CHAPTER 4

RESULTS AND DISCUSSION

This chapter describes the results obtained from steady-state simulations and model calibrations based on automated parameter estimation scheme. Parameter sensitivity analysis, after calibration, using both traditional method and a new approach based on parameter estimation scheme will also be discussed. Lastly, the result from uncertainty analysis of water budget using Monte Carlo analysis will be presented.

4.1 Steady-State Model Calibration Results

4.1.1 Initial Model Execution

After the model was successfully executed with initial parameter values, the model outcome was checked whether it could, at least, simulate comparable hydraulic heads observed in the field. Figure 4-1 shows scattered plot between model-calculated heads vs. field-measured heads. It appeared that model simulation with initial parameter values resulted in a comparable hydraulic heads although the goodness-of-fit indicative parameters were relatively high. These goodness-of-fit parameters refer to objective function (F), root-mean-square error (RMS), and normalized root-mean-square error ($NRMS$) and they can be calculated from Equations (4-1) to (4-3), respectively.

Objective Function: $$F = \sum_{i=1}^{N} w_i (h_{obs} - h_{calc})^2 \qquad (4\text{-}1)$$

Root-Mean-Square Error: $$RMS = \sqrt{\frac{\sum_{i=1}^{N} [h_{obs} - h_{calc}]^2}{N}} \qquad (4\text{-}2)$$

Normalized RMS Error: $$NRMS = \sqrt{\frac{\sum_{i=1}^{N} \left[\frac{h_{obs} - h_{calc}}{h_{obs}}\right]^2}{N}} \times 100 \qquad (4\text{-}3)$$

The objective function is a quantity that is normally used to indicate how much error of the model is. It is usually used, as its name indicated, as a target for calibration procedure which is trying to minimize the objective function by changing model's parameter values. The value of weight, w_i, refers to the reliability of the observation data and it gives a relative confidence level of the observed value. If all observations are equally reliable or important, weight can be identical and, typically, it is set equal to one (1.0). In some cases, different observation can have different value of weight because the reliability of the measurement is different. This could also be due to the fluctuations in head measurements. In that case, the value of weight is normally an inverse of the variance of measurement or $w_i = 1/s_i^2$ where s_i is the standard deviation of head measurement.

4.1.2 Model Calibration Using PEST

Using initial parameter values, the objective function of the model simulation is still relatively high. The automated model calibration using PEST program was used to reduce objective functions, hence, to calibrate the model. The method, facilitated by nonlinear least squares regression and associated statistics, defines the optimal parameter set as that for which the sum of squared deviations between model-calculated heads vs. field-measured heads (see Equation (4-1)). The calibration target results were described in terms of hydraulic head and water budget that can be

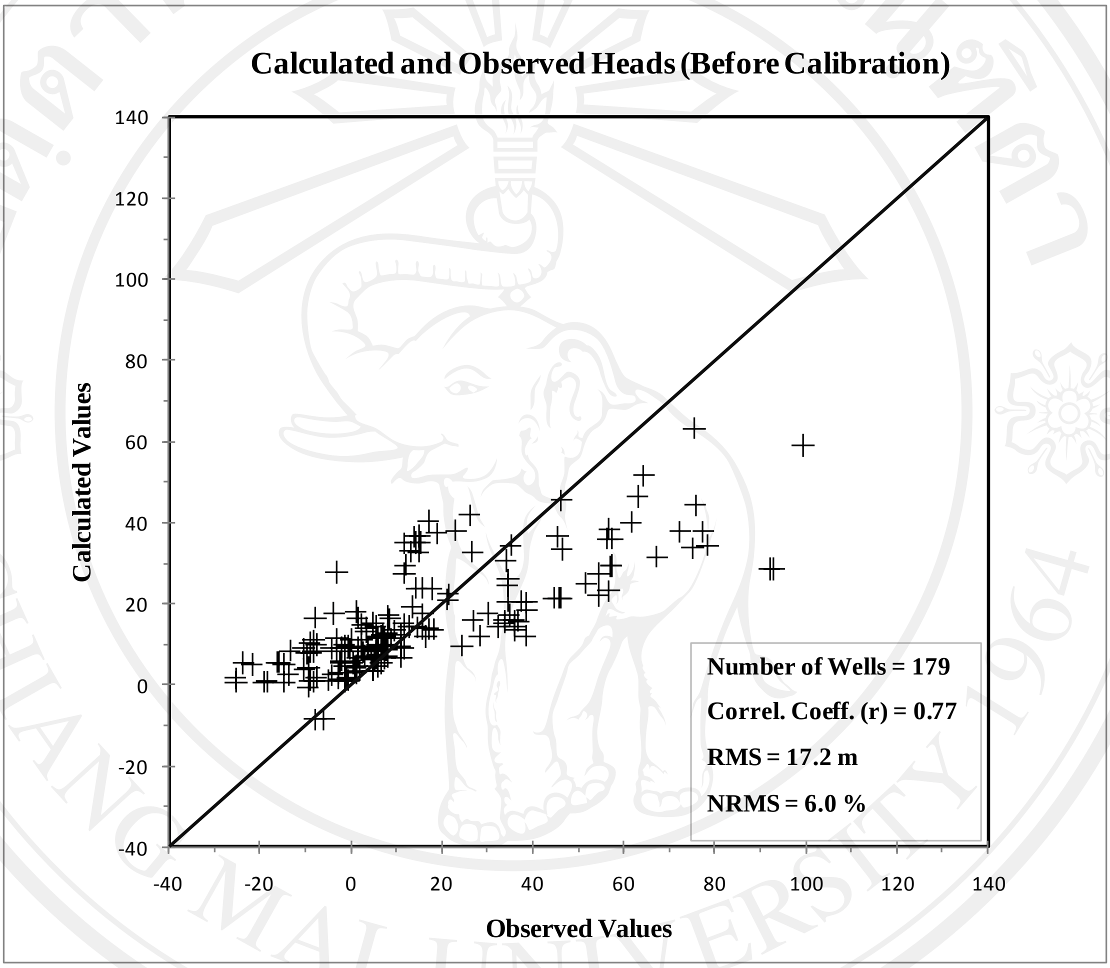

Figure 4-1 Field-observed heads vs. model-calculated heads using initial parameter values (i.e., *before* calibration).

displayed both qualitatively and quantitatively. Presentation of calibration results can be done in several ways. In this study, model calibration results were reported by expressing the difference between model-calculated and field-measured by using maps, graphs, or tables.

