Phatcharasak Arlai

Numerical Modeling of possible Saltwater Intrusion Mechanisms in the Multiple-Layer Coastal Aquifer System of the Gulf of Thailand
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ABSTRACT

The lower central plain region of Thailand that consists of Bangkok Metropolis and the vicinity provinces, namely, Samut Prakan, Samut Sakhon, Nonthaburi, Pathum Thani, Nakhon Pathom, Chachoengsao, and Phra Nakhon Si Ayutthaya are economically the fastest growing territory of Thailand. As a consequence, this region has faced an incredible increase of groundwater withdrawal during the last few decades, especially, during the recent economic boom which has induced a multiple augmentation of both population and industrial factories in both Bangkok and its neighboring provinces, the more so since the surface water supply is insufficient. Accordingly, the groundwater demand has accrued considerably and thus uncountable discharge wells have been drilled into the Bangkok multiple aquifers system - until 1983 free of any financial groundwater charge and often without government permission. Hence, this has led to the present moribund situation where the actual groundwater pumping shows evidence of overdraw beyond the natural aquifer yield, with the consequence, that the piezometric heads in the productive aquifers have rampantly decreased, especially in the second, the third and the fourth aquifer layer, and steep head gradients have built up that are inducing encroachments of saltwater from its sources into the producing aquifers, leading to heavy saltwater pollution there.

However, in spite of much research activities in recent years, the mechanisms of saltwater intrusion in the Bangkok aquifers system are not yet fully grasped, namely, it is still a matter of dispute whether the saline contamination found in some areas is due to either classical seawater intrusion or to vertical seepage of saline water from the uppermost marine clay layer that is prevalent over most of the area of the Lower Chao-Praya river basin.

The understanding of these saline intrusion mechanisms would help to establish sustainable groundwater management scenarios that are resilient to the present fatal circumstances and that allow, consequently, to sustain groundwater use in the Bangkok aquifers in the long run or, even better, to revert some of the detrimental effects by aquifer restoration.
All of these facets of facts lead to the topic of the present Dr.-Ing dissertation and where the author is attempting through state-of-the art numerical flow and transport modeling to better understand the sources and dynamics of the severe saline contamination in the Bangkok aquifers system and, based on that, to develop resilient groundwater management strategies for the efficient future restoration of this heavily stressed aquifer.

The contexts and basic conclusions of the 10 chapters of the present dissertation are as follows:

**Chapter 1** summarizes a statement of the problem, the objectives, the scope of study and its expected advantages.

**Chapter 2** reviews the literature on the relevant research work done up-to-date in the study area.

**Chapter 3** describes the hydrogeological and hydroclimatic specifics of the study area.

**Chapter 4** describes the model set-up of the Bangkok aquifers model using the MODFLOW-96 groundwater model and illustrates the important steps necessary to reasonably assess calibrated hydraulic parameters which are, namely, (1) the conventional trial-and-error forward analysis, (2) a new approach of the zone-wise calculation of sensitivity- and correlation coefficients for each parameter through nonlinear inverse regression which indicates those estimated parameters that are well-determined and unique in each of the sub-zones – a critical calibration aspect which a common groundwater modeler often neglects and, (3) the pure stochastic approach which consists in applying Monte-Carlo (MC)-simulations. This is done in two steps: Firstly, a theoretical stochastic formula which describes how $\sigma^2_Y$ of the heterogeneous transmissivity field contributes to $\sigma^2_H$ of the observed head and/or residuals is validated. Secondly, it is examined which factors affect the residual error of the model estimation. The results of this task indicate that both transmissivity variations and errors in the head measurements are mostly responsible for a non-zero estimated residual
head, while the uncertainties in the pumping rates play only a minor role for the success of the model-fit to the observed data.

**Chapter 5** deals with the applicability of the sustainable yield concept to the Bangkok aquifers system, using basically two scenarios of future groundwater withdrawal. Succinctly, the results show that the sustainable yield cannot serve the demand, and there is a so-called unmet demand that must be supplemented by surface water. It is listed for each province affected. Although the sustainability condition for the piezometric head might be satisfied, contamination inside layers 3, 4 and 5 could not be significantly alleviated, since (a) saline water is driven downward from the uppermost marine clay layer into the lower ones and, (b) the pump-induced hydraulic gradients cannot push back the saltwater to its source regions. Indeed the water balance shows that 34% of the inflow to the aquifer system originates in the uppermost marine clay layer, while only 6% of the inflow intrudes from the Gulf of Thailand.

In **Chapter 6** the author discloses from the analyses of the available groundwater quality data and by numerical modeling that two synchronous saltwater cradles co-exist for the aquifer-system, namely, one from seawater intrusion and another one from vertical saltwater leakage from the uppermost marine clay layer that has protruded to the lower aquifer layers. The author is able to draw an innovative map that allows to discriminate between four types of contaminated zones from the two sources. This map clearly shows that seawater dominantly intrudes along the coastline west of the Chao-Praya River, while vertical saltwater intrusion mainly pollutes groundwater in the vicinity of Bangkok, Nonthaburi, Pathum Thani and some parts of Samut Prakan. Moreover, the author indicates that, because of the dual origins of the saline waters above, a classical groundwater recharge alone is not able to improve the groundwater quality in the Bangkok aquifer system in the future, but that more complex water management strategies are needed, such as “policy”- or “non-constructive” measures, as well as a combination of “policy”- and “constructive” (use of recharge- and clean-up wells) measures. For that purpose a set of 31 different schemes is analyzed by means of the flow and transport model MODFLOW/MT3DMS. It turns out that the best scenarios are the ones where all pumps in the lower layers are shut off, or where the pump rates are reduced to 60% of their 2002- values. An even more efficient, but also costlier scenario is one which uses such a water policy change in conjunction with several recharge and clean-up wells.
In Chapter 7 it is explained how urgently a density-dependent flow and solute transport model is needed to model the Bangkok aquifers system, given the high salinity concentrations found there. For the achievement of this goal the author uses, in addition to the constant-density MODFLOW-96&MT3DMS model, the SEAWAT-2000 variable-density model. As an important result of these investigations it is unveiled that, at least for the present application, both the density-dependent and the density-constant model result basically in similar saline plume migrations. The author explains this astounding outcome by the fact that the groundwater pumping in the Bangkok multilayered aquifers plays the most important role in the plume movement, overshadowing the density (buoyancy) -effects. As an add-on to this study part a detailed sensitivity analysis of the hydrodynamic dispersion and of the aquifer anisotropy is performed. From all of these results it is concluded that the variable density of the contaminant saline plumes does not appear to have a significant feedback effect on the hydraulic flow itself in the Bangkok multilayered aquifers. Thus, a complicated and computationally time-consuming density-dependent flow and solute transport model may pragmatically not function better than a simple tracer (constant-density) model and may be duly forsaken for practical groundwater management purposes.

In Chapter 8 the author explores seven different groundwater management schemes for the best sustainable future groundwater restoration of the Bangkok aquifers system. The first three “non-constructive” schemes are taken from a previous chapter where they have been simulated only by the constant-density MODFLOW-96&MT3DMS model and they are re-run by the newest version of the variable-density model SEAWAT-2000, allowing for a more realistic determination of the saline plume effects on the flow due these schemes. In a second part of this chapter the author employs, for the first time, a highly complex groundwater management optimization tool, the GWM-model—which uses techniques of linear programming and nonlinear optimization---, to optimize various other recharge- and clean-up well configurations of the best integrated non-constructive and constructive schemes investigated earlier and, in addition, optimizes three new schemes that use a “water supply trade-off concept” for the in-lieu water supply cells of the recharge wells. Next, all seven schemes are re-simulated with the variable-density flow and solute transport model SEAWAT-2000 to see how their efficiency is impacted by saline density effects. Finally, the author is doing a very careful evaluation and comparison of the hydraulic- and the
groundwater-quality efficiency and of the total financial costs of all schemes investigated and proposes one of them as the best alternative for realization.

Finally, the author investigates in an Appendix in more detail, as part of a case study of classical coastal seawater intrusion, the importance of using a density-dependent flow and transport model for this purpose. The results of these investigations unveil that, although the variable-density flow and transport model is computationally much more time-consuming than the density-independent (tracer) one, it mimics the physical mechanisms of coupled flow and solute transport much better than the latter and thus should be used for such applications.
KURZFASSUNG


Trotz vieler Forschungstätigkeiten in den letzten Jahren wurden die Umstände und Mechanismen der Salzwasserintrusion im Aquifersystem von Bangkok noch nicht völlig geklärt. In der Diskussion ist ob die örtliche gefundene Salzwasserverschmutzung des Grundwassers durch klassische Meerwasserintrusion oder aber durch vertikale Versickerung salzigen Wassers aus dem Hangenden der obersten Tonschicht, die im Bereich des unteren Chao-Praya Flußbeckens weit verbreitet ist, verursacht wird.

Das Verständnis dieser Mechanismen der Salzwasserintrusion würde zur Erstellung von Grundwassermanagement-Szenarien beitragen, die der gegenwärtigen fatalen Umstände entgegenwirken, die längerfristige schonende Nutzung des Grundwasserdargebotes des
Bangkok Aquifer-Systems sichern können und, mehr noch, eine Wiederherstellung und Sanierung des Aquifers ermöglichen.


Der Inhalt und die grundlegenden Ergebnisse der zehn Kapitel dieser Forschungsarbeit lassen sich wie folgt beschreiben:

Im ersten Kapitel werden der Problemzustand, die Zielsetzung, das Bereichsfeld der Studie und die zu erwartenden Ergebnisse beschrieben.

Das zweite Kapitel fasst den Stand der Forschung anhand der relevanten Literatur und der bisher im Untersuchungsgebiete durchgeführten Studien zusammen.

Das dritte Kapitel beschreibt detailliert die hydrogeologischen und hydrologischen Besonderheiten des Untersuchungsgebiets.

Das vierte Kapitel beschreibt die Konfiguration des MODFLOW-96 Modells für das Aquifers-System von Bangkok und veranschaulicht die wichtigsten Schritte, die notwendig sind, kalibrierte hydraulische Parameter zu erhalten. Diese sind (1) die herkömmliche „trial-and-error“ Vorwärtsanalyse, (2) ein neuer Ansatz der zonenweise Berechnung der Empfindlichkeits- und Korrelationskoeffizienten durch nichtlineare inverse Regression, die es gestattet, die gut geschätzten Parameter kenntlich zu machen - ein kritischer Aspekt der Kalibrierung, der häufig in der Grundwassermodellierung vernachlässigt wird und, (3) der rein stochastische Ansatz, der in der Anwendung von Monte-Carlo (MC)-Simulationen besteht. Dies geschieht in zwei Schritten: Erstens wird eine theoretische stochastische Formel, die eine Aussage macht wie $\sigma_Y^2$ eines heterogenen Transmissivitätsfeldes zu $\sigma_H^2$ der beobachteten Standrohrspiegelhöhen und/oder den Residuen beiträgt, validiert. Zweitens wird
überprüft, welche der Faktoren den residualen Fehler des Modells beeinflussen. Die Resultate dieser Methoden zeigen dass meistens beide, Variationen der Transmissivität und Fehler bei der Messung der Standrohspiegelhöhen, für eine ungleich-null geschätzte residuale Standrohspiegelhöhe verantwortlich sind, während Ungewissheiten über Pumpraten nur eine kleine Rolle bei der Modellanpassung an die beobachteten Werte spielen.


zum Zwecke des praktischen Grundwassermanagements leichten Herzens aufgegeben werden.


## CONTENTS

**Chapter 1: Introduction**

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>Motivation</td>
<td>1</td>
</tr>
<tr>
<td>1.2</td>
<td>Objectives</td>
<td>4</td>
</tr>
<tr>
<td>1.3</td>
<td>Scope of study</td>
<td>5</td>
</tr>
<tr>
<td>1.4</td>
<td>Expected advantages</td>
<td>6</td>
</tr>
<tr>
<td>References</td>
<td></td>
<td>7</td>
</tr>
</tbody>
</table>

**Chapter 2: Literature Review**

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Deterministic modeling of saltwater intrusion</td>
<td>11</td>
</tr>
<tr>
<td>2.2</td>
<td>Saltwater intrusion investigations in the multiple-aquifers system underneath Bangkok and adjacent provinces</td>
<td>13</td>
</tr>
<tr>
<td>2.3</td>
<td>Density effects on solute transport</td>
<td>17</td>
</tr>
<tr>
<td>References</td>
<td></td>
<td>20</td>
</tr>
</tbody>
</table>

**Chapter 3: Hydrogeological Overview of Study Area**

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1</td>
<td>Topography</td>
<td>24</td>
</tr>
<tr>
<td>3.2</td>
<td>Geology</td>
<td>24</td>
</tr>
<tr>
<td>3.3</td>
<td>Hydrogeology</td>
<td>27</td>
</tr>
<tr>
<td>3.4</td>
<td>Climatic characteristics and groundwater recharge</td>
<td>30</td>
</tr>
<tr>
<td>3.4.1</td>
<td>Rainfall</td>
<td>30</td>
</tr>
<tr>
<td>3.4.2</td>
<td>Evaporation</td>
<td>30</td>
</tr>
<tr>
<td>3.4.3</td>
<td>Recharge</td>
<td>31</td>
</tr>
<tr>
<td>References</td>
<td></td>
<td>32</td>
</tr>
</tbody>
</table>
Chapter 4: Statistical and stochastic Approaches to assess reasonable calibrated Parameters in a complex Multi-Aquifer System ................................................................. 33

4.1 Motivation ........................................................................................................................................... 33

4.2 Study area and model implementation .................................................................................................. 36

4.3 Mathematical formulation .......................................................................................................................... 37
  4.3.1 Groundwater flow equation and numerical approach ........................................................................ 37
  4.3.2 Statistics of sensitivity analysis ........................................................................................................... 43
  4.3.2 Stochastic formulation .......................................................................................................................... 46

4.4 Effective approaches to assess the reliable parameters in the Bangkok aquifers model.. .......................................................... .................................................................................... 47
  4.4.1 Conventional (forward) trial-and-error approach ................................................................................. 47
  4.4.2 Statistical regression (inverse) approach ............................................................................................... 49
  4.4.3 Stochastic modeling using MC-simulations and validation of stochastic theory ............................. 56

4.5 Summary ............................................................................................................................................... 62

References ..................................................................................................................................................... 64

Chapter 5: Modeling Flow and Transport for sustainable Yield Estimation of Groundwater Resources in the Bangkok Aquifer System................................................. 66

5.1 Statement of problem ................................................................................................................................. 66

5.2 Study area and model implementation ..................................................................................................... 67

5.3 Calibration of reliable parameters in the model ........................................................................................ 68
  5.3.1 Flow calibration ..................................................................................................................................... 68
  5.3.2 Solute transport calibration ................................................................................................................... 69

5.4 Sustainable yield estimation ....................................................................................................................... 71

5.5 Summary ............................................................................................................................................... 76

References ..................................................................................................................................................... 78
Chapter 6: Numerical Modeling as a Tool to investigate the Feasibility of artificial Recharge to prevent possible Saltwater Intrusion into the Bangkok coastal Aquifer System

6.1 Introduction .................................................................................................................. 79
6.2 Study area and model implementation ....................................................................... 80
6.3 Investigation of the origins of the saline sources ......................................................... 80
  6.3.1 Water balance study ............................................................................................... 80
  6.3.2 Vertical saltwater intrusion .................................................................................. 81
  6.3.3 Horizontal seawater intrusion .............................................................................. 81
  6.3.4 Contamination type zones ................................................................................... 81
6.4 Numerical study of the possibility of aquifer restoration............................................. 85
  6.4.1 Non-feasibility of recharge alone .......................................................................... 85
  6.4.2 Optimal design of possible aquifer restoration schemes ....................................... 85
6.5 Conclusions .................................................................................................................. 91
References ................................................................................................................................ 92

Chapter 7: Numerical Investigation of Density-driven Flow Effect in transient State to the Seawater and vertical Saltwater Intrusion of the Bangkok-Multilayered Aquifers System

7.1 Introduction .................................................................................................................. 93
7.2 Numerical method ......................................................................................................... 94
  7.3.1 Governing equations ............................................................................................. 94
  7.3.2 MODFLOW- and SEAWAT models implementation ........................................... 96
  7.3.3 Conversion and import of reliable parameters into SEAWAT-2000 ..................... 97
  7.3.4 Verification of the SEAWAT-2000 model ........................................................... 98
7.4 Density-driven flow effects on horizontal seawater- and vertical saltwater intrusion 103
  7.4.1 Comparison of constant density- and variable density model of the calibrated parameters .................................................................................................................. 103
  7.4.2 Sensitivity analysis of hydrodynamic dispersion ................................................. 105
7.4.3 Sensitivity analysis of hydraulic anisotropy...................................................... 106

7.5 Effects of density-dependent flow and transport on the effectiveness of the trial & error aquifer restoration management schemes ................................................................. 109

7.6 Conclusions and outlook .......................................................................................... 111

References .......................................................................................................................... 113

Chapter 8: Integrating an Groundwater Management Optimization Module and a variable Density Flow and Transport Model to investigate sustainable Restoration Schemes for the Bangkok Aquifers ..................................................................................... 114

8.1 Motivation .................................................................................................................. 114

8.2 Study area and model implementation ................................................................... 116

8.3 Theoretical statement of the groundwater management problem ....................... 116

8.3.1 Linear programming formulation ...................................................................... 116

8.3.2 Nonlinear constrained optimization approach .................................................. 117

8.3.3 Formulation of the objective function and the constraints for the Bangkok aquifers GWM problem ................................................................................................. 117

8.4 Discussion of the various groundwater management schemes ............................ 121

8.4.1 1st scheme - sustainable yield ........................................................................... 121

8.4.2 2nd scheme - non-constructive scheme ............................................................. 122

8.4.3 3rd scheme - non-constructive scheme ............................................................. 122

8.4.4 4th scheme - optimized integrated non- and constructive scheme ................. 122

8.4.5 5th scheme - applied “water trade-off concept” to the integrated non-and constructive scheme (4th scheme) .......................................................... 122

8.4.6 6th scheme - applying “water trade-off concept” to the 2nd scheme ............... 123

8.4.7 7th scheme - applying “water trade-off concept” to the 3rd scheme ............... 123

8.5 Results ...................................................................................................................... 123

8.5.1 Optimization results for the 4th scheme ............................................................ 123

8.5.2 Optimization results for the 5th to 7th schemes ............................................... 126

8.5.3 Quantitative analysis of variable-density effect of all schemes ....................... 126

8.5.4 Detailed cost-analysis of the various schemes ................................................... 128
8.6 Discussion ............................................................................................................................. 129
8.7 Summary ............................................................................................................................. 130

References .................................................................................................................................. 132

Appendix A .................................................................................................................................. 134

Numerical Investigation of the Need for Density-dependent Flow and Transport Modeling on a Case-Study of a real coastal Aquifer System ................................................................................. 134

A1. Motivation and statement of the problem ............................................................................. 134
A2. Ghyben-Herzberg approximation for the fresh-seawater interface .................................. 136
A3. Analytical expression based on Dupuit’s assumptions ......................................................... 137
A4. Steady-state simulation ....................................................................................................... 138
A5. Transient simulation ........................................................................................................... 140
A6. Summary ............................................................................................................................. 146

References .................................................................................................................................. 147
List of Figures

Figure 1.1. Hydrogeological north-south profile of the Bangkok aquifers system..............2
Figure 3.1. Study domain (a) and 3-D geological map of the Lower Central Plain (b)........27
Figure 3.2. Hydrogeological north-south profile of the Bangkok aquifers system.............30
Figure 3.3. The average annual rainfall distribution in Thailand (1975 to 2004)..................31
Figure 4.1. 3D hydrogeological map (a) and FD grid in the fifth layer of the model (b)....35
Figure 4.2. A discretized hypothetical aquifer system; ------ aquifer boundary, active cell,
inactive cell, dimension of cell along the row direction; subscript (J) indicates the number
of the column, dimension of cell along the column direction; subscript (I) indicates the
number of row, and dimension of the cell along the vertical direction; subscript (K) indicates
the number of the layer.............................................................................................................38
Figure 4.3. Cell i, j, k and indices for the six adjacent cells.............................................39
Figure 4.4. Flow into cell i, j, k from cell i, j-1, k...............................................................39
Figure 4.5. Observed versus steady-state computed heads (m) for 1999
in (a) layer 3, (b) layer 4 and (c) layer 5..................................................................................47
Figure 4.6. Observed versus computed heads for 1999 (a), with upper and lower 95%
confidence limits; ME, MAE, RMS obtained when transmissivities T and vertical leakances
V_k are varied percentally from their optimal calibrated values (b).........................................48
Figure 4.7. Subzones of transmissivity in layer 3, Phra Padeang; 4, Nakhon Luang;
and 5, Nonthaburi Aquifer.......................................................................................................49-50
Figure 4.8. Sub zones of vertical leakance in layer 3, Phra Padeang; 4, Nakhon Luang; and 5,
Nonthaburi Aquifer...................................................................................................................51-52
Figure 4.9. Relative composite scale sensitivity analysis for transmissivity (a) and vertical
leakance in the various sub-zones (b).......................................................................................54
Figure 4.10. Correlation coefficient matrix of (a) transmissivity and (b) vertical leakance in
layer 3, 4 and 5..........................................................................................................................55
Figure 4.11. Examples of realizations which are generated by using Monte Carlo simulations
for layer 3 (a), 4 (b) and 5 (c) obtained using \( \sigma_Y^2 = 0.55, 0.77 \) and 0.59.........................58
Figure 4.12. Simulated variograms of head in layer 3 (a), 4 (b) and 5 (c) with variances $\sigma^2_y$ and correlation lengths $\lambda_y$ as specified in Table 4.3...............................................................59

Figure 4.13. Similar to Figure 4.9, but with $\sigma^2_y$ in layer 3 (a), 4 (b) and 5 (c) twice as big and as specified in Table 4.4.....................................................................................................61

Figure 5.1. Observed versus computed heads in layers 3, 4 and 5 (a); observed - - - and computed --- , head (m) isolines in 1999 for layer 3 (b), layer 4 (c), and layer 5 (d)..............68

Figure 5.2. The 2000 to 2002 monthly observed and computed heads at monitor wells PD 93 (a), NL2 (b), and NB61 (c) in layers 3, 4 and 5, respectively.................................................................69

Figure 5.3. Observed (red) and computed (blue) NaCl concentrations (mg/l) in 1995 in layers 3 (a), 4 (b) and 5 (c)..................................................................................................................70

Figure 5.4. Discharge-, storage- and recharge- changes in the aquifer system between 1993 and 2002.............................................................................................................................71

Figure 5.5. Unmet water demand (“umd”) in 2012 (a), 2022 (b) and 2032 (c) in various provinces when projecting the 1983-2002 pumping rate over the next 30 years (1st scenario). SMS (Samutsakorn), SMP (Samut- prakarn), BK (Bangkok), NB (Nonthaburi), NP (Nakhon Pathom), PT (Pathumthani) and PNAU (Phra Nakhonsri Ayutthaya)......................72-73

Figure 5.6. Salt plume concentration (mg/l) distribution in layer 3 (a), layer 4 (b) and layer 5 (c) in 2032. Saline contamination inside these upper layers cannot significantly be alleviated, due to saline intrusion from the thick top clay layer ................................................................74

Figure 5.7. Saltwater intrusion profiles in 1990 and 1995 (b).............................................75

Figure 5.8. The velocity vectors and piezometric heads in layer 3 (a), layer 4 (b) and layer 5 (c) in 2032. The major direction of the groundwater flow is from the boundaries to the center of the aquifer.............................................................................................................................75

Figure 5.9. Steady state water budget in 1999.................................................................76

Figure 6.1. Monitor wells and profile lines (a) and sensitive leakage areas obtained from 1990 measured data (b).................................................................82

Figure 6.2. Observed chloride (mg/l) fingerprints for several profiles (see Fig. 6.8) in 1990..................................................................................................................82

Figure 6.3. Snapshots of simulated saltwater intrusion plume from the upper clay layer for 1993, 1995 and 1997.................................................................83

Figure 6.4. Simulated seawater intrusion front along profile 2 in June 1995.................83
Figure 6.5. Map of delineating four types of contamination zones, drawn from simulated chloride distributions. Blue color marks the area of seawater intrusion; dark, the green area of mixing between horizontal seawater- and vertical saltwater intrusion; green, the area of vertical, shallow saltwater intrusion; and red, the area of deep saltwater intrusion, i.e. the highly sensitive intrusion zone.

Figure 6.6. Flow velocity vectors and piezometric heads in layer 3 (a), layer 4 (b) and layer 5 (c) in 2032. The major direction of the groundwater flow is from the boundaries to the center of the aquifer. The pump-induced hydraulic gradients cannot push back the saltwater to its source regions, leading to permanent saline pollution there.

Figure 6.7. Results of the WOS scheme: Head distribution in the 3rd layer (a), 4th layer (b), 5th layer (c); Saltwater plume distribution in the 3rd layer (d), 4th layer (e), 5th layer (f); and along the 2nd profile (g) in 2032.

Figure 6.8. Results of the 19th scheme: Head distribution in the 3rd layer (a), 4th layer (b), 5th layer (c); Saltwater plume distribution in the 3rd layer (d), 4th layer (e), 5th layer (f); and along the 2nd profile (g) in 2032.

Figure 6.9. Results for the 31st scheme: Head distribution in the 3rd layer (a), 4th layer (b), 5th layer (c); Saltwater plume distribution in the 3rd layer (d), 4th layer (e), 5th layer (f); and along the 2nd profile in 2032.

Figure 7.1. FD grid in the 5th layer of groundwater flow and solute transport (a) and the 3D finite difference grid of the multilayered model of the Bangkok aquifers.

Figure 7.2. Comparison of observed versus computed heads of SEAWAT-2000 (variable-density flow); observed and computed head contours in 1999 for layer 3 (a), layer 4 (b), and layer 5 (c).

