CHAPTER 1

INTRODUCTION

1.1 Statement and Significances of the Problems

The Bang Pakong river is one of the four major rivers of Thailand's Central Plain. The basin is economically important in terms of industrial and agriculture production for Thailand. Apart from its strategic location, the basin supports a great number of communities through its rich natural resources and biodiversity. It also contains important estuarine ecosystems with remarkable biological diversity that supports a highly profitable shrimp industry and a coastal tourism industry. The basin has also had rapid industrial and agriculture development. However, lack of capacity and coordination in surface water management of the river basin as well as coastal area has led to issues that affect the natural resources and well-being of people. This therefore leads to an increase in groundwater usage in the Bang Pakong river basin.

In 2005, some parts of the basin had been shortage of water supply for industrial activities because of the amount of surface water could not support the demand. In addition the Office of The National Economic and Social Development Board (DGR, 2006) estimated that there will be insufficiency of surface water in this basin during the year of 2007 to 2015. Consequently a large number of groundwater wells have been drilled and water has been pumped and used as additional sources for industrial and domestic used. Although groundwater is frequently regarded as a secondary source of water supply for domestic use and agricultural activities, there is unfortunately no record of groundwater usage or regulations with respect to groundwater abstraction. As a result there is an increasing concern regarding rapid depletion of groundwater resources in this basin and a better management plan for effective and sustainable usage is required.

During the last few decades, Division of Groundwater of the Department of Mineral Resources (DMR) and the Department of Groundwater Resources (DGR) initiated a detailed hydrogeologic investigation which included assessment of groundwater resources potential and development of groundwater map of the Bang Pakong river basin. Groundwater potential in this area was assessed using both traditional and innovative methods. In traditional method groundwater potential was evaluated using aquifer thickness and its hydraulic properties, groundwater yield, types and number of hydrogeologic units, and annual recharge rate (DGR, 2006; 2008). On the other hand, the innovative groundwater assessment was evaluated using groundwater flow modeling technique (DGR, 2006). In this method, the mathematical model was constructed and used to predict future impact of groundwater abstraction, and also to determine sustainable yield. However the accuracy of the developed model is still in doubt because the model had normally been calibrated using trial-and-error method rather than a systematic calibration (Hill, 1998). In addition almost all groundwater models may not necessarily capture all complexities associated with naturally heterogeneous aquifers. Hence, there is always uncertainty in reserve calculation and this uncertainty or model error must be quantified and reported.

The Bang Pakong aquifer system is complex and groundwater model that is constructed by using zonal hydraulic conductivity fields may not be sufficient in representing naturally heterogeneous aquifers. Moreover, hydraulic conductivities and storage coefficients from pumping tests are available only at points rather than heterogeneous subsurface structure. A single site conceptual model based on local estimates of hydraulic conductivities and storage coefficients can be quite uncertain and satisfied model calibration may not be obtained. Monte Carlo modeling technique can make key model parameters uncertain by specifying a distribution type and associated statistical characteristics (Gelhar, 1993). Instead of making one simulation, Monte Carlo technique makes hundreds or thousands of simulations. In each simulation, a different set of parameter values is selected to simulate flow regime. When processing the results, one will look for the probability that something may happen by evaluating, organizing and summarizing statistics from the Monte Carlo simulation outcomes. It is believed that this type of simulation could be used to evaluate the envelope of model uncertainty in the context of groundwater reserve calculation.

The use of Monte Carlo simulation will be helpful to construct a well-calibrated groundwater flow model for future planning to determine reserve potential and especially its uncertainty. Consequently safe yield can be obtained and effective groundwater management actions can be achieved.

1.2 Location of the Study Area

The Bang Pakong river basin is located in eastern Thailand, between latitudes 13º09′N to 14º32′N and longtitudes 100º 52′ E to 102º 00′ E. The study area covers approximately 8,614 square kilometers covering five provinces: Chachoengsao (11 districts), Nakhon Nayok (4 districts), Prachin Buri (2 districts), Chon Buri (7 districts), and Saraburi (4 districts). A location of the study area shown in Figure 1-1. The study area is bounded by:

The west	The major part of the Lower Central Plain (Bangkok Plain) which is a large flat plain of the Chao Phraya delta and Gulf of Thailand.
The east	The Prachin Buri river basin which is almost relatively flat and highlands.
The north	A mountain range, Upper Plain, and Khorat Plateau.
The south	The East Coast river basin which is highlands, and terraces.

1.3 Purposes and scopes

The main purpose of this study was to construct a large, regional complex groundwater model of the Bang Pakong river basin based on comprehensive hydrogeologic study. A well-calibrated groundwater flow model will be developed and used to evaluate model uncertainty in the context of groundwater reserve calculation. Specifically, this research attempts:

1. To perform a hydrogeologic study and to construct a well-calibrated groundwater flow model of the Bang Pakong river basin, and
2. To evaluate groundwater potential as well as its uncertainty using Monte Carlo simulation technique.