First, a scatter plot showing model-calculated heads against observed heads is illustrated in Figure 4-2. If the model fits perfectly to real situation, all data points should fall along a 1:1 (or 45°) straight line. In reality, however, the model can never capture all aspects of groundwater system; hence, there are still some discrepancies between model-simulated and observed hydraulic heads. Presenting a scattered diagram for a goodness-of-fit is usually associated with some statistical parameters such as correlation coefficient (r), root-mean-square error (RMS), and normalized root-mean-square error ($NRMS$). All of these parameters were calculated and reported as shown in box of Figure 4-2. The scatter plot shows a relatively good fit where most data points do not significantly deviate from the 1:1 straight line. The reduction of RMS and $NRMS$ errors, after PEST calibration, is significant where RMS error is reduced from 17.2 m to 15.5 m and $NRMS$ error is reduced from 6.0 % to 5.3 %. The optimized parameter values are listed in Table 4-1 and these set of parameters will subsequently be used in further studies where uncertainty of groundwater budget will be evaluated.

Second, the reduction of objective function (Φ; see Equation (4-1)) which is the sum of squared weighted residuals was used as another indicator for a goodness-of-fit. This parameter is a measure of total error from model and the ultimate goal of model calibration is to minimize Φ. During calibration the model is repeatedly executed with new set of parameter values until the objective function is minimize. Figure 4-3 presents how PEST adjusts the best parameter set in each iteration to minimize the objective function (Φ). It shows the plot of objective functions vs. iteration number. Clearly, after the third iteration of automated calibration, the objective function decreases drastically following the gentle change until the third iteration. This result represents slight changes due to the convergence of the model by achieving the calibration target of the final optimal parameter values (Table 4-1). Such table shows the result of calibrated steady-state model reporting the final optimized parameter values and its associated sensitivity.

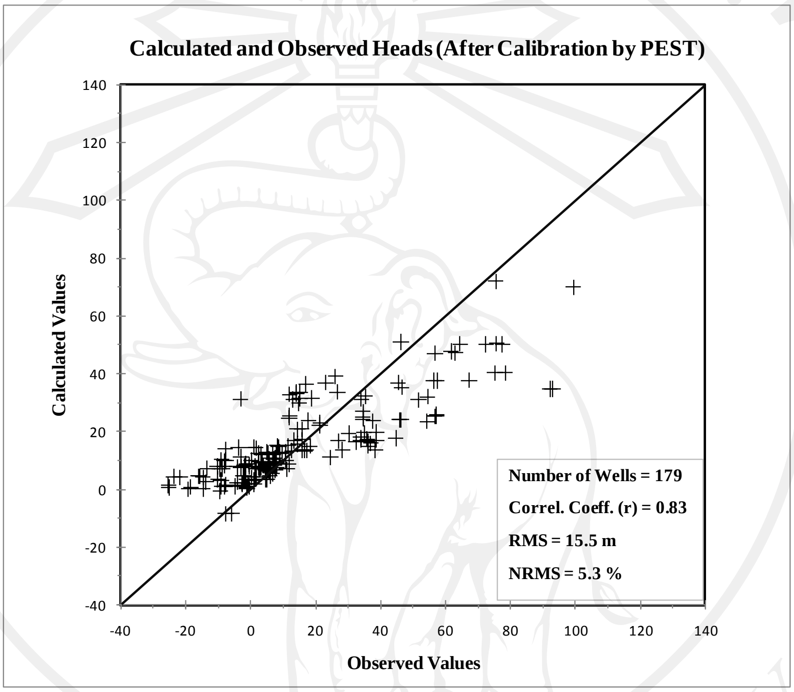

Figure 4-2 Field-observed heads vs. model-calculated heads *after* calibration using PEST algorithm.

Table 4-1 Final parameter values and its sensitivity after calibration using PEST.

Parameter group	Parameter name	Optimized parameter value	Sensitivity results
Hydraulic Conductivity; (m/d)	hk_1 (Qfd)	0.220	0.023
	hk_2 (Qyt)	3.105	0.417
	hk_4 (Qot)	0.522	0.207

Table 4-1 (Continued)

Parameter group Hydraulic Conductivity; (m/d)	Parameter name	Optimized parameter value	Sensitivity results
Hydraulic Conductivity; (m/d)	hk_5 (Qcl)	0.849	0.114
	hk_6 (SDmm)	0.076	1.221E-03
	hk_7 (Jmk)	3.920	2.315E-06
	hk_8 (Cms)	0.081	4.040E-02
	hk_9 (Trpn)	0.401	0.936
	hk_10 (Gr)	0.199	0.421
	hk_11 (Vc)	0.429	0.968
Vertical Anisotropy, K_v/K_h; (-)	vani_12	5.006	0.120
Evapotranspiration Rate; (m/d)	evt_13	2.112E-05	1.185E-02
	evt_14	6.462E-06	9.106E-06
	evt_15	1.138E-04	0.251
	evt_16	1.110E-06	1.856E-03
	evt_17	8.692E-05	1.281E-02
Recharge Rate; (m/d)	rch_18	7.335E-05	0.996
	rch_19	2.926E-05	0.680
	rch_20	1.440E-05	1.020
	rch_21	8.143E-05	0.793
	rch_22	7.023E-05	0.417
	rch_23	1.103E-05	3.206E-02

Table 4-1 Final (Continued)

Parameter group	Parameter name	Optimized parameter value	Sensitivity results
Recharge Rate; (m/d)	rch_24	8.831E-07	1.732E-02
	rch_25	6.185E-09	2.997E-04
General Head Conductance; (m^2/d)	ghb_27	3.493E+06	2.272E-03
	ghb_28	5645.29	4.507E-04
	ghb_29	74.24	0.399
	ghb_30	34.61	0.192
	ghb_31	546.94	3.445E-03
River Bed Conductance; (m^2/d)	riv_32	3.275E+06	2.343E-03
	riv_33	36451.6	1.113E-03
	riv_34	208.96	0.121
	riv_35	2643.28	5.805E-03
	riv_36	3881.88	1.376E-03

Lastly, another way to present the calibration result is to generate hydraulic head contour maps of model-calculated vs. field-measured values. This shows the spatial distribution of error in the calibration. The difference in head distribution patterns represents a quantitative measure of the goodness-of-fit between the simulation results and field observed. It is very helpful for identifying of the model where the calibration weakest, and determining the calibration result is significant.