Figure 7.3. Scatter plot of observed versus SEAWAT – 2000 - computed heads of in layer 3, 4 and 5 in steady-state mode for calibration year 1999; 95% confidence limit.

Figure 7.4. Observed versus computed head (m) of SEAWAT-2000 (variable-density flow); observed and computed, head contours in June, 1995 for layer 3 (a), layer 4 (b), and layer 5 (c).

Figure 7.5. The scattered diagram of observed- versus computed head of SEAWAT – 2000 of layer 3, 4 and 5 in 1993 to 1997.

Figure 7.6. Observed (white solid line) and SEAWAT-2000- computed (black dashed line) saline concentrations in 1995 in layers 3(a), 4(b) and 5(c).
Figure 7.7. Scatter plots of observed and computed saline water in layer 3 (a), 4 (b) and 5 (c) in transient mode for years for calibration years 1993 to 1997..........................102

Figure 7.8. Piezometric head contours computed with the constant-density MODFLOW-96 model (solid line) versus those of the variable-density SEAWAT-2000 model (dashed line) and flow vectors with pump scheme in December, 2032 in the 3rd (a), 4th (b), and the 5th (c) layer............................................................104

Figure 7.9. Computed saline distributions using the constant-density MODFLOW-96&MT3DMS model modeled (solid line) versus those of variable density model – SEAWAT-2000 (dashed line with chloride concentration values in mg/l underlined) with pump (circles) scheme in Dec. 2032 at column 21 of model or UTM-X = 662000 m........105

Figure 7.10. Simulated saline concentrations of density-independent (solid line) versus density-dependent (dashed line) model after 30 years (Dec, 2032) under various conditions for the hydrodynamic dispersivity and the pumping; 0.5, 2, 10 folds of the calibrated $A_L$ and $A_T$ with pumping (a),(b) and (c); and 0.5, and 2 fold of the calibrated $A_L$ and $A_T$ without pumping (d) and (e), respectively..........................................................107

Figure 7.11. Simulated saline concentrations of constant-density- (solid line) versus variable-density (dashed line) model after 30 years (Dec, 2032) under different conditions of the vertical hydraulic conductivity and the pumping; 0.1 and 10 folds of the calibrated $K_z$ with pumping (a) and (b); and 10 fold of the calibrated $K_z$ without pumping (c) and (d), respectively..............................................................................................108

Figure 7.12. Snapshots of simulated saline plumes for Dec, 2032, using the “constant-density”—MODFLOW&MT3DMS (a, c, e) and “variable-density”—SEAWAT-2000 (b,d,f) model for three kinds of remediation schemes: “WOS” (top), “best policy” (middle), and “best integrating policy- and –constructive” (bottom), respectively, Concentrations in kg/m$^3$.................................................................................................................................110

Figure 8.1. Trial-and error well scheme: Orange area shows the distribution of the present day pumps, blue area the line of recharge wells, with the clean-up wells located 4 cells northward of the former.........................................................................................................................119

Figure 8.2. An example of in lieu delivered water supply cell (white cell), recharge well(blue cell) candidates and withdrawal cells (orange cell) in layer 3 (a), 4(b) and 5 (c) of the scheme 5 to 7..................................................................................................................................121
Figure 8.3. Trial-and-error well scheme: Orange area shows the distribution of the present day pumps, blue area the line of recharge wells, with the clean-up wells located 4 cells northward of the former...

Figure 8.4. 2032-heads for the “trial & error”- (solid lines) and “optimized” (dashed lines) well scheme in layers 3(a), 4(b) and 5(c); a blue circle is an optimized clean-up well, a yellow triangle is an optimized recharge well, a red plus is a head constraint.

Figure 8.5. Summary of % averaged reduction of vertical saline plume pollution area, seawater intrusion area and head recovery in layers 3 to 8 relative to the WOS scheme.

Figure 8.6. Comparison of unmet water demand, averaged reduction of saline pollution area and total costs of each scheme.

Figure 8.7. Saline concentration (kg/m$^3$) profile (UTM-X = 662000 m.) of the WOS-scheme (a) and the 3$^{rd}$ scheme (b) located at the western side of the Chao Praya river.

Figure A1. Domain and boundary conditions in the coastal aquifer.

Figure A2. Ghyben-Herzberg stationary interface.

Figure A3. Shape of a stationary interface by the Dupuit-Ghyben-Herzberg approximation.

Figure A4. Steady-state saline concentrations (kg/m$^3$) at Y = 250 m. of constant-density- (dashed line), variable-density model (solid line), Ghyben-Herzberg interface location (circles), and interface location based on Dupuit’s assumptions (diamonds). Also shown is the phreatic water table (triangles).

Figure A5. Flow vectors for steady-state seawater intrusion at Y = 250 m. of density-independent model (a) and density-dependent model (b). Blue lines envelop approximately the flow vector area affected by the sea boundary and/or the density driven flow.

Figure A6. Phreatic water tables at Y = 250 m. of density-dependent and density-independent models at different times. Abbreviations: n Yr = water table at n years for density-dependent model; n_wod Yr = water table of a model without density at n year.

Figure A7. Exaggerated size of flow vectors (for better viewing) in transient state at Y = 250 m and time = 30 years of density independent (a) and density-dependent model (b). Blue box shows position of pump cells and ←→ a flow vector; a diamond at its left-hand side is a basement of that vector and the line that is shot out from that basement represents the flow direction and magnitude of that vector.
Figure A8. Transient saline distributions of density independent- (solid lines) and density-dependent model (dash lines). Blue box shows the pump position.................................143

Figure A9. Breakthrough curves at X = 750 m, Y = 250 m, Z = -15 m (a), -45 m (c), -95 m (e), at X = 500 m (same line of pump position), Y = 250 m, Z = -15 m (b), -45 m (d) and -95 m (f).........................................................................................................................................145
List of Tables

Table 4.1 The composite scaled sensitivity and relative composite scaled sensitivity for calibrated transmissivity sub-zones in Bangkok Multilayered system ..........................................................53

Table 4.2 The composite scaled sensitivity and relative composite scaled sensitivity for calibrated vertical leakance sub-zones in Bangkok Multilayered system ........................................53

Table 4.3. Comparison of $\sigma_H^2$ obtained from Gelhar’s Eq. (4.5) and MC-simulations ........................................................................................................................................60

Table 4.4. Similar to Table 4.3, but with $\sigma_H^2$ twice as big...............................................................................................................................60

Table 6.1. Summary of the effectiveness of a particular aquifer restoration scheme as evaluated along the 2nd profile...................................................................................................................86

Table 8.1. Comparison of head recovery and values of cost-funciton (hydraulic costs and monetary costs) for implementation and operational & maintenance of the two restoration schemes proposed .............................................................................................................................................125

Table 8.2. Summary of optimization results for the 5th to 7th scheme .........................................................................................................................126

Table 8.3. Summary of costs in each scheme ........................................................................................................................................128
List of Terminologies

A  a matrix of coefficients defining the form of the constraints

A  a coefficient matrix assembled by MODFLOW using user-specified model data

\( A_L \)  the longitudinal dispersivity (L)

\( A_T \)  transversal dispersivity (L)

\( b \)  a column vector of right-hand-side coefficients associated with the constraints

\( b \)  a vector of defined flows, terms associated with head-dependent boundary conditions and storage terms at each cell

\( b \)  a vector containing values of each of the NP parameters being estimated

\( b \)  aquifer thickness (L)

\( b_j \)  the \( j^{th} \) estimated parameter of the parameter vector \( b \)

\( \beta_a \)  the cost or benefit per unit volume of water withdrawn or recharged at well site \( n \)

\( \beta_R \)  the operational recharged water cost per CMD

\( \beta_W \)  \textit{in-lieu} delivered water cost per CMD

\( c \)  a transposed column vector of objective-function coefficients associated with the decision variables

\( C \)  solute concentration (M/L^3)

\( C \)  a coefficient that depends on the dimensionality of the flow, and possibly other parameters of the flow configuration

\( C_s \)  the solute concentration of water entering from sources or sinks (M/L^3)

\( \text{cc}(i, j) \)  the covariance between parameter \( i \) and \( j \)

\( \text{css}_j \)  the composite scaled sensitivity for the \( j^{th} \) parameter

\( D \)  the hydrodynamic dispersion tensor (L^2/T)

\( D^* \)  is the molecular dispersion (L^2/T)

\( D_m \)  the mechanical dispersion, related to the linear fluid velocity \( \bar{v} \) (L/T)

\( h \)  the potential metric head (L)
\( h_f \) the fresh water head (L)
\( h_{i,j,k,2} \) the modeled head at the 42 head constraint locations at col. = i, row = j, layer = k and stress period 2
\( h_{i,j,k} \) the head at col. = i, row = j, layer = k
\( H_{i,j,k,2} \) the named head constraint acting as a flow barrier
\( J \) average hydraulic gradient
\( KR_{i,j-1/2,k} \) the hydraulic conductivity along the row between nodes i, j, k and i, j-1, k (L^3\(T^{-1}\))
\( K_{xx}, K_{yy}, K_{zz} \) hydraulic conductivity along the x, y and z coordinate axes (LT\(^{-1}\))
\( K_{ff}, K_{ff}, K_{fc} \) equivalent freshwater hydraulic conductivities in the three coordinate directions (LT\(^{-1}\))
\( K_{xy} \) hydraulic conductivity in the plane x and y
\( L \) the seawater intrusion length
\( \lambda \) an integral scale (L)
\( M \) the preconditioned form of \( A \)
\( N_x \) surface recharge (L/T).
\( ND \) the number of observations
\( NP \) the number of estimated parameters
\( NPR \) the number of prior information values
\( \nu \) the iteration level
\( \xi_{\Delta} \) the change in head
\( P_p \) the \( p^{th} \) prior estimate included in the regression
\( P_p(b) \) the \( p^{th} \) simulated value
\( q_{i,j-1/2,k} \) the volumetric fluid discharge through the face between cells i, j, k and i, j-1, k (L^3\(T^{-1}\))
\( q_b \) \( b_k - A_k x_{k-1} \)
\( Q_0 \) lateral freshwater discharge
\( q_s \) the volumetric flow rate of sources and sinks per unit volume of aquifer (T\(^{-1}\))
\( Q_i \) a flow rate into the cell \( (L^3 T^{-1}) \)
\( Q_{ln} \) the clean-up (discharge) rate in layer \( k \) and well site \( n \) \( (n = 31 \) is max. number of flux decision variables for layer \( k \))
\( Q_{kn} \) the in-lieu delivered water rate cell in layer \( k \) and well site
\( \Delta r_{j-1/2} \) the distance between nodes \( i, j, k \) and \( i, j-1, k \) \( (L) \)
\( rcs_j \) the relative composite scaled sensitivity
\( R_k \) \( (k=1, ..., N) \) the rate of solute production or decay in reaction \( k \) of \( N \) different reactions \( (M/(L^3 T)) \)
\( R_{ln} \) the recharge rate \( (L/T) \)
\( R_{kn} \) the recharge rate \( (L/T) \)
\( \rho \) density of native aquifer water \( (M/L^3) \)
\( \rho_f \) density of freshwater \( (M/L^3) \)
\( \rho_s \) the density of water entering from a source or leaving through a sink \( (M/L^3) \)
\( S \) the coefficient of storage
\( S_f \) specific storage in term of equivalent fresh water head \( (L^{-1}) \)
\( S(b) \) the weighted least-squares objective function
\( S_s \) the specific storage of the porous media \( (L^{-1}) \)
\( SS_{ij} \) the scaled sensitivities
\( \sigma^2_H \) the head variance
\( \sigma^2_Y \) the variance of \( \ln K \) or \( \ln T \)
\( t \) time \( (T) \)
\( T \) Transmissivity \( (L^2/T) \)
\( T_{Qwn} \) the total active duration of the flow-rate \( (T) \)
\( \theta \) effective porosity
\( \Delta V \) the volume of the cell \( (L^3) \)
\( \text{var}(i) \) the variance of parameter \( i \)
\( \text{var}(j) \) the variance of parameter \( j \)
\( W \) a volumetric flux per unit volume representing sources or sinks of water \( (T^{-1}) \)
\( \omega \) the weight for the \( i^{th} \) observation
ωₚ  the weight for the pᵗʰ prior estimate

ωᵢ  the weight of iᵗʰ observation

x  a column vector of decision variables with upper bounds u

x  a vector of hydraulic heads at each cell. One value of the hydraulic head for each cell is computed at the end of each time step

x_{k-1}  initial head

yᵢ  the iᵗʰ observation being matched by the regression

yᵢ  the simulated value associated with the iᵗʰ observation

yᵢ(b)  the simulated value from MODFLOW which corresponds to the iᵗʰ observation

Z  the value of the objective function
Chapter 1: Introduction

1.1 Motivation

Bangkok Metropolis and the vicinity provinces, namely, Samut Prakan, Samut Sakhon, Samut Songkram Nonthaburi, Pathum Thani, Nakhon Pathom, Chachoengsao, and Phra Nakhon Si Ayutthaya are economically the fastest growing regions of Thailand and, as a consequence, have experienced a tremendous increase of groundwater consumption in recent years. As a matter of fact, groundwater has been developed for use in the Bangkok region over the past six decades, starting with the first large-scale public water supply works by Metropolitan Waterworks Authority in 1954. During the industrial boom with its subsequent increase in population and industrial factories in the suburbs of Bangkok, the demand for groundwater water has increased tremendously and, thus, numerous wells---many of these without government enactment control---have been drilled into the multiple aquifers system underlying the Central Plain region to supplement the limited amount of available surface water.

The coastal aquifers system underneath Bangkok and adjacent provinces consists of 8 water-bearing units, namely, Bangkok aquifer (BK - 50m.), Phra Pradang aquifer (PD - 100m.), Nakhon Luang aquifer (NL - 150m.), Nonthaburi aquifer (NB - 200m.), Sam Khok aquifer (SK- 300m.), Phaya Thai aquifer (PT - 350m.), Thon Buri aquifer (TB – 450m.) and Pak Nam aquifer (PN - 550m.) (Fig.1.1). These aquifers are made primarily of sand and gravel, separated by aquitard clay layers. Among these aquifers, groundwater has been mainly
extracted from PD, NL and NB which are very productive and of relatively good water quality. However, with the aforementioned higher rates of groundwater pumping experienced in recent decades, this benevolent situation is being deteriorating. In fact, whereas the total groundwater withdrawal was around 8,360 m$^3$/day in 1954, 1.3 million m$^3$/day were extracted in 1982 (Buapeng, 1985) and 1.5 million m$^3$/day in 1992 (Kokusai Kogyo Co., Ltd, 1995). Such high pumping rates may have exceeded the natural yield of the aquifer system for several decades and there is enough evidence now that saline water is being drawn from its sources towards the producing areas (Gupta and Yapa, 1982; Buapeng, 1985; Gupta, 1986; Gangopadhyay, 1993; Kokusai Kogyo Co., Ltd., 1995; Chaowiwat, 1999; Buapeng, 1999); i.e. the fresh groundwater is being contaminated by saline water. This classical problem of saltwater intrusion has resulted in diminishing quantities of clean groundwater being available for drinking purposes in the Lower Chao Praya river basin.

![Figure 1.1. Hydrological profile of North-South section of the Bangkok aquifers system.](image)

Facing these problems, the Thai Government and other researchers have attempted to develop strategies to mitigate these adverse effects on the present and future drinking water supply. In developing such effective strategies numerical groundwater models which can simulate both
flow and solute transport occurring in the aquifer system under natural and forced (pumping) conditions are of great help. However, in spite of much research and numerous case studies, many of the mechanisms of saltwater intrusion are not yet fully understood. The situation is even more complicated in the Bangkok coastal aquifer system, since, as will be discussed in more detail further down, the origins of the saline waters in some of the productive aquifer units are not yet clear, i.e. it is still at debate whether the saline pollution is due either to classical seawater intrusion or to vertical seepage of connate saline water from the upper clay-rich layers that are persistent over much of the Lower Chao Praya river basin.

Originally, the classical seawater intrusion problem was conceptualized by assuming hydrostatic balance, immiscible fluids and the existence of a sharp interface between the fresh- and the saltwater as, for example expressed in the famous Ghyben and Herzberg relation (cf. Bear, 1979). Many recent studies still use this classical approach to simulate the phenomenon of saltwater intrusion in aquifers (William, 1982; Essaid, 1990; Varut et al., 2000; Cheng and Chen, 2001). In reality, however, due to molecular diffusion and hydrodynamic dispersion, fresh water and saltwater are actually miscible liquids and therefore the zone of contact between the two fluids will be a transition zone, rather than a sharp interface (Todd, 1976; Merritt, 1996; Gambolati et al. 1999; Cheng and Chen, 2001). The situation is further intricate by the fact that the saltwater intrusion itself changes the fluid density and, to a lesser extent, the viscosity, so that these parameters vary in space and time as a function of changes in the concentration, the temperature, or the pressure in the fluid and, finally, that the porous medium itself is usually stochastically heterogeneous. Therefore, to properly mimic the mechanism of saltwater encroachment, a variable density flow and transport modeling approach has to be used (Voss and Souza, 1987; Koch, 1992, 1993; Koch and Zhang, 1992, 1998; Voss and Koch, 2001; Koch and Starke, 2001, 2002, 2003, Koch and Sharma, 2003). However, past studies of saltwater intrusion in Thailand (see Chapter 2) have not yet been dealing properly with the use of such variable fluid density and viscosity flow and transport models. The present thesis will attempt to overcome this deficiency.

One of the newest and very attractive density-dependent flow and transport model to be used in the present thesis is SEAWAT-2000 (Langevin et al., 2003). The source code for SEAWAT-2000 was developed by combining MODFLOW-2000 (Harbaugh et al. 2000) and
MT3DMS (Zheng and Wang, 1999) into a single program that can simulate either constant- or variable-density groundwater flow or solute transport in a three dimensional aquifer system. Up-to-date there is prior no any published application of the SEAWAT-2000 model; this research work would be the first pragmatic application of this code. One of the major advantages of SEAWAT-2000 is that is able to use to a large extent the powerful and versatile tools of MODFLOW to set up complicated 3D aquifer models and, additionally, can simulate more realistic groundwater flow and solute transport situations in real aquifers by using its variable density option. The SEAWAT-2000 simulation is run through the cooperation between the graphic user interface-MODFLOW-GUI (Winston, 2000), Model Viewer (Hsieh and Winston, 2002) and Argus One GIS (Argus Holding Ltd., 2005), so these three software codes allow the sophisticated density model-SEAWAT-2000 is more flexible to be set up, simulated and visualized the post processing for the 3D of finite difference of complex Bangkok multilayered aquifers model. Therefore the SEAWAT-2000 model evidences all features that are particularly useful for the numerical modeling of possible saltwater intrusion mechanisms in the multiple-layer coastal aquifer system of the Gulf of Thailand.

1.2 Objectives

According to the previous studies mentioned of saltwater intrusion in the multiple aquifer system underlying Bangkok and its vicinities, saline contamination sources may be mainly classified into two categories, namely, (1) horizontal seawater intrusion originating in the Gulf of Thailand and, (2) vertical saltwater leakage from the upper marine aquifer clay layers, adjoining aquifers or connate water (Gupta and Yapa, 1982; Buapeng, 1985; Gupta, 1986; Gangopadhyay, 1993; Kokusai Kogyo Co., Ltd., 1995; Chaowiwat, 1999). Nowadays, however, the real sources of this saline contamination are still obscure and at a question being discussed within the group of Thai water resources scientists. Moreover, the previous studies were fraught of several limitations in the numerical modeling approach of the saltwater intrusion simulation:

1. Density-dependent transport simulation which means that the migration of the miscible phase is not only due to forced advection by the hydraulic gradients and to dispersion, but also driven by free convective motions as a consequence of density variations in the
flow (Koch and Zhang, 1992). Up-to-date the investigations in the study area have not yet considered density effects in the saltwater transport simulations (Gupta and Yapa, 1982; Sabanathan, 1984; Gupta, 1986; Gangopadhyay, 1993; Kokusai Kogyo Co., Ltd., 1995; Chaowiwat, 1999).

2. Numerical distortion due to limitations in the methodology of the former studies, namely the physics of the saltwater intrusion mechanism.

3. The investigation of the transitional band between saltwater and fresh water has only been part of one investigation in the study area (Kokusai Kogyo Co., Ltd., 1995), and this approach is only two-dimensional (2D). As more data has become available at the present time, a 3D numerical-model approach is now feasible.

The above mentioned questions and issued lead to the topic of my Ph.D. dissertation: “Numerical modeling of possible Saltwater Intrusion Mechanisms in the Multiple-Layer Coastal Aquifer System of the Gulf of Thailand”. In this study I will endeavor to discriminate unequivocally the sources of saltwater contamination in the aquifer system through the use of the aforementioned density-dependent model SEAWAT-2000. By properly duplicating numerically the mechanism of saltwater intrusion it will be investigated the cradles of contamination underneath Bangkok and adjoining provinces is either due to seawater intrusion or to saltwater intrusion from contamination sources. Based on these results, future possible sustainable management strategies for the present and future safeguard of the groundwater resource for the larger Bangkok region will be simulated using trial and error approaches, as well as techniques of optimization theory. As such, this Ph.D. study should help to alleviate some of the ever-increasing problems of the diminishing clean groundwater resources in Thailand.

1.3 Scope of study

Essentially the study will involve the following consecutive steps

1. Setting up a comprehensive 3D groundwater flow model for the Bangkok multiple aquifer system using the MODFLOW-96 program, incorporating newly available data on the geology and on the external hydraulic stresses on the aquifer (recharge and pumping rates).
2. Using the density-independent MODFLOW-96 (Harbaugh and McDonald, 1996) and MT3DMS embedded in PMWIN (Chiang and Kinzelbach, 2001; 2005) and variable density–dependent flow and transport SEAWAT 2000 (Langevin, et al., 2003) investigations of the saltwater intrusion mechanisms will be performed. Results of the two models will be compared and the applicability of the models to the Bangkok aquifer system be tested.

3. Applying the model to data of well observations in the Phra Pradang, Nakhon Luag and Nonthaburi Aquifer underneath Bangkok and adjoining provinces, the 3rd, 4th and 5th modeled aquifer, respectively, to simulate (1) the present-day situation of seawater intrusion or/and saltwater from vertical leakage sources in these coastal aquifers and (2) the future migration of the saline plumes and of the saltwater-freshwater interface under several water usage scenarios and to set up possible management strategies, using trial and error approaches, as well as techniques of optimization theory, to prevent and alleviate a future deterioration of the coastal groundwater resources.

1.4 Expected advantages

The expected advantages of the present Ph.D. thesis can be summarized as follows:

1. Grasp the phenomenon of fresh- and saltwater intrusion in the coastal aquifer by using deterministic and stochastic techniques,
2. Learn exactly where the saline contamination sources invade from?
3. Understand the present-day situation of saltwater intrusion in the Phra Pradang, Nakhon Luang and Nonthaburi aquifers by first-time application of a numerical model that includes density-dependent effects,
4. Get a picture of the transient advancements of the saltwater intrusion fronts and learn of ways of optimal strategies for the mitigation of possible future saline groundwater contamination through simulation of various management variants under present-day and future groundwater exploitation scenarios,
5. Obtain a new understanding on how to alleviate some of the ever-increasing problem of diminishing clean groundwater resources in the study area.
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Chapter 2: Literature Review

2.1 Deterministic modeling of saltwater intrusion

Deterministic modeling considers that the model parameters describing the aquifer system are known and that the response of the system to stresses can be determined through the modeling effort. The most classical deterministic modeling of saltwater intrusion is based on the Ghyben-Herzberg (1901) (GH) relation of the position of the (sharp) interface between the fresh and the saline water (cf. Todd, 1976; Bear, 1979). The GH-relationship was conceptualized by assuming hydrostatic balance, immiscible fluids and the existence of a sharp interface between the fresh and the saltwater. Numerical saltwater intrusion models have traditionally been developed for areal- and cross-sectional simulations by assuming this sharp interface-approach between fresh- and saltwater (Todd, 1976; Merritt, 1996; Cheng and Chen, 2001). Mercer et al. (1980) were one of the first authors to present a numerical model that solves the partial differential equations describing the motion of saltwater and freshwater separated by such a sharp interface. Their 2D areal approach was based on the Dupuit approximation. Voss (1984) developed SUTRA which simulates fluid movement and transport of either energy or solute in a subsurface environment. It employs a two-dimensional hybrid finite-element and integrated-finite-difference method. Essaid (1990) presented a quasi-three-dimensional, finite difference sharp interface model in a multiple-layered coastal aquifer system. Gangopadhyay (1993) modified the SUTRA model to a quasi-
three-dimensional model to simulate saltwater encroachment in a multiple-aquifer system. A preliminary groundwater flow model was constructed using the SWIP code as modified by Merritt (1994). The model solved groundwater flow equation accounting for fluid density and viscosity dependence on temporal changes of pressure, temperature and solute transport. Putti and Paniconi (1995) applied Picard and Newton linearization for the coupling between the flow and transport equations of saltwater intrusion. Craig et al. (2004) used SUTRA for an idealized evaporating salt lake, the results of which are compared with an equivalent laboratory Hele-Shaw cell system.

Koch and Zhang (1998) investigated saltwater seepage from coastal brackish canals in Southeast Florida with the SUTRA model. Cheng and Chen (2001) developed a three-dimensional variable density flow and transport model to study saltwater intrusion. Its transport equation is solved by a coupled Eulerian-Lagrangian method. Guo and Langevin (2003) developed the SEAWAT-2000 model to simulate three-dimensional, variable-density, transient ground-water flow in porous media. The source code for SEAWAT-2000 was developed by combining MODFLOW-2000 (Harbaugh et al., 2000) and MT3DMS (Zheng and Wang, 1999) into a single program that either solves the coupled flow and solute-transport equations or uncoupled ones.