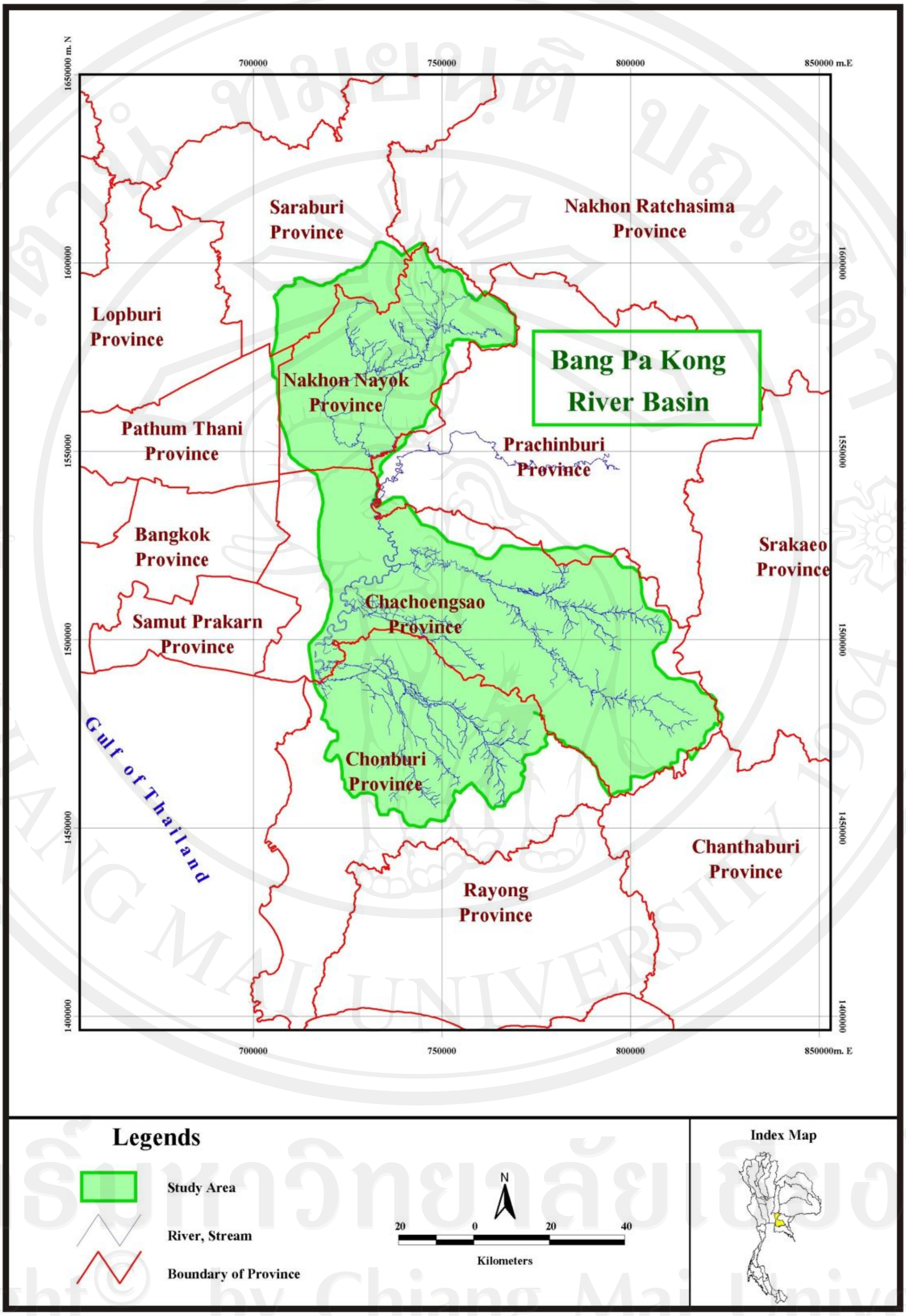


Figure 1-1 Location map of the study area (Bang Pakong river basin).

The scope of this study includes a review detailed groundwater exploration and potential assessment of the Bang Pakong river basin Project conducted by the Department of Groundwater Resources. The groundwater flow model is constructed and calibrated using automated parameter estimation method and evaluated its uncertainty in outcome using Monte Carlo simulation technique. The calibration process utilized sets of field-measured piezometric heads and chemical properties data from 173 transient observation wells.

1.4 Methods and Materials

This research was achieved using several methods or techniques as described below. Steps for evaluating model uncertainty in predicting groundwater potential are shown in Figure 1-2.

1. Establishing a pictorial representation of the groundwater flow system by reviewing and reconstructing fourteen hydrogeologic cross-sections from previously collected and interpreted data from geologic map, topographic map, drilling logs, resistivity surveys, etc.
2. Measuring water level every four months to obtain an annual average of well head from 179 representative observation wells that extend over every aquifer and are evenly distributed over the basin.
3. Constructing a groundwater flow model by converting a conceptual model to a finite-difference model used MODFLOW program (Harbaugh et. al, 2000). Selecting appropriate grid spacing and number of layers. Applying suitable boundaries conditions including specified head or flux (e.g., pumping wells) or head-dependent flux (e.g., rivers).
4. Calibrating the model as well as analyzing its sensitivity used a computer

program PEST (Doherty, 1994).

5. Evaluating model uncertainty in predicting groundwater potential using Monte Carlo technique after completion of model calibration.

Several material compilations were used in this study, their comprised of documentations from previous studied, field work, maps, software programs, and GIS databases.

1.5 Theory

Groundwater flow modeling is an important tool that can be used to analyze and predict the large scale impact of interference in the hydrologic equilibrium of groundwater. It is a necessary step in hydrogeological study which is used in effective groundwater resources management. The origin of groundwater flow modeling was dated far back at the beginning of this century. The foundation of groundwater modeling is Darcy's Law, which was published in 1856, is still used today. Freeze (1994) reports that Darcy's famous sand column experiments were performed and subsequently the Laplace equation is relevant to groundwater flow came later when Forcheimer (1886) in Europe and Slichter (1985) in the United States independently applied the Laplace equation to groundwater problems. Numerical modeling was introduced in the mid 1960s and quickly became a standard tool for analyzing groundwater flow problem.

Mathematical models are simply representations of reality where the complexity of hydrostratigraphic units, variable hydraulic properties of aquifer units, and cause and effect relationships are translated into mathematical terms.

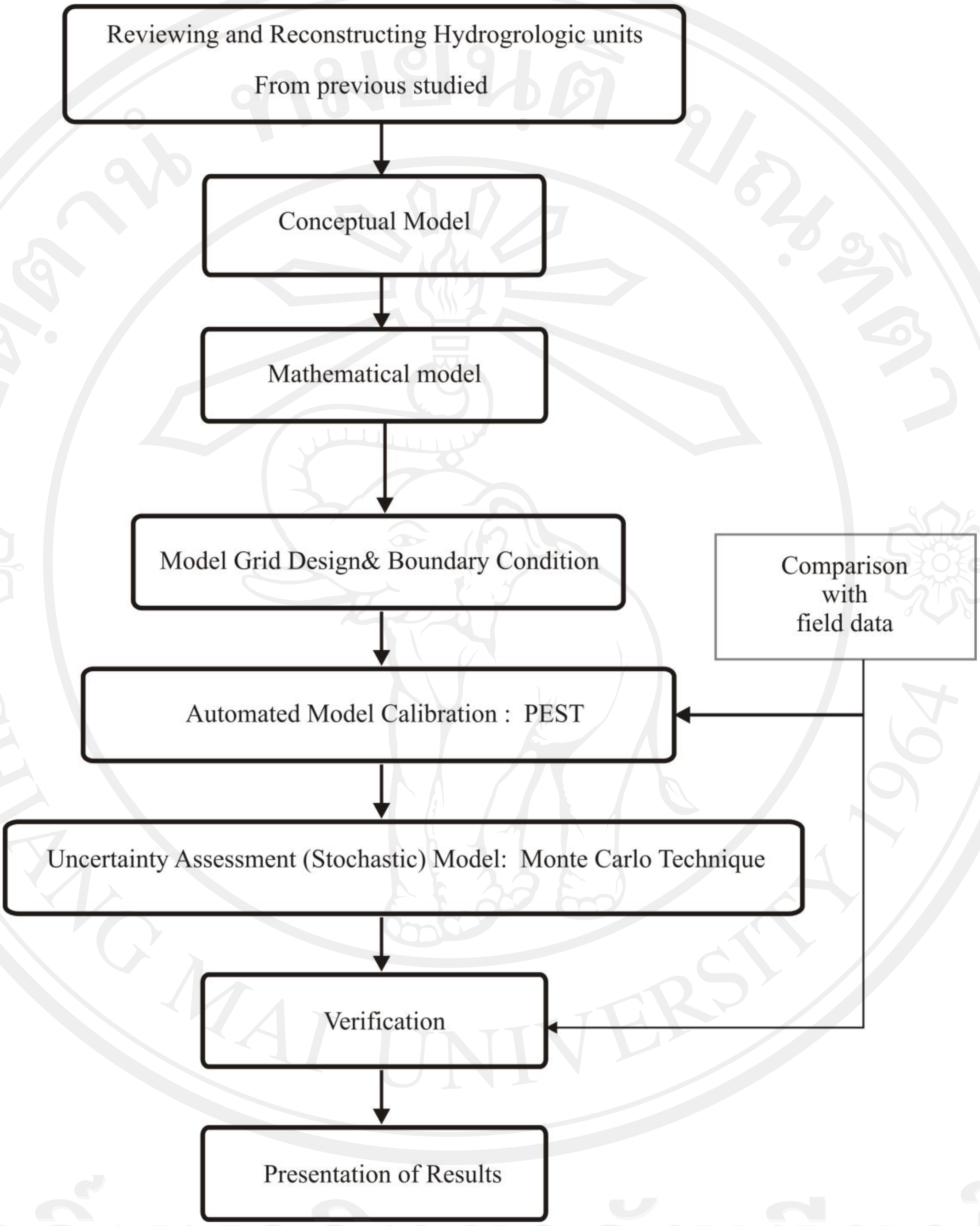


Figure 1-2 Flowchart showing steps for evaluation of model uncertainty in predicting groundwater potential.