Figure 4-4 shows the contour maps of hydraulic head distribution after automated calibration. It displays a head contours pattern that can depict the groundwater flow

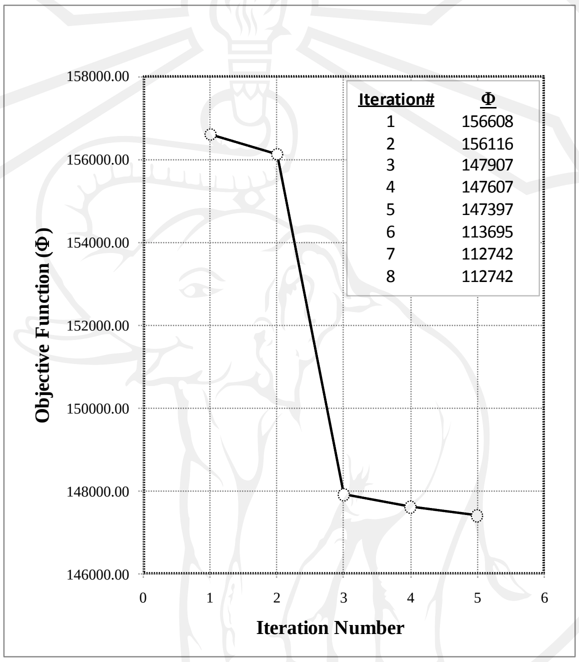

Figure 4-3 Progression of the sum of square of weighted residuals during automated model calibration by PEST.

directions. It shows groundwater flowing towards the central and the central-west direction (coastline) from northern and lower-southeast and heads declined from the northern and the lower-southeast to central-west direction. Figure 4.4 and 4.5 illustrate the similarity between before calibration vs. after calibration of hydraulic head distribution patterns. In this figure, it was found that the spatial variation of hydraulic heads is low near the coast (west) and higher in the mountains (north & southeast). Although head distribution in some areas showed high residual error but these can be justified due to the lack of data (i.e., observation wells) in the high mountainous areas. Nevertheless, this result indicates that a relatively good fit of the model considering highly complex groundwater system at a regional scale.

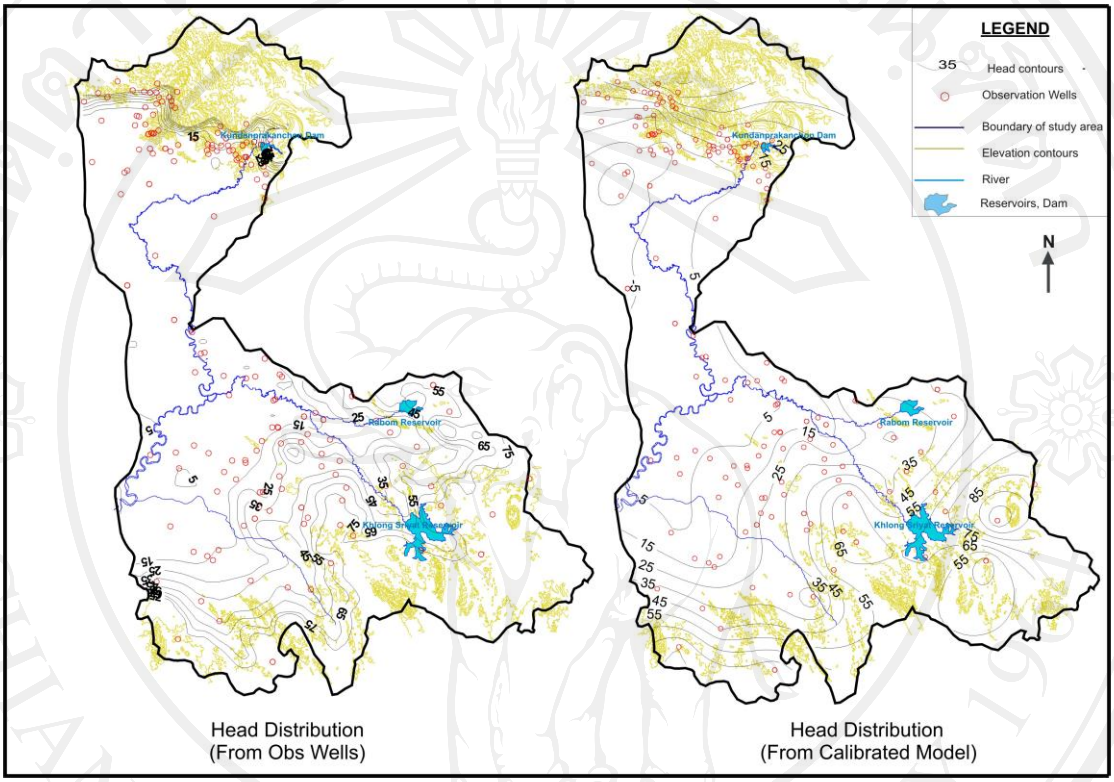

Figure 4-4 Steady-state hydraulic head distribution from observation wells (left) and after calibration with PEST (right).

Water budget analysis is important in calibration because it can be quantified on the basis of the calibrated model output. This measurement is one of the key indicators of a successful calibration result. If an error in difference of the water budget is less than 0.1% that can indicates perfectly balance between inflow and outflow. The error in the water budget of 2% is usually considered acceptable on regional groundwater system (Konikow, 1978). The results of water budget are given in Table 4-2. The error in water budget, after model calibration, is 0.28% which can be assumed zero groundwater change $(\Delta S = 0)$ under steady state condition. Then, this result (with acceptable error) indicates fairly well calibrated model. Total estimated groundwater flow through groundwater basin was 125.54 Mm^3/yr. Precipitation which provided the primary net recharge of the system was estimated to be 101.79 Mm^3/yr which is approximately 7.63% of the annual rainfall. Groundwater usage was about 14.59% and evapotranspiration was about 67.78% of annual groundwater recharge. Net recharge difference between water-balance calculation (DGR, 2006) and from this model is as small as +1.09% indicating that the model was considered sufficiently and successfully calibrated.