Voss and Koch (2001) simulated effects of groundwater pumping on saltwater upconing in the state of Brandenburg, Germany, using several 2D and 3D flow and transport models, with and without density effects included. This, in order understands their origins, namely, if they are (1) derived from a major leaching salt dome in the study area or, (2) are just ancient regional formation water. They found that, due to the shallowness of the aquifer system, the surficial topography has a large effect on the flow and migration patterns and, especially, gives rises to upwelling flow underneath the discharge area underneath the major river in the region. Comparing models with and without density effects included, they then investigated possible saltwater upconing due this natural discharge flow pattern. Eventually the accentuated effects of a newly proposed well field on the upconing process were simulated, using both classical non-density-dependent and density-dependent models. Based on these results, their final objective of the investigation was to provide the water agencies with a proper management plan to secure the long-term quality of the extracted groundwater in that part of the country.
Bakker (2003) adopted the Dupuit approximation for the simulation of three-dimensional regional seawater intrusion, but diffusion and dispersion are not taken into account. The formulation is based on a vertical discretization of the groundwater into zones of either constant density (stratified flow) or continuously varying density (piecewise linear in the vertical direction). During a simulation both the change of the elevations of the surfaces and the change in head are computed through consistent application of continuity of flow; a simple tip and toe tracking algorithm is applied to simulate the horizontal movement of the surfaces. The main advantage is the tremendous reduction of the number of cells needed for a simulation because every aquifer may be represented by a single layer of cells.

2.2 Saltwater intrusion investigations in the multiple-aquifers system underneath Bangkok and adjacent provinces

The investigation of groundwater resources in the Bangkok area started in 1969 by Camp, Dresser and McKee (1970) who reported that chloride concentrations in some wells had increased from 10 ppm in 1959 to 600 ppm in 1969 and that they were ranging from 500 ppm to thousands of ppm in depths of only about 35 m.

Bashir (1978) applied a 1D finite-difference (FD) model to investigate saltwater intrusion in the Nakhon Luang aquifer. His results showed that saltwater had intruded into the aquifer from a connate water body located on the western side of Chao Praya River and also from the Gulf of Thailand.

Yapa (1979) formulated a 2D FD model and investigated the saltwater intrusion in the Phra Pradang Aquifer and provided an approximate location for the connate water bodies. He further stated that the saltwater contamination may not only be due to seawater intrusion, but also due to vertical leakage of saline water from adjoining aquifers.

Gunasekara (1980) developed a saltwater intrusion model by coupling the 2D hydrodynamic and 2D convection-diffusion equations to simulate saltwater movement in the aquifer. The model was calibrated and applied to different pumping scenarios in the Nakhon Luang aquifer.
to study the response of the aquifer system and the saltwater intrusion.

*De Mel (1982)* formulated a multiple-aquifer solute transport model which takes into account the interaction between aquifers. A multi-aquifer hydrodynamic model is coupled with the solute transport model to study the cause of saltwater intrusion in the Bangkok and Phra-Padang aquifers considering intrusion caused by sea, seepage from Tha-Chin and Chao-Praya River and connate water bodies. The study results showed that the seepage of saltwater from the two rivers is not the only cause of contamination in the aquifers, but the connate water bodies entrapped in both aquifers may also be responsible. Especially, for the Phra-Padang aquifer the seepage of saline water from the overlying Bangkok clay aquifer is found to be significant in areas where the two layers interconnect as evidenced by a detailed geological investigation.

*Gupta and Yapa (1982)* applied both analytical and numerical models for assessing the saltwater intrusion phenomenon in the Phra Pradaeng aquifer. They considered only longitudinal dispersion to assess the contamination sources and used also numerical modeling to identify the sources of contamination and to evaluate the effectiveness of the present water quality monitoring network. From their study they could conclude that saltwater intrusion in the Phra Pradaeng aquifer does not occur only from the sea but also from the infiltration of connate water bodies entrapped in sediments from the time of deposition under marine conditions, leading to a contamination of fresh water supplies. These bodies are to the west and southwest of the Chao Praya River. Either vertical leakage of saltwater from the upper aquifer of brackish-water content occurs, or some wells from which water samples had been collected were improperly grouted. Possibly both of these conditions have prevailed.

*Sabanathan (1984)* developed a computer program which solved the partial differential equation describing the process of solute transport in the groundwater flow and coupled it to the flow model. This model was applied to the Bangkok, Phra-Pradaeng and Nakhon Luang aquifers and the results showed that the main sources of saltwater intrusion into these aquifers are the connate water body entrapped in the western side of Chao Praya river and the vertical leakage of salt water from the Chao Praya itself, especially in places where the aquifers are vertically interconnected. Furthermore, this connate water body had a very high concentration
in the southwest corner of the model area. This may be because of its location closer to the sea where horizontal seawater intrusion becomes more influential.

*Buapeng (1985)* reviewed the previous studies and the observed data in the Bangkok aquifer system. According to these publications he concludes that the groundwater is mainly withdrawn from the Phra Pradaeng, Nakhon Luang and Nonthaburi aquifers. The water levels have dropped around 50-51 m below the ground surface in the Nakhon Luang aquifer, 34-35 m in the Phra Pradaeng aquifer and 50-51 m in the Nonthaburi aquifer. In the Bangkok aquifer, water was found to be salty with a chloride content ranging from 500 mg/l to several thousands mg/l throughout most of the area. The Nakhon Luang and Nonthaburi aquifers contained freshwater in the east bank of the Chao Praya river and in the extreme westerly parts of the multiple-aquifer system. Salty water has been found almost all along the north-south direction of the western bank of the Chao Praya river. From the observations and the interpretation of the hydrochemistry of the water it was deduced that actual sea water intrusion occurs only in areas near the shore, whereas connate water entrapped under marine conditions after the time of their deposition is the predominant contaminating source of the fresh groundwater supply.

*Gupta (1986)* applied analytical and numerical modeling procedures to simulate hydrodynamic dispersion and analyzed the saltwater contamination in the Nakhon Luang aquifer. A preliminary evaluation of the approximate locations of the contaminating sources was performed by simulating one-dimensional transport along selected streamlines. The study showed that (1) the connate water bodies were the predominant source of contamination; (2) the contaminating sources are widespread and located on the western side of the Chao Praya River and, (3) with the current pumping rates, the highest rate of intrusion is from the northwest direction towards the main pumping center. The author recommended further studies to investigate the possibility of contamination due to vertical leakage of saltwater from the Bangkok aquifer through the abandoned deep wells.

*Gangopadhyay (1993)* modified the SUTRA to a quasi-three-dimensional model and then applied it to simulate groundwater flow and chloride movement in the Phra Pradaeng and Nakhon Luang aquifers. His study results revealed that in both aquifers the predominant
saltwater front invades from the west, south-west, and north-west toward the central Bangkok region where the maximum pumped zones are located. Also, the critical regions can be identified to be in the south-west, south-east and north of the Chao Phraya River, namely, Samut Sakorn province, Samut Prakarn province and the western part of Prathumtani province.

*Kokusai Kogyo (1995)* has performed the most comprehensive study up to date. They investigated groundwater flow, land subsidence and saltwater intrusion in the Bangkok area and its vicinity, in order to establish a groundwater management system and to set up scenarios to mitigate land subsidence and saline water intrusion in the study area. The results of this exhaustive study revealed that, (1) according to a well inventory database, the total groundwater extraction rate in the Bangkok aquifers system amounts to around 1.5 million m$^3$/day, (2) piezometric heads in the Phra Pradaeng, Nakhon Luang and Nonthaburi aquifers have declined from 30 m to 60 m below MSL in Pathum Thani, Samut Sakhon and from eastern Bangkok to Samut Prakarn, (3) land subsidence occurred at a rate of more than 20 mm/year underneath Bangkok metropolis, Samut Prakarn, Samut Sakhon, and the central part of Pathum Thani and parts of Nonthaburi and, (4) high chloride concentrations exist underneath the areas from Samut Sakhon to Pathum Thani along the western side of Chao Praya River and in the coastal area of Samut Prakarn. In some areas of the Phra Pradaeng aquifer these saline concentrations are over 5,000 mg/L, between 3,000 to 16,000 mg/L in the Nakhon Luang aquifer and between 2,400 to 13,000 mg/L in the Nonthaburi aquifer.

*Chaowiwat (1999)* used a coupled version of the MODFLOW and MT3D program to simulate groundwater flow and saltwater intrusion in the Nonthaburi aquifer. The study results revealed that the total salt mass transport in the Nonthaburi aquifer is due to seawater intrusion for as much as 84%, and by vertical leakage from the Nakhon Luang aquifer by only 16%. The author recommended that a further study should investigate the possibility of artificial groundwater recharge along the coast of gulf of Thailand to remedy seawater intrusion which, as stated, is one of the major objectives of the present Ph.D. thesis.
2.3 Density effects on solute transport

Experimental effects of the impacts of density dependence on the migration of a contaminated plume have been discovered by Paschke and Hoopes (1984) who investigated the leaching of a sodium chloride plume of very high concentration in a sand tank model. Schincariol and Schwartz (1990) investigated the mixing of a variable density plume in a porous medium, Hayworth et al. (1991), show significant vertical plume movements for already relatively low concentrations. The observed plume delineations of these experiments also disclosed several significant features of hydrodynamic instability and viscous fingering phenomena in a porous medium.

Koch (1992) investigated numerically interface instabilities for unfavorable density contrasts between (a) two superposed immobile layers and (b) at boundaries of advected solute plume which is of some environmental interest. The numerical results showed, at least qualitatively, agreement with some of the predictions of a theoretical scaling analysis and with experiments. He disclosed that the onset and evolution of these interface instabilities is mostly affected by the competition of the unfavorable density contrast (destabilizing) and the hydrodynamic dispersion (destabilizing). The latter and here especially the transversal dispersion governs morphology and growth of the finger regime in a non-deterministic way. The author indicated, additionally, that the problem of interface instabilities has to be treated as a classical nonlinear dynamical system.

Koch and Zhang (1992) illustrated that the migration of a miscible solute phase is not only due to forced advection by hydraulic gradients and to dispersion, but is also driven by free convective motions due to the density differences. Whether density effects are important or not depends on a variety of hydraulic parameters of the aquifer model. Furthermore, they found that the combined influence of the various model parameters above can be very different, depending on whether the plume is still near the source or has already extended into the region far away from it. In some cases, variable density might have an effect on the plume migration for even moderate density contrasts of ~ 0.3% (which corresponds to a concentration of ~ 2160 mg/l NaCl). Again, hydrodynamic dispersion tends to reduce the density effects.
Koch (1993) investigated numerically the dynamics of viscous fingering arising at a miscible interface in a unstably density-stratified fluid in porous media. The study results unveiled that the onset, evolution and morphology of the instability are mostly affected by the dispersivity of the porous medium. The analysis of S-curves of the vertical plume movement demonstrated that the onset of instability is mainly governed by the longitudinal dispersion, whereas transversal dispersion is more responsible for the dynamics of the mature fingers. The finger instabilities show the typical behavior of a nonlinear dynamical system whose response depends essentially on the initial conditions imposed.

Koch (1994) extended his earlier study to include stochastic heterogeneity of the porous media. Both a deterministic and a random heterogeneous (stochastic) porous medium are considered. The results of the simulations showed that unlike in a homogeneous porous medium where the evolution and the morphology of finger instabilities are mostly affected by the initial perturbation, for a random medium it is its stochastic realization that determined the fate of the fingers; i.e., the medium has an ordering effect on the finger pattern and fingers are essentially channeled through local sections of reduced hydraulic conductivity.

Koch and Zhang (1998) modeled the phenomenon of density-driven vertical saltwater intrusion from a brackish, tidally-affected open sea-canal in southeast Florida with the density-coupled groundwater flow and transport model SUTRA. Their results showed that brackish canal water intrusion depends on the adjacent groundwater table elevation: lowering the latter during a dry season may trigger the seepage process which then becomes essentially irreversible. Moreover, the authors reveal a significant influence of the short-term tidal fluctuations on the long-term dispersion of the vertical saltwater plume in the aquifer. Then possible mitigation plans were simulated which show that a minimum of threshold water level must be maintained in the well field during dry seasons. However, raising the water table can not be achieved by artificial injection of reclaimed wastewater, but may be succeeded by placing a freshwater canal along the brackish tidal canal.

Voss and Koch (2001) modeled the effects of groundwater pumping on saltwater upconing in the state of Brandenburg, Germany, using several 2D flow and transport models, with and
without density effects included. A sensitivity study of the hydrodynamic dispersion and of the hydraulic anisotropy of the aquifer was carried out. The model results revealed that density effects are diminishing for large values of the dispersivity and high anisotropy ratios.

*Koch and Starke (2001; 2002; 2003; 2006)* investigated the macro-dispersion in density-dependent transport in a heterogeneous medium by both experiments and numerical modeling. Their results showed that both experiments and numerical models exhibit for the same density contrast a larger sinking of the mixing layer with decreasing inflow velocity and, at the same time, an apparent increase of the lateral dispersion coefficient $D_T$.

All of these studies above do, indeed, indicate that density effects on solute transport are, in principal not to be dismissed. Even so, as density-dependent flow and transport modeling poses, at least in many practical applications, a tremendous burden on the computational resources available, the question still remains as for their indispensable need in the every-day modeling of groundwater quantity and quality in a particular real aquifer situation, i.e. to forgo exact representation of the physical system dynamics for computational expediency. The present thesis will attempt to provide some further arguments in this debate.
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Chapter 3: Hydrogeological Overview of Study Area

3.1 Topography

The study area is located in the Lower Central Plain (Figure 3.1.) or so-called “Lower Chao Phraya River Basin” and has a size of approximately 150 km in the E-W- and 200km in N-S- direction. The plain is demarcated in the west by the Tanaosri range, in the north by small hills in Nakhon Sawan province, in the east by the Khorat Plateau and small hills in Chantaburi province and in the south by the Gulf of Thailand. The plain is the largest flat plain of Thailand and consists of young fluvial and marine sediments. Fans and terraces exist in the peripheral zones of the plain. A peneplain and a structural terrace in the eastern part of the plain are the oldest landforms of the region. The average altitude of the plain is ranged from 20 m (MSL) in the northern part to only 1.5 m (MSL) in the Bangkok area. From there on the plain forms a deltaic marine plain that extends until the Gulf of Thailand and which can divided further into the tidal zone, the tidal flat of marine clay, the tidal flat of brackish clay and the barrier (Kokusai Kogyo, 1995).

3.2 Geology

With the topographic characteristics as stated above, the landform of the Lower Central Plain
can be mainly divided in parts that are *mountains*, *high terraces*, *peneplain*, *middle terraces*, *old and young alluvial fans*, *delta*, *tidal flats* and *barriers* (Figure 3.1.b). The main geological properties of each of these landforms can be summarized as follows:

**Mountains:** These are made mostly of marl and forming gentle slopes. In the northeast of the plain the mountains consist mainly of Palaeozoic limestone.

**High terraces:** These from roughly a 40 km-wide N-S stretching band in the western part of the plain. The altitude of these terraces varies from 30 m to 150 m. Monadnocks which consisted of Palaeozoic to Mesozoic rocks are scattered throughout the terrace. The un-/consolidated units inside the terraces are comprised of laterite, sand, silt and granular sand which formed in the Pliocene to early Pleistocene age.

**Middle terraces:** They are located narrowly in between the high terraces and the peneplain and have altitudes of 3 m to 40 m. This formation mainly consists of clay, sand and gravel which are spatially intervened by laterite, deposited in the Middle Pleistocene.

**Peneplain:** It is mainly located in the east of the Bang Pakong river (in the east of the plain) with an elevation ranging from 10 m to 100 m. The basis of the Peneplain is made of laterite and weathered granite, covered by depositions of the early Pleistocene to Pliocene age.

**Old alluvial fans:** Those situated in the west of the plain are, namely, the Nong Chang fan (altitude: 20 m to 100 m) and the Don Chedi fan (altitude: 5 m to 45 m). Another fan in the east is the Pasak fan (altitude: 5 m to 40 m). The un-/consolidated rock are composed of clay, silt, sand and gravel which are intercalated by laterite, also of Middle Pleistocene age.

**Young alluvial fan:** It occupies mainly the west of the plain and is inclining gently toward east, namely, the Mae Klong fan (altitude: 5 m to 20 m). Here the deposits are rather thick, with a total height of more than 80 m, and are comprised primarily of sand, clay, silt and gravel of the middle to late Pleistocene.

**Delta:** The delta formed by the Chao Phraya River can be divided into two zones:
(1) The *Delta of fluvial sediments* located in the northern part of plain is about 60 km wide and 80 km long, varies from 6 m to 18 m in altitude, and inclines by 3° towards the south. The deposits are comprised of silty clay and sandy loam whose major petrological constituents are pisolitic concretion and iron oxide, can be dated back to the late Pleistocene, was formed in the shallow sea and deltaic environment of high sea level (Monastirian Stage: 8 m. to 15 m. above MSL). It may connect to the water-bearing-facies at a depth of 60 m.

(2) The *Delta of Brackish Sediments* extends north of Ayuttaya. Its elevation ranges between 4 m to 12 m and leans at a rate of 3° southward. The depositions are of late Pleistocene and are mainly comprised of dark or black grayish clay and whose major minerals are manganese and iron pisolitic nodules. This delta correlates with the Bangkok stiff clay.

*Tidal flat:* Again, two tidal flat areas can be defined:

(1) The *Tidal Flat of Brackish Clay* stretches to the south of the plain is 120 km wide and 80 km long and has an altitude of 2 to 3 m. The formation is composed of dark or black clay which is an ingredient of shell and crab fossils and has a thickness of 2 to 3 m in Ayutthaya and of 20 m in Bangkok. This clay layer is correlated with Bangkok soft clay.

(2) The *Tidal Flat of Marine Clay* lies along the coast, has an elevation of 0 m to 3 m and is composed of dark/black or brown/blue clay. This deposit correlates with the upper part of the Bangkok clay (top clay).

*Barrier:* It is located along the south and southeast borders of the plain, has an elevation of 1 m to 3 m and is mainly comprised of shell fragments. The barrier originated in the Holocene at a temporal stagnant stage of the sea level during regression of the sea from the maximum transgression.
3.3 Hydrogeology

Examining former geological studies, *Kogkusai Kogyo* (1995) and *Gangopadhyay* (1997) concluded that Bangkok and its vicinities are underlain by a prevalent layer of blue or grey marine clay, the so-called “Bangkok Clay” of 15 m to 30 m thickness. Underneath this clay-layer one finds unconsolidated and semi-consolidated sediments with a total thickness of 400 m to 1800 m. The coring-logs of the groundwater wells allow to discriminate the unconsolidated and semi-/consolidated sediments into the one top clay layer and up to 8 water bearing formations (aquifers) down to a depth of 550 m. These aquifers are comprised primarily of sand and gravel separated by clay layers and lenses are as follows (Figure 3.2.):

![Figure 3.1. The study domain (a) and 3-D geological map of the Lower Central Plain (b).](image-url)
(a) **Bangkok Clay** varies in between 15 to 30 m depth. The layer is divided into the upper, soft clay and the lower stiff clay. The soft clay is very soft, black and its primary constituents are shell fragments locally intercalated with fine sand along the Chao Phraya River. However, locally one encounters also some sediment sand originating from flooding events. The stiff clay, the other hand, is comprised of brown sandy silt and clay.

(b) **Bangkok Aquifer** (50 m zone) – The thickness of this aquifer varies from 20 to 60 m and it contains thick alluvial deposits of coarse sand, gravel and pebble intervened with brown or black calcareous clay lenses. The Bangkok clay above is confining this aquifer on its top and has been contaminating the groundwater in this aquifer since the transgression period from vertical leakage of saline formation water. As a consequence, the groundwater in this aquifer is of poor quality and has a brackish to salty taste. Normally, it is not able to be used for any utilization.

(c) **Phra Pradaeng Aquifer** (100 m zone) – It is separated from the Bangkok aquifer by a bed of dark stiff clay. The porous medium contains white to pale-gray gravel and sand, with grains rounded and fairly well-sorted, but interspersed with carbonized woods and peat in the lower part. There are clay lenses intercalated in between unconsolidated formations. Phra Pradaeng is a main productive water-bearing unit and a common discharge well yields in between 50 – 100 m$^3$/hr, but the groundwater quality was brackish to rather salty, except fresh groundwater in the south and southwest of Bangkok. However, the groundwater presently has been contaminated to be brackish water or salty water in those areas.

(d) **Nakhon Luang Aquifer** (150 m zone) – A thick and hard clay bed overlie a sand-gravel formation that are moderate- to well-sorted but are interspersed by clayish formations of whitish, yellowish or grayish brown color. This aquifer has been heavily developed for utilization. A general well-pump can produce groundwater yields of 100 - 250 m$^3$/hr, with a high water quality, except in the west, south and southwest of Bangkok where the water gets salty.

(e) **Nonthaburi Aquifer** (200 m zone) – The basic characteristics of this aquifer are the same as those of the Nakhon Luang aquifer. This formation is comprised of rather uniform sand and gravel with intervening sandy clay lenses. The groundwater yields in this aquifer characterize it as a most-productive water-bearing unit, the more so,
since water quality was excellent. There was less number of wells which has been drilled into this layer before 1975, after expanding area of contaminated groundwater in Nakhon Luang aquifer, numerous wells have been developed into the Nonthaburi aquifer, as that consequence, it has drawn saline water to pollute in this aquifer.

(f) **Samkok Aquifer** (250 m. zone) – The unconsolidated formation is comprised of sand gravel and clay characterized by yellowish to dirty brown. The unconsolidated unit is locally intervened by calcareous clay. The yields of this aquifer are slightly less than those of the Nakhon Luang and Nonthaburi aquifers, but, nevertheless water quality is good.

(g) **Phaya Thai Aquifer** (350 m. zone) – This formation is sand-gravel which are poorly- to fairly-well graded and angular, while the intervening clay lens are brown to dark brown, calcareous, lateritic and compacted. Most of the discharge wells in central and southern Bangkok yield brackish to salty water, whereas others in the north of Bangkok produce fresh water. Because of its large depth, the aquifer is commonly not favorable to groundwater development.

(h) **Thonburi Aquifer** (450 m. zone) – The hard and compacted clay is the upper confining bed of this aquifer which generally contains sand and gravel with intercalating clay lenses. The groundwater is generally fresh but slightly brackish southwest of Bangkok.

(i) **Paknam Aquifer** (550 m zone) – It is demarcated from the upper layer by a leaky clay to sandy clay. Its porous media comprises of sand and gravel which is intervened by clay lens. The unconsolidated formation is normally characterized as white, gray and well-graded. The groundwater yields are of quantity and good quality. The water temperature is approximately 43 °C. Anyhow, the aquifer formation is just too deep for a common well development, except in the area where contaminated groundwater in upper aquifers are not useable and main industrial factories are located, i.e. Samutprakran (south of Bangkok).
3.4 Climatic characteristics and groundwater recharge

3.4.1 Rainfall

The rainfall in the lower Chao Phraya basin is influenced by the southwestern monsoon and some typhoons. The frequency of typhoon which gusts through Thailand is around 2 typhoons per annum and occurs normally in between May to December. Around 85% of rain in Chao Phraya basin is falling in May to October and the high intensity of rain falling occurs in September, meanwhile drought period generally occurs in November to April. The average annual rainfall is around 1200 mm (Suvanpimol, 2003). Figure 3.3 shows the annual rainfall distribution in Thailand.

3.4.2 Evaporation

The average annual evaporation is 1080 mm (Hirota, 2001), highest evaporation rate is at 190 mm. in April which is the hottest month of Thailand; meanwhile the lowest one occurs in November at the rate of 126 mm (Chaowiwat, 1999).

Figure 3.2. Hydrological profile of North-South section of the Bangkok aquifer.
3.4.3 Recharge

Based on the landforms and deposits, the recharge to the aquifers system is likely flowed via mountains, hills, terraces and fans which are mainly located in the western and eastern boundaries of plain. While the recharge through Chao Praya river is likely insignificant, as the most of sediments along Chao Praya river is fine grain materials and generally intercalated by clay beds and consolidated calcareous layers. Furthermore, the Bangkok clay and confining beds of lower layers are significantly thick and commonly overlaid all over in each artesian. Hence, it could be mentioned “the surface recharge within plain is likely too low or insignificant”. Moreover, the isotope-hydrogeology-study and particle tracking simulation (Sandford and Buapeng, 1996) disclosed that the groundwater age is approximately in between 10000 and 30000 YBP which could be interpreted that recharge inside the plain is very low or/and groundwater circulates really slow in the aquifers system.
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Chapter 4: Statistical and stochastic Approaches to assess reasonable calibrated Parameters in a complex Multi-Aquifer System

4.1 Motivation

Prediction reliability is a fundamental problem in groundwater modeling (Anderson and Woessner, 1992; Poeter and Hill, 1997; Yobbi, 2000). Usually a trial-and-error approach is employed to estimate the relevant geohydraulic parameters of the aquifer system under question during the calibration process, but this may turn out to deliver non-unique solutions, i.e. different combinations of parameters produce identical head distributions, precluding a successful prediction of the behavior of the groundwater system under future possible stresses. Another problem of this common trial-and-error method is that the solution may only deliver a local instead of a global minimum of the, generally, multidimensional head distribution. As neither the observed heads nor the geohydraulic parameters of the aquifer system are known precisely, this might not be too much of a drawback in many practical
studies. Nevertheless, better results and a more thorough investigation of the response surface can be achieved through the additional use of statistical methods (Poeter and Hill, 1997; Yobbi, 2000) and, namely, methods based on stochastic theory (Gelhar, 1993), with the latter also being able to quantify the effects of errors in both the objective and subjective data.

In this chapter I will present an application of these three different approaches to the complex Bangkok multi-aquifer system, Thailand, which is the major groundwater resource for about a third of the population of that country. In addition to the conventional trial-and-error modeling approach with the well-known MODFLOW model, as embedded in the PMWIN-WINDOWSURFACE (Chiang and Kinzelbach, 2001), the calibration for the relevant geohydraulic parameters, namely, transmissivity and leakance fields, but also uncertain pumping rates, will be done by using a statistical technique, the automated non-linear regression program, UCODE (Poeter and Hill, 1998) in conjunction with MODFLOW. Advantages of non-linear regression inverse modeling are that, firstly, the data shortcomings and further needs can be evaluated, secondly, better confidence in estimates and predictions are obtained and, thirdly, parameter correlations and low sensitivities which are indicators of non-unique solutions can be computed, providing a better statistical understanding of the overall system behavior.