Groundwater modeling is the art and science of applying various investigative methods, checking the results against one another, and representing the complexity of nature in a simplified form that allows mathematical treatment. There are three purposes of groundwater model: it is used to predict the future, used as a framework for studying system dynamics and/or organizing filed data, and used to analyze flow in hypotetical hydrogeologic systems (Boonstra and Ridder, 1981; Anderson and Woessner, 2002)

Groundwater in a basin is not at rest but is in a state of continuous movement. Its volume is increased by the downward percolation of rain and surface water causing the rise of the water table or potentiometric surface. At the same time this volume is decreased by evapotranspiration, discharge to springs, outflow to streams, and other natural drainage channels, all of which cause the fall of water table. When considered over a long period, the average recharge equals the average discharge and a state of hydrologic equilibrium exists. The water table is virtually stationary, with mere seasonal fluctuations around an average basin level.

Any interference in the hydrologic equilibrium may create undesirable side-effects. Abstraction of groundwater allows the increase in natural recharge from surface water bodies. A decrease in abstraction on the other hand causes natural discharge. If the abstraction is kept within certain limits, the increase in recharge and the decrease in discharge will balance the abstraction and a new hydrologic equilibrium will be established. The water table will again be almost stationary, although at a deeper level than before. If this level is too deep, it may affect agriculture and the ecosystem in the area. Excessive abstraction from wells can cause a continuous decline in the water table, which means that the groundwater reserves will be depleted.

Groundwater models can be divided broadly into two categories: groundwater flow models and solute transport models. Groundwater flow models solve for the distribution of head, whereas solute transport models solve for concentration of solute as affected by advection, dispersion, and chemical reaction. Several types of models have been used to study groundwater flow systems. These can be divided into three broad categories: physical models, analog models, and mathematical models (Wang and Anderson, 1982). Physical models include sand tanks or a laboratory sand tanks simulate groundwater flow directly, analog models include viscous fluid models and electrical models, and mathematical models include analytical and numerical models simulate groundwater flow indirectly by means of a governing equation thought to represent the physical processes that occur in the system, together with equations that describe heads or flows along the boundaries of the model (Mercer and Faust, 1980; Anderson and Woessner, 2002; Pusshpa and Ashim, 1993; Engelen and Kloosterman, 1996; Boronia et al., 2003).

A mathematical model is a simplification of real groundwater system and it is usually necessary to solve the mathematical model approximately using numerical techniques. There are four types of numerical models, a finite difference model (FDM), a finite element model (FEM), method of characteristics (MOC), and random walk model (RW) (Spitz and Moreno, 1996). The models are capable of solving the more complex equations that describe flow models and solute transport and the accuracy of mathematical models depends upon the accuracy of the model input data, the size of space and time discretization, and the numerical method used to solve the model equations.

When it has been determined, a numerical model is necessary for helping to evaluate groundwater potential. The next steps in design and construction of model are including establishing the purpose, developing the conceptual model, designing the model, model calibration, sensitivity analysis, and model verification. All steps in constructing model process have been made error and the mathematical model not represented of real groundwater system. Thus the error tolerance for the numerical closure should be small enough and was verified. Therefore the models with many parameters and the large regional scale models might require the model calibration methods for help address issues of reliability and uncertainty to achieve an acceptable real-groundwater system. Because many aspects of groundwater system are unknown, most models are calibrated. Thus a present day the calibration method is becoming commonly necessary efficiency stages of applying in mathematical groundwater model and it must be need to be calibrated prior to use in prediction.

After groundwater flow model setup is completed. Calibration is one of essential stages to a site-specific problem. Calibration is the process of refining the model representation of the hydrogeologic framework, hydraulic properties, and boundary conditions to achieve a desired degree of correspondence between the model simulations and observations of the groundwater flow system. The method is designed to promote accuracy when simulating complex systems with mathematical models that need to be calibrated. These calibration methods can be divided broadly into two main categories: manual method (trial-and-error) and an automatic (inverse) method for calibrating a flow model. A trial-and-error approach is most commonly classic manual method in real applications but this is very time consuming and depends to experience of user. In addition, this solving does not give information on the degree of uncertainty in the final parameter selection and guarantee the statistically best solution. Besides the trial-and-error process is influenced by the modeler's expertise and biases (Anderson and Woessner, 2002). Then last three decades, the automatic calibration method is becoming widely a new approach to use. It is called "inverse modeling" that it is used to calibrate model parameters with the help of historical time series of hydraulic head data. In automatic calibration method has many a computer codes that there are widely used UCODE and PEST. Traditionally groundwater flow model was calibrated using trial-and-error approach which is time-consuming and sometimes discouraging. Recently the calibration process began to utilize a more systematic approach called inverse modeling. An inverse modeling posed as a parameter-estimation normally utilized a nonlinear regression technique (Poeter and Hill, 1998) to estimate the model's input parameters so that satisfactory matching between observed and model simulated heads/flows can be obtained.

Although inverse modeling had been explored earlier by Stallman (1956) and Nelson (1960), the modelers gave this methodology new impetus. Groundwater flow modeling developed with sense of euphoria over the realization that with computers we could now solve complex problems. In the 1970s, skepticism about modeling arose because contaminant transport models did not live up to expectations and calibrations of flow models was now recognized to be highly uncertain process owning to uncertainty over parameter values. In the 1990s, there are increasing questioning the reliability of our modeling results. The usual calibration procedure is by trial-and-error adjustment of parameter values until simulated heads are in some sense close to measured heads. However, calibration procedures frequently are not well documented; in most calibrations the justification for the final selection of parameter values is not well defined. Hence, there is a lot of uncertainty in most calibrated models. Parameter estimation models for solving the inverse problem guide the modeler through the calibration process and help the modeler make informed decision, leading to better calibrations. Then current interest in parameter estimation models as a way of improving model reliability was evident during a recent.

