

APPLIED FINITE DIFFERENCE METHOD FOR GROUNDWATER FLOW MODELING IN XAYSOMBOUN PROVINCE, LAO PDR

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Abstract

Groundwater modeling has become a popular approach and common of conducting groundwater flow and contaminant transport simulation. Consequently, in order to understand the behavior of groundwater flow, this study has established and developed conceptual model of groundwater at Phukham Copper - Gold operations mining. In addition, this study is applied Groundwater Modeling System (GMS) 6.5 software and using MOFLOW Package which employs advanced mathematics as Finite Difference Method (FDM). Steady Flow model is set up and calibrated within target ± 2 meters; then the model is run in MOFLOW in order to obtain acceptable observed and simulated hydraulic head by adjusting hydraulic conductivities and recharge values. Recharge rate is adjusted between 2% to 12% from annual rainfall 0.00475 m/d and it is found out to be 7.22 % or 0.00034 m/d. Model has come up with reasonable finding. Hence, root mean square error of steady state: layer1, 2, 3 and 4 are 1.840 m, 1.767 m, 1.963 m and 0.574 m, respectively. The coefficient of determination of steady state for layer1, 2, 3 and 4 are 0.965, 0.96, 0.959 and 0.985, respectively.

Keyword: *Groundwater, Finite Different Method, MODFLOW, Calibration.*

1. INTRODUCTION

This study conducted on groundwater flow modeling in Xaysomboun Province at Phu kham Copper - Gold operations in Lao PDR. MODFLOW is numerical modeling that is very useful and necessary for dealing with groundwater, it was programmed in order to encode by FORTAN language approach,

Groundwater modeling is a significant model to visualize the natural phenomenon aquifer and bring some of those related data to the computer modeling system. Consequently, The objectives of the study are to built the conceptual model of groundwater system, simulate and calibrate groundwater flow modeling in steady state, however, the target of the study is to obtain properly between observed and computed hydraulic head values based on the component of the model; besides this simulation will be automatically retrieved groundwater balance from the conceptual model, by adjusting recharge, horizontal hydraulic conductivity and horizontal anisotropy.

Conceptual model is built based on borehole geological data which is quite complex geology, according to fifteen boreholes logging data are input to GMS 6.5 to create solid and grid model then the model is converted into conceptual model with 3 dimensions in MODFLOW-2000 package which consists of limestone, schist, redbed siltstone and braccia aquifer as shown in Fig.2, including boundary condition of groundwater modeling.

FDM is a technique of advanced mathematical model which be applied partial differential equation (PDE) to simulate and solve problem that are cognate to groundwater. MODFLOW is also numerical model with employing Finite Difference method in order to deal with groundwater modeling which comprises of steady state package.

The study is monitored and traced groundwater level in order to deal with groundwater flow which includes fifteen boreholes as shown in Fig.1 and detail of those data will be illustrated in Table.3. This study will be useful and also being a reference for other proposed future study in groundwater within this vicinity.

2. THE STUDY AREA.

The study site lies at 279924.53E, 2088841.57N latitude and longitude, respectively, which is located in Xaysomboun Province in Center of Laos, it is far away from Vientiane capital about 120 km, and most of the area is covered with mountain and forest (Phu Bia Mining Annual review, 2009). Hence, the highest elevation is 2800m and the lowest is 240m of mean sea level (Geography department, 2010).

The study site has surface area approximately 693.3 hectares or 6.933 square kilometers within the boundary; these area has been operated and developed copper and gold mines since 2008 (Phu Bia Mining Annual review, 2009), within the area consists of monitoring groundwater level as shown in Fig.1 various color of the symbols.

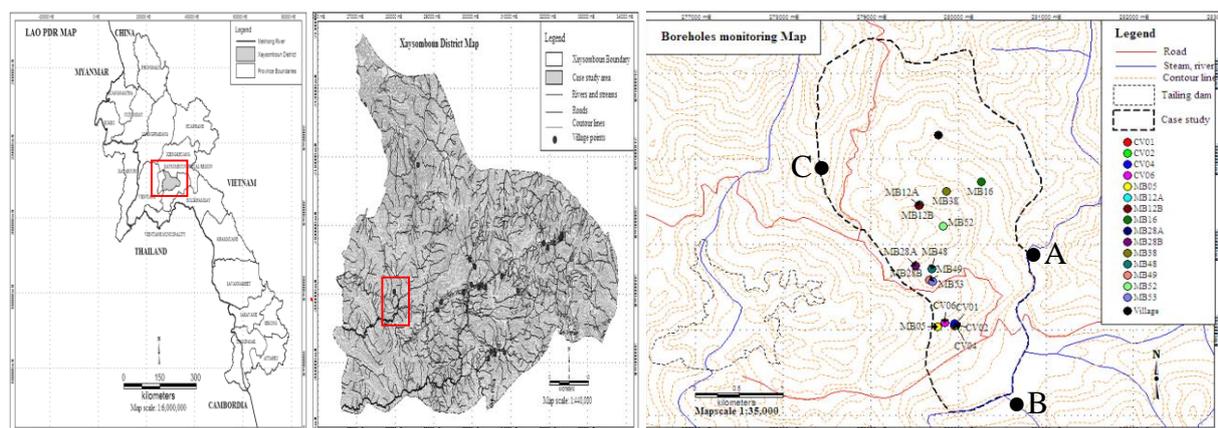


Figure.1. Study site and observation points in Xaysomboun Province.