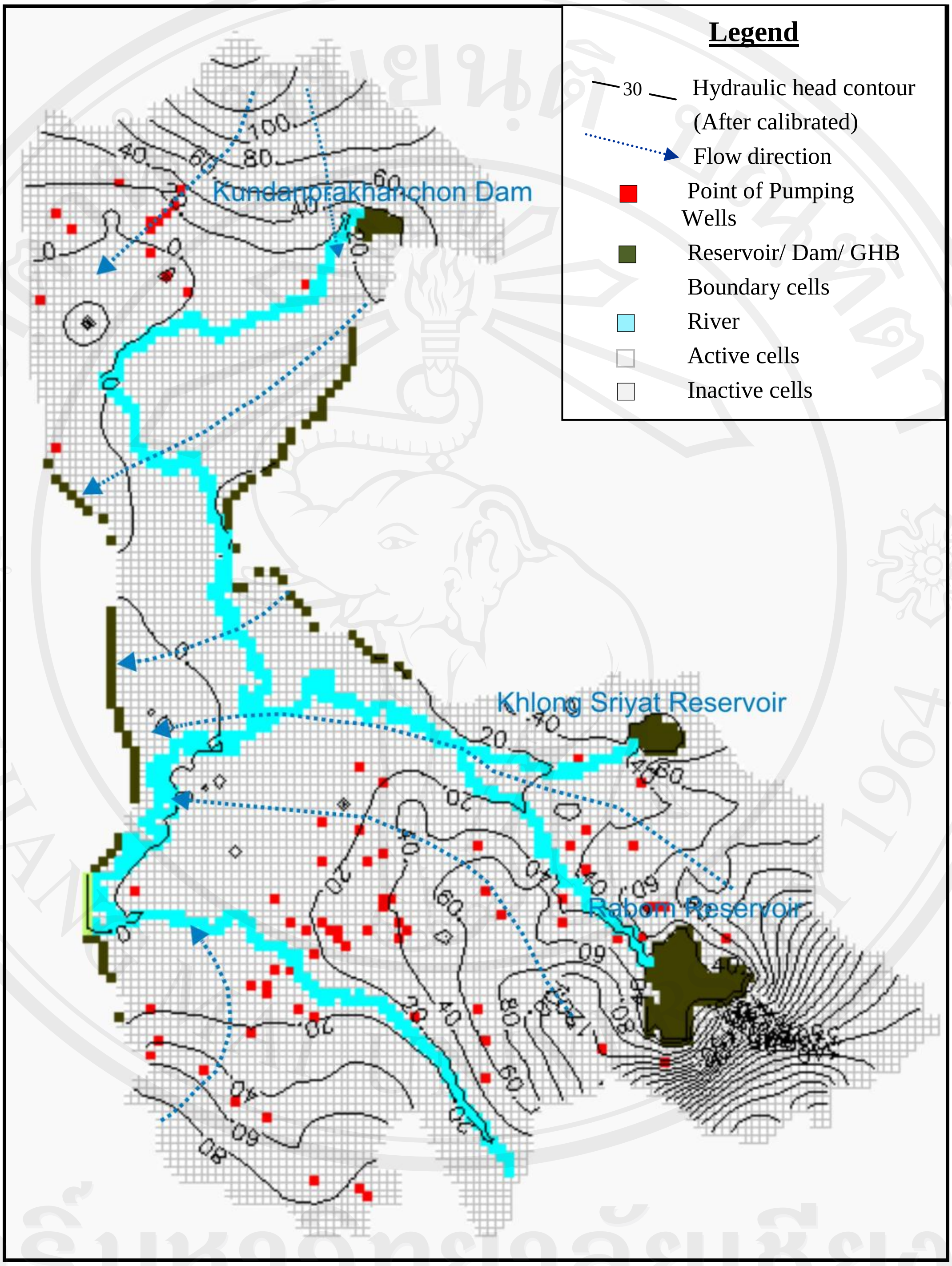

Figure 4-5 Steady-state hydraulic head distribution after calibration.

Table 4-2 Water budget at calibration target.

	Inflow (**Mm^3/yr**)	**Outflow** (**Mm^3/yr**)	**Percentage of recharge (%)**
Storage	-	-	-
Recharge	101.79	-	0
Evapotranspiration	-	56.69	67.78
Pumping Wells	-	14.85	14.59
Constant Head Boundary	0.11	0.02	0.02
General Head Boundary	18.21	19.67	19.32
River	5.43	33.96	33.36
Total, (Mm^3/yr)	**125.54**	**125.19**	
Error, (Mm^3/yr)	**0.35 (0.28 %)**		

4.2 Parameter Sensitivity Analysis

There are two approaches of representing parameter sensitivity; a traditional approach and the new approach. The latter is based on the determination of absolute sensitivity from parameter estimation process using PEST. In traditional method, the sensitivity of parameter is calculated by changing parameter values by a factor designated by modeler and the corresponding objective function is calculated from model simulation. The parameter sensitivity is normally used to indicate how sensitive or how *important* the parameter in the context of available set of observations. Figures 4-6 to 4-10 show the sensitivity of five parameter groups:

hydraulic conductivity, recharge rate, evapotranspiration rate, general head conductance, and river-bed conductance, respectively.

The sensitivities for all parameter groups showed the model was more sensitive to recharge rate and hydraulic conductivity. This is perhaps because the recharge is the primary source of inflow groundwater. While the other parameter groups (i.e., evapotranspiration, general head conductance and river-bed conductance) were less sensitive have small influence to this model as there were almost no changes in the objective function even when large parameter multiplier was used. The results of sensitivity analysis are summarized in Figure 4-11, shown that the model was the most sensitive to recharge rate and was insensitive to general head conductance and river-bed conductance.