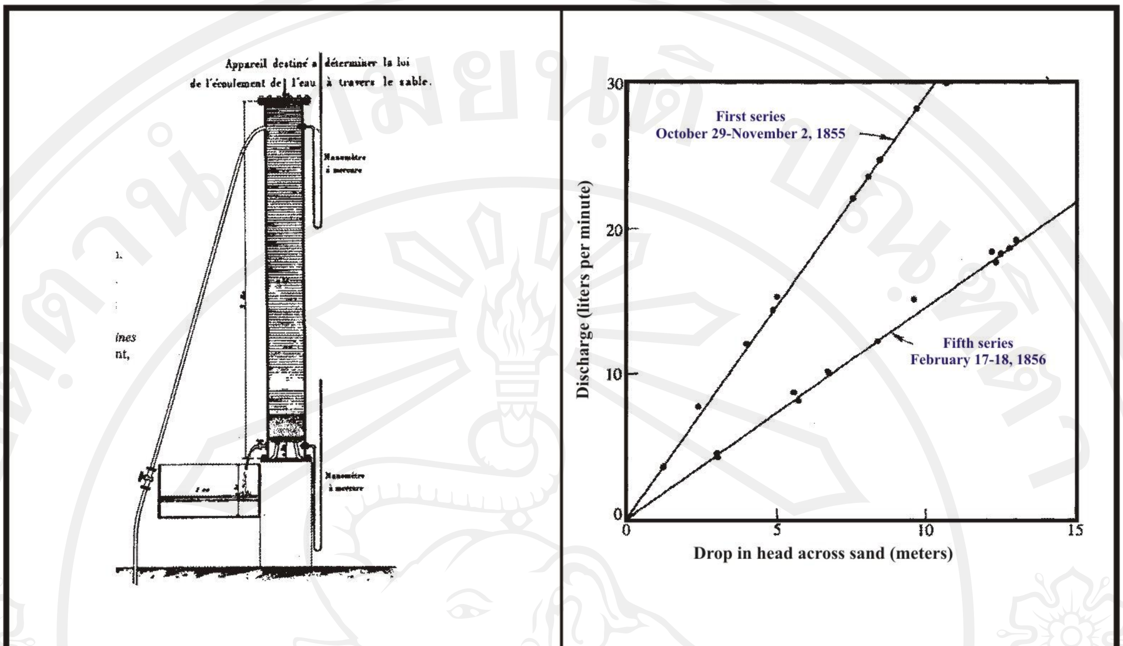
A stochastic methods and statistical concepts in hydrogeology brought together a number of researchers who were already thinking about uncertainty and the use of stochastic methods. The roots of the major research directions in groundwater modeling for the last quarter of the 20th century and for the coming century grew out of this. The major directions for groundwater modelers in the 21th century include using parameter estimation codes to help with calibration, using good modeling protocols to improve model reliability, and developing field techniques to help with geological characterization of heterogeneity. Using of stochastic methods in hydrogeology is as a way of dealing with uncertainties in the geological description of aquifers. A rational approach of quantifying values (Gelhar et al., 1992) requires information on geological heterogeneity. Proponents of the stochastic approach represent heterogeneity using random hydraulic conductivity fields with specified statistical properties in the hope of capturing the relevant features in the subsurface that govern movement. There are four main approaches including reliance on effective parameters, geo-statistics, Monte Carlo Simulation, and conditional simulation (Yeh, 1993). Models quantifying uncertainty should be advanced, most appropriately within a stochastic framework that links the modeling process to available data.

1.5.1 Principles and Theories of Groundwater Movement

Groundwater in its natural state is in variably movement. This movement is governed by established hydraulic principles. The flow through aquifers, most of which are natural porous media, can be expressed by what is known as Darcy's law. Hydraulic conductivity which is a measure of the permeability of the media is an important constant in the flow equation. Determination of hydraulic conductivity can be made by several laboratory or field techniques. Applications of Darcy's law enable groundwater flow rates and directions to be evaluated. In the zone of aeration, the presence of air adds a complicating factor to the flow of water. A mathematical model of groundwater flow through porous media relies upon the solution of equations that include Darcy's law and mass conservation, which is the water balance equation (Freeze and Cherry, 1979; Todd, 2005; Fetter, 1988; Karanth, 1994).

(1) Darcy's Law in Three Dimension

More than a century ago Henry Darcy, a French hydraulic engineer investigated the flow of water through a horizontal bed of sand to be used for water filtration in 1856 (Todd, 2005). Figure 1-3 illustrates Darcy's original model design and its extension to study flow in a one-dimensional flow column.



(a) Darcy's experimental sand column

(b) Darcy's data showing that discharge in proportional to head drop for two different sands

Figure 1-3 Pressure distribution and head loss in flow through a sand column.

Darcy's Law is a generalized relationship for flow in porous media. It shows the volumetric flow rate (Q) is a function of the flow area (A), elevation (*h*), fluid pressure (Δh) and a proportionality constant (*K*, *L*). It may be stated in several different forms depending on the flow conditions. Since its discovery, it has been found valid for any Newtonian fluid. Likewise, while it was established under saturated flow conditions, it may be adjusted to account for unsaturated and multiphase flow. The following outlines its common forms and assumes water is the working fluid unless otherwise stated.

$$Q = -KA\frac{(\Delta h)}{L} \tag{1-1}$$

Expressed in general terms

$$Q = -KA\frac{dh}{dl} \tag{1-2}$$

or simply

$$v = \frac{Q}{A} = -K\frac{dh}{dl} \quad , \tag{1-3}$$

where dh/dl is known as the hydraulic gradient.

The three-dimensional generation of Darcy’s law(see in Figure 1-4) requires that the one dimensional from equation 1-2 be true for each of the x, y, and z components of flow (Ashraf, 2008). According to Darcy’s law may be expressed in general term for a spatial discretization of an aquifer system with a mesh of block call cells. Using Darcy’s law, the Darcy flux in each direction is (Todd, 2005):

$$q_X = -K\frac{\partial h}{\partial x} \qquad q_y = -K\frac{\partial h}{\partial y} \qquad q_Z = -K\frac{\partial h}{\partial z} \tag{1-4}$$

(2) Mass Conservation or Continuity Equation

The mass conservation, which is known in terms of continuity principle, states that fluid involved in a change of volume or in a change in the mass stored in the fluid, or both, cannot result in a net change in the mass. Any change in mass flowing into the small volume of the aquifer must be balanced by a corresponding small volume change or both (Freeze and Cherry, 1979). The conservation of fluid mass statement is,

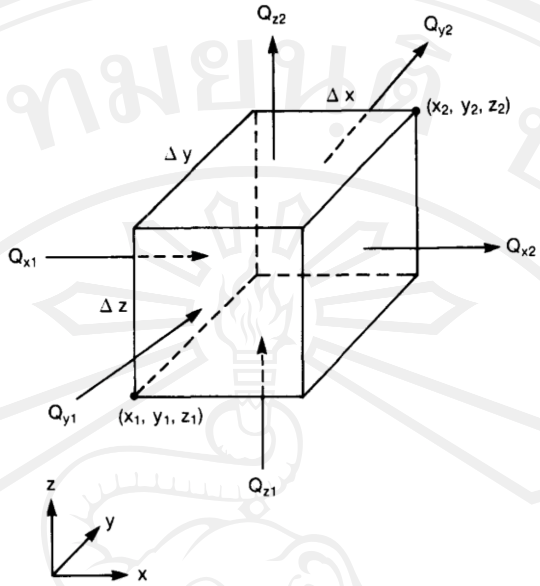


Figure 1-4 Flow into three dimensional finite difference grids. (Source: http://www.predictionprobe.com/generic/mode_f17.jpg; last accessed 17 Jan 2011)

$$GW_{inflow} - GW_{outflow} = \pm \Delta GW_{storage} \qquad (1\text{-}5)$$

The groundwater flow equation, in its most general form, it describes the movement of groundwater in porous medium. It is know in mathematics as the diffusion equation and has many analogs in other fields. It is often derived from a physical basis using Darcy's law and a conservation of mass for a small control volume. It is mathematical expression which is used to describe the behavior of groundwater flow through an aquifer. The groundwater flow equation is often derived for a small representative elemental volume (REV), where the properties of the medium are assumed to be effectively constant. To use the groundwater flow equation to estimate the distribution of hydraulic heads, or the direction and rate of groundwater flow that it must be solved.

