport or chemically reactive single species solute transport. US Geological Survey Water Resources Investigation Report 84-4369, 1984.

APPENDIX: Description of the SALTFLOW Model

SALTFLOW is a numerical model for solving complex density-dependent groundwater flow and mass transport problems. The model can be used to solve one, two, or three-dimensional mass transport problems within a variety of hydrogeological systems.

Finite elements are employed for high accuracy and to allow deformable domain geometry. The model includes an efficient preconditioned conjugate gradient solver to solve the matrix equations. In this model the equation of conservation of mass of fluid is expressed as:

$$\frac{\partial}{\partial x_i}\left[K_{ij}\left(\frac{\partial\psi}{\partial x_j}+\gamma c n_j\right)\right]-\sum_{k=1}^{N} Q_k(t)\cdot\delta(x_k,y_k,z_k) = S_s\frac{\partial\psi}{\partial t} \qquad (1)$$

where x_i are the 3D spatial coordinates $(x_i = x, y, z)$, t is time (T), K_{ij} is the hydraulic conductivity tensor (L T^{-1}) and ψ is the equivalent freshwater head (L). The constant γ is defined by $\gamma = (\rho_{max}/\rho_o - 1)$ where ρ_{max} (ML^{-3}) is the maximum fluid density and ρ_o (ML^{-3}) is the reference freshwater density (Frind, 1982), c is the relative concentration, n_j is the unit vector, $Q_k(t)$ is the volume flux (L^3T^{-1}) for the sources/sinks located at (x_k, y_k, z_k), N is the number of sources/sinks, δ (x_k, y_k, z_k) is the Dirac delta function (L^{-3}) and S_s is the specific storage coefficient (L^{-1}).

The equation of conservation of mass of salt is represented by:

$$\frac{\partial}{\partial x_i}\left[\left(\frac{D_{ij}}{R}\right)\frac{\partial c}{\partial x_j}\right]-\frac{\partial}{\partial x_i}\left(\frac{v_i}{R}c\right)-\lambda c+ \sum_{k=1}^{N}\frac{Q_k(t)c_k(t)}{R\theta}\cdot\delta(x_k,y_k,z_k)=\frac{\partial c}{\partial t} \qquad (2)$$

where D_{ij} is the hydrodynamic dispersion tensor (L^2T^{-1}), v_i is the average linear groundwater velocity (L T^{-1}), R is the retardation factor (dimensionless), λ is the first order decay term (T^{-1}) and θ is the porosity of the saturated media (dimensionless).

Further details regarding the theoretical basis of the SALTFLOW model, spatial and temporal discretisation criteria, and example applications are available in Molson and Frind (1994).