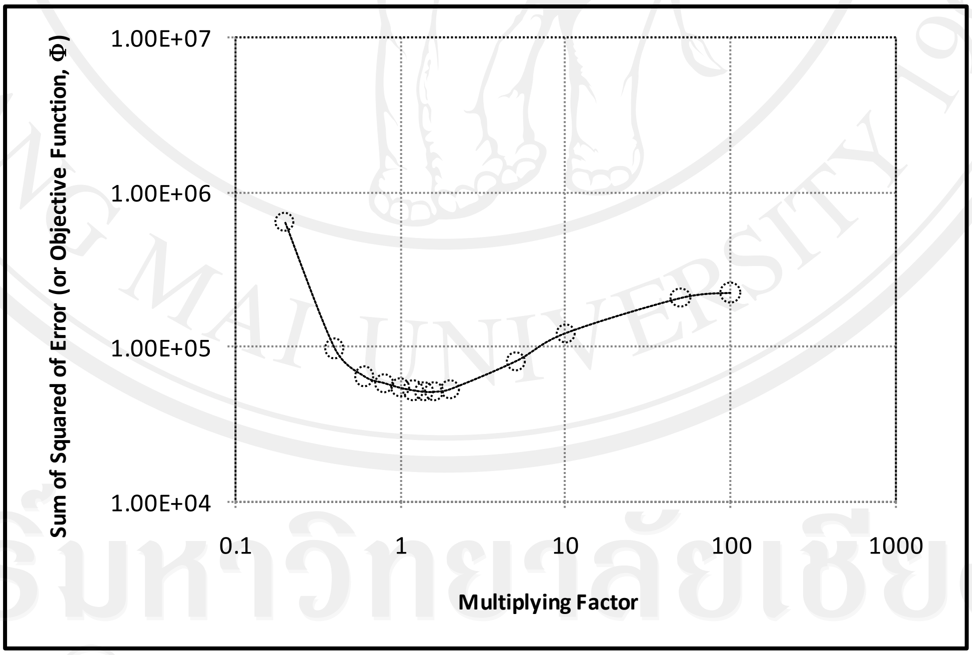

Figure 4-6 Sensitivity analysis of hydraulic conductivity group.

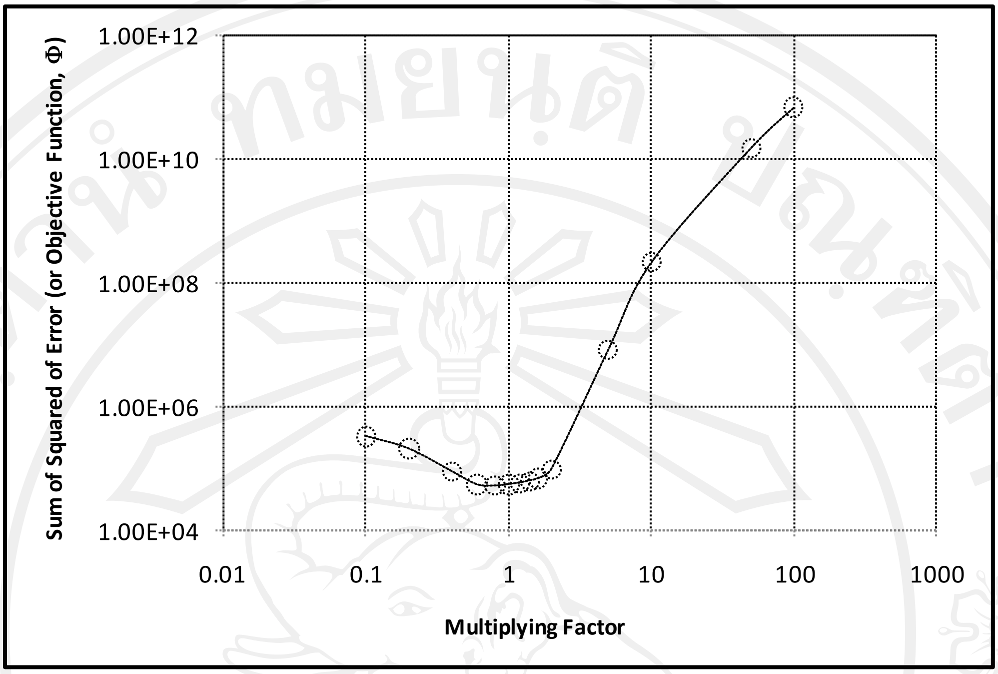

Figure 4-7 Sensitivity analysis of recharge rate group.

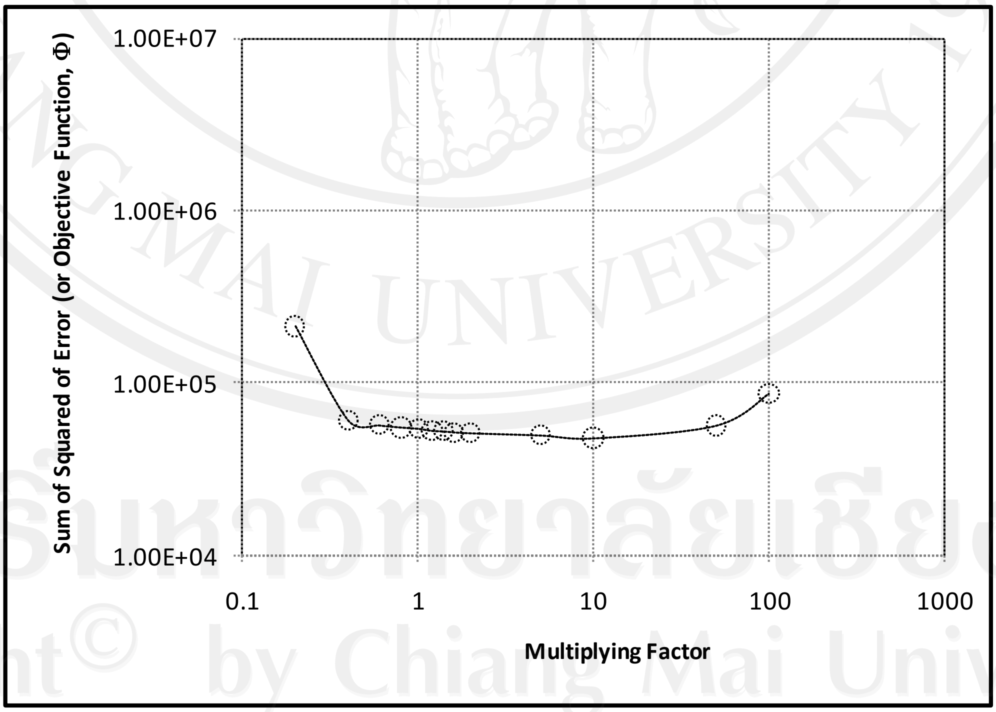

Figure 4-8 Sensitivity analysis of evapotranspiration rate group.