However, neither the trial-and error, nor the inverse method, both of which are still deterministic techniques, work satisfactorily when the “objective” head and/or pumping data and/or the “subjective” aquifer calibration parameters (hydraulic conductivity, transmissivity) are prone to a high degree of uncertainty, as is the case in the present application. For this reason stochastic modeling using Monte-Carlo simulations of realizations of the Y= In T transmissivity field and, subsequently, of the pumping rates are performed. A formula based on Gelhar’s stochastic theory (Gelhar, 1993) that predicts how the uncertainty (variance) $\sigma^2_Y$ projects into the variance $\sigma^2_H$ of the head and/or the residual head is validated through the MC simulations. Using this stochastic approach, I should be able to provide the best calibration of the aquifer system under the present constraints of erroneous head data, local transmissivities and pumping rates.
Figure 4.1. 3D hydrogeological map (a) and FD grid in the fifth layer of the model (b).
4.2 Study area and model implementation

The Bangkok multi-aquifer system is located underneath the lower Chao Praya river basin which is bordered in the east, north and west by ridges of hills and mountains and in the south by the Gulf of Thailand (Figure 4.1a.). Hydrogeologically, the aquifer system can be divided into a topmost soft and stiff clay layer and 8 lower principle confined aquifers (Kokusai Kogyo, 1995). The groundwater flow model for the Bangkok multilayered aquifers is implemented by the quasi 3D finite-difference model MODFLOW (McDonald and Harbaugh, 1988), with 9 aquifer layers, whereby the topmost clay layer is treated as an unconfined aquifer and the 8 lower ones as confined. The model is divided into 55 rows and 52 columns with grid sizes varying from 2*2 km$^2$ to 16*16 km$^2$, following the MODFLOW modeling approach of Kokusai Kogyo (1995) (Figure 4.1b.).

The top boundary of the model is specified as constant head, representing the water table. The main recharges into the aquifer system are at the outcropping basin flanks and are simulated also as constant head that is set equal to the terrain altitude. Because the topmost clay layer has a thickness varying from 15 to 30 meters, recharge inside the basin is basically zero. The bottom of the 9th layer is assigned as a no-flow boundary. Cells in the southern 55th row of the model that are connected to the Gulf of Thailand are treated as constant head at sea level. The initial transmissivities and vertical leakances have been taken from a former study of Kokusai Kogyo (1995), Gangopadyay (1997) and new geological profiles (Kasetsart University, 2003). Head and pumping data have been provided by the Water Resources System Research Unit, Chulalongkorn University.

Using the three different approaches mentioned, the piezometric data from about 179 monitoring wells in 1999 are used to calibrate mainly, among others, zonal transmissivities and leakances under steady state flow conditions. The results of these calibrations form the basis of the subsequent study of saltwater intrusion and management.
4.3 Mathematical formulation

4.3.1 Groundwater flow equation and numerical approach

Groundwater flow equation

The three dimensional movement of groundwater of constant density through porous earth media may be described by the partial – differential equation (MODFLOW, McDonald and Harbaugh, 1988):

\[
\frac{\partial}{\partial x} \left( K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{zz} \frac{\partial h}{\partial z} \right) - W = S_s \frac{\partial h}{\partial t}
\]

(4.1)

where \( K_{xx}, K_{yy} \) and \( K_{zz} \) are values of hydraulic conductivity along the x, y and z coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity (LT\(^{-1}\)); \( h \), the potentiometric head (L); \( W \), a volumetric flux per unit volume and represents sources and/or sinks of water (T\(^{-1}\)); \( S_s \), the specific storage of the porous media (L\(^{-1}\)) and \( t \), time (T).

A spatial discretization of an aquifer system with a mesh of blocks called cells, the locations of which are described in term of rows, columns and layers. An i, j, k indexing system is used. For a system consisting of “nrow” rows, “ncol” column, and “nlay” layers, i is the row index, \( i = 1,2,...,\text{nrow} \); j is the column index, \( j = 1,2,...,\text{ncol} \); and k is the layer index, \( k = 1,2,...,\text{nlayer} \) (Figure 4.2.).

Finite difference formulation

The groundwater flow equation in finite difference form follows from the application of the continuity equation: the sum of all flows into and out of the cell must be equal to the rate of change in storage within the cell. Under the assumption that the density of groundwater is constant, the continuity equation expressing the balance of flow for a cell is

\[
\sum Q_i = SS h \Delta V
\]

(4.2)
Figure 4.2. A discretized hypothetical aquifer system; -------- aquifer boundary, ● active cell, ○ inactive cell, $\Delta r_j$ dimension of cell along the row direction; subscript $(J)$ indicates the number of the column, $\Delta c_i$ dimension of cell along the column direction; subscript $(I)$ indicates the number of row, and $\Delta v_k$ dimension of the cell along the vertical direction; subscript $(K)$ indicates the number of the layer.

where $Q_i$ is a flow rate into the cell (L$^3$T$^{-1}$); $SS$ has been introduced as notation for specific storage in the finite difference formulation; its definition is equivalent to that of $S_s$ in equation (4.2)—i.e., it is the volume of water which can be injected per unit volume of aquifer material per unit change in head (L$^{-1}$); $\Delta V$ is the volume of the cell (L$^3$); and $\Delta h$ is the change in head over a time interval of length $\Delta t$.

Figure 4.3 depicts a cell $i, j, k$ and six adjacent aquifer cells, $i-1, j, k; i+1, j, k; i,j-1,k; i,j+1,k; i, j, k-1; and i, j, k+1$. To simplify the following development, flows are considered positive if they are entering cell $i, j, k$; and the negative sign usually incorporated in Darcy’s law has been dropped from direction from cell $i, j, k$ (Figure 4.4), is given by Darcy’s law as

$$q_{i,j-1/2,k} = KR_{i,j-1/2,k} \Delta c_j \Delta v_k \frac{(h_{i,j-1,k} - h_{i,j,k})}{\Delta r_{j-1/2}} \quad (4.3)$$
where $h_{i,j,k}$ is the head at node $i,j,k$ and $h_{i,j-1,k}$ that at node $i,j-1,k$; $q_{i,j-1/2,k}$ is the volumetric fluid discharge through the face between cells $i,j,k$ and $i,j-1,k$ (L$^3$T$^{-1}$); $KR_{i,j-1/2,k}$ is the hydraulic conductivity along the row between nodes $i,j,k$ and $i,j-1,k$ (LT$^{-1}$); $A_{c}A_{v}$ is the area of the cell faces normal to the row direction; and $\Delta r_{j-1/2}$ is the distance between nodes $i,j,k$ and $i,j-1,k$ (L).

![Figure 4.3. Cell i, j, k and indices for the six adjacent cells.](image)

![Figure 4.4. Flow into cell i, j, k from cell i, j-1, k.](image)
General aspects of finite difference techniques

MODFLOW calculates heads in each cell of the finite difference grid through setup of one finite difference (FD) equation for each cell. Each of this FD equation expresses the relationship between the head at a node and the heads at each of the six adjacent nodes at the end of a time step, i.e. an implicit solution technique is used which, by default, has the appealing property that it is unconditionally stable, irrespective of the time step, unlike in explicit technique which is plagued by the need for small time steps, in order to achieve numerical stability. However, the huge drawback of an implicit method is, since the head values at the coupled neighboring nodes in each of the FD equation is not known at that time, all equations for the whole grid must be solved simultaneously at each time step. This leads to a system of simultaneous finite difference linear equations which can be written in matrix notation as

\[ A \cdot x = b \]  \hspace{1cm} (4.4)

where \( A \) is a coefficient matrix assembled by MODFLOW using user-specified model data; \( b \) is a vector of defined flows, terms associated with head-dependent boundary conditions and storage terms at each cell; \( x \) is a vector of hydraulic heads at each cell. One value of the hydraulic head for each cell is computed at the end of each time step.

Solver options

The MODFLOW package offers various solvers options for the solution of the system of simultaneous linear equations (4.4), namely, the Strongly Implicit Procedure (SIP) package, the Slice-Successive Over Relaxation (SSOR) package (McDonald and Harbaugh, 1988), the Preconditioned Conjugate-Gradient 2 (PCG2) package (Hill, 1990) and the Direct Solution (DE45) package (Harbaugh, 1995). Here is will only explain briefly DE45 and PCG2 as they have been mainly used in the present study.
The DE45 direct solver

The direct solver requires more memory and typically requires more computational effort than the other iterative solvers, but produces the exact solution in a fixed number of flops and is also attractive for the nonlinear problem which may cause an iterative solver to fail in convergence. The DE45 direct solver uses Gaussian elimination with an alternating diagonal equation numbering scheme that is more efficient than the standard method of equation numbering. Equation 4.4 can be rewritten as an equation in which unknown values are the change in head from one solution to the next. If equation 4.4 is written for solution \( k \), and \( A_k x_{k-1} \) is subtracted from the both sides, the result is

\[
A_k \xi_k = q_k
\]  

(4.5)

where \( \xi_k \) is the change in head, \( x_k - x_{k-1} \) and \( q_k \) is \( b_k - A_k x_{k-1} \). The head for solution \( k \) is calculated as

\[
x_k = x_{k-1} + \xi_k
\]  

(4.6)

For the first solution of a simulation (\( k=1 \)), \( x_{k-1} \) is defined to be initial head, which is specified as part of the input data for MODFLOW. In Gaussian elimination, equation 4.5 is modified systematically so that all elements of \( A \) that are on the left side of the diagonal are transformed to zero, which is called upper triangular form. When Gaussian elimination has been performed, the value of \( \xi \) are solved for using a method called back substitution. In back substitution, the value of \( \xi \) is solved for in reverse order starting with the last value. Because \( A \) is in the upper triangular form and reverse order is used, each individual equation represented by matrix equation 4.5 contains only one unknown value of \( \xi \) that can be readily solved for. The ordering equations in back substitution are mainly affecting the computer time and memory. The D4 ordering found by Price and Coats (1974) can improve this drawback by eradicating the back substitution, so that D4 can work 50% to 80% more efficiently than the standard direct method. The DE45 is to be added in the Picard iteration to the D4 scheme in order to solve the non-linear problem. Since Bangkok aquifers system is a complex non-linear system with an upper unconfined aquifer, at the early stage of the calibration process using
MODFLOW-96 with a common iterative solver was not successful, thus the author changed to the DE45 solver, however at the expense of prohibitive computational execution times.

**The PCG2 (preconditioned conjugate gradient2 method)**

The preconditioned conjugate-gradient method for solving a set of linear equations is iterative. In iterative methods, it is assumed that the matrix $A$ can be split into the sum of two matrices; that is $A = M + N$. $M$ is called the preconditioned form of $A$, and the goal is to define $M$ so that it is easy to invert and resembles $A$ as much as possible. In the preconditioned conjugate-gradient method, $M$ must always be symmetric and positive definite.

When $M$ has been defined, the basic iterative equation is developed from Equation 4.4 and the splitting of $A$, and can be written as

$$Mx_{k+1} = Mx_k + b - Ax_k$$

where $k$ is the iteration index. Noting that $b - Ax_k$ is the residual ($r_k$) of the original set of equations at the $k^{th}$ iteration, and setting $s_k = x_k + 1 - x_k$ gives

$$Ms_k = r_k$$

$$s_k = M^{-1}r_k$$

The new heads may then be calculated as $s_{k+1} = s_k + s_k$. More generally, some function of $s_k$ may be used to calculate $x_{k+1}$.

Conjugate-gradient methods are second-order iterative techniques because at each iteration the new change in $x$, which is called $p_k$, is calculated using the change from the prior iteration, $p_{k-1}$, in addition to the vector $s_k$ of equation 4.9. Conjugate-gradient methods begin
by calculating \( \mathbf{r}_k = \mathbf{b} - \mathbf{A} \mathbf{x}_k \). The following steps are executed for each iteration, starting with \( k = 0 \):

\[
\mathbf{s}_k = \mathbf{M}^{-1} \mathbf{r}_k \quad \text{(4.10a)}
\]

for \( k = 0 \)

\[
\mathbf{p}_k = \mathbf{s}_k \quad \text{(4.10b)}
\]

for \( k > 0 \)

\[
\beta_k = \frac{\mathbf{s}_k^T \mathbf{r}_k}{\mathbf{s}_{k-1}^T \mathbf{r}_{k-1}} \quad \text{(4.10c)}
\]

\[
\mathbf{p}_k = \mathbf{s}_k + \beta_k \mathbf{p}_{k-1} \quad \text{(4.10d)}
\]

\[
\alpha_k = \frac{\mathbf{s}_k^T \mathbf{r}_k}{\mathbf{p}_k^T \mathbf{A} \mathbf{p}_k} \quad \text{(4.10e)}
\]

\[
\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k \quad \text{(4.10f)}
\]

\[
\mathbf{r}_{k+1} = \mathbf{r}_k + \alpha_k \mathbf{A} \mathbf{p}_k \quad \text{(4.10g)}
\]

where the superscripted \( T \) indicates the transpose of the vector. Because \( \mathbf{r}_{k+1} \) can be calculated using the last statement, \( \mathbf{b} \) need not be saved within the solver. Iteration parameters \( \beta_k \) and \( \alpha_k \) are calculated internally such that successive updating vectors, \( \mathbf{p}_k \) are \( \mathbf{A} \) orthogonal to previous \( \mathbf{p}_k \) vectors—that is, \( \mathbf{p}_k^T \mathbf{A} \mathbf{p}_l \neq 0, k \neq l \). It was found that the convergence of the PCG2 method is critically dependent on the proper choice of the relaxation parameter. Using a value of latter between 0.97 and 0.99 as reported by Ashcraft and Grimm (1988) turned out to be a good choice, with the PCG2 solver then to be 10 times as fast as the DE45 method.

### 4.3.2 Statistics of sensitivity analysis

The UCODE is a universal inverse code that can be used with any application model and performs inverse modeling, posed as a parameter-estimation problem, by calculating parameter values that minimize a weighted least-squares objective function using nonlinear
regression. The UCODE can also report the plagues of inverse modeling field, i.e. data shortcomings or needs and nonuniqueness by (1) using relative scaled sensitivity and (2) correlation coefficient matrix, respectively.

During a calibration process, UCODE searches for a parameter set for which the sum of squared residuals between model-calculated and measurement values at the observed wells is reduced to attain a minimum by using non-linear regression. For this dissertation, the UCODE cooperates with MODFLOW to optimize the initial optimal set of calibrated parameters, and then this set of parameters is finer-tuned by using trial-and-error. Again, cooperating UCODE and MODFLOW is used to assess the data shortcoming and nonuniqueness from the trial-and-error set of calibrated parameters. These two models are embedded in PMWIN (Chiang and Kinzelbach, 2001) and the details of involved theories can be read in Poeter and Hill, 1997; Hill, 1998; Poeter and Hill, 1998. This work will only mention on the statistical parameters which are used to determine the data shortcoming and nonuniqueness problem.

**Weighted least-squares objective function**

The weighted least-squares objective function $S(b)$ is a measure of the fit between simulated values and the observations that are being matched by the regression can be expressed as:

$$ S(b) = \sum_{i=1}^{ND} \omega_i [y_i - y'_i(b)]^2 + \sum_{p=1}^{NPR} \omega_p [P_p - P'_p(b)]^2 $$  \hspace{1cm} (4.11)

where $b$ is a vector containing values of each of the NP parameters being estimated; ND is the number of observations; NPR is the number of prior information values; NP is the number of estimated parameters; $y_i$ is the $i^{th}$ observation being matched by the regression; $y'_i(b)$ is the simulated value from MODFLOW which corresponds to the $i^{th}$ observation; $P_p$ is the $p^{th}$ prior estimate included in the regression; $P'_p(b)$ is the $p^{th}$ simulated value; $\omega_i$ is the weight for the $i^{th}$ observation; and $\omega_p$ is the weight for the $p^{th}$ prior estimate.
**Dimensionless scaled sensitivities**

When the diagonal matrix is used, the scaled sensitivities $ss_{ij}$ can be formulated as (Hill, 1998):

$$ss_{ij} = \left( \frac{\partial y_i'}{\partial b_j} \right) b_j \omega_i^{1/2} \quad \text{(4.12)}$$

where $y_i'$ is the simulated value associated with the $i^{th}$ observation; $b_j$, the $j^{th}$ estimated parameter of the parameter vector $b$; $\frac{\partial y_i'}{\partial b_j}$, the sensitivity of the simulated value associated with the $i^{th}$ observation with respect to the $j^{th}$ parameter and $\omega_i$, the weight of $i^{th}$ observation.

Because the problem is nonlinear with respect to most of the geohydraulic parameters of interest, the value of the sensitivity will be different for the different components of $b$. The scaled sensitivity $ss_{ij}$ can be used to compare the importance of different observations to the estimation of a single parameter or the importance of different parameters to the calculation of a simulated value. In both cases, greater absolute values are associated with greater importance.

**Composite scaled sensitivities**

Composite Scaled Sensitivities are calculated for each parameter using the scaled sensitivities for all observations, and indicate the total amount of information provided by the observations for the estimation for one parameter. The composite scaled sensitivity for the $j^{th}$ parameter (Poeter and Hill, 1998),

$$css_j = \left[ \frac{\sum_{i=1}^{ND} (ss_{ij})^2}{ND} \right]^{1/2} \quad \text{(4.13)}$$
where \( ND \) is the number of observations which are used in the nonlinear regression. Finally, the statistical sensitivity is reported in terms of the relative composite scaled sensitivity (Poeter and Hill, 1998; Yobbi, 2000)

\[
rcs_j = \left\{ \frac{(css_j)}{\max (css_j)} \right\}^{1/2} 
\]

(4.14)

**Correlation coefficients**

Correlation coefficients are determined as the covariance between two parameters divided by product of their standard deviations (Poeter and Hill, 1998),

\[
cc(i, j) = \frac{\text{cov}(i, j)}{\text{var}(i)^{1/2} \text{var}(j)^{1/2}} 
\]

(4.15)

where \( cc(i, j) \) is the covariance between parameter \( i \) and \( j \); \( \text{var}(i) \), the variance of parameter \( i \); and \( \text{var}(j) \), the variance of parameter \( j \).

### 4.3.2 Stochastic formulation

As part of his famous and, nowadays, well-known stochastic theory of flow and transport processes in stochastically random media, Gelhar (cf Gelhar, 1993) has proposed a stochastic formula which is of great use in the present study. This formula applies to saturated groundwater flow and basically states that if the head process is locally stationary, then the head variance \( \sigma_H^2 \) for a steady-state flow process can be written as

\[
\sigma_H^2 = C \sigma_Y^2 \lambda^2 J^2 
\]

(4.16)
where $C$ = a coefficient that depends on the dimensionality of the flow, and possibly other parameters of the flow configuration; $\sigma_y^2$ = the variance of $\ln K$ or $\ln T$; $\lambda$ = an integral scale; $J$ = average hydraulic gradient. A more detailed discussion of this very important equation is provided in Section 4.4.3

4.4 Effective approaches to assess the reliable parameters in the Bangkok aquifers model

4.4.1 Conventional (forward) trial-and-error approach

A qualitative evaluation of the calibration success is provided by the visual inspection of similar patterns between computed and observed heads in the 3rd, 4th and 5th model layer which are the key productive groundwater layers and where most observed wells are located (Figure 4.5.).

A quantitative assessment is carried out by an analysis of the scatter plot of measured against computed heads (Fig. 4.6a) and by a measure of the residual error quantified by

![Figure 4.5. Observed versus steady-state computed heads (m) for 1999 in (a) layer 3, (b) layer 4 and (c) layer 5.](image)
Figure 4.6. Observed versus computed heads for 1999 (a), with upper and lower 95% confidence limits; ME, MAE, RMS obtained when transmissivities T and vertical leakances $V_k$ are varied percentally from their optimal calibrated values (b).

(1) the mean error (ME),
(2) the mean absolute error (MAE) and,
(3) the root mean squared error (RMS).

The scatter plot reveals a well-posed calibration, since all points are closed to the diagonal line, with the coefficient of determination $R^2 = 0.92$, i.e. being close to one. Moreover, the diagrams of the sensitivities for ME, MAE and RMS (Figure 4.3b) disclose that this set of
calibrated hydraulic parameters is optimal in the sense that it provides the best result among the manifold of slightly perturbed parameter values.

One point of particular importance to the modeler should be to examine how large a model error, i.e. residual is acceptable for a calibrated model to be considered satisfactory. Usually, the maximally acceptable error depends on the magnitude of the head change over the model domain and is formulated as the ratio of the RMS to the former (Anderson and Woessner, 1992). In our case these ratios are 4%, 3% and 4% in layers 3, 4 and 5, respectively, which is quite satisfactory given the uncertainties in the data as will be discussed further down.

4.4.2 Statistical regression (inverse) approach

Combining the forward MODFLOW model with the nonlinear regression (inverse) model UCODE (Poeter and Hill, 1998) offers a more versatile exploration of the model calibration space than is possible by the trial-and-error method above. In addition to allow for area

(a) Sub zones of transmissivity in layer 3, Phra Padeang Aquifer

Figure 4.7. Subzones of transmissivity (m²/day) in layer 3, Phra Padeang; 4, Nakhon Luang; and 5, Nonthaburi Aquifer.
Figure 4.7. Subzones of transmissivity (m$^2$/day) in layer 3, Phra Padeang; 4, Nakhon Luang; and 5, Nonthaburi Aquifer (continued).
(a) Sub zones of vertical leakance in layer 3, Phra Padeang Aquifer,

Figure 4.8. Sub zones of vertical leakance (day$^{-1}$) in layer 3, Phra Padeang; 4, Nakhon Luang; and 5, Nonthaburi Aquifer.
zoning of hydraulic parameters, UCODE computes sensitivity and correlation coefficients for each of these, resulting in an estimate of the uncertainties in the calibration and providing a scrutiny of the overall piezometric response surface.

In the present application, the model domain is divided into 5, 6 and 5 sub-zones for the transmissivity and 5, 5 and 4 sub-zones for the vertical leakance in layers 3, 4 and 5, respectively. Figure 4.7 and 4.8 shows the zoning used for layers 3, 4 and 5 which are the major producing aquifer. The composite scaled sensitivity (css) (equation 4.13) computed by UCODE expresses how well the parameters are designated by the observations and reflects how well the parameters can be calibrated. In order to interpret this sensitivity easier, the relative composite scaled sensitivity (rcs) (equation 4.14) obtained by normalizing all css-values by the largest one will be represented. A parameter with larger rcs is likely to have a smaller uncertainty, a broader confidence interval and, thus, be more informative for the calibration. Although the lower cut-off value for rcs to characterize a parameter value as

(c) Sub zones of vertical leakance in layer 5, Nonthaburi Aquifer,

**Figure 4.8** Sub zones of vertical leakance (day$^{-1}$) in layer 3, Phra Padeang; 4, Nakhon Luang; and 5, Nonthaburi Aquifer (continued).
**Table 4.1** The composite scaled sensitivity and relative composite scaled sensitivity for calibrated transmissivity sub-zones in Bangkok Multilayered system.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Zone Number</th>
<th>Composite Scaled Sensitivity</th>
<th>Relative Composite Scaled Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1</td>
<td>13.600</td>
<td>0.701</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>5.000</td>
<td>0.425</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>4.570</td>
<td>0.406</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>8.090</td>
<td>0.540</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>1.530</td>
<td>0.235</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>13.000</td>
<td>0.685</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>5.620</td>
<td>0.450</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>6.280</td>
<td>0.476</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>3.610</td>
<td>0.361</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>2.340</td>
<td>0.291</td>
</tr>
<tr>
<td></td>
<td>11</td>
<td>0.603</td>
<td>0.148</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>9.810</td>
<td>0.595</td>
</tr>
<tr>
<td></td>
<td>13</td>
<td>27.700</td>
<td>1.000</td>
</tr>
<tr>
<td></td>
<td>14</td>
<td>14.200</td>
<td>0.716</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>2.410</td>
<td>0.295</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>0.962</td>
<td>0.186</td>
</tr>
</tbody>
</table>

**Table 4.2** The composite scaled sensitivity and relative composite scaled sensitivity for calibrated vertical leakance sub-zones in Bangkok Multilayered system.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Zone Number</th>
<th>Composite Scaled Sensitivity</th>
<th>Relative Composite Scaled Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1</td>
<td>0.013</td>
<td>0.074</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.000</td>
<td>0.654</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>2.340</td>
<td>1.000</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>1.340</td>
<td>0.757</td>
</tr>
<tr>
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<td>5</td>
<td>0.192</td>
<td>0.286</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>0.129</td>
<td>0.235</td>
</tr>
<tr>
<td></td>
<td>7</td>
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<tr>
<td></td>
<td>8</td>
<td>0.577</td>
<td>0.497</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>0.605</td>
<td>0.508</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>0.068</td>
<td>0.170</td>
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<td>0.610</td>
<td>0.511</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>0.179</td>
<td>0.277</td>
</tr>
<tr>
<td></td>
<td>13</td>
<td>0.622</td>
<td>0.516</td>
</tr>
<tr>
<td></td>
<td>14</td>
<td>0.349</td>
<td>0.386</td>
</tr>
</tbody>
</table>
Figure 4.9. Relative composite scale sensitivity analysis for transmissivity (a) and vertical leakance in the various sub-zones (b).
Figure 4.10. Correlation coefficient matrix of (a) transmissivity and (b) vertical leakance in layer 3, 4 and 5.
totally uncertain is rather arbitrary, Yobbi (2000) sets the former to 0.02. Using the nonlinear regression model UCODE (Poeter and Hill, 1998) the various sensitivity parameters are calculated for 16 sub-zones of transmissivity and 14 sub-zones of vertical leakance. The results are analyzed and listed in Tables 4.1 and 4.2 and Figure 4.9 and 4.10.