3. METHODOLOGY.

3.1. MATHEMATICAL MODEL.

The formula below is expressed to three dimensional groundwater flow, which includes hydraulic conductivities, hydraulic head boundary and initial condition, in this case, it explains to transient three dimension (groundwater hydrograph) in difference of aquifer layers and direction of flow (Heterogeneous and anisotropic medium) and hydraulic conductivity will be aligned with the coordinate directions Eq(1), (McDonald and Harbaugh, 1988). The governing partial differential equation solved numerically in MODFLOW is given in the following form:

$$\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial h}{\partial z} \right) + W = S_s \frac{\partial h}{\partial t} \quad (1)$$

Where

K_{xx} is hydraulic conductivity a long x axe LT^{-1} , K_{yy} is hydraulic conductivity a long y axe (LT^{-1}), K_{zz} is hydraulic conductivity a long z axe (LT^{-1}), h is hydraulic head(L), W is volume metric flux per unit volume represented to sink and or/source of water if $W < 0.0$ flow out of groundwater system and if $W > 0.0$ flow into groundwater system (T^{-1}), S_s is specific storage of the porous material (L^{-1}) and t is time of movement (T) (Peter Szucs, et al, 2011).

3.2. FINITE DIFFERENCE MODEL

Finite Difference Method (FDM) is a technique of advanced mathematical model, in terms of mathematical model, the model is used partial differential equation to simulate and solve problem (Gerald W. Recktenwald, 2011), in fact, FDM is a grid system, including row (i), column(j) and layer(k) of a interested domain, the grid system will be identified and developed by super imposing a system of nodal point over the problem domain. (Philip B. Bediet et al, 1994). In addition, nodes can be located inside cells (block centered or intersection of grid system (mesh centered)). Hence, aquifer properties and head values will be assumed to be constant value in a block centered, and finite difference model will not be evaluated the node points, because the model will not develop that surrounding area (Philip B. Bediet et al., 1994). Therefore, behind of the model there is an equation term of the mathematical model by employing Laplace' equation in three dimensions for steady state groundwater flow to evaluated the head of the grid system.

$$\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial h}{\partial z} \right) + W = 0 \quad (2)$$

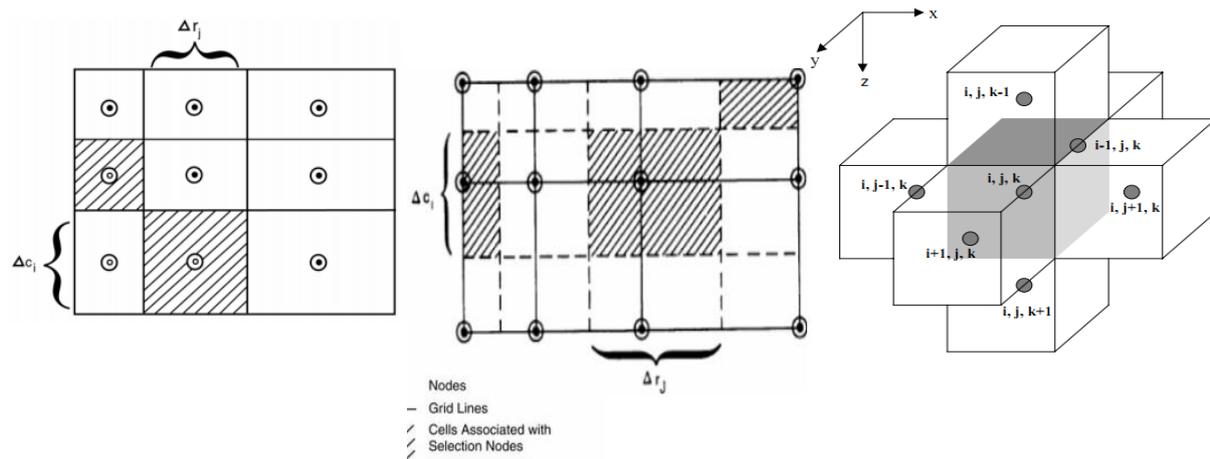


Figure.2. The index system used for the finite difference (finite-volume) grid.

The interfaces between node (i, j, k) and the six adjacent nodes are shown as shaded surfaces.

3.3. CONCEPTUAL MODEL

3.3.1. GRID DESIGN MODEL

Surface area of the study site approximately 693.3 hectares. Therefore, the case study is subdivided into various small grids with finite difference in order to easily comprehensive and more accuracy. In general, the model consists of x , y and z in real projection or i , j and k in the model as three dimensions which means row, column and thickness of the aquifer layer, respectively.