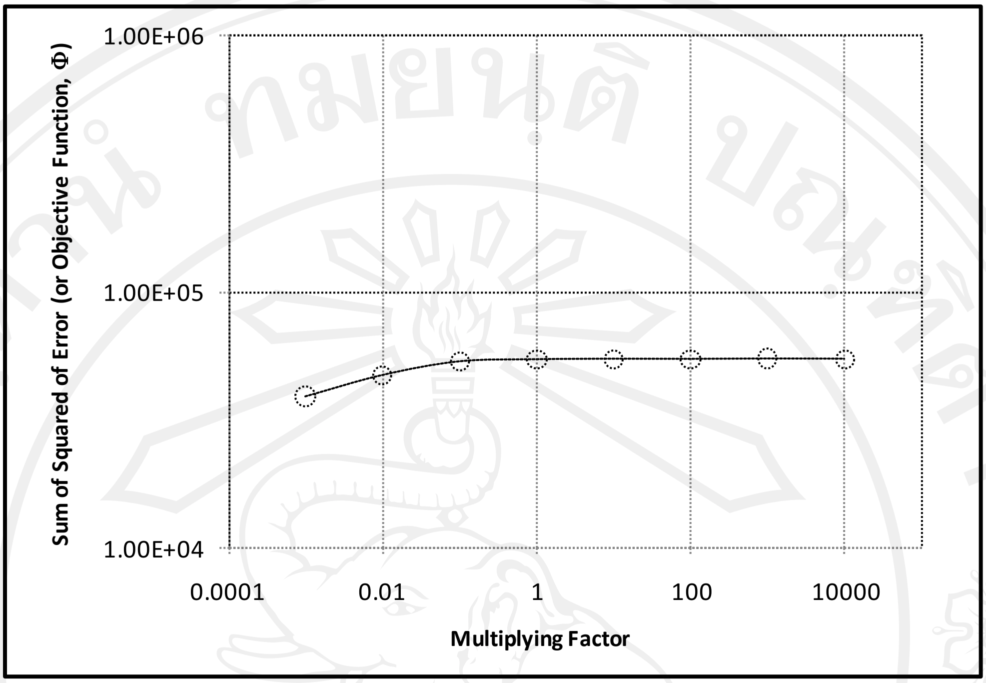

Figure 4-9 Sensitivity analysis of general head conductance group.

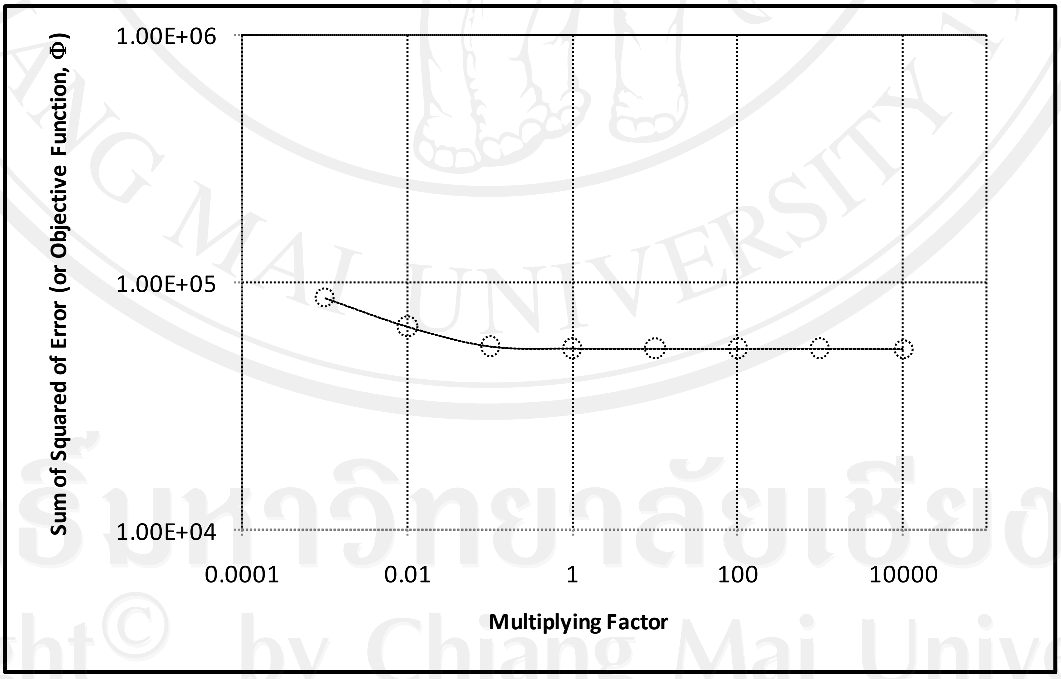

Figure 4-10 Sensitivity analysis of river bed conductance group.