Figure 4.9 and 4.10 show in more detail the matrix of the correlation coefficients \( (cc) \) between the various sub-zonal parameters, providing information on which of the sub-zones can be determined independently of the other. It can be seen that the \( cc \) are unity along the diagonal lines and that they have only small values in the off-diagonal elements of the matrix, particularly for the transmissivity, whereas for the leakance the zoning is slightly less optimal. According to the statistical criteria assumed previously, I would consider our zoning choice for the vertical leakance and, more so, for the transmissivity as satisfactory.

### 4.4.3 Stochastic modeling using MC-simulations and validation of stochastic theory

Although the two deterministic modeling approaches used previously, namely, the trial-and-error and the statistical nonlinear inverse methods have resulted in satisfactory calibrations, none of them has been able to perfectly fit the observed “objective” piezometric head data, leaving a nonzero residual as quantified by the RMS (see Figure 4.6b.). There are two reasons for this:

1. the “objective” head and/or the pumping data are not exactly measured and/or
2. the particular, “deterministic” calibration parameters obtained represent only a local instead of a global minimum of the piezometric response surface.

On the other hand, one has to assume that the Bangkok aquifer system is more heterogeneous than is pictured by the zonal calibrated transmissivity \( T \) and leakance fields \( V_k \) obtained so far. Moreover, given that local estimates of \( T \) from pump tests and of \( V_k \) from geological borehole profiles are available that point to a rather heterogeneous subsurface structure, one would like to condition the model calibration on these extra “subjective” model observations.
For this purpose I will present in the following a stochastic modeling approach using Monte-Carlo (MC) simulations of realizations of the \( Y = \ln T \) transmissivity field and partly conditioned on the observed “subjective” \( T \)-data. I will look into the question as to how the uncertainty (variance) \( \sigma^2_Y \) projects into the variance \( \sigma^2_H \) of the heads and/or the residual heads. Recall Equation 4.16, using stochastic theory, Gelhar (1993) developed the following relationship between these two variances (assuming steady state saturated groundwater flow):

\[
\sigma^2_H = C \cdot \sigma^2_Y \cdot \lambda^2 \cdot J^2
\]

where \( C = \) a coefficient that depends on the dimensionality of the flow (\( C = 0.46 \) for 2D); \( \sigma^2_Y \) = the variance of \( \ln K \) or \( \ln T \); \( \lambda \) = an integral or correlation scale; and \( J \) = average hydraulic gradient.

This equation shows that the residual head variance \( \sigma^2_H \) is directly proportional to the variance \( \sigma^2_Y \) and the square of the correlation scale \( \lambda^2 \) of the transmissivity field. Thus, the head variance \( \sigma^2_H \) provides a lower bound for a calibration target which means that the model should be calibrated such that the simulated \( \sigma^2_H \text{ (sim)} \) attains approximately the theoretical value \( \sigma^2_H \text{ (Gelh.)} \) of Equation (4.16).

Firstly, I validate Eq. (4.9) by comparing it with MC simulations of random realizations of a logarithmic transmissivity field \( Y = \ln T \). Using a classical random field generator (Chiang and Kinzelbach, 2001), 180 realizations of \( Y = \ln T \) with a set of variances \( \sigma^2_Y \) for each layer, namely, \( \sigma^2_Y = 0.55, 0.77, 0.59 \), in the layers 3, 4 and 5, respectively, and two sets of correlation lengths \((\lambda_x, \lambda_y)\) (with \( x \) and \( y \) corresponding to the EW and NS-direction, respectively) that represent 63% and 95% of the sill of the observed variograms, namely, \( \lambda_x = 9000, 6000, 5500 \) and \( \lambda_y = 12500, 23000, 7500 \) for the 63% -sill and \( \lambda_x = 26000, 21500, 17500 \) and \( \lambda_y = 33000, 56000, 22500 \) for the 95%-sill --which appears to characterize the possible stochastic range of the \( \ln T \)-field in the multi-aquifer system—are performed.
Figure 4.11. Examples of realizations which are generated by using Monte Carlo simulations for layer 3 (a), 4 (b) and 5 (c) obtained using $\sigma_Y^2 = 0.55, 0.77$ and 0.59.

Using these MC-Carlo simulations we investigate how the input $\sigma_Y^2$ projects through the groundwater system onto the head variance $\sigma_H^2$. It turns out that the $\sigma_H^2$ obtained for the 95%-sill correlation length conforms well with that of the stochastic formula, while that for the 65%-sill length results in biased (too low) values. The variograms of the MC-simulated heads are shown in Figure 4.12. The results obtained theoretically and from the MC-simulations are summarized in Table 4.3 and they show rather unanimously that the $\sigma_H^2$ Gelhar conform well to the $\sigma_Y^2$ simulated.

For further clarification and in order to alleviate the problem of the poorly-known flow factor $J^2$ in Equation 4.16, results of MC-calculations with $\sigma_H^2$ twice as big as those in Table 4.4 are presented in Figure 4.13. As expected, the simulated $\sigma_H^2$ are about two times higher than in the first case. This clearly provides further evidence of the applicability of the analytical stochastic theory of Gelhar (1993) in the present case. As mentioned earlier, the lower bound of an acceptable error of calibration should be equal to $\sigma_H^2$ calculated with Gelhar’s formula. The accepted error targets for $\sigma_H$ computed stochastically are 5.36, 7.89 and 5.84 m in layers 3, 4, and 5, respectively.
Figure 4.12. Simulated variograms of head in layer 3 (a), 4 (b) and 5 (c) with variances $\sigma^2_Y$ and correlation lengths $\lambda_Y$ as specified in Table 4.3.
Table 4.3. Comparison of $\sigma_H^2$ obtained from Gelhar’s Eq. (4.16) and MC- simulations.

<table>
<thead>
<tr>
<th>Layer</th>
<th>$C$</th>
<th>$\sigma_Y^2$</th>
<th>$\lambda_y$ (m)</th>
<th>$J$</th>
<th>$\sigma_H^2$ (Gel.) (m$^2$)</th>
<th>$\sigma_H^2$ (sim) (m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
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<td>0.55</td>
<td>33000</td>
<td>3.24E-04</td>
<td>28.9</td>
<td>29</td>
</tr>
<tr>
<td>4</td>
<td>0.46</td>
<td>0.77</td>
<td>56000</td>
<td>2.37E-04</td>
<td>62.3</td>
<td>60</td>
</tr>
<tr>
<td>5</td>
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<td>0.59</td>
<td>22500</td>
<td>5.00E-04</td>
<td>34.1</td>
<td>35</td>
</tr>
</tbody>
</table>

Table 4.4. Similar to Table 4.3, but with $\sigma_Y^2$ twice as big.

<table>
<thead>
<tr>
<th>layer</th>
<th>$C$</th>
<th>$\sigma_Y^2$</th>
<th>$\lambda_y$ (m)</th>
<th>$J$</th>
<th>$\sigma_H^2$ (Gel) (m$^2$)</th>
<th>$\sigma_H^2$ (sim) (m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.46</td>
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<td>33000</td>
<td>3.24E-04</td>
<td>57.9</td>
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<tr>
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<td>2.37E-04</td>
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<td>22500</td>
<td>5.00E-04</td>
<td>68.1</td>
<td>70</td>
</tr>
</tbody>
</table>

The set of calibrated parameters obtained using the trial and error approach, resulted in MAE values 1.97, 2.14 and 2.11m, respectively, i.e. are lower than the ones above obtained from the stochastic representation of the aquifer’s transmissivity. Basically this means that the deterministic trial and error approach resulted in a calibration which is not conditioned enough on the transmissivity-information available.

Finally, it is investigated which factors affect the model residual errors the most. In addition to the stochastic transmissivity variations $\sigma_Y^2$ which result in head variations $\sigma_H^2$ as given by Equation 4.16, there will be intrinsic errors in the head measurements (noise) $\sigma_n^2$ that should add up to the first ones. Hence, the $\sigma_H^2$ obtained from stochastically generated transmissivities and the intrinsic errors of the head measurements were determined. The average $\sigma_H$ of all monitoring stations are 3.73, 11.23, 7.17 m in the layers 3, 4 and 5, respectively which is higher than predicted by Eq. (4.9). A major reason for this might be that erroneous pumping rates are used. Indeed, pumping rates in the study area are not always correctly reported by well owners. To investigate the effects of varying pumping rates on the residual head variance, 180 Monte Carlo simulations with randomly disturbed pumping rates of varying magnitudes (30 - 80 % of the reference value) are performed. The average $\sigma_H$ of
Figure 4.13. Similar to Figure 4.12, but with $\sigma^2_y$ in layer 3 (a), 4 (b) and 5 (c) twice as big and as specified in Table 4.4 (continued).
all monitoring stations results in 3.40, 7.53, 6.23 m in layers 3, 4 and 5, respectively. It is evident that although the residual head variances due to stochastic pumping are lower than those due the stochastic transmissivity-field, pumping is still a significant factor contributing to the model error.

4.5 Summary

Effective assessment of reasonable calibrated aquifer parameters can be mainly divided into three categories: firstly, the conventional trial-and-error forward analysis, secondly, the calculation of sensitivity- and correlation coefficients through nonlinear inverse regression and, thirdly, the pure stochastic approach applying well-known stochastic formulae. I have applied these three approaches to the Bangkok multi-aquifer system that consists of 8 complex water bearing layers underneath the Chao Phraya river basin. First, using the MODFLOW code in the conventional forward trial-and-error manner, the hydraulic parameters, namely, the transmissivity for this aquifer system are estimated by visually comparing observed and calculated heads. Next, the estimated parameters are assessed by combining MODFLOW with the automated non-linear regression program, UCODE. Sensitivity and correlation coefficients for each of the parameters are calculated zone-wise.

The results indicate that the estimated parameters are well-determined and unique in each of the sub-zones. In a third step, the full stochastic approach is used. Applying a random field generator, realizations of a logarithmic transmissivity-field \( Y = \ln T \) with various sets of variances \( \sigma^2_H \) and correlation lengths \( (\lambda_x, \lambda_y) \) for each layer that characterize the possible stochastic range of the \( \ln T \)–field in the multi-aquifer system are simulated. Using these Monte Carlo MODFLOW simulations the study investigates how \( \sigma^2_Y \) contributes to the \( \sigma^2_H \) of the observed head and/or residuals. Stochastic theory predicts that \( \sigma^2_H \) and \( \sigma^2_Y \) are related to each other as \( \sigma^2_H \sim \sigma^2_Y \times \lambda^2 \).
Finally, I investigated which factors affect the residual error of the model estimation. Obviously, both transmissivity variations and errors in the head measurements are mostly responsible for a non-zero estimated residual head. Hence, the variances of head that are obtained from stochastically generated transmissivities and the intrinsic errors of the head measurements were determined. The results show that the stochastically predicted variances of the head are still somewhat lower than the variances of the residual head, indicating additional uncertainties in the fitted model. Indeed, the pumping rates turn out to be very evasive. To investigate the effects of the latter on the residual head variance, Monte Carlo simulations with randomly disturbed pumping rates of varying magnitudes are performed. The results show that pumping plays a smaller but still significant role for the estimation of the residual error, as the residual head variances obtained from stochastic pumping are lower than those of the stochastic transmissivity field.
References


(10) McDonald, M.G. and A.W. Harbaugh (1988), A modular three dimensional finite different ground-water flow model, *Water-Resources Investigations Report 83-875*, USGS.


Chapter 5: Modeling Flow and Transport for sustainable Yield Estimation of Groundwater Resources in the Bangkok Aquifer System

5.1 Statement of problem

The complex Bangkok coastal multilayered system has been tremendously exploited over the last several decades. As a consequence, the piezometric heads in the aquifer system have dropped significantly, especially in the 3rd, 4th and 5th aquifer layer and head gradients have built up that have induced intrusion of saltwater from its source regions into the producing areas of the aquifers system. Thus it is clear that the groundwater aquifer system is being overused, leading to the adverse effects on the groundwater mentioned. As a matter fact, as one can expect the observed increased pumping trend of the past to continue well into the future, the detrimental situation is bound to even deteriorate more. It is at this stage where the concept of sustainable yield of the aquifer enters the game and this will be at the center of present chapter.
This concept of sustainable yield is of fundamental importance in long-term groundwater management and can aid groundwater resources authorities to identify and design viable water supply alternatives. Basically, the sustainable yield defines the maximum amount of groundwater that can be drawn from the aquifer, in order to prevent long-term deterioration of both the quantity and the quality of the groundwater, usually measured in terms of a maximally allowed head drop in the aquifer and/or concentrations of dissolved solids (i.e. salt) in the groundwater. Of course, the exact limits of sustainable yield depend on the particular hydraulic circumstances in an aquifer, but also on the regional and national environmental standards which can be different in a “first-world” country like the US (Hays, 2000; McKee et. al., 2004) than in a “developing” country like Thailand. In spite of this somewhat arbitrary definition of sustainable yield, for the sake of a quantitative analysis, I have set the following definition in the present application of the Bangkok aquifers system:

*Sustainable yield* is “the maximal groundwater yield that may be withdrawn so that the water levels in the third, forth and fifth layer do not decrease by more than 25% of their current water levels (Dec, 2002) and/or that their chloride concentration stays beneath 250 mg/l.” As for the water quality standard mentioned, 250 ppm is the generally accepted upper level of dissolved solids in drinking water as recommended by the UN Health Organization (WHO), although in many overpopulated coastal areas of the world, higher levels of up to 1000 ppm, defining nearly brackish water, may have to be accepted by the local people.

Using the above definition of sustainable yield, the 3D finite difference MODFLOW96 model, coupled with the solute transport model MT3DMS is set up for the Bangkok aquifer system in the present chapter.

### 5.2 Study area and model implementation

The details of the study area and model implementation have already been described in Chapter 4 and are thus omitted here.
5.3 Calibration of reliable parameters in the model

5.3.1 Flow calibration

179 monitoring wells are applied to calibrate the hydraulic parameters for steady state in 1999 (Figure 5.1). Transient state calibration is pursued from 1993 to 1997 and 2000 to 2002 (Figure 5.2). Three main methods, namely (1) the conventional misfit-error approach, (2) sensitivity- and correlation analysis by automatic non-linear regression-UCODE (Poeter and

Figure 5.1. Observed versus computed heads in layers 3, 4 and 5 (a); observed and computed head (m) isolines in 1999 for layer 3 (b), layer 4 (c), and layer 5 (d).
Figure 5.2. The 2000 to 2002 monthly observed (red) and computed (blue) heads at monitor wells PD 93 (a), NL2 (b), and NB61 (c) in layers 3, 4 and 5, respectively.

Hill, 1998) and (3) pure stochastic analysis (Gelhar, 1993) and MC random simulations are used to calibrate the hydraulic parameters (transmissivity and leakance) in steady state model (cf. Arlai et al., 2006, for details).

5.3.2 Solute transport calibration

Solute transport calibration is done from 1993 to 1997 (Figure 5.3) using MODFLOW coupled with the transport module MT3DMS. Dirichlet BC conditions with the seawater concentration are set at cells along the Gulf of Thailand and saline concentration for cells in the upper clay layer that acts as a source of saline pollution, with both concentration boundaries are set equal to concentration data which obtained from Kogkusai Kogyo, 1995.
Figure 5.3. Observed (red) and computed (blue) NaCl concentrations (mg/l) in 1995 in layers 3 (a), 4 (b) and 5 (c).
5.4 Sustainable yield estimation

From the flow calibration, total stress, storage and recharge, changes in the aquifer system from 1993 to 2002 are calculated (Figure 5.4.). Sustainable equilibrium results in a total recharge of $\approx 1.01 \times 10^6 \, \text{m}^3/\text{d}$.

The maximum sustainable yield is estimated under two scenarios of pumping in the 6th to 9th aquifer, namely

(1) by projecting into the future for the next 30 years the 1983 – 2002 accelerated pumping rate and
(2) by doubling the average 1983-2002 pumping rate over the next 30 years.

Meanwhile the pumping in layer 3 to 5 are trial-and-error tuned to meet the sustainable yield conditions for the next 30 years, as the groundwater quality in these layers are adversely affected from the upper saline clay formations and their piezometric heads have been severely dropped from massive pumping since last few decades, they are likely to be non-utilizable in the next few years.

Figure 5.4. Discharge, storage and recharge changes in the aquifer system occurring between 1993 and 2002.
Summarizing the most salient results of the task at hand, it is found out that, in order to meet the sustainability condition for the first scenario, pumping in layers 3, 4 and 5 is to be decreased at the rate of 1.2%, 1.2% and 1.9% per year, respectively. Hence, the sustainable yield in 2032 is $4.86 \times 10^5$ m$^3$/d. On the other hand, the second scenario is impossible to realize, as the groundwater discharge is too high.

In any case, the sustainable yield calculated in this way cannot serve the expected future demand, and there is a so-called “unmet demand (umd)” that must be supplemented by surface water. The umd at different times is calculated by the total pumping rate in layer 3, 4 and 5 at that time which can attain the sustainability conditions minus the present pumping rate (2002) in those layers. Because it is expected that if it does not have any remediation plan in the Bangkok aquifers system, the pumping discharge in layer 3, 4 and 5 would remain rather constant in the future, thus the present pumping rate is the reference pumping scheme for umd. The exact values of umd are listed in Figure 5.5, for each province affected. This can give a water management view for the relevant policy makers.

(a)

**Figure 5.5.** Unmet water demand in 2012 (a), 2022 (b) and 2032 (c) in various provinces when projecting the 1983-2002 pumping rate over the next 30 years (1st scenario). SMS (Samutsakorn), SMP (Samut- prakarn), BK (Bangkok), NB (Nonthaburi), NP (Nakhon Pathom), PT (Pathumthani) and PNAU (Phra Nakhonsri Ayutthaya).
Figure 5.5. Unmet water demand (umd) in 2012 (a), 2022 (b) and 2032 (c) in various provinces when projecting the 1983-2002 pumping rate over the next 30 years (1st scenario). SMS (Samutsakorn), SMP (Samut-Prakan), BK (Bangkok), NB (Nonthaburi), NP (Nakhon Pathom), PT (Pathumthani) and PNAU (Phra Nakhonsri Ayutthaya) (continued).
Although the sustainability condition for the piezometric head might be satisfied, the MT3DMS solute transport simulation show that the contamination inside layers 3, 4 and 5 could not be significantly alleviated (Figure 5.6). I find out two reasons for this, namely,

(a) saline water is driven downward from the uppermost marine clay layer into the lower ones (Figure 5.7),

(b) owing to the major direction of the groundwater flow that is from the boundaries of the model towards the central aquifers (Fig.5.8), the pump-induced hydraulic gradients cannot push back the saltwater to its source regions.

Indeed the water balance (Figure 5.9) shows that 34% of the inflow to the aquifer system originates in the uppermost marine clay layer, while only 6% of the inflow intrudes from the Gulf of Thailand. By that, it implies that the vertical invasion of saline water in the topmost marine clay layer is the major cradle of contamination in Bangkok aquifers system, while horizontal seawater intrusion is only the minor source.

Figure 5.6. Salt plume (mg/l) distribution in layer 3 (a), layer 4 (b) and layer 5 (c) in 2032. Saline contamination inside these upper layers cannot be significantly alleviated, due to saline intrusion from the thick top clay layer.
Figure 5.7. Salt water intrusion profiles in 1990 and 1995.

![Figure 5.7](image)

**Remark:**
- **Salt front in 1990**
- **Invasion front in 1995**

Figure 5.8. The velocity vectors and piezometric heads in layer 3 (a), layer 4 (b) and layer 5 (c) in 2032. The major direction of the groundwater flow is from the boundaries to the center of the aquifer.
Figure 5.9. Steady state water budget in 1999

5.5 Summary

The sustainable yield of an aquifer is of fundamental importance to groundwater resource authorities to get an understanding of the long-term sustainability of the aquifer and, thus prepare them to identify and to design viable water supply alternatives.

From the MODFLOW/MT3DMS modeling investigations it is found out that one scenario which can meet the sustainability conditions consists in diminishing the groundwater
withdrawal rate in layers 3, 4 and 5 at the annual rate of 1.2%, 1.2% and 1.9%, respectively. Hence, the sustainable yield in 2032 is \(4.86 \times 10^5\) m\(^3\)/d. In fact, the sustainable yield cannot sufficiently serve the demand, and this difference defines a so-called “unmet demand (umd)” that must additionally be supplied by surface water. It is reported for each province affected.

Even though a further future drop of the piezometric heads in aquifer layers 3, 4 and 5 might be contained under the specified sustainability conditions, the saline pollution within these layers could not be significantly relieved. Two main reasons are made responsible for this flaw, namely,

(a) saline water leaks downward from the uppermost marine clay layer into the lower ones,

(b) because of the principle direction of the groundwater flow that streams from the model boundaries toward the center of aquifers, consequently hydraulic gradients that have built by the pumping cannot push back the saline water to its original sources.

Moreover, the numerical water balance calculation discloses that 34% of the inflow to the aquifer system cradles in the uppermost marine clay layer, while only 6% of the inflow invades from the Gulf of Thailand.
References


Chapter 6: Numerical Modeling as a Tool to investigate the Feasibility of artificial Recharge to prevent possible Saltwater Intrusion into the Bangkok coastal Aquifer System

6.1 Introduction

The depleted groundwater situation in Bangkok aquifers system which is mentioned in earlier chapters is a crucial problem in Thailand, as this problem adversely impacts to the freshwater resource which is the fundamental need for human, industrial sectors, and welfares in the central region - the biggest economic hub of Thailand. Notwithstanding much research activities in recent years, the mechanisms of saltwater intrusion in the Bangkok aquifers system are not yet fully grasped, namely, i.e. it is still a matter of debate whether the saline pollution encountered in some areas is due to either classical seawater intrusion or to vertical seepage of saline water from the uppermost clay layer that is prevalent throughout much of
lower Chao-Praya river basin. The understanding of contamination cradles and mechanism which is the principle step is significantly for set up the sustainable management scheme for the Bangkok aquifers system.

Thus the objective of the present paper is to investigate through numerical flow and transport modeling the saline groundwater contamination and, in particular, the origins of the saline water that are crucial for the implementation of efficient groundwater management schemes for the future mitigation of this problem. As Thai water authorities are presently considering the installation of an Aquifer System Recovery (ASR) program which relies dominantly on artificial recharge, one specific aim of the present paper is a numerical feasibility study of possible recharge schemes and, if so, to provide clues for their optimal design.

6.2 Study area and model implementation

The details of the study area and model implementation have already been described in Chapter 4 and thus omitted here.

6.3 Investigation of the origins of the saline sources

6.3.1 Water balance study

As mentioned, vertical seepage of saltwater from the upper marine clay layer and horizontal seawater intrusion are the most likeable contamination sources in the Bangkok aquifers, though their relative importance is not yet clear. As indicated by the water balance study of the previous chapter (see Figure 5.9.) 34\% of the inflow into the lower aquifer layers originates in the clay layer, while only 6\% of the inflow intrudes from the sea, providing evidence that the saline water in the marine clay is indeed the main pollution source in the Bangkok aquifers.
6.3.2 Vertical saltwater intrusion

Additional support of the dominant adverse effect of the vertical saltwater intrusion on the groundwater quality comes from the inspection of observed saline concentrations, illustrated in Figure 6.1 and 6.2. The 2D vertical cross-sections of Cl\textsuperscript{−} (Figure 6.2) illustrates firstly that the primary contamination source is the topmost enriched saline clay layer and, secondly, a finger-like structure of the vertical plume movement, most likely due to high-conductivity channels in the heterogeneous aquifer, but also due to local pumping effects in the middle and lower layers of the aquifer. Based on these profiles, they have delineated an area of sensitive saltwater leakage in the aquifer system (Figure 6.1b).

Using the (density-independent) flow and transport model, it has approximately simulated the downward migration of the saltwater emanating from the top clay layer. Results, though they must be taken with a “grain of salt”, as the negative buoyancy effects of the salinity are not taken into account in the present model, with the consequence that the adverse pollution effects might be somewhat underestimated (cf. Koch and Zhang, 1992, 1998), are shown in Figure 6.3. and appear to - at least qualitatively- corroborate the observations. This will be re-modeled with the density dependent groundwater flow and transport model-SEAWAT-2000 in Chapter 7.

6.3.3 Horizontal seawater intrusion

Since there are no monitoring stations offshore and nearby the shoreline available, seawater intrusion could observationally not be tracked and we have to rely on the numerical flow and transport model. Figure 6.4. shows a snapshot of the simulated encroaching seawater intrusion front in 1995. One notes that the intrusion is mainly in horizontal direction in the 1\textsuperscript{st} to 3\textsuperscript{rd} aquifer layer which are directly connected to the open Gulf, but is also directed vertically downward via hydraulically connected zones in the lower water bearing formations, especially, in the shoreline section of the 4\textsuperscript{th} and 5\textsuperscript{th} layer

6.3.4 Contamination type zones

Using the results of the saltwater transport modeling of the previous sections, it can delineate particular zone types of contamination, with respect to their sources and effects. Such a
classification appears to be indispensable for a successful future groundwater management of the Bangkok aquifer system.

Figure 6.1. Monitor wells and profile lines (a) and sensitive leakage areas obtained from 1990 measured data (b).

Figure 6.2. Observed chloride (mg/l) fingerprints for several profiles (see Fig. 6.1a) in 1990.
Figure 6.3. Snapshots of simulated saltwater intrusion plume from the upper clay layer for 1993, 1995 and 1997.