The model is constructed based on lithological (boreholes) data which consists of limestone, schist, redbed siltstone and breccia lithology, and then grid model is designed and consists of 89 rows, 53 column and 4 layers, the length are 2650 m and 4450 m in x and y respectively, and the horizontal spacing is uniformly with thickness is 247.8 m. Based on this the original cell starts from 278370 m easting and 2087009 m northing, as groundwater model has classified into 4 layers, thickness of each layer between 1.2 m to 108.9 m ,1.5 m to 59.6m ,2 m to 57.3m and 7.8 m to 37.6 m , first , second , third and fourth layer, respectively. Hence numbers of cells are 18868 cells design and numbers of nodes are 24300 nodes as shown in Fig.3 and Fig.4, the model is applied boundary matching method to create the 3D MOFLOW modeling.

3.3.2. INITIAL CONDITION

Starting hydraulic head model is very important for groundwater water modeling they have shown in Fig.5, if determining the starting hydraulic head is so big and too small, it will take long time to calibrate and very difficult to have the actual hydraulic head and simulated head to meet as the purpose of calibration. Therefore, the study has applied elevation from

3dimensional grid model, in this case after input elevation value of the grid cell model, it needs to do interpolation from the model in order to have very proper starting hydraulic head, and the model achieves four difference values on individual grid layer.

3.3.3. BOUNDARY CONDITION

In general, boundary conditions represent to the physical or hydraulic feature of terrain. Therefore, before establishing the model, boundary condition should be clearly defined and identified in order to do groundwater modeling. However, there are three different types of the boundary conditions (Rana Amin Sulaiman Kharmah, 2007) as following:

TYPE-1 Specified head boundaries condition will be used to model boundaries when knowing the hydraulic head values, in other words know as Dirichlet boundary condition of the model.

$$1. \text{ Specified head boundaries (Dirichlet)} \quad h(x, y, z, t) = \text{Constant} \quad (3)$$

TYPE-2 Specified flux boundaries condition are used to model boundary if flux are known values, it sometimes is also known as Neumann boundary condition of the model

$$2. \text{ Specified flux boundaries (Neumann)} \quad \frac{dh(x, y, z, t)}{dn} = \text{Constant} \quad (4)$$

TYPE-3 Head dependent boundaries are used to model boundaries condition; it is depending on the changing of the hydraulic head for instance: river, stream, lake at the external boundary condition of the region, and it is also known as Cauchy boundary condition.

$$3. \text{ Head dependent boundaries (Cauchy)} \quad \frac{dh}{dn} + ch = \text{Constant} \quad (5)$$

In fact, among of three boundaries condition are only general concepts of boundary condition in the model. Therefore, in order to define boundary condition in the groundwater model, it needs to know the environment of the case study and then can determine the boundary according to phenomenon of terrain or topography.

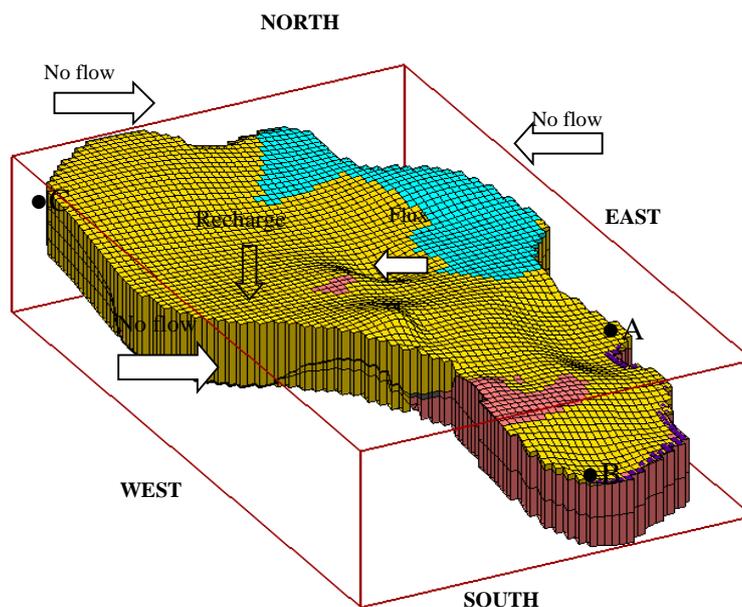


Figure.3. 3D conceptual model

changing hydraulic conductivities with trial and error values until it become acceptable values as calibration target as intended ,they have shown from Fig.6.

3.5.1. Recharge calibration in the model

Groundwater balance is a part of groundwater modeling, due to inflow and out flow need to be the same in final summary or difference is not much. Thus, groundwater balance is $-0.002 \text{ m}^3/\text{d}$ and percent discrepancy is $0.00007 \text{ m}^3/\text{d}$, Recharge rate has adjusted from 2% to 12% from annual rainfall and it is found 7% is reasonable recharge to groundwater modeling.