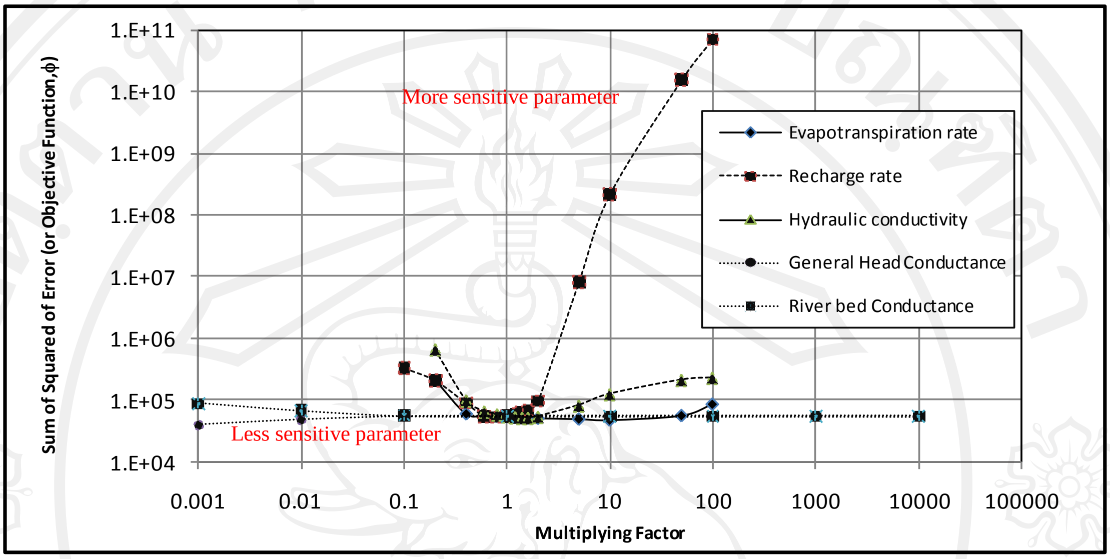

Figure 4-11 Resulting of all parameter groups on sensitivity analysis at the calibration target (i.e., steady state condition).

In the new approach of sensitivity analysis, the absolute parameter sensitivity is calculated after model calibration was successfully achieved. The inverse model algorithm (PEST) automatically calculates the value of sensitivity (which is actually, a derivative of objective function with respect to the parameter value or S_i = ¶F/¶ P_i where S_i is the sensitivity of parameter P_i. The values of S_i is listed in Table 4-1. These results of values of the sensitivity of parameters (S_i) identified the recharge rate was the most sensitive than other parameter groups and parameters rch_20, rch_18, and rch_15 were more sensitive than other recharge zones. The general head conductance and river bed conductance were the lowest sensitive values for the aquifer parameters and the boundary conditions. The results showed that recharge rate and hydraulic conductivity are the most sensitive parameters.

During PEST execution, the sensitivity of parameter can vary significantly. As shows in Figure 4-12, the model was less sensitive to the general head conductance and river bed conductance. This result corresponds to the traditional approach of sensitivity analysis method. It also shows the objective function tends to decrease as iteration progresses (and, objective function decreases too). At the end of PEST run, the program produces optimal parameter set with the lowest objective function (see Table 4-1). The optimum values determined by PEST can be found in the PESTCTL.REC file in Appendix B.

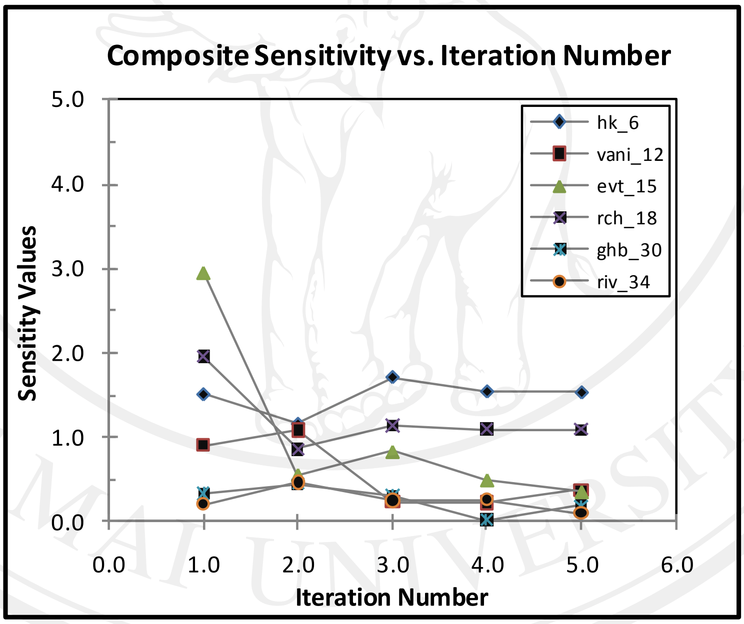

Figure 4-12 Showing how PEST adjusts the all parameters with each iteration to minimize the objective function.

4.3 Uncertainty Analysis of the Model

In previous section, model calibration and sensitivity analysis results shows the calibrated model still, at its best, produces some discrepancies between measured and calculated heads. In fact, this indicates that model is still associated with some error. In other words, there is still an uncertainty in model calculation. In this section, the uncertainty of the model described in terms of water budget and heads will be quantified based on Monte Carlo method.

In order to determine the appropriate number of multiple runs in Monte Carlo analysis, multiple sets of steady-state simulations were performed. In this case, the number of model runs of 50, 100, 250, 500, 750, 1000 and 1,500 realizations were executed (see Appendix C for the distribution or histogram of parameter values). These simulations generally take weeks to months to complete. The average water budget (INFLOW or OUTFLOW) for each case was computed and plotted against the number of realizations. Figure 4-13 shows the change in water budget and its associated error with each Monte Carlo set of simulation and, as can be clearly seen, the water budget became stabilized after approximately 100 realizations. This implies random sampling process has generated a sufficiently representative set of parameter values, and it is not necessary to execute the flow model more than 100 realizations to evaluate model uncertainty.

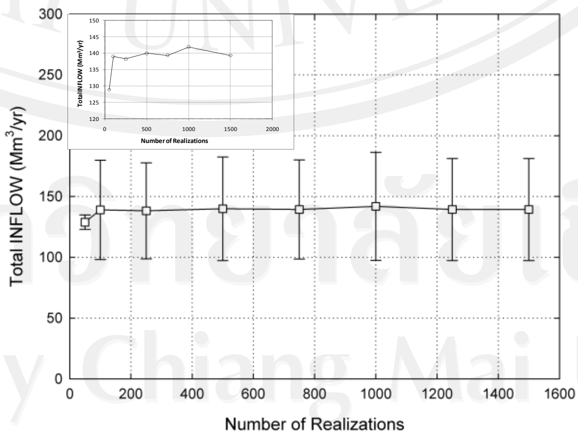

Figure 4-13 The predicted water budget (Inflow) resulting from range in uncertainty analysis on calibrated model.