Figure 6.4. Simulated seawater intrusion front along profile 2 in June 1995.
Four types of contamination zones have been demarcated, namely, (1) a zone of seawater intrusion (concentration, $c > 4000$ mg/l nearby the shoreline), (2) a mixing zone between horizontal seawater and vertical saltwater intrusion, (3) a zone of shallow vertical saltwater intrusion ($c > 1000$ mg/l in the $3^{rd}$ layer) and, (4) a zone of deep saltwater intrusion ($c > 1000$ mg/l in the aquifer down to the $5^{th}$ layer), the latter actually defining a highly sensitive intrusion zone (HSI-Z). Figure 6.5 shows this innovative type-zone map constructed in this way. This map is obviously able to clarify the sources and effects of most of the saline contamination in the Bangkok aquifer system. The map discloses, for example, that seawater intrudes heavily into the coastal aquifer near Samut Sakhon, southwest of Bangkok, but less so along the Samut Prakan shoreline, while vertical saltwater pollution occurs mainly in a band that extends from west of Bangkok in northeastern direction up to Pathum Thani, Lam Luk Ka.

**Figure 6.5.** Map of delineating four types of contamination zones, drawn from simulated chloride distributions. Blue color marks the area of seawater intrusion; dark, the green area of mixing between horizontal seawater- and vertical saltwater intrusion; green, the area of vertical, shallow saltwater intrusion; and red, the area of deep saltwater intrusion, i.e. the highly sensitive intrusion zone.
Contamination is especially prevalent in the highly sensitive intrusion zone southwest of Pathum Thani.

6.4 Numerical study of the possibility of aquifer restoration

6.4.1 Non-feasibility of recharge alone

From the investigation of the possible origins of the saline waters above, we conjecture that classical groundwater recharge alone is not able to improve the groundwater quality in the Bangkok aquifer system but, on the contrary, that it would even accelerate the landward movement of the seawater plume and, more so, of the vertically seeping saline plumes emanating from the uppermost clay layer. There are two reasons for this, namely, (1) well-recharge may push existing saline water horizontally to the sides, thus polluting other areas of the aquifer and, (2) the major direction of the groundwater flow is from the boundaries of the model towards its center, as shown in Figure 6.6.

6.4.2 Optimal design of possible aquifer restoration schemes

Because of the likely impossibility of a pure recharge scheme for successful aquifer restoration, we are numerically analyzing in the following sections a vast set of other possible management options to that regard, some of which include simple policy-, or “non-constructive” measures--through either by shutting off pumps in the lower layers or to completely stop pumping in the deep saltwater intrusion zones or by decreasing the pumping rates by different percentages relative to the present situation (Dec, 2002)--, others a combination of policy- and constructive (use of recharge- and clean-up wells) measures, whereby the number of recharge- or clean-up wells has been varied in various fashions, details of which are omitted here for the sake of brevity. Table 6.1 summarizes the most salient results obtained for the total of 31 restoration schemes tested. The table shows the effectiveness of each type (column 12) by, (1) the delineation of the cross-sectional area of contamination along the 2nd profile (column 8), (2) the extent of the landward-directed seawater intrusion (column 9) and, (3) the effective reduction of the contaminated area (column 10) and of the intrusion extent (column 11) by the corresponding scheme with respect to a passive (“laissez-faire”) reference scheme (see below).
Figure 6.6. The velocity vectors and piezometric heads in layer 3 (a), layer 4 (b) and layer 5 (c) in 2032.

Table 6.1 Summary of the effectiveness of a particular restoration scheme as evaluated along the 2nd profile

<table>
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<th>layer4</th>
<th>layer5</th>
<th>layer6</th>
<th>layer7</th>
<th>layer8</th>
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<th>Total area Landused seawater intrusion (hm$^2$)</th>
<th>%Reduction of contaminated area</th>
<th>%Reduction of seawater intrusion</th>
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Abbreviations: WOS = without any scheme (see text), NCM = non-constructive measure, INCM = integration of non- and constructive measure.
Because of the page limitation of the present paper which precludes a complete discussion of all options in Table 1, the study will concentrate here only on the 1\textsuperscript{st} (the “laissez-faire”) scheme and two successful schemes that are representatives of a non-constructive measure (10\textsuperscript{th} or 19\textsuperscript{th} scheme), and of an integration of non- and constructive measures (31\textsuperscript{st} or 32\textsuperscript{nd} scheme).

First (WOS) Scheme: This “without any scheme, WOS”, i.e. “laissez-faire”, or “do-nothing” scheme serves as the baseline to assess the effectiveness of the other model schemes tested. This WOS consists in leaving the future pump rates in the 3\textsuperscript{rd} to 5\textsuperscript{th} aquifer layer as in 2002, but increasing future pumping in the 6\textsuperscript{th} to 9\textsuperscript{th} layer by the same average growth rate as has been encountered in the last two decades, 1983 to 2002. Figure 6.7 clearly illustrates that the groundwater quality in the upper (3\textsuperscript{rd} to 5\textsuperscript{th}) layers will be more and more adversely affected by the infiltration of the saline clay-formation water, making them most likely non-utilizable in the near future. Fig. 6.7 reveals also that the minimum piezometric head obtained with the WOS in 2032 is -52, -68 and -76 m (MSL) in layers 3, 4 and 5, respectively. Moreover, in some sections of the aquifer the saltwater plume migrates deeply downward, whereas seawater intrudes landward over 12 km in layer 3, clearly limiting the usable aquifer yield.

The Nineteenth Scheme: This is a “non-constructive” measure that consists in keeping the present pump rate in each layer until 2011, decrease the pumping thereafter to 60% of today in low-sensitive zones, but shut off completely the pumps in high-sensitive zones (Figure 6.5). This scheme has the appeal to give 5 more years for law enactment. It turns out that this option is the best among the “non-constructive” measures, with recovered heads of -29, -37 and -42 m (MSL) in layers 3, 4 and 5, respectively, in 2032. Meanwhile the saltwater plume area is reduced by 1.6 km\textsuperscript{2} and seawater invades 2 km less than with the WOS (Figure 6.8).

The Thirty-First Scheme: This scheme turns out to be the best among the class of “integrated non- and constructive” measures and is; of course, by design overall the best in terms of aquifer restoration, since it includes an active recharge and clean-up component. Here all pump rates are kept at the values of 2002, with the pumps in the deep layer 6 completely shut off in year 2012.
Figure 6.7. Results of the WOS scheme: Head distribution in the 3\textsuperscript{rd} layer (a), 4\textsuperscript{th} layer (b), 5\textsuperscript{th} layer (c); Saltwater plume distribution in the 3\textsuperscript{rd} layer (d), 4\textsuperscript{th} layer (e), 5\textsuperscript{th} layer (f); and along the 2\textsuperscript{nd} profile (g) in 2032.
Figure 6.8. Results for the 19th scheme: Head distribution in the 3rd layer (a), 4th layer (b), 5th layer (c); Saltwater plume distribution in the 3rd layer (d), 4th layer (e), 5th layer (f); and along the 2nd profile (g) in 2032.
Figure 6.9. Results for 31st scheme: Head distribution in the 3rd layer (a), 4th layer (b), 5th layer (c); Saltwater plume distribution in the 3rd layer (d), 4th layer (e), 5th layer (f); and along the 2nd profile in 2032.
Recharge wells are set up along the seawater intrusion front, \( c > 4000 \text{ mg/l} \), and a clean-up well penetrating to the depth of the saltwater front \( c < 1000 \text{ mg/l} \) that extracts saline water which, after treatment, is recharged back into the aquifer. Figure 6.9 shows that this scheme results in minimum water levels of -49, -65 and -76 m (MSL) in layers 3, 4 and 5, respectively, in 2032. Moreover, the saltwater plume area is decreased by 1.2 km\(^2\) and seawater intrusion is pushed back by 4 km compared with the reference WOS.

### 6.5 Conclusions

Through numerical modeling of flow and solute transport in the Bangkok aquifer system we have been able to testify the feasibility of an aquifer system restoration (ASR) program, using a combination of policy (non-constructive), and active (recharge and clean-up) measures. The restoration success is partly hampered by the fact that there are essentially two kinds of sources of the observed saline groundwater contamination, namely, one that originates in the saline formation-waters of the upper, widespread marine clay layer and which makes up about 34\% of the inflow to the aquifer system, and another, minor one, that is classical seawater intrusion from the Gulf of Thailand. With regard to the first source, which induces vertical seepage of saltwater extending to the deepest layers in some areas of the aquifer, high saline concentrations are found in a band that stretches from southwest of Bangkok northeastward to Pathum Thani, Lam Luk Ka. Seawater intrusion, the second source, is mostly limited to the coastline of Samut Sakon.

As for the ASR schemes tested, water pollution in the 3\(^{rd}\) to 5\(^{th}\) aquifer layer could not be significantly reduced by any scheme, as these layers are being concurrently contaminated by vertical saltwater seepage and seawater intrusion. It turns out that a scheme of artificial recharge alone is not successful for the remediation of the saline contamination. For this reason, numerous combination schemes of water policy changes and constructive measures have been tested that appear to be more promising for, at least, some aquifer restoration in the future. For example, shutting off the presently active pumps in the 5\(^{th}\) to 9\(^{th}\) layer (10\(^{th}\) scheme, Table 1) or reducing the pump rates by 60\% of their present-day values and completely shutting off the pumps in highly sensitive areas after 2012 (19\(^{th}\) scheme) gives the best results in terms of both water level- and water quality recovery.
References


(3) Buapeng, S. (1999), Special Lecture on Groundwater Crisis and Land Subsidence in Bangkok Areas and Suburban, at Department of Water Resources Engineering, Chulalongkorn University, Bangkok, Thailand.


Chapter 7: Numerical Investigation of Density-driven Flow Effect in transient State to the Seawater and vertical Saltwater Intrusion of the Bangkok-Multilayered Aquifers System

7.1 Introduction

In a practical groundwater management problem, the modeler must often make a decision about to either realistically represent the basic physics/geology of the groundwater flow system---with the caveat of prohibitive computer modeling times---, or to forego such details and use a more crude model that is easier to handle and delivers practical results faster. A typical example of this dilemma is the modeling of groundwater flow and transport in coastal aquifers or where groundwater pollution due to dense contaminants needs to be modeled as appears to be the case in the Bangkok aquifer system which is adversely affected by both horizontal coastal saltwater intrusion and vertical seepage of saline waters from upper marine clay layers (Arlai et al., 2006a). Although the use of a density-dependent coupled flow and transport model is clearly indicated in such situations (cf. Koch and Zhang, 1992), many groundwater modelers opt, instead, particularly, for large-scale 3D complex aquifers, for a
computationally much simpler classical (tracer) groundwater and transport flow model, with
the benefit of obtaining practical results much faster while, possibly, lacking some important
physics of the transport problem. The major question to be answered in the present chapter, is
then as to how and to what extent density effects will play an important role in the dynamics
and the quality of the groundwater in the heavily stressed Bangkok aquifer system and,
consequently, if the sole use of a tracer model there is acceptable, at least for practical
purposes.

Using the density-independent flow and transport model MODFLOW-96&MT3DMS (Zheng
and Wang, 1999, Arlai et al. (2006a;b;c) have simulated the long-term transient behavior of
saline transport in the Bangkok-Multi-aquifers under present-day and future pumping
conditions. Based on these results, the next milestone is to numerically investigate if the
effects of variable density on plume migration are to be important and, thus, are to be
included in models of present and future groundwater management of the region. This is the
objective of the present chapter. To that avail, the study will use the 3D density-dependent
groundwater flow and solute transport model SEAWAT-2000 (Langevin et al., 2003) which is
based on the MODFLOW-2000 model and, therefore, has the appealing property that most of
the geometric and parametric set-up and calibration of Arlai et al. (2006a;b;c) for
MODFLOW96 can be directly incorporated into SEAWAT-2000. The main differences for
these two flow and transport model approaches with regard to the modeled plumes will be
presented and some issues of their sensitivity to various flow and transport parameters will be
discussed.

7.2 Numerical method

7.3.1 Governing equations

The study uses two groundwater and solute transport models, i.e., firstly the coupled
MODFLOW-96 (Harbaugh and McDonald, 1996) & MT3DMS (Zheng and Wang, 1999)
which is a standard widely known density-independent code and secondly, SEAWAT-2000
(Langevin et al., 2003) is the newest release of the computer program for the simulation of
three-dimensional, variable density, transient groundwater flow and solute transport in porous
media. The variable density expressions which are applied in SEAWAT-2000 as follows:
The density-dependent groundwater flow equation:

\[
\frac{\partial}{\partial x} \left[ \rho K_{fx} \left( \frac{\partial h_f}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[ \rho K_{fy} \left( \frac{\partial h_f}{\partial y} \right) \right] + \frac{\partial}{\partial z} \left[ \rho K_{fz} \left( \frac{\partial h_f}{\partial z} \right) + \left( \frac{\rho - \rho_f}{\rho_f} \right) \frac{\partial Z}{\partial z} \right]
\]

\[
= \rho S_f \frac{\partial h_f}{\partial t} + \theta \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} - \rho_s q_s
\]

where \( h_f \) = is the fresh water head; \( K_{fx}, K_{fy}, K_{fz} \) are equivalent freshwater hydraulic conductivities in the three coordinate directions \((LT^{-1})\); \( \rho \) = density of native aquifer water \((M/L^3)\); \( \rho_f \) = density of freshwater \((M/L^3)\); \( S_f \) = specific storage in term of equivalent fresh water head \((L^{-1})\); \( C \) = solute concentration \((M/L^3)\); \( \theta \) = effective porosity (dimensionless); \( t \) = time \((T)\); \( \rho_s \) = the density of water entering from a source or leaving through a sink \((M/L^3)\) and \( q_s \) = the volumetric flow rate of sources and sinks per unit volume of aquifer \((T^{-1})\).

The variable density solute transport equation:

Groundwater movement is consequent to the redistribution of solute concentration, and the redistribution of solute concentration changes the density field, hence, affecting groundwater flow. Therefore the groundwater flow and the transport of solute in the aquifer are coupled processes, and the two equations must be solved jointly. The solute transport in groundwater can be governed by the partial differential equation as follows:

\[
\frac{\partial C}{\partial t} = \nabla \cdot (D \cdot \nabla C) - \nabla \cdot (\bar{v} C) - \frac{q_s}{\theta} C_s + \sum_{k=1}^{N} R_k
\]

where \( D \) is the hydrodynamic dispersion tensor \((L^2/T)\), with \( D = D_m + D^* \), where \( D^* \) is the molecular dispersion and \( D_m \), the mechanical dispersion, related to the linear fluid velocity \( \bar{v} \) \((L/T)\) through \( D_m = (A_L, A_T)^* \bar{v} \), (cf. Bear, 1979, for details) where \( A_L \) and \( A_T \) are the longitudinal and transversal dispersivities \((L)\), \( C_s \) is the solute concentration of water entering from sources or sinks \((M/L^3)\); and \( R_k \) \((k=1,...,N)\) is the rate of solute production or decay in reaction \( k \) of \( N \) different reactions \((M/(L^3*T))\), which in the present case of saltwater concentration is set to zero.
Equation of state between density and concentration

For isothermal condition, fluid density is predominantly affected by the solute concentration and fluid pore pressure. The empirical equation between the density of saltwater and concentration can be written as follows:

$$\rho = \rho_f + \frac{\partial \rho}{\partial C} * C$$  \hspace{1cm} (7.3)

where $\frac{\partial \rho}{\partial C} \approx 0.7143$ is the empirically determined slope of the linear relationship between density and salt concentration. Equation (7.3) establishes the coupling between the concentration equation (7.2) and the flow equation (7.1).

7.3.2 MODFLOW- and SEAWAT models implementation

Flow model

The Bangkok multi-aquifer system is located underneath the lower Chao Praya river basin which is bordered in the east, north and west by ridges of hills and mountains and in the south by the Gulf of Thailand (referred to chapter 3). Hydrogeologically, the aquifers system is conceptualized as 9 layers, i.e., the topmost clay layer and eight lower principle confined aquifers (Arlai et al., 2006a). The groundwater flow model for the Bangkok multilayered aquifers is implemented by the 3D finite-difference model MODFLOW-96 and SEAWAT-2000, with 9 modeled layers whereby the topmost clay layer is treated as an unconfined aquifer and the 8 lower ones as confined aquifers. The model is divided into 55 rows and 52 columns with grid sizes varying from 2*2 km$^2$ to 16*16 km$^2$, following the approach of Arlai et al. (2006a) (Figure 7.1). The top boundary of the model is specified as constant head, representing the water table. The main recharges into the aquifer system are at the outcropping basin flanks and are simulated also as constant head that is set equal to the terrain altitude. Because the topmost clay layer has a thickness that varies from 15 to 30 meters, then recharge rate inside the basin is zero. The bottom of 9th layer is assigned as a NEUMAN boundary. All offshore cells in the uppermost layer are set as Dirichlet BC based on bathymetry is specified. Cells at the southern 55th row of the lower modeled layers that are connected to the Gulf of Thailand are treated as DIRICHLET boundary condition at sea level.
Figure 7.1. The FD grid in the 5th layer of the groundwater flow and solute transport model (a), and the 3D FD grid of the 9-multilayered model of Bangkok aquifers system (b).

Solute transport model:

Dirichlet constant-concentration BC’s for the saline concentrations are set at all active cells for the 1st layer reflecting the upper enriched saline clay layer that acts as a source of saline pollution inland over much of the extent of the model domain. Another intrusion source is the seawater offshore. Here some cells at the 55th row of the 2nd and 3rd layer which intersect the Gulf of Thailand have also been attributed a constant-concentration BC.

7.3.3 Conversion and import of reliable parameters into SEAWAT-2000

Many of the SEAWAT-2000 calibration parameter can be taken from the set of calibrated parameters of the coupled MODFLOW-96&MT3DMS model (Arlai et al., 2006a; b; c), as both codes are 3D FD, with SEAWAT-2000, furthermore, originally modified from MODFLOW-2000&MT3DMS. Therefore much of the input data which is reasonably calibrated by MODFLOW-96&MT3DMS is basically compatible with SEAWAT-2000, except for the transmissivity ($T$), vertical leakance ($V_k$), and the coefficient of storage ($S$), that are not used in the same form in SEAWAT as in MODFLOW. In fact, the new density dependent flow package embedded in SEAWAT-2000, namely the Layer-Property Flow (LPF) package, uses other forms of these three parameters, so that they must be converted to horizontal hydraulic conductivity ($K_{xy}$), vertical hydraulic conductivity ($K_z$) and specific
storage \( (S_s) \), respectively. The horizontal hydraulic conductivity and specific storage can be calculated from the calibrated transmissivity and the coefficient of storage through the well-known formulae \((\text{Anderson and Woessner, 1992})\)

\[
\begin{align*}
T &= b * K_{xy} \\
S &= b * S_s
\end{align*}
\]

(7.5) \hspace{1cm} (7.6)

where \( b \) = thickness (m). The vertical hydraulic conductivity \( K_z \) used in SEAWAT-2000 is obtained from the steady state calibration.

### 7.3.4 Verification of the SEAWAT-2000 model

The verification of the SEAWAT-2000 models proceeds in two main stages, steady state and transient

#### Steady-state validation

In the steady-state validation SEAWAT-2000 models the variable-density heads for the steady-state year 1999 and these are compared with the observed ones. A qualitative and a quantitative measure are used to validate the reliability of the code. The qualitative measure consists in a comparison of steady-state modeled isolines (Figure 7.2), and the quantitative one in the regression analysis of the scattered modeled and observed heads (Figure 7.3). One notices from both figures that the SEAWAT-2000 model can reasonably well mimic the observed heads as the isolines conform well (Figure 7.2), and that the correlation coefficient of the scatter plot is close to one (Figure 7.3), with the points of observed-against computed heads located closed to the diagonal line and inside the 95% confidential lines.

#### Transient validation

The validation in transient state is divided into two parts, firstly, groundwater flow (head) and, secondly the solute transport validation. For the flow part this done similar to the steady-. The second stage is the transient state verification; SEAWAT-2000 simulates the variable-density head and solute transport from 1993 to 1997 when the data was rather completely measured in all observed stations. And then it’s computed head and chloride concentration is compared to the measured data.
Figure 7.2. Comparison of Observed versus computed head of SEAWAT-2000 (variable-density flow); observed and computed head contours in steady state for 1999 for layer 3 (a), layer 4 (b), and layer 5 (c).

Figure 7.3. Scattered plot of observed head against computed head of SEAWAT – 2000 in layer 3, 4 and 5 in the steady state year 1999; –– 95% confidence limit.
Figure 7.4. Observed versus computed head (m) of SEAWAT-2000 (variable-density flow); observed and computed head contours in June, 1995 for layer 3 (a), layer 4 (b), and layer 5 (c).

\[ R^2 = 0.96 \]

Figure 7.5. The scattered diagram of observed-versus computed head of SEAWAT – 2000 of layer 3, 4 and 5 in 1993 to 1997.

Transient state validation, by comparing isolines (Figure 7.4) and the scatter plot (Figure 7.5), this time for the, arbitrary, target date, June, 1995. These two figures show the SEAWAT-2000 can mimic reasonably well the groundwater flow in the Bangkok aquifers system.

For the solute transport validation, the spatial plots of measured- and simulated saline concentrations for layers 3, 4 and 5 are selected for year 1995 as an example (Figure 7.6.).
Figure 7.6. Observed (white solid line) and computed (black dashed line) Saline concentrations in 1995 of SEAWAT-2000 in layers 3(a), 4(b) and 5(c).
Figure 7.7. Scatter plots between observed and computed saline concentrations in layer 3 (a), 4 (b) and 5 (c) in transient mode, 1993 to 1997.

These and the corresponding scatter plots are illustrated in Figure 7.6 and Figure 7.7, respectively. These two figures show that, likewise to the hydraulic heads, the modeled chloride concentrations in all these three layers conform well to the observed ones.

In conclusion of this section, one can be confident that SEAWAT-2000 is able to simulate satisfactorily both groundwater heads and saline plume distribution in the Bangkok aquifers.
7.4 Density-driven flow effects on horizontal seawater- and vertical saltwater intrusion

The numerical simulations of density-driven flow and transport in transient state (years 2003 to 2032) in the Bangkok-Aquifers system are to mainly simulate both the horizontal seawater and the vertical saltwater intrusion. As such we will discuss in the following in more detail three aspects of this modeling effort, namely (1) a comparison of the constant-density- and variable-density model of the calibrated parameters; (2) sensitivity analysis of the influence of hydrodynamic dispersion; and (3) of the hydraulic anisotropy.

7.4.1 Comparison of constant density- and variable density model of the calibrated parameters

3D model simulations are performed with the calibrated hydraulic parameters and projected pump rates for the next 30 years (2003 to 2032) condition, i.e., withdrawal rates in 3rd, 4th and 5th layer are kept constant at the rates of 2002, while the pumps and their rates in the other lower layers are to follow the pumping trend experienced between 1983 to 2002. The longitudinal to transversal dispersivity ratio is $A_L/A_T = 10$ with $A_L = 5, 25, 32, 35, 72, 25, 25, 25$ and $10 \text{ m}$ in the 1st to 9th layers, respectively; with calibrated parameters for the heterogeneous hydraulic conductivity; specific yield and storage coefficient taken from Arlai et al. (2006c).

Using these parameters in both the constant density-MODFLOW96&MT3DMS model and the variable density- SEAWAT-2000 model flow and transport for the target date December, 2032 are computed and compared. Figure 7.8. and 7.9. show the differences for the piezometric heads and the saline concentrations, respectively. Basically one notes that these differences are only minor but, yet, do reflect the different physics represented by these two models. For example, the piezometric head comparison of Figure 7.8. qualitatively unveils that the head contours of the variable-density model envelop those of the constant-density model, which means that the drawdown cone of the former is deeper than that of the latter. This situation becomes even clearer from the inspection of the saline plume concentration isolines in Figure 7.9. where the “variable-density” – plumes extend slighter deeper than their “constant-density”- homologues.
While this denoted behavior of the “variable-density” plumes is in agreement with the physical phenomenon of “density-driven flow or buoyancy-induced flow”, one might be surprised about the somewhat small effects detected here, unlike in simulations of the migration of density-dependent plumes of Koch and Zhang (1992; 1998) where density effects were much more prevalent, even at small concentrations.

Indeed the visual comparison of the computed saline concentrations for the two model cases (Figure 7.9) discloses that the saline isolines > 1000 mg/l which are mostly situated within the productive pumped layers (depth range 70-300 m) are rather identical, whereas the 250 mg/l-contour-which is located mainly in a section with fewer pumps-of the variable-density model is driven down more than that of the constant-density model. Thus it appears that the large groundwater pumping in the middle section of the model wipes out to a large extent the usually observed differences in the plume migrations for the two model approaches.

Indeed the massive groundwater withdrawal in the polluted layers, with a subsequent rise of the hydraulic gradient induces, by virtue of Darcy’s law, an increase of the average flow

![Figure 7.8](image)

**Figure 7.8.** The piezometric head contour of computed head of invariable density-MODFLOW-96 model (solid line) versus variable density-SEAWAT-2000 model (dashed line) and flow vectors with pump scheme in December, 2032 at the 3rd (a), 4th (b) 5th (c) layer.
velocity $v$, the more as the transmissivities in these productive sand aquifers are already rather large (Arlai et al., 2006a;c). These high velocities then lead to a large hydrodynamic dispersion coefficient $D$. As a higher $D$ leads to a spreading of the saline plume, its negative buoyancy will diminish, in agreement with earlier numerical studies on density-dependent solute transport (Koch and Zhang, 1992; Voss and Koch, 2001), and the difference to a “constant-density” plume disappears.