Consequently, the ground-water flow equation is solved using the finite-difference approximation. The three dimensional movement of groundwater use in MODFLOW of constant density through porous material may be described by the partial differential equation (McDonald and Harbaugh, 1988). Then development of the groundwater flow equation in finite difference term follows from the application of continuity equation that it is the sums of all flows into and out of the cell must be equal to the rate of change in storage within the cell. In the more simply the general groundwater flow equation is expressed as:

$$\frac{\partial}{\partial x}\left(K_{XX}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)+W=S_s\frac{\partial h}{\partial t} \qquad (1\text{-}6)$$

where K_{xx}, K_{yy} is K_{zz} are value of hydraulic conductivity along axes x, y and z; which are assumed to be parallel to the major axes of hydraulic conductivity [LT^{-1}]

S_s is the specific storage of the porous material [L^{-1}]

W is a volumetric flux per unit volume and represents sources/sink of water

h is the potentiometric head [L]

t is time [t]

For steady state conditions, continuity requires that the amount of water flowing into a representative elemental volume be equal to the amount flowing out. The existence of steady-state conditions implies that head is independent of time. Then, the Laplace’s equation is the governing equation for groundwater flow through an isotropic homogeneous aquifer under steady-state conditions (Ashraf, 2008).

In transient-state, heads change with time. Transient problem are also called time dependent, unsteady, non-equilibrium, or non-steady-state problems. In the derivation of the governing equation for transient conditions, the continuity equation is modified such that the volume outflow rate equals the volume inflow rate plus the rate of release of water from storage (Ashraf, 2008). The Poisson's equation uses the governing equation under transient-state of three dimensional.

(3) Groundwater Flow System

Groundwater is part of the hydrologic cycle and it is constantly moving along the hydrologic cycle. Water can move rapidly through the atmosphere and cover long distances from the oceans to the continents. After precipitation water may run off to a stream or seep into the soil. Surface runoff can carry water through the watershed back to the ocean. Along the way, the water may evaporate or be transpired by plants. This seepage may also move deeper into the subsurface to recharge an aquifer. Once in the subsurface, groundwater may flow along a local or regional flow path (Figure 1-5). The local flow path may end at the local stream or lake, while the regional flow path may end at a major river. Groundwater flow is slow so it can take years or decades to move along some of the longer flow paths in Figure 1-5. The connection between surface water and groundwater is also shown in Figure 1-5. Groundwater discharges to surface water at various scales, from the local to regional scale. This groundwater flow sustains surface flows during periods with no precipitation including annual dry periods or even during droughts.

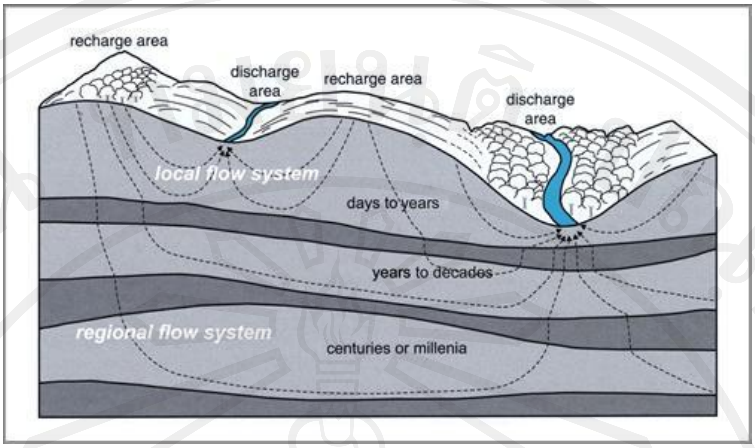


Figure 1-5 A cross-section showing local and regional groundwater flow Systems. (Source: http://www.mahometaquiferconsortium.org/ Edmats_2Hcycle _0605_files /image002.jpg*; last accessed 10 October 2010*)

1.5.2 Numerical Solution of Groundwater Flow Equation

(1) Numerical Models

A numerical groundwater flow model is the mathematical representation of an aquifer in a computer. Using the basic laws of physics of govern groundwater flow that it is based on groundwater flow equations. There are differential equations that can often be solved only by approximately methods using a numerical analysis. It is a key tool assisting in resolving concerns related understanding the groundwater flow system. There are usually used to simulate and predict the effects of aquifer conditions. Narasimhan (1982) identified the two fundamental tasks of numerical model: (1) to partition the flow domain into a finite number of subsets whose geometry and bounding surface is defined, and (2) to evaluate fluxes across each identified surface segment over a discrete time interval. Because flux is related to the spatial gradient of potential (head), task (2) is to evaluate head gradients across each surface segment defined in task (1). Differences in the numerical formations common to hydrologic model (i.e. finite difference method (FDM) and finite element method (FEM)) can be discussed in terms of these tasks, and recognition of these differences provides us with a base for evaluating their relative strengths and weaknesses (Narasimhan, 1982). Thus there exist various types of numerical models that are widely used by hydrologists in present-day. One such approach is the finite difference method, wherein the continuous system described by equation and derived from Darcy's law of conservation of mass.

(2) Description of Finite Difference Model

The first finite difference groundwater models that found fairly widespread usage were developed for two dimensional. Even through the use of these models has been superseded by the U.S. Geological Survey MODFLOW model. Thus, probably a Three-Dimensional Finite-Difference Ground-Water Flow Model (FDM) is the most widely applied numerical formation in groundwater hydrology. FDM is easy to understand and well suited for solving many groundwater flow problems. The aim of numerical modeling is to evaluate in a small-volume by integration in space and time. The FDM method consists of subdividing the flow region in of the aquifer to finite number of rectangular blocks shaped (see Figure 1-6) wherein uniform values of hydraulic conductivity (K), specific storage (S_s), and source/sink terms (R) are assigned to represent the average of K, S_s, and the integral of R over the block, representatively. Located in the center of each block is a node, where hydraulic head (h) is computed to represent the average value of the true head in the block.

In FDM discretization, one reduces the continue boundary value problem described by 1 to a finite set of discrete points in space and time. Partial derivatives at a point are then approximated by differences between variables over a small but finite interval. This leads to system of *N* linear, algebraic, finite difference equations in *N* unknowns, one for each node, where *N* is the number of equations on a computer. As is indicated above, the finite difference methods make use of approximations. However, the resulting inaccuracies can be made negligibly small through proper use of the methods.