Based on this Monte Carlo analysis the uncertainty in water budget was calculated and shown in Table 4-3. The uncertainty in total budget of the Bang Pakong river basin is 139.0±40.8 Mm^3/yr. It should be noted that the majority of the error or uncertainty arises from river and general-head boundary conditions. This finding agrees with the sensitivity analysis where river and general-head boundary conductance were the less sensitive to head observations than other parameters. This means the available information on head observations does not reflect the importance of river and general-head boundaries. More information on observation such as flow measurements between surface and groundwater at the river boundaries and the flow exchange along the general-head boundaries should be provided to increase parameter sensitivity of RIV and GHB conductance and, hence, model's reliability.

Table 4-3 Water budget calculation from Monte Carlo analysis.

	Inflow **(Mm^3/yr)**	**Outflow** **(Mm^3/yr)**
Storage	-	-
Recharge	106.9±0.03	-
Evapotranspiration	-	54.5±9.6
Pumping Wells	-	14.9±0.18
Constant Head Boundary	1.1±2.5	2.15±11.6
General Head Boundary	11.0±5.8	28.9±39.2
River	20.0±34.7	38.6±11.0
Total, (Mm^3/yr)	**139.0±40.8**	**139.0±40.8**
%Error	**0.0**	

Figure 4-14 shows the map of observation well locations that have high uncertainty (*CV* > 0.5 for head) in *head prediction* from the model (red symbol; larger symbol size refers to larger *CV*) while other wells are shown in blue symbol. These high uncertainty wells should be re-investigated whether the water level measurements were performed correctly or whether the information on the depth of well screen, screen length, and screen interval were obtained correctly. This indicative (Monte Carlo) simulation is very powerful because it can be used to delineate the area(s) where head measurements require more careful attention. In this case, the upper part of the basin may need more accurate information on head observation to increase model's reliability.

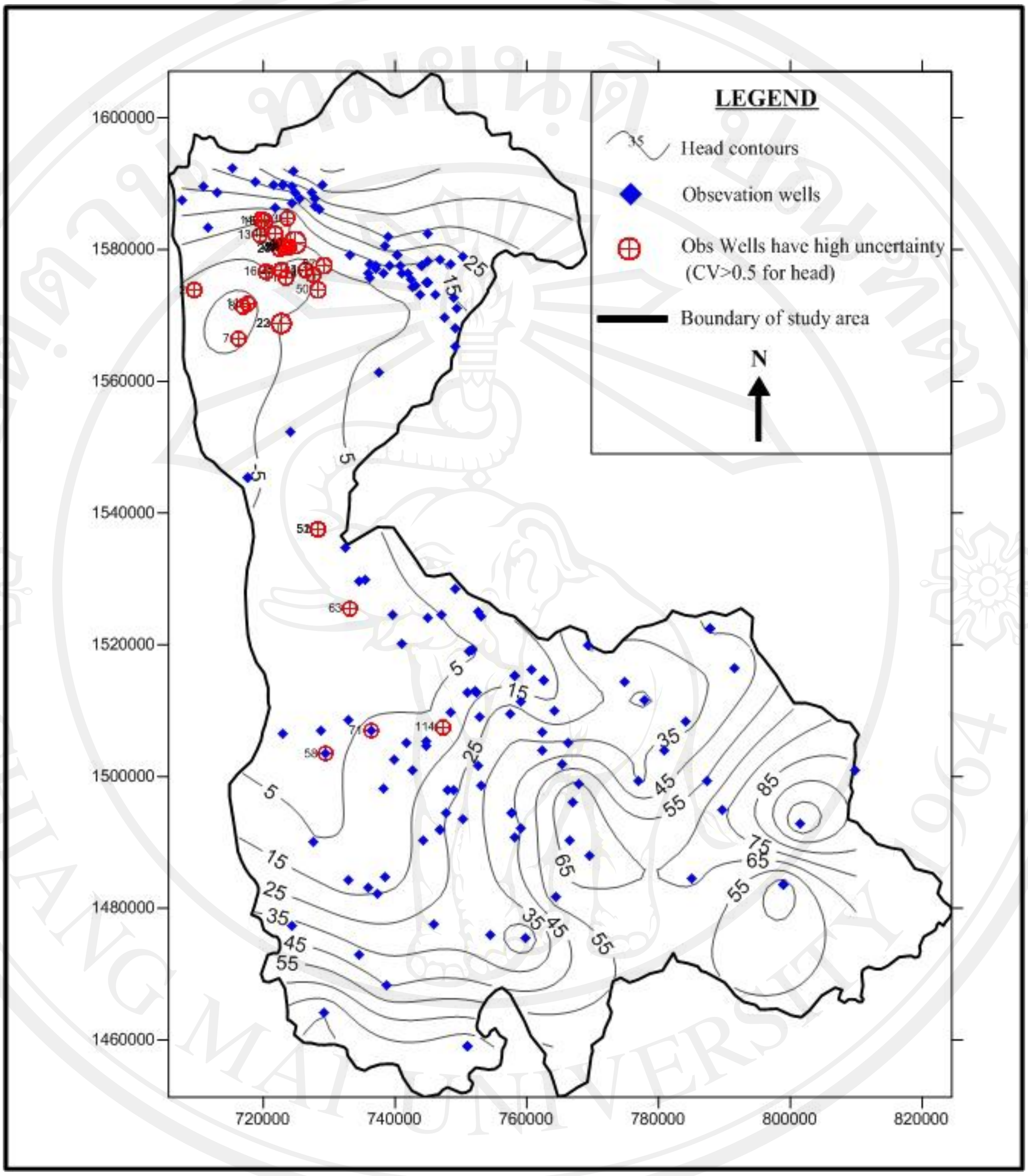

Figure 4-14 Observation wells having high uncertainty in prediction (red symbol).