### 7.4.2 Sensitivity analysis of hydrodynamic dispersion

As seen above, hydrodynamic dispersion appears to be a key factor of the behavior of density-dependent solute migration. In this section it will carry out a more detailed sensitivity analysis of the influence of hydrodynamic dispersion $D$, or more specifically, the dispersivity $A$. This is the more important as the latter is usually not known for real aquifers and, therefore, has to be approximated, taking into account the so-called spatial scale-effect (cf. Gelhar, 1993), whereby the size of $A$ scales roughly linearly with the aquifer size to be modeled. The following simulations are performed with various values of the dispersivity $A$, namely 0.5, 2 and 10 times the calibrated $A_L$ and $A_T$ and with future pumping rates fixed at their 2002-values (cf. Arlai et al., 2006b), or with no pump stresses at all over the next 30 years. All other parameters are kept invariable. The salt concentrations simulated by both the constant- and the variable-density model are illustrated in Figure 7.10. Firstly, take a look at the simulation cases that include pumping until 2032 (Figure 7.10 a, b and c). As can be expected
and has already been noted in the previous section, for all dispersivity cases and outside the major pumping zones the density-dependent plumes sink deeper than the tracer ones. Also, larger values of the dispersivity lead to an increased downward movement of the salt plume, and this for both the constant- and the variable-density. As for the horizontal movements of the plumes edges, differences are less notable for the various dispersivities, which could be a consequence of the rather small scale of the horizontal dispersivities (several tens of meters) relative to the horizontal model scale (several thousand meters), so that the model grid is not able to completely resolve all the relevant features of the present flow and transport system.

For the second simulation-set that has the pumps shut-off until 2032, Figure 7.10 (d) and (e) show that the delineation of both the tracer- and the density-dependent plumes is essentially identical. This behavior may be explained such that after ceasing of the pumping stress after year 2002, the depletive piezometric heads will be restored from their lowest values of -44, -57 and -52 m . (MSL) in layers 3, 4 and 5, respectively to -1, -2 and -2 m. (MSL) in December, 2032. This significant uplift of the piezometric surfaces induces a strong vertical advective flow that appears to over-compensate the negative buoyancy of the density driven flow so that no visual effects are discerned.

### 7.4.3 Sensitivity analysis of hydraulic anisotropy

Understanding the vertical sinking of the density-dependent solute plume is of utmost importance in variable density transport. As shown by Koch and Zhang (1992) through a scaling analysis, vertical sinking is proportional to \( K_{fz} \delta \rho \), i.e. the vertical hydraulic conductivity \( K_{fz} \) plays a dominant role in the downward migration of the plume.

In order to grasp this mechanism in more detail, \( K_{fc} \) is varied in the following simulations, while keeping \( K_{xx} \) and \( K_{yy} \) invariable, i.e. the effects of anisotropy of the hydraulic conductivity are investigated. Two cases of \( K_{fc} \) are examined, namely, 0.1 and 10 fold of the calibrated \( K_{fc} \) for a set of simulations with and without transient pumping withdrawal, while keeping all other parameters invariant.

Solute concentration contours obtained in this way for the two model approaches are drawn in Figure 7.11. One notes that the variable density plays a central role outside the pumping influence zone (at a depth lower than 300 m MSL), as the unstable edge of the variable-
(a) 0.5 times of calibrated $A_L$ and $A_T$ with 30 years-pumps

(b) 2 times of calibrated $A_L$ and $A_T$ with 30 years-pumps

(c) 10 times of calibrated $A_L$ and $A_T$ with pump

(d) 0.5 times of calibrated $A_L$ and $A_T$ without pump

(e) 2 times of calibrated $A_L$ and $A_T$ without pump

**Figure 7.10.** The simulated saline concentration of density independent (solid line) versus density-dependent (dashed line) model after 30 years (Dec, 2032) under various conditions; 0.5, 2, 10 folds of calibrated $A_L$ and $A_T$ with pump (a),(b) and (c) 0.5, and 2 folds of calibrated $A_L$ and $A_T$ without pump (d) and (e), respectively.
Figure 7.11. The modeled saline concentration of density independent (solid line) versus–dependent (dashed line) model after 30 years (Dec, 2032) under different conditions; 0.1 and 10 folds of calibrated $K_z$ with pump (a),(b), 0.1 and 10 folds of calibrated $K_z$ without pump (c) and (d), respectively.
density plume moves deeper than that of the tracer plume. On the other hand, within the pumping zone the differences in the concentration isolines for the two models are negligible. The reasons for this are the same as explained in the previous section.

Moreover, the first two plots of Figure 7.11 also illustrate that, at least of the present application of a strongly-pumped aquifer, the vertical hydraulic conductivity seems to have a lower impact on the sinking of the solute plume than the hydrodynamic dispersion, unlike in the cases studied by Koch and Zhang (1992). It turns out that this peculiar behavior is the consequence of the multi-layered aquifer system which has aquitards with rather low leakance values sandwiched between the separate aquifer layers and which inhibit significantly vertical groundwater flow across, giving rise to the visual impressions of Figure 7.11.

7.5 Effects of density-dependent flow and transport on the effectiveness of the trial&error aquifer restoration management schemes

As the “constant-density” flow and transport model MODFLOW-96&MT3DMS used so far in Chapter 6 for the determination of the best “non-and constructive” schemes may not be able to accurately represent the real physical mechanism of density-dependent flow and transport of “dense” solutes encountered in the present application, a revision of the results obtained so far is in order using the 3D “variable- density” groundwater flow and solute transport model SEAWAT-2000 (Langevin et al., 2003). In the following this model will be applied for the simulation of some of the same aquifer remediation analyzed earlier.

Figure 7.12 compares the results of the two model approaches for three remediation schemes (see Chapter 6, for details) with respect to the saline plume distribution for the target date Dec. 2032. Most strikingly, one observes from the two columns representing respectively constant- and variable density computations that the salinity plume migrations for both model-approaches do not show any significant difference, i.e. the inclusion of variable density into the model does not appear to have any noticeable effect, at least, with regard to the future saline plume evolution. However, a more detailed inspection of the piezometric heads obtained for the two model approaches reveals that these are about 5 m lower for the variable-than for the constant-density model in the producing layers indicated in the previous section which is conformed to what is explained in section 7.4.1.
Figure 7.12. Snapshots of simulated saline plumes for Dec, 2032, using the “constant-density”—MODFLOW&MT3DMS (a, c, e) and “variable-density”—SEAWAT-2000 (b,d,f) model for three kinds of remediation schemes: “WOS” (top), “best policy” (middle), and “best integrating policy- and –constructive” (bottom), respectively, concentrations in kg/m$^3$. 
7.6 Conclusions and outlook

Results of both a tracer- and a variable-density flow and transport model in transient mode with regard to the proper simulation of saline plume migration in the large-scale Bangkok multilayered aquifer system are evaluated. The fundamental question has been if, and to what extent density effects play a significant role as to alter the conclusions drawn for the transport from a simplified constant-density model which one might favor for every-day groundwater management purposes. For the achievement of this goal, two 3D-finite difference flow and transport models are employed, namely (1) the density-independent MODFLOW96&MT3DMS- model and, (2) the SEAWAT-2000 variable-density model. Based on the heterogeneous subsurface structure- and the computed saline contamination in the years 2003 to 2032 of the Bangkok aquifers system, various simulations with the tow approaches are performed.

The 3D FD flow and solute transport model SEAWAT-20000 has been set up by using reasonably calibrated input data from the earlier MODFLOW96&MT3DMS simulations in Chapter 4. (Arlai et al., 2006). The objectives of the modeling efforts and sensitivity studies are three-fold: (1) a comparison of the calibrated parameters for the constant-density and the variable-density model; (2) a sensitivity analysis of the influence of hydrodynamic dispersion and; (3) a sensitivity analysis of the impact of aquifer anisotropy.

The results of the investigations unveil that, although the variable-density flow and transport model is computationally much more time-consuming than the density-independent (tracer) one, it mimics the physical mechanisms of coupled flow and solute transport much better than the latter. Nevertheless, in the present application, both the density-dependent and the density-constant model result basically in similar saline plume migrations. This astounding outcome is due to the fact that the groundwater pumping in the Bangkok multilayered aquifers plays the most important role in the plume movement, i.e., density (buoyancy) –effects have less of an impact on the saltwater movement than the hydraulic gradients induced by the pumps. Indeed, in those zones which are less affected by pumping the saline plumes computed by the density-dependent model sink deeper than those of the density-constant one, in agreement with basis physics. As for the effects of hydrodynamic dispersion, the results show that for both model approaches vertical downward movement of the plumes increases somewhat with increasing dispersion coefficients and, expectedly, with the effect accentuated for the variable-density
model and in those areas that are less affected by pumping. In the pump-dominated zones, on the other hand, the differences are negligible. As for the effects of hydraulic aquifer anisotropy, the results indicate that increasing the ratio of vertical to horizontal hydraulic conductivity leads to a stronger vertical intrusion of the saline plumes and, again, with the effects more pronounced for pump-free zones and the density-dependent model.

Furthermore, the investigation of the effects of density-dependency of the flow and transport on the trial-&-error management schemes investigated earlier does not show any significant difference for the SEAWAT-2000 model, at least, with regard to the effectiveness of the proposed aquifer remediation schemes to alter the saline plume intrusion for the target date December 2032.

From the above results one may conclude that the variable density of the contaminant saline plumes does not appear to have a significant feedback effect on the hydraulic flow itself in the Bangkok multilayered aquifers. As such a complicated and time-consuming density-dependent flow and solute transport model may pragmatically not function better than a tracer model. Thus, for the groundwater pollution prevalent in the Bangkok aquifer system, the use of a tracer model may be reasonably sufficient for practical groundwater management purposes.
References


(9) Langevin, C.D., W.B. Shoemaker and W. Guo (2003), Documentation of SEAWAT-2000 version with the variable-density flow process (VDF) and the integrated MT3DMS transport process (IMT). USGS report 03-426.


Chapter 8: Integrating an Groundwater Management Optimization Module and a variable Density Flow and Transport Model to investigate sustainable Restoration Schemes for the Bangkok Aquifers

8.1 Motivation

Even though the simultaneously acting two cradles of the major saline pollution in the Bangkok aquifer system have already been clarified and some sustainable aquifer remediation concepts, consisting in both non-constructive and integrating policies & constructive measures have been proposed in Chapter 6, the latter may globally not be optimal, neither in terms of hydraulics nor of economics, as they have exclusively been determined by human judgment or so-called “trial & error”. Furthermore, the numerical method used there, i.e.
MODFLOW-96&MT3DMS, did not yet take into account the density-dependent effects of the saline concentrations on the flow and solute transport. In the present chapter I will overcome these two limitations partly by

a) application of the groundwater management optimization module GWM (Ahlfeld et al., 2005), which embedded in MODFLOW-2000, to further optimize hydraulically and economically the number of recharge-,clean-up wells and three new water trade-off concepts for the given set of head targets,

b) use of the variable-density model SEAWAT-2000 to investigate the density effects on the optimized schemes proposed in a) and on the non-constructive schemes from chapter 5 and 6.

It should be noted that this consecutive approach is, theoretically, not completely wishful, as neither the solute transport, nor the density-dependency of the groundwater flow are incorporated a priori in the GWM analysis. Nevertheless it is the best that can be achieved with the modeling resources available at the present time. Given these caveats, I will re-evaluate in the present chapter the three most efficient non-constructive schemes found earlier in Chapters 5 and 6 by means of the MODFLOW-96 & MT3DMS trial & error simulations and will examine, additionally, 4 more new optimal groundwater schemes, i.e. a total of 7 schemes. These 7 schemes are, namely, the

(1) 1st scheme - the sustainable yield scheme (Chapter 5),
(2) 2nd scheme – a non-constructive scheme (the 19th scheme from Chapter 6),
(3) 3rd scheme – another non-constructive scheme (the 10th scheme from Chapter 6),
(4) 4th scheme–optimizing the number of recharge- and clean-up wells of the best integrated non- and constructive scheme (the 31st scheme from Chapter 6),
(5) 5th scheme- applied “water trade-off concept” to the best non-and constructive 4th scheme (new scheme)
(6) 6th scheme– applying “water trade-off concept” to the 2nd scheme (new scheme)
(7) 7th scheme– applying “water trade-off concept” to the 3rd scheme (new scheme).

The first three schemes are only re-modeled using the variable-density model-SEAWAT-2000 in order to reflect more realistically the density-dependent effects on the groundwater
movements and saline transport resulting from these schemes. The 4th scheme is directly obtained from applying GWM, to optimize the number of recharge-and clean-up wells which can attain the same head targets from the previous trial&error simulations. The 5th to 7th “water trade off concept” schemes are simulated with GWM to examine the least-cost effective means to raise the water levels along the front of the seawater intrusion up to zero meter (MSL)--- as the modeled 2032 water levels in the productive water bearing units of these previously simulated remediation schemes are below sea level,---, either by shutting off the discharge wells or increasing freshwater injection close to the shoreline through in-lieu water supply, in order better restrain seawater intrusion or to reduce the polluted area of the “without scheme”. This approach may particularly appeal to the Thai water authorities who are interested in a recharge concept for the Bangkok aquifers system, to prevent further saltwater encroachment. However, as the GWM-model cannot take into account the density-dependent solute transport into the optimization process, these; firstly, optimized schemes 4 to 7 are re-simulated by SEAWAT-2000. Eventually, the best remediation scenario for the Bangkok aquifer system will is extracted from a comparison of these 7 schemes, based on their effectiveness with respect to (1) the saline pollution reduction, (2) the groundwater-use policy to existing groundwater users and, (3) the scheme’s implementation and operational costs.

### 8.2 Study area and model implementation

The details of the study area and model implementation have already been explained in Chapters 4 (MODFLOW) and 7 (SEAWAT-2000) and are, hence, disregarded here.

### 8.3 Theoretical statement of the groundwater management problem

#### 8.3.1 Linear programming formulation

The ground-water management (GWM) problem is set into a form that can be solved using so-called linear programming techniques. As such the GWM problem consists of a (linear) objective function \( Z \) of the decision variables \( x \) that is either maximized or minimized, subject to constraints of these decision variables, i.e. (cf. Ahlfeld et al., 2005)
Maximize (minimize) \( Z = c^T x \) (8.1)

subject to \( Ax = b \) (8.2)

and \( 0 < x < u \) (8.3)

where \( Z \) is the value of the objective function; \( c \) is a transposed column vector of objective-function coefficients associated with the decision variables; \( x \) is a column vector of decision variables with upper bounds \( u \); \( A \) is a matrix of coefficients defining the form of the constraints; and \( b \) is a column vector of right-hand-side coefficients associated with the constraints. The constrained linear programming problem (8.2) to (8.3) is solved by the well-known Simplex method.

8.3.2 Nonlinear constrained optimization approach

As the topmost modeled layer of the Bangkok aquifer system is fully convertible between a confined and an unconfined aquifer (setting the parameter LAYCON = 3 in MODFLOW), there will be a nonlinear relation between the position of the water table and the discharge- or injection stresses. Thus the constrained optimization problems become nonlinear which is more intricate to handle computationally. The usual approach consists then in linearizing the nonlinear objective function through a Taylor series expansion and to obtain a linear programming problem as above that can be solved as stated by the simplex method. This technique is also called sequential linear programming (SLP).

8.3.3 Formulation of the objective function and the constraints for the Bangkok aquifers GWM problem

According to the goals of the GWM optimization schemes for the Bangkok aquifers explained above, the constrained groundwater management optimization problem is formulated in two ways:

(1) For the optimization of the 4\(^{th}\) scheme the objective function is to minimize the rates \( Q \) (or costs) of possibly 93 recharge and 93 clean-up well-candidates (Figure 8.1), subject to the
constraints that (a) the maximum recharge and extraction well rates $Q$ are less than 12000 CMD, (b) the total recharge rate cannot be greater than the extraction rate and, (c) the computed heads $h$ at 42 spatially-fixed locations along the two lines of the proposed recharge wells and clean-up well barrier in layers 3 to 5 are not dropping below specified values $H----$ obtained from an earlier MODFLOW calibration of the “non-optimized” well scheme within the Bangkok Aquifers system (Arlai et al., 2006b)--- and that appears to be appropriate to repel future seawater intrusion (cf. Reichard et al., 2003). With these goals the GWM-problem is mathematically stated as follows:

$$
\text{Min} \left( \sum_{n=1}^{31} \beta_n \cdot (R_{3n} + Q_{3n} + R_{4n} + Q_{4n} + R_{5n} + Q_{5n}) \cdot T_{Qwn} \right)
$$

subject to the constraints

$$
\begin{align*}
0 & \leq R_{kn} \leq 12000; k = 3,4,5; n = 1,...,31 \\
0 & \leq Q_{kn} \leq 12000; k = 3,4,5; n = 1,...,31
\end{align*}
$$

$$
\sum_{k=3}^{5} \sum_{n=1}^{31} R_{kn} \leq \sum_{k=3}^{5} \sum_{n=1}^{31} Q_{kn}
$$

and

$$
h_{i,j,k,2} \geq H_{i,j,k,2} \quad (\sum i + j + k = 42)
$$

where $R_{kn}$ is the recharge rate, $Q_{kn}$, the clean-up (discharge) rate in layer $k$ and well site $n$ ($n = 31$ is max. number of flux decision variables for layer $k$); $\beta_n$ is the cost or benefit per unit volume of water withdrawn or recharged at well site $n$, (if only flow-rate is optimized, $\beta_n$ is set to a dimensionless value of 1.0); $T_{Qwn}$ is the total active duration of the flow-rate that is taken here as identical with $T_{Qwn} = 7665$ days (for the stress period 2 between year 2012 and 2032) at all well sites; $h_{i,j,k,2}$ is the modeled head at the 42 head constraint locations at col.$= i$, row $= j$, layer $= k$ and stress period 2; and $H_{i,j,k,2}$ is the named head constraint acting as a flow barrier.

(2) For the optimization of the 5th to 7th scheme- the objective function is to minimize the monetary costs $\beta Q$ of the “water trade-off concept” of possible 93 recharge wells and 123 in-
(a)    (b)          (c)

Figure 8.1. Trial-and error well scheme: Orange area shows the distribution of the present
day pumps, blue area the line of recharge wells, with the clean-up wells located 4 cells
northward of the former.

\textit{lieu} delivered water supply cells ---with the number of recharge wells and \textit{in-lieu}-delivered
water supply cells taken from those cells whose discharge wells have rates are greater than
500 CMD (Figure.8.2), subject to the constraints that, (a) the maximum recharge and
extraction well rates \( Q \) are, in turn, equal or less than 12000 CMD, their existing pumping
rates of selected discharged cells \( Q_{exn} \) and, (b) the computed heads \( h \) at 42 spatially-
head constraints along of the proposed recharge wells in layers 3 to 5 do not decline below
specified values \( H = 0 \) meter (MSL) and that which appears to be appropriate to avert future
seawater invasion (\textit{cf.} Reichard et al., 2003). By that, the objective function and the
constraints can be formulated mathematically as follows:

\begin{equation}
\min \left( \sum_{n_k=1}^{N_k} 31; 3N_w = 31; 4N_w = 60; 5N_w = 32 \right) \left( \beta_R \left[ R_{3n_k} + R_{4n_k} + R_{5n_k} \right] + \beta_W \left[ Q_{3n_k} + Q_{4n_k} + Q_{5n_k} \right] \right) T_{Q_{W_k}} \right) (8.8)
\end{equation}

subject to the constraints

\begin{equation}
0 \leq R_{n_k} \leq 12000, k = 3, 4, 5, n = 1, \ldots, 31
\end{equation}

\begin{equation}
0 \leq Q_{exn} \leq Q_{exn}, k = 3, 4, 5, n = 31, 60, 32
\end{equation}

\begin{equation}
h_{i,j,k,n} \geq 0
\end{equation}

(8.10)
and \( (\sum i + j + k = 42) \) (8.11)

where \( R_{kn} \) is the recharge rate, \( Q_{kn} \), the in-lieu delivered water rate cell in layer \( k \) and well site \( n \) (\( n = 31 \) for \( R_{kn} \) and 31, 60, 32 for \( Q_{kn} \) are max. number of flux decision variables for layer \( k=3,4 \) and 5; \( \beta_R \) and \( \beta_W \) are the operational recharged- (approximate 0.43 USD; modified from Pyne, 1995) and in-lieu delivered water cost per CMD (approximate 0.4 USD; modified from the Bangkok Metropolitan Water Work Authority; assumed 40 Baht ~ 1 USD) at well site \( n \); \( T_{Qmn} \) is the total active duration of the flow-rate that is taken here as identical with \( T_{Qmn} = 7665 \) days (for the stress period 2 between year 2012 and 2032) at all well sites; \( h_{i,j,k} \) is the modeled head at the 42 head constraint locations at col. = \( i \), row = \( j \), layer = \( k \) and stress period 2.

As stated, the GWM problem for the present application is nonlinear, i.e. the hydraulic heads depend in a nonlinear manner on the well-pumping (recharge or discharge). Therefore the problem is solved through SLP, once the head constraints are linearized through 1\(^{st}\) -order Taylor series expansion with respect to the flow-rate decision variables \( (R, Q) \) as follows:

\[
h_{i,j,k}^{\nu}(R_{kn}^{\nu} and Q_{kn}^{\nu}) = h_{i,j,k}^{\nu}(R_{kn}^{\nu} and Q_{kn}^{\nu}) + \sum_{n=1}^{N} \frac{\partial h_{i,j,k}^{\nu}}{\partial (R_{kn}^{\nu} and Q_{kn}^{\nu})} - ((R_{kn}^{\nu} and Q_{kn}^{\nu}))((R_{kn}^{\nu} or Q_{kn}^{\nu}) - (R_{kn}^{\nu} and Q_{kn}^{\nu})) \quad (8.12)
\]

where the superscript \( \nu \) denotes the iteration level, \( h_{i,j,k} \) is the head at col. = \( i \), row = \( j \), layer = \( k \) and stress period 2 obtained when the set of withdrawal and in lieu water supply rates \( (R_{kn}^{\nu} and Q_{kn}^{\nu}) \) is applied, \( (R_{kn}^{\nu} and Q_{kn}^{\nu}) \) is the new set of withdrawal and in lieu water supply rates and \( \frac{\partial h_{i,j,k}^{\nu}}{\partial (R_{kn}^{\nu} and Q_{kn}^{\nu})} \) are the response coefficients. The SLP algorithm recalculates the response coefficient for the heads at each iteration \( \nu \) from a new set of optimal withdrawal- and in-lieu water supply rates which are obtained from the linear programming solution of the previous iteration using the simplex algorithm.
8.4 Discussion of the various groundwater management schemes

As mentioned 7 schemes will be evaluated in this chapter, and for practical purposes, are to be compared to the reference scheme, the so-called “laissez-faire” scheme (Chapter 6).

8.4.1 1st scheme - sustainable yield

The sustainable yield is defined as “the maximal groundwater yield that may be withdrawn so that the water levels in the third, forth and fifth layer do not decrease by more than 25% of their current water levels (Dec, 2002)”. This scheme constrained pumping in the 6th to 9th aquifer by projecting into the future for the next 30 years (2003 to 2032) the acceleration rate of pumping from 1983 to 2002. Finally, the sustainability condition for the above conditions can be met if the pumping in layers 3, 4 and 5 is to be decreased at the rate of 1.2%, 1.2% and 1.9% per year, respectively (Arlai et al., 2006a).
8.4.2 2nd scheme - non-constructive scheme

It consists in keeping the present pump rate (2002) in each layer from 2012 to 2032, but decrease the pumping thereafter to 60% of today in low-sensitive zones and shut off completely the pumps in high-sensitive zones. This scheme is allowed to give 5 more years for law enactment.

8.4.3 3rd scheme - non-constructive scheme

It comprises maintaining the pump rates in layers 3 and 4 at the same rates than those of the WOS scheme from 2012 to 2032, as they are the main aquifer layers exploited, but completely stopping groundwater pumping in layers 5 to 9 which should retard vertical sinking mechanism of the salt plume from the upper source layers. This pump-shutoff in the lower layers will be executed from 2012 to 2032, leaving 5 more years for legal enactment.

8.4.4 4th scheme - optimized integrated non- and constructive scheme

The scheme is to minimize the least cost of “trial & error” integrated non- and constructive management scheme which combines recharge, clean-up wells and a cease of groundwater pumping in the 6th modeled layer. 31 recharge wells and 31 clean wells along the tongue of seawater intrusion in each layer are specified, resulting in a total of 93 recharge- and 93 clean-up wells (Figure 8.3) in order to attain the heads at the 42 head constraint locations with a complete cease of the groundwater withdrawal in layer 6, and keeping the extraction rates in layers 7 to 9 at the present-day rate (2002). The scheme will be operated from 2012 to 2032 leaving 5 years for realization.

8.4.5 5th scheme- applied “water trade-off concept” to the integrated non-and constructive scheme (4th scheme)
This scheme is to optimize the “water trade off concept”: 93 recharge wells and 123 in-lieu delivered water supply cells candidates are applied (with no clean-up wells) and keeping the 21 head constraints equal to zero meter height (MSL) at the end of 2032. The in-lieu delivered water supply cells are selected from those pumping cells located closed to the shoreline (UTM Y: 694000 to 720000) that have the pump rates in a FD-cell 500 CMD---as the author has tested and found that if the existing pumping rates in a cell are specified to less than 500 CMD, the dimension of the optimized problem becomes too huge to be treated computationally in an acceptable time---. The GWM-optimization of this scheme is to ensure least costs for construction, operation and maintenance for its realization. This optimized scheme operates from 2012 to 2032, allowing 5 more years for governmental ruling (Figure 8.2).

8.4.6 6th-scheme- applying “water trade off concept” to the 2nd scheme

It applies the “water trade off concept” as described in the 5th scheme with the 2nd scheme.

8.4.7 7th-scheme- applying “water trade off concept” to the 3rd scheme

It applies the “water trade off concept” in 5th scheme with the 3rd scheme.

8.5 Results

8.5.1 Optimization results for the 4th scheme

For the “trial & error” well scheme which combines recharge, clean-up wells and a cease of groundwater pumping in the 6th modeled layer, 31 recharge wells and 31 clean wells along the tongue of seawater intrusion in each layer are specified, resulting in a total of 93 recharge- and 93 clean-up wells (Figure 8.3). Each of these wells is operated at a rate of 7000 CMD. Hence the total water circulation rate in this scenario is $6.51 \times 10^5$ CMD. On the other hand, using the MODFLOW-GWM optimization code to solve the GMW-objective function and
constraints, results in a total of only 37 recharge-(15, 10, 12 wells in layer 3, 4 and 5) and 27 clean-up (16, 6, 5 wells in layer 3, 4 and 5) wells to control the heads at the 42 head constraint locations. And the water circulation rate is merely $3.17 \times 10^5$ CMD. Hence, compared with the “trial & error” well scheme, the MODFLOW-GWM “optimized” scenario results in a significant reduction in both the number of wells and total water circulation rate (a 51% reduction), i.e., obviously a tremendous cost-saving, as discussed below.