(3) Groundwater Flow Process in MODFLOW

MODFLOW is a three-dimensional finite-difference ground-water model that was first published in 1984. It is the name that has been given the USGS. It has a modular structure that allows it to be easily modified to adapt the code for a particular application. Many new capabilities have been added to the original model. Then MODFLOW has become the worldwide standard groundwater flow model. Because of its ability simulate a wide variety of systems and its extensive publicly available documentation. Groundwater flow within the aquifer is simulated in MODFLOW

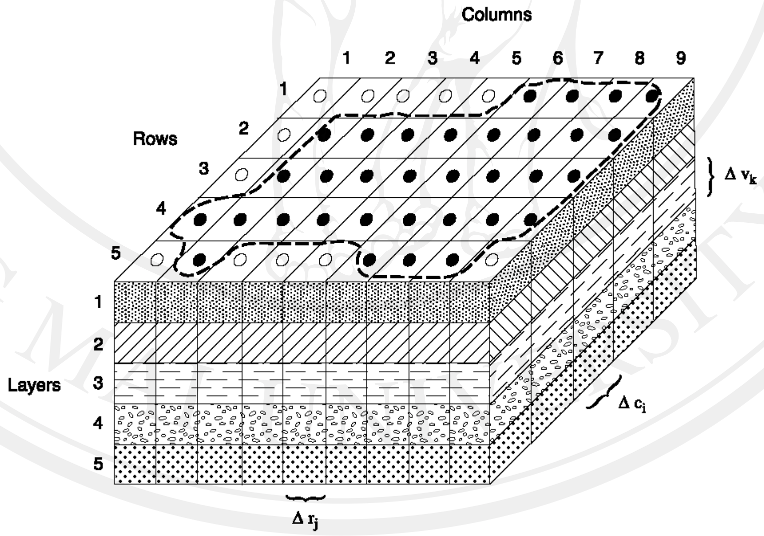


Figure 1-6 A FDM discretized hypothetical aquifer system. (Source; Todd , 2005)

using a block-centered finite-difference approach. In order to use MODFLOW, initial conditions, hydraulic properties, and stresses must be specified for every model cell in the finite difference grid. MODFLOW simulates steady and non-steady flow in an irregularly shaped flow system in which aquifer layers can be confined, unconfined, or a combination of confined and unconfined. Flow from external stresses, including flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through river beds, can be simulated. Hydraulic conductivities or transmissivities for any layer may differ spatially and be anisotropic (restricted to having the principal directions aligned with the grid axes), and the storage coefficient may be heterogeneous. Specified head and specified flux boundaries can be simulated as can a head dependent flux across the model's outer boundary that allows water to be supplied to a boundary block in the modeled area at a rate proportional to the current head difference between a "source" of water outside the modeled area and the boundary block.

1.5.3 Model Calibration

When simulating natural and engineered groundwater flow and transport systems, one objective is to produce a model that accurately represents important aspects of the true system. This can be achieved through the use of automatic model calibration. There are currently two famous external model calibration software UCODE or PEST. There perform inverse modeling calibration, using nonlinear regression. Calibration is difficult because values for aquifer parameters and hydrologic stresses are typically known at only a few nodes and, even then, estimates are influenced by uncertainty. Nevertheless parameter estimation is essentially and there are two classic calibration methods for solving the inverse problem. Firstly, the manual trial-and-error adjustment of parameters but it does not give information on the degree of uncertainty in the final parameter selection and guarantee the statistically best solution. Secondly, an automated estimation model calibration statistically based solution of the inverse problem quantifies the uncertainty in parameter estimates and gives the statistically most appropriate solution for the given input parameters provided, it is based on an appropriate statistical model of errors (Anderson and Woessner, 2002).

The automated estimation calibration is a widely valuable tool for finding the best fit to field observations. This method is the automated inverse modeling that is performed using specially developed codes. It is used either a direct or indirect approach to solve the inverse problem.

(1) Model-Independent Parameter Estimation Software: PEST

However, using direct measurements of system characteristics, hydraulic conductivity, to construct a model often poorly produces simulated values that match observations of the system state, including hydraulic heads, flows and concentrations (Barth et al., 2001). This occurs because of inaccuracies in the direct measurements and because the measurements commonly characterize system properties at different scales from that of the model aspect to which they are applied.

PEST is a general purpose automated parameter estimation utility developed by John Doherty of Watermark Computing. PEST is a model-independent nonlinear parameter estimation technique known as the Gauss-Marquardt-Levenberg method. During the past decades PEST has become the industry standard in calibration of groundwater modeling because of the time required for calibration of complex models with long run times can be significantly reduced through the use of PEST's powerful, operating-system-independent, parallelization capability. Besides the aspects of reality that may not be amenable to direct measurement and it can generally using fewer model runs than any other estimation method. Hence the PEST interface in GMS® (Aquaveo, 2010) can be used to perform automated parameter estimation for MODFLOW. One of the tools provided in GMS® for model calibration is automated parameter estimation. With automated parameter estimation, an external utility, sometimes called an "inverse model", is used to iteratively adjust a set of parameters and repeatedly launch the model until the computed output matches field-observed values. Parameter estimation is used in conjunction with the head observations and the flow observations. This Figure 1-7 describes the steps and guidelines for model calibration using PEST. Using automated parameter estimation to model calibration take greater advantage of construct a model and estimate model input values. The benefits of this step include (1) clear determination of parameter values that product the best possible fit to the available observations; (2) diagnostic statistics that quantify (a) quality of calibration, (b) data shortcomings and needs; (3) inferential statistics that quantify reliability of parameter estimates and predictions; and (4) identification of issues that easily overlooked during non-automated calibration (Hill, 1998).

1.5.4 Model Uncertainties

(1) Stochastic Methods Applications in Hydrogeology

There are two general approaches to modeling groundwater flow: deterministic and stochastic. The deterministic approach has a long and proven history of applications, where its success is clearly based on its ability to explain field observations in physical terms. Stochastic models treat aquifer parameters as random

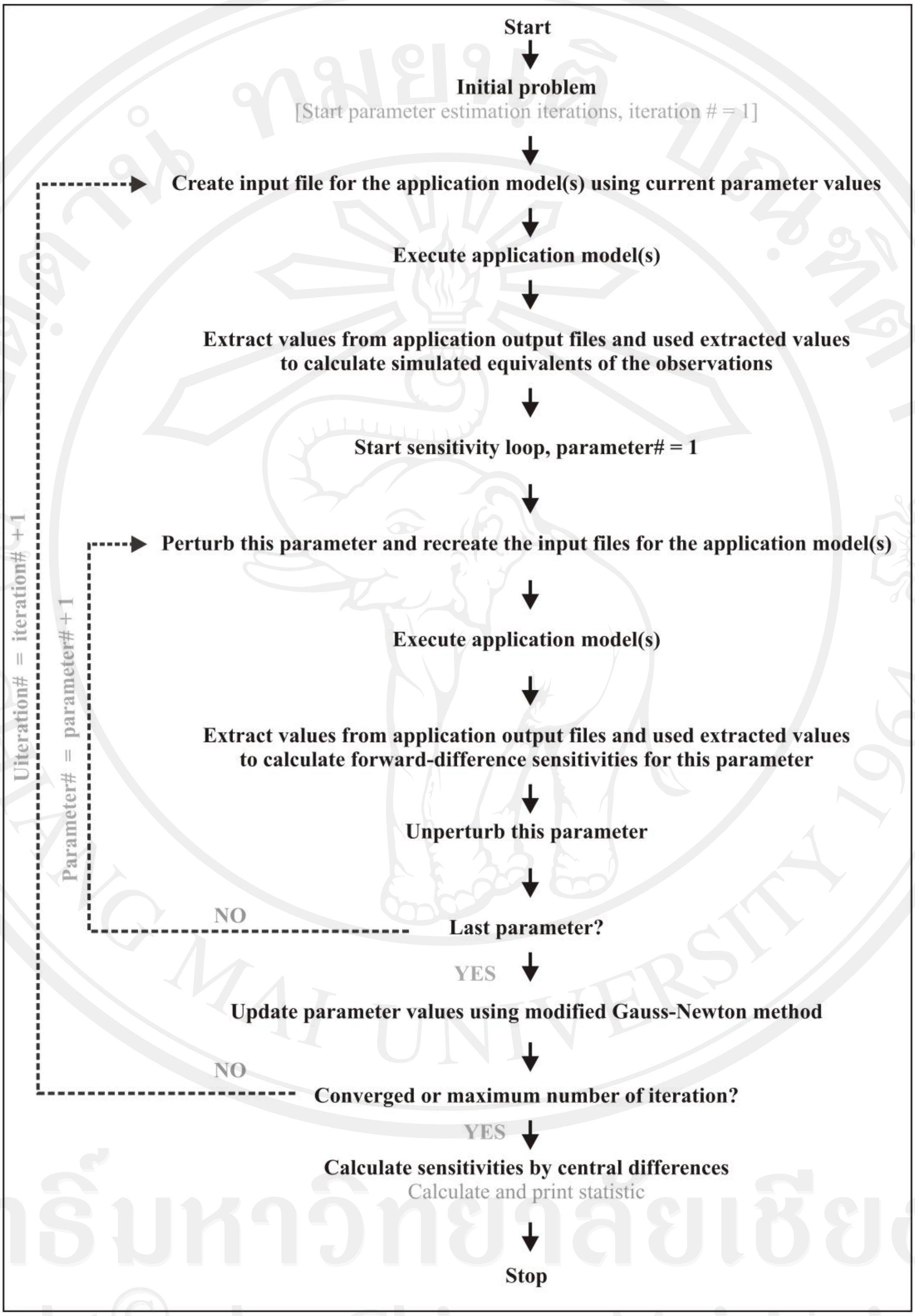


Figure 1-7 Flowchart for estimating parameter with PEST (Modified from; Hill, 1998).

functions in a probabilistic sense. Moreover, it is a well known that at a field scale, geological formations are heterogeneous, and the groundwater flow and solute transport processes in the formation are considerably affected by the heterogeneity of the formation properties. The Stochastic approach in subsurface hydrology has undergone a tremendous development in the last thirty years and a large body of knowledge has accumulated, many stochastic theories have been developed for groundwater flow and solute transport in heterogeneous porous media (e.g., Dagan, 1989; Gelhar, 1993; Cushman, 1997; Zhang, 2002). In development of the theories, it is common to assume that the spatial distributions of the medium properties can be characterized by one single correlation scale. The stochastic approach in modeling groundwater flow and solute transport regards the aquifer properties and the parameters that influence flow and transport as random. The randomness reflects the uncertainty of their values: the most common example is the hydraulic conductivity (K) that varies in space by orders of magnitude in seemingly erratic manner. The field data based on measurements are generally scarce and permit estimating K in statistical terms only. The same is true for many other properties of heterogeneous formations (e.g., storativity, pore-scale, dispersivity, reactive properties, natural recharge, transport initial condition, aquifer geometry, etc). The probability density function of properties and parameters serve as input to the quantitative modeling of flow and transport, resulting in stochastic differential equations for the dependent variables (pressure head, water Darcian velocity, solute concentration) (Dagan, 2002). Moreover, multiple realizations that are conditioned to borehole data provide modelers with a rational approach for dealing with uncertainty associated with site characterization. Stochastic simulations can be applied to regional representations of the aquifer behavior in addition to local scale simulations. As a result, the latter can also be characterized only statistically by their probability density function or in a more restricted manner by a few moments (mean, variance, etc). Prediction is therefore subjected to uncertainty and aquifer management under risk is appropriate approach. This is in contrast with the traditional deterministic modeling of groundwater flow and transport (Dagan, 2002; Dagan, 2004).

There are two methods for stochastic modeling using MODFLOW 2000. First, parameter zonation, uses either a Random Sampling, Latin Hypercube Sampling, or Gaussian Fields to generate the different sets of parameters. The second approach is indicator simulation which uses a set realizations generated by T-PROGS.

(a) Parameter Zonation

- *Random Sampling*: Random Sampling is the most widely used approach for generating multiple random model simulation. It supports both normal and uniform distribution. To set up the Random Sampling, it is needed to specify the mean, standard deviation, upper and lower bounds for each parameter, and finally, choose how many realizations you want to generate.

- *Latin Hypercube Sampling:* The Latin Hypercube randomization approach is a method that tries to efficiently probe the probability space for each parameter in a simulation in such a way that there is at least one simulation that represents every probability area for each parameter. First, specify the number of segments for each parameter. The total probability, defined by distribution, mean, standard deviation, and upper and lower bounds, is divided up into parts with equal probability (area). Then program generates a random parameter value so that there is one value that lies within each probability segment (Figure 1-8).

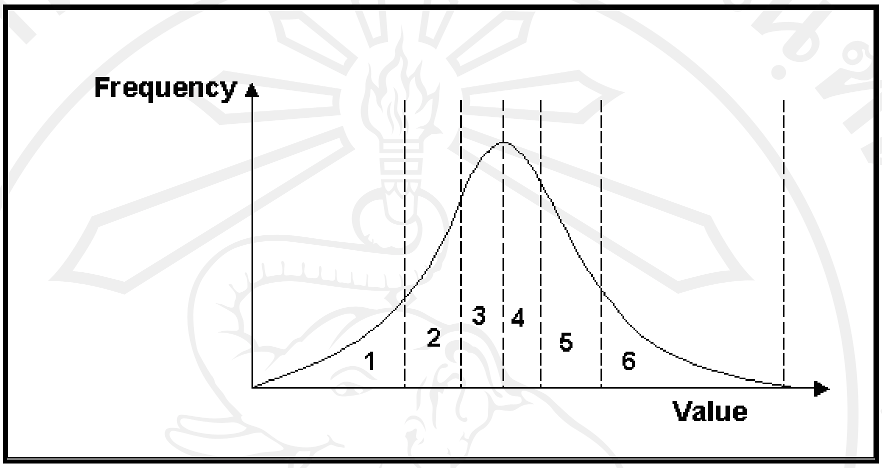


Figure 1-8 Showing generates a random parameter value within each probability segment. (Modified from; Aquaveo, 2010)

This is repeated in a combinatorial fashion for each parameter so that there are number of simulations. Using the Latin Hypercube method has the benefit of needing a fewer number of runs to achieve the same level of confidence than the number required for the Monte Carlo approach.

(2) Monte Carlo Technique

Stochastic theories of subsurface flow have changed the way about heterogeneity but have not had much impact on practical groundwater modeling. Most numerical models still provide no information on predicting uncertainty. This gap between theory and practice is due largely to the excessive computational demands of available numerical methods for solving stochastic problems. The alternative, Monte Carlo methods requires solving large numbers of equations on fine grids spacing that are smaller than the log conductivity correlation length, no matter how smooth the mean flow and variance dynamics of interest are. This result in computational times that are many orders of magnitude greater than those required for conventional deterministic simulations.

In a deterministic model, a fixed set of parameters and boundary conditions were used to calibrate model. When making predictions, the stresses were changed in the model to simulate what will happen to the groundwater system in the future. Only one run was made and the result was presented in the report. In some cases, bracket of the deterministic solution was performed with a best and worst case. This method does not really address the issue of uncertainty in parameters distributions in the model and how that uncertainty effects predictions. Although the deterministic modeling approach using trial-and error method has resulted in satisfactory calibrations, the observed "objective" piezometric head data could not be fitted perfectly, leaving a nonzero residual as quantified by the RMS. 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. The Monte Carlo technique can make key model parameters uncertain by specifying a distribution type and associated statistical characteristics. Instead of making one simulation, it makes hundreds or thousands of simulations. In each simulation, a different value is selected for uncertain parameters. When processing the results of a Monte Carlo simulation, it looks at the probability that something will happen by evaluating of the hundreds or thousands of simulations.

1.6 Literature Review

1.6.1 Hydrogeology of the Bang Pakong river basin

Piancharoen (1970) described six groundwater provinces in Thailand based on the areal extent of important aquifers and physiographic features. The Bang Pakong river basin was included in the eastern provinces. The aquifers of the Bang Pakong river basin are unconsolidated sediments and fracture of consolidated rocks. These aquifers have an average yield of about 50 to 70 m^3/hr and their water quality is suitable for domestic purposes, but some part of the area is brackish with a yield less than 5 m^3/hr.

Chuamthaisong and Intrasutra (1992) also described six groundwater provinces in Thailand based on physiographic features. The Bang Pakong river basin was classified as one of these basins. Groundwater occurs in beach sand deposits, decomposed rocks, granitic and metamorphic rocks. These sediments have average depths of 10 meters and yield of about 2-3 m^3/hr which water quality is fresh to brackish, besides, fractured rocks have averaged depths of 35 meters and yield of about 10 m^3/hr which water quality is generally suitable for domestic purposes but the water is iron-rich in many places.

The Department of Mineral Resources: DMR (1996a&b, 2001a&b) mapped groundwater occurrence of Chachoengsao and Chonburi provinces at a scale of 1:100,000. The map illustrates the types of aquifers, groundwater quality, and groundwater quantity. From the groundwater availability map of Chachoengsao and Chonburi provinces, it can be seen that the groundwater in the some part of study area occurs in an unconsolidated aquifer that is the floodplain aquifer (Q_{fd}) which is composed of gravel, sand, silt, and clay and its thickness ranges from 15 to 60 meters.

Its yield is less than 5 m^3/hr. The groundwater generally has Total Dissolved Solids (TDS) content less than 500 mg/L.

The Department of Mineral Resources: DMR (1996c and 2001c) mapped groundwater occurrence of Nakhon Nayok province at a scale of 1:100,000. The map shows the types of aquifer, groundwater quality, and groundwater quantity. From the groundwater availability map of Nakhon Nayok province, it consists of unconsolidated and consolidated aquifers. The unconsolidated aquifers deposited in the middle long to the south whereas the consolidated aquifers occurs in the north and in the northeast and it can be seen that the groundwater in the some part of study area occurs in an unconsolidated aquifer that is the floodplain aquifer (Q_{fd}) and high terrace aquifers (Q_t). There are composed of gravel, sand, silt, and clay and its thickness ranges from 50-120 meters. It yields less than 5-10 m^3/hr. The groundwater quality is generally good and moderate and it generally has Total Dissolved Solids content less than 500 mg/L.

Ramnarong and Wongsawat (1999) and Wongsawat (1999) reported important groundwater units and groundwater potential provinces of Thailand. The Bang Pakong river basin, included in the eastern provinces can be divided into two hydrogeologic units: consolidated and unconsolidated aquifers. Unconsolidated aquifers unit has an averaged depth 3-8 meters with yield of 10-30 m^3/hr with good water quality whereas consolidated aquifers from fracture of metamorphic rocks and granite rocks has an average yield of about 10-40 m^3/hr with good water quality.

Klueabthong (2005) studied hydrogeology of Bang Khla Royal Development Project in order to determine its groundwater resources potential in Bang Khla District, Chachoengsao province which is a part of Bang Pakong river basin. Its hydrogeologic units can be divided into 3 units including clay unit, sand unit, and shale interbeded sandstone unit which have transmissivity in the range of from 0.252 m^2/d to 2.232 m^2/d, storage coefficient in the range of 8.7×10^{-3} to 1.41×10^{-2}, and hydraulic conductivity in the range of 3.07×10^{-3} m/d to 0.02 m/d. Groundwater recharge has been estimated using two methods: hydrologic budget method, and a combination of Geographic Information System database and permeability testing method. The results show that recharge estimated from hydrologic budget method, it is 18,988 m^3/yr which is about 7.43 % of the annual rainfall, whereas the other method gave recharge estimate of 16,642.7 m^3/yr or about 6.52 % of the annual rainfall. Groundwater flow pattern indicated flow direction is from the central to the rim of the area.

1.6.2 Groundwater Flow Model in the Bang Pakong River Basin

During the last few decades methods for groundwater potential assessment and groundwater usage prediction in Thailand have been developed rapidly. Groundwater modeling technique was one of several methods used in those applications. There are a number of government-funded projects applied groundwater flow model to resource management studies.

Department of Groundwater Resources: DGR (2006) explored and assessed groundwater resource potential, predicted future impact, and developed groundwater map of the Bang Pakong river basin. Visual MODFLOW® program was used to simulate the three-dimensional groundwater flow under both steady-state and transient conditions with no use of automatic calibration. Hydrogeologic units were divided into 2 units including unconsolidated and consolidated aquifers. Unconsolidated aquifers have an average depth 15-200 meters, average yield of about

5-10 m^3/hr, TDS of 500-1,500 mg/L, transmissivity ranging from 0.3-50 m^2/d, storage coefficient ranging from 0.01-0.003, and hydraulic conductivity ranging from 0.03-10.0 m/d. Consolidated aquifers have an average depth 10-30 meters, water quality is generally good, average yield of 2-5 m^3/hr, transmissivity ranging from 0.5-50 m^2/d, storage coefficient ranging from 0.001-0.007, and hydraulic conductivity range from 0.07-10 m/d. Shallow and deep groundwater flow patterns have the direction from the east to the west and the central of basin. The amount of recharge from annual rainfall is 146.2 Mm^3/yr and have groundwater budget as follows: (1) total inflow to groundwater system is 215.8 Mm^3/yr (2) total outflow from groundwater system is 32.3 Mm^3/yr, as a result of groundwater storage is 183.5 Mm^3/yr.

1.6.3 Recent Application of The Stochastic Modeling in Hydrogeology

Koch and Arlai (2007) studied deterministic and stochastic modeling of groundwater flow and solute transport in the heavily stressed Bangkok coastal multi-aquifer system, numerical simulations of the relevant groundwater flow and transport processes under the present and future stress conditions. The major objectives of these investigations, as follows: (1) 3D steady-state and transient calibration of the aquifer flow system using MODFLOW, including automatic parameter estimation code UCODE; (2) stochastic simulations to take into account uncertainties of aquifer parameters, observed heads and reported pumping rates and comparison with analytical stochastic theory; (3) MTD3MS solute transport modeling and determination of the cradles of saline groundwater pollution; (4) analysis of the present-day and future sustainability of the groundwater resources in the aquifer; (5) investigation of feasible aquifer restoration (remediation) schemes through groundwater management strategies and, (6) investigation of density effects of the saline plume concentrations on the results obtained above, using the SEAWAT model. The ultimate goal of this analysis was to understand 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 showed that the stochastically predicted variances of the head are still lower than the variances of the residual head, indicating additional uncertainties in the fitted model. 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.