Figure 8.4. illustrates that the modeled heads for year 2032 of the “trial & error”- and “optimized” well schemes coincide pretty well at the locations of the head constraints—but less so in the seaward zone where the named water circulation rate differences are prevalent, with the effect that the “trial & error”- computed heads in the gulf area are higher than those of the “optimized” one (Figure 8.4.). The minimum head recoveries in 2032 for the two schemes are listed in Table 8.1. One notes that the head recovery for the “optimized” scenario is better than that of the “trial & error” one which is due to the fact that some of the, evidently redundant clean-up wells of this somewhat arbitrary scenario have a detrimental effect on the head recovery. Table 1 lists also the economic benefits of employing the “optimized” instead of the “trial & error” – scheme---the former being calculated by associating a unit price in the objective function (4)---. One clearly observes that, not only is the “optimized” well scheme

![Figure 8.3.](image)

(a) (b) (c)

**Figure 8.3.** Trial-and error well scheme: Orange area shows the distribution of the present day pumps, blue area the line of recharge wells, with the clean-up wells located 4 cells northward of the former.
Figure 8.4. 2032-heads for the “trial & error”- (solid lines) and “optimized” (dashed lines) well scheme in layers 3(a), 4(b) and 5(c); a blue circle is an optimized clean-up well, a yellow triangle is an optimized recharge well, a red plus is a head constraint.

Table 8.1. Comparison of head recovery and values of cost-function (hydraulic costs) and monetary costs for implementation and operational & maintenance for the two restoration schemes proposed.

<table>
<thead>
<tr>
<th>Aspect</th>
<th>Original well scheme</th>
<th>Optimized well scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Layer3</td>
<td>Layer4</td>
</tr>
<tr>
<td>1. Head recovery</td>
<td></td>
<td></td>
</tr>
<tr>
<td>a. Yes</td>
<td>-54.79</td>
<td>-64.82</td>
</tr>
<tr>
<td>b. -54.79 -64.82 -82.26 -31.99 -28.56 -82.26 -55.00 -59.66 -67.82 -31.61 -28.06 -67.82</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2. Cost</td>
<td></td>
<td></td>
</tr>
<tr>
<td>a. 31</td>
<td>31</td>
<td>31</td>
</tr>
<tr>
<td>b. -54.79 -64.82 -82.26 -31.99 -28.56 -82.26 -55.00 -59.66 -67.82 -31.61 -28.06 -67.82</td>
<td></td>
<td></td>
</tr>
<tr>
<td>c. 2.17</td>
<td>2.17</td>
<td>2.17</td>
</tr>
<tr>
<td>d. 2.17</td>
<td>2.17</td>
<td>2.17</td>
</tr>
<tr>
<td>e. 100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>f. 49.90</td>
<td>49.90</td>
<td>49.90</td>
</tr>
</tbody>
</table>

Remark

- Unit Cost of clean-up project implementation 251 US Dollar/CMD, cf. Henthorne, 2003
- Unit Cost of O&M of recharge project 0.43 US Dollar/CMD, cf. Reichard et al., 2003
- Unit Cost of O&M of clean-up project 0.2 US Dollar/CMD, cf. Henthorne, 2003

1. Piezometric head
   a. Similarity along the head constraints
   b. Minimum head (m. MSL)
2. Cost
   a. Number of recharge well
   b. Number of clean-up well
   c. Total recharge rate (10^3 CMD)
   d. Total clean-up rate (10^3 CMD)
   e. Project implementation cost (Million USS)
   f. Operational & Maintenance Cost/year (Million USS)
cheaper by 154 million US Dollars for the project implementation, it results also in annual operation and maintenance cost savings of 76.7 million US Dollar compared to the latter scheme.

8.5.2 Optimization results for the 5th to 7th schemes

Table 8.2 lists the optimization results obtained for three new schemes (5th-7th scheme), namely, the cell candidates for the recharge-wells and the in-lieu delivered water supply wells which are able to recover the piezometric heads up to the constraints of zero meter (MSL), and the least costs achieved. The table illustrates that the 7th scheme is the most effective, at least with regard to the costs of installation and operation of the recharge wells, as both the number of recharge wells and the recharge rates are at a minimum while satisfying the zero meter (MSL) head constraint as a water barrier layers 3 to 5. However, at this current stage, it cannot be concluded that this is really best scheme, since, in principle, for each optimized recharge well and in-lieu delivered water supply cell configuration the models should be re-simulated using SEAWAT-2000 to check for possible solute density effects on the schemes’ groundwater flow effectiveness, neglected so far.

Table 8.2. Summary of optimization results for the 5th to 7th scheme

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Recharged well candidates</th>
<th>In lieu well cells candidates</th>
<th>Optimized recharged wells</th>
<th>Optimized in lieu delivered water supply</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Number of wells</td>
<td>Total recharge rate (CMD)</td>
<td>Annual operational cost (10^6 USD)</td>
<td>Number of cells</td>
</tr>
<tr>
<td>5th</td>
<td>93</td>
<td>123</td>
<td>30</td>
<td>229035</td>
</tr>
<tr>
<td>6th</td>
<td>93</td>
<td>123</td>
<td>30</td>
<td>163612</td>
</tr>
<tr>
<td>7th</td>
<td>93</td>
<td>123</td>
<td>23</td>
<td>160570</td>
</tr>
</tbody>
</table>

8.5.3 Quantitative analysis of variable-density effect of all schemes

As the GWM-MODFLOW-2000 module could no simulate the density-dependent groundwater flow and solute transport, the WOS-scheme and all other schemes will be re-run using SEAWAT-2000. The most salient results obtained in this manner---with respect to
those of the WOS-scheme---are summarized in terms of groundwater hydraulics, quantity and quality for layers 3 to 8 of the aquifer in Figure 8.5. The vertical saline plume pollution and horizontal seawater intrusion extent in Figure 8.5 are, in turn, defined as that contaminated area where the salinity concentrations are higher than 250 and 4000 mg/l-locates nearby/closed to shoreline, with the reduction measured relative to original polluted area of the WOS-scheme. The % head recovery is specified by the ratio of the minimum head of each scheme to that of the WOS-scheme. The diagram shows that the 6th scheme is clearly the best one to reclaim both the piezometric heads and the groundwater quality, in as much as the average head recovery is 68%, and the area polluted by vertical saline plume intrusion is reduced by 9% and that affected by horizontal seawater intrusion by 18%. Not surprisingly, all the 5th to 7th --- the “water trade off concept” schemes--- reduce both polluted areas better and result in better head recoveries than all other schemes.

Figure 8.5. Summary of % averaged reduction of vertical saline plume pollution area, seawater intrusion area and head recovery in layers 3 to 8 relative to the WOS scheme.
8.5.4 Detailed cost-analysis of the various schemes

The schemes discussed can be divided into three categories, namely, (a) non-constructive schemes- 1st to 3rd scheme, (b), optimized non-and constructive scheme- 4th scheme and (c) applied water trade off scheme-5th to 7th scheme. For the category (a) schemes, the unmet water demand ($umd$) and which is defined as the difference between the total withdrawal rate difference between the WOS-scheme and the pumping rate under the policy of that scheme is assumed to be served by surface water supply from Bangkok Metropolitan Water Authority (BMWA). Hence, the costs for the non-constructive scheme must be estimated by taking into account the construction costs of the delivering water supply pipe, connected to a water supply distributor station of BMWA, i.e. construction costs of a 8 inch diameter – pipe, 20 meters long are 5350 USD (including 7% VAT) which can provides water supply 934 CMD (assuming flow velocity in a pipe 1 m/s and operating 8 hrs/day), meanwhile the costs for the use of the additional water supplied are assumed to be covered by existing groundwater users there, namely 0.4 USD for a cubic meter of water supplied (BMWA- service rate and assuming 1 USD ~ 40 Baht).

These assumptions apply also for the unmet demand of the other two scheme-categories. The costs of scheme-category (b) are taken from Arlai et al. (2007a). The costs of the scheme-category (c) are determined by calculating the implementation as well as the operational expenses for the recharge wells using the values of (Arlai et al., 2007a), while the costs of

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Unmet water Demand 10^6CMD</th>
<th>Cost of water supply implementation for unmet demand in 2032 Million USD</th>
<th>Cost of Recharge wells Implementation in 2032 Million USD</th>
<th>Annual Operational cost of Recharge well in 2032 Million USD</th>
<th>Total Cost in 2032 Million USD</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.39</td>
<td>2.22</td>
<td></td>
<td></td>
<td>2.22</td>
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<tr>
<td>2</td>
<td>0.86</td>
<td>4.91</td>
<td></td>
<td></td>
<td>4.91</td>
</tr>
<tr>
<td>3</td>
<td>0.88</td>
<td>5.02</td>
<td></td>
<td></td>
<td>5.02</td>
</tr>
<tr>
<td>4</td>
<td>0.16</td>
<td>0.94</td>
<td>146</td>
<td>73</td>
<td>220</td>
</tr>
<tr>
<td>5</td>
<td>0.72</td>
<td>4.14</td>
<td>48</td>
<td>36</td>
<td>88</td>
</tr>
<tr>
<td>6</td>
<td>1.00</td>
<td>5.74</td>
<td>34</td>
<td>26</td>
<td>66</td>
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<tr>
<td>7</td>
<td>1.00</td>
<td>5.73</td>
<td>34</td>
<td>25</td>
<td>65</td>
</tr>
</tbody>
</table>
the *in-lieu* water supply is taking into account only the costs of delivering water pipe construction as stated above. The total costs are then defined as the sum of the initial costs of implementation plus annual operational cost in the target year 2032. The cost summary of Table 8.3 unveils that the *sustainable yield*-scheme requires the smallest investment among all the other schemes, namely 2.22 million USD, while the investment costs of the 7th scheme are the lowest among the group of integrated *non- and constructive* schemes, i.e. 65 million USD. One an interesting point to mention is that the 6th scheme—-which has been the best with respect to the efficiency in recovering the groundwater heads and the – quality---requires only one million USD more than the 7th scheme. On the other hand, if the schemes’s impact on the groundwater use policy is taken into account, one must consider also the unmet water demand (*umd*), since a higher *umd* would be more affecting existing groundwater users. From this point of view, the 4th scheme would be the least painful for them.

### 8.6 Discussion

From the results obtained, it is difficult to give a clear “cut” for the best aquifer restoration scheme when considering the recovery of the groundwater quality, the costs of implementation & operation, and the impact of the groundwater use policy of each scheme on the existing groundwater users. As a trade-off and possible guidance to the water authorities of Thailand to choose among the various options proposed, these three relevant parameters, i.e. reduction of total pollution area, total cost and unmet water demand of each scheme are plotted in Figures 8.6.

Figure 8.6. discloses that the 3rd scheme appears to be the optimal one for sustainable groundwater management and restoration of the Bangkok aquifers system. This is because the 3rd scheme can not only reclaim the total saline pollution area up to about two third of that of the best schemes---the 6th and 7th scheme---and also retard the vertical sinking of the salinity plume from the upper marine clay layers (as shown in Figure 8.7), but it also requires also an investment of only 5.02 million USD for construction costs which is 92% cheaper than the total costs of the 6th and 7th scheme. Even this 3rd scheme may considerably impact the existing groundwater users, they latter may get a compensation from the construction costs saved of the water supply pipe connecting to the BMWA distributor and may thus pay only the unit costs of the water used.
Figure 8.6. Comparison of unmet water demand, averaged reduction of saline pollution area and total costs of each scheme.

8.7 Summary

Seven different groundwater management schemes are investigated for the best sustainable future groundwater restoration of the Bangkok aquifers system. The first three non-constructive schemes that have been selected from a previous chapter where they have been simulated only by the constant-density groundwater flow and solute transport model MODFLOW-96 & MT3DMS (Chapters 5 and 6) are re-run by the newest version of the variable density groundwater flow and solute transport model-SEAWAT-2000, allowing for a more realistic determination of the flow and saline transport due these schemes. The 4th scheme is set-up by applying GWM-optimized recharge- and clean-up wells to the best non-constructive scheme investigated earlier, and the 5th, 6th and 7th scheme uses also GWM to optimize “the water supply trade-off concept” with the 4th, 2nd and 3rd scheme, respectively. After optimizing the 4th to 7th scheme, the optimal non-and constructive- and the in-lieu water supply concept schemes are re-simulated with the variable-density flow and solute transport model SEAWAT-2000. Next, the hydraulic- and the groundwater-quality efficiency and the total financial costs of all schemes are evaluated and compared. Eventually, the 3rd scheme
appears to be the optimal scheme in all points of views and it is the one that may be recommended to the Thai water resources authorities for possible realization.

**Figure 8.7.** Saline concentration profile (UTM-X = 662000 m.) of the WOS-scheme (a) and the 3\textsuperscript{rd} scheme (b) located at the western side of the Chao Praya river, concentrations in kg/m\textsuperscript{3}.
References


(8) Langevin, C.D., W.B. Shoemaker and W. Guo (2003), Documentation of SEAWAT-2000 version with the variable-density flow process (VDF) and the integrated MT3DMS transport process (IMT). USGS report 03-426.

Appendix A

Numerical Investigation of the Need for Density-dependent Flow and Transport Modeling on a Case-Study of a real coastal Aquifer System

A1. Motivation and statement of the problem

The modeling of a case-study of seawater intrusion in a coastal aquifer in Israel by J. Bear (Bear, 2001) by means of a 3D finite element model will be used in the appendix of this thesis as an example to test the importance of density effects in a real coastal groundwater system. The problems investigated, in particular, are seawater intrusion and upcoming. Here I will apply both the MODFLOW-2000&MT3DS (a constant density code) and the SEAWAT-2000 (a newest variable density code) 3D model to the case-study of Bear using the same model-setup and the same flow and transport parameters and attempt to understand the importance of density-dependent effects in this problem.

The modeling approach used can be divided into two steps:

First, assuming no groundwater withdrawal (pumping), a simulation over 30 years (until a steady state is reached) is carried out and modeled salinities of both constant- and variable density models are compared.

The second step consist in a transient simulation of the seawater encroachment and of the up-coning induced by a pumping well located closely to the shoreline with and without density effects included.
The computational domain is a rectangular prism 1000 m long, 500 m wide and 105 m thick and discretized by 20 m x 20 m cells x 15 and 10 m for layer 1 and the others (in the z direction), respectively (Figure A1.). Thus the model comprised of 10 modeled layers. The aquifer is recharged horizontally by a constant freshwater influx at a rate of \( q_0 = 0.0215 \) m/day on the inland boundary, while on the seawater boundary heads and concentrations are set to seawater conditions. Note that for the constant-density code MODFLOW-2000&MT3DMS the seawater boundary head must be adjusted to comply with the higher seawater- than fresh water pressure. This is done by calculating the so-called equivalent fresh water head, using the following formula

\[
h_f = \frac{\rho}{\rho_f} h - \frac{\rho - \rho_f}{\rho_f} Z
\]  

(A1)

where \( h_f \) is the equivalent fresh water head (m); \( \rho \), the density of saline aquifer water (~1.025 kg/m\(^3\)); \( \rho_f \), the density of fresh water (~1 kg/m\(^3\)); \( h \) the head (0 m at sea boundary); and \( Z \) is the elevation, taken for each layer of the model in the middle. For the variable-density code SEAWAT-2000, on the other hand, the transformation (A1) is not needed explicitly, as all equations are internally already written in terms of the equivalent fresh-water head. To wrap up the boundary conditions, the bottom boundary is assumed to be impervious to flow and transport. The aquifer is recharged surficially through natural replenishment by precipitation at a rate of 0.15 m/year.

\[\text{Figure A1. Domain and boundary conditions in the coastal aquifer (Bear et al, 2001).}\]
The hydraulic- and solute transport parameters used are follows: Porosity = 0.25, horizontal conductivity = 20 m/day, vertical conductivity = 2 m/day, density of pure freshwater = 1000 kg/m$^3$, density of pure seawater = 1025 kg/m$^3$, longitudinal dispersivity = 10 m, transversal dispersivity = 1 m and the molecular diffusivity = 0 m$^2$/day.

A2. Ghyben-Herzberg approximation for the fresh-seawater interface

Ghyben and Herzberg (cf. Bear, 1979) have derived a well-known, the Ghyben-Herzberg formula for the approximate location of stationary (sharp) interface between the fresh- and the seawater, namely (Figure A2)

$$h_s = \frac{(\rho_f/l)(\rho_s - \rho_f)\times h_f}{\rho_s - \rho_f} \tag{A2a}$$

which, using standard values, results in

$$h_s = 40 \times h_f \tag{A2b}$$

where

![Figure A2. Ghyben-Herzberg stationary interface.](image-url)
$h_s$ = the depth of stationary interface below sea level,

$h_f$ = freshwater table above sea level,

$\rho_s = 1025\text{kg/m}^3$, the density of seawater,

$\rho_f = 1000\text{kg/m}^3$, the density of fresh water.

**A3. Analytical expression based on Dupuit’s assumptions**

A phreatic aquifer with uniform natural replenishment ($N$), where it is assumed that the steady flow in the aquifer is essentially horizontal and $h(x) = \delta h_f(x); \delta = \rho_f/ (\rho_s - \rho_f)$, the application of continuity equation results in (Figure A3, from Bear, 1979):

$$Q_0 + N_x = -K(h + h_f) \partial h_f / \partial x = -K(1 + \delta) h_f \partial h_f / \partial x$$

(A3)

where

$Q_0$ = lateral freshwater discharge,

$N_x$ = surface recharge.

**Figure A3.** Shape of a stationary interface by the Dupuit-Ghyben-Herzberg approximation
Eq. A3. is integrated from \( x=0 \), \( h_f = \phi_0 \) to \( x \), \( h = B \) (depth from the sea level to the bottom of the aquifer) which results in

\[
\phi_0^2 - h_f^2 = (2Q_0 x + Nx^2) / K(1 + \delta) \tag{A4}
\]

At \( x = L \) (horizontal extension of the seawater intrusion) \( h_f = 0 \), which gives:

\[
Q_0 = \frac{KB^2}{2L} (1 + \delta) - \frac{NL}{2}, \phi_0 = \frac{B}{\delta} \tag{A5}
\]

Thus the size of \( L \) of the seawater intrusion can be determined from Eq. A5 which, using the values of the present model setup, results in \( L = 1080.5 \) m. Using a parabolic shape in X-directional symmetry and \( L \) value (Bear, 1979), the position \( y(x) \) of the interface can be written as parabolic equation of the form:

\[
(y - 0)^2 = 4 * (-2.3137) * (x - 1000) \tag{A6}
\]

### A4. Steady-state simulation

Results of the steady-state simulations with no pumping, using both the constant-density (MODFLOW-2000&MT3DMS) and the variable-density model SEAWAT-2000 are plotted together with the Ghyben-Herzberg interface location and the interface location based on Dupuit’s assumptions in Figure A-4. The figure illustrates unequivocally the importance of the incorporation of density-dependent into the seawater intrusion modeling problem, as the density-driven intrusion plume moves further landward and conforms better to the two analytical approximation solution) than that of the constant-density model.
**Figure A4.** Steady-state saline concentrations (kg/m$^3$) at $Y = 250$ m. of constant-density- (dashed line), variable-density model (solid line), Ghyben-Herzberg interface location (circles), and interface location based on Dupuit’s assumptions (diamonds). Also shown is the phreatic water table (triangles).

This behavior can be understood from Darcy’s law;

$$
q_x = -\frac{K_x}{\mu} \frac{\partial P}{\partial x}, q_y = \frac{K_y}{\mu} \frac{\partial P}{\partial y}, q_z = \frac{K_z}{\mu} \left( \frac{\partial P}{\partial z} + \rho g \right)
$$

(A7)

With the density $\rho$ of the fluid taken at the point and time for which the specific discharge $q$ is to be determined.

Even though Eq. (A7) predicts at first sight that density effects act only in vertical direction, one must consider that the whole pressure distribution in a porous media is partly influenced by the overall fluid density distribution and, hence, also the horizontal specific discharge is affected by the variable densities in the groundwater system. This is clearly manifested also by the results for the flow vectors shown in Figure A5.
Figure A5. Flow vectors for steady-state seawater intrusion at $Y = 250$ m. of density-independent model (a) and density-dependent model (b). Blue lines envelop approximately the flow vector area affected by the sea boundary and/or the density driven flow.

A5. **Transient simulation**

For this transient model case, a pump is applied onto the aquifer at the location $X = 500$ m., $Y = 250$ m. with a screened length of the pump of 10 m and centered at $Z = -10$ m. (Figure A1).
Figure A6. Phreatic water tables at Y = 250 m. of density-dependent and density-independent models at different times. Abbreviations: n Yr = water table at n years for density-dependent model; n_wod Yr = water table of a model without density at n year.

The results of these simulations with the two model approaches for the phreatic water tables, the flow vector regimes, and the seawater intrusion fronts are plotted for different times in Figure A6, A7 and A8, respectively.

One notices from Figure A6 that the phreatic water tables of the density-independent and density-dependent models are different only at the initial time, but these differences disappear more or less for later times. This phenomenon might be explained by the fact that the strong convective flow due to the pumping increases considerably the averaged linear velocity flows in the system inducing, consequently, higher dispersion coefficients which diminish the density effects lesser. This behavior seems to be similar to what has been found in Chapter 7 for the zones of the Bangkok aquifer system where large pumping was occurring.
Figure A7. Exaggerated size of flow vectors (for better viewing) in transient state at Y = 250 m and time = 30 years of density independent (a) and density-dependent model (b). Blue box shows position of pump cells and a flow vector; a diamond at its left-hand side is a basement of that vector and the line that is shot out from that basement represents the flow direction and magnitude of that vector.
Figure A8. Transient saline distributions of density independent- (solid lines) and density-dependent model (dash lines). Blue box shows the pump position.
The flow vectors for the transient state (Figure A7b.) show an important thing, namely, that for the variable-density model the flow vectors affected by the sea boundary disappear after 30 yrs, whereas those of density-dependent model are still affected by the sea boundary after that time.

The saline distributions shown in Figure A8 illustrate that the seawater intrusion bands are inaugurated downstream of the pump, then the isochlors steadily move toward the withdrawal well, turning into up-coning in the 2\textsuperscript{nd} year for the density-dependent model, whereas for the density-independent model the up-coning commences only in the 4\textsuperscript{th} year. Furthermore, while for the density-dependent model, the 3.5 kg/m\(^3\) - isochlor has already reached the withdrawal well at that time this happens for the density-independent one only in the 8\textsuperscript{th} year.

Simultaneously, the seawater intrusion bands are continually driven further landward with progressing times, especially those of the density-dependent model, which is in agreement with the analytical relation between \((Q_0 + N)\) and \(L\) of Eq. (A4), that is, a net replenishment rate \((Q_0 + N)\) which inflows into the aquifer is decreased by the a pumping well rate, consequently, the seawater intrusion length \(L\) extends further landward.

From the breakthrough curves of Figure A9 one can observe that (1) for the isochlors at \(X = 750\) m (Figure A9a; -c; -e), after 2 years, the density-independent modeled ones have a higher concentration than those of the density-dependent model at \(Z = -15\) (Figure A9a.) and -45 m (Figure A9c.) and, after 8 years, they are equal to the density-dependent ones at \(Z = -95\) m (Figure A9e.); (2) the isochlors of the density-dependent model at \(X = 500\) (Figure A9b; -d, -f), where the pump is located, are always greater than the ones of the constant-density model.

Recalling Figure A4 for the steady state simulation, one can notice there that the seawater intrusion of the density-dependent model has extended farther landward than that of the density-independent model. Thus, when the pump starts to operate, it will have stronger up-coning impact on the longer seawater tongue of the density-dependent model than on the less-developed tongue of the constant-density model (Figure A9b, -d, -f).
Figure A9. Breakthrough curves at X = 750 m, Y = 250 m, Z = -15 m (a), -45 m (c), -95 m (e), at X = 500 m (same line of pump position), Y = 250 m, Z = -15 m (b), -45 m (d) and -95 m (f).
A6. Summary

The most salient results obtained can be summarized as follows:

(a) The steady-state simulations show that a density-dependent flow and solute transport model mimics seawater intrusion in a coastal aquifer more realistically than a constant-density model, as the intrusion band of the former conforms closer to the two analytical solutions for the location of the salt–fresh water interface (Bear, 1979) than the latter.

(b) Strong convective flow due to pumping diminishes the effect of density-dependence on the flow regime as shown in Figures A6. and A7..

(c) The band of seawater intrusion of the density-dependent model is wider than the one of the constant-density model. This can be explained by basic physics (Figure 8A.).

(d) From these entire results one may conclude that one does need to use a density-dependent flow and transport model to simulate realistically seawater intrusion in a coastal aquifer.
References


(2) Bear, J., Q. Zhou, and J. Bensabat (2001), Three Dimensional Simulation of Seawater Intrusion in Heterogeneous Aquifers, with Application to the Coastal Aquifer of Israel, presented at 1st International Conference on Saltwater Intrusion and Coastal Aquifers Monitoring, Modeling, and Management, Essaouira, Morocco, April 23-25.
Biography

Mr. Phatcharasak Arlai was born at Nikom-a small village in the coastal district-Cha-Am of Phetburi province which is located in the upper part of the southern peninsula of Thailand. He received his B.Eng. in Water Resources Engineering from Kasetsart University, Bangkok, in 1997, obtained the first level of the civil engineering professional certificate and his M.Eng in Water Resources Engineering from Chulalongkorn University, Bangkok in 2000. He has been a faculty member of the Program of Construction Technology, Faculty of Sciences and Technology, Nakhon Pathom Rajabhat University since 2000 and commenced his Dr.-Ing study in 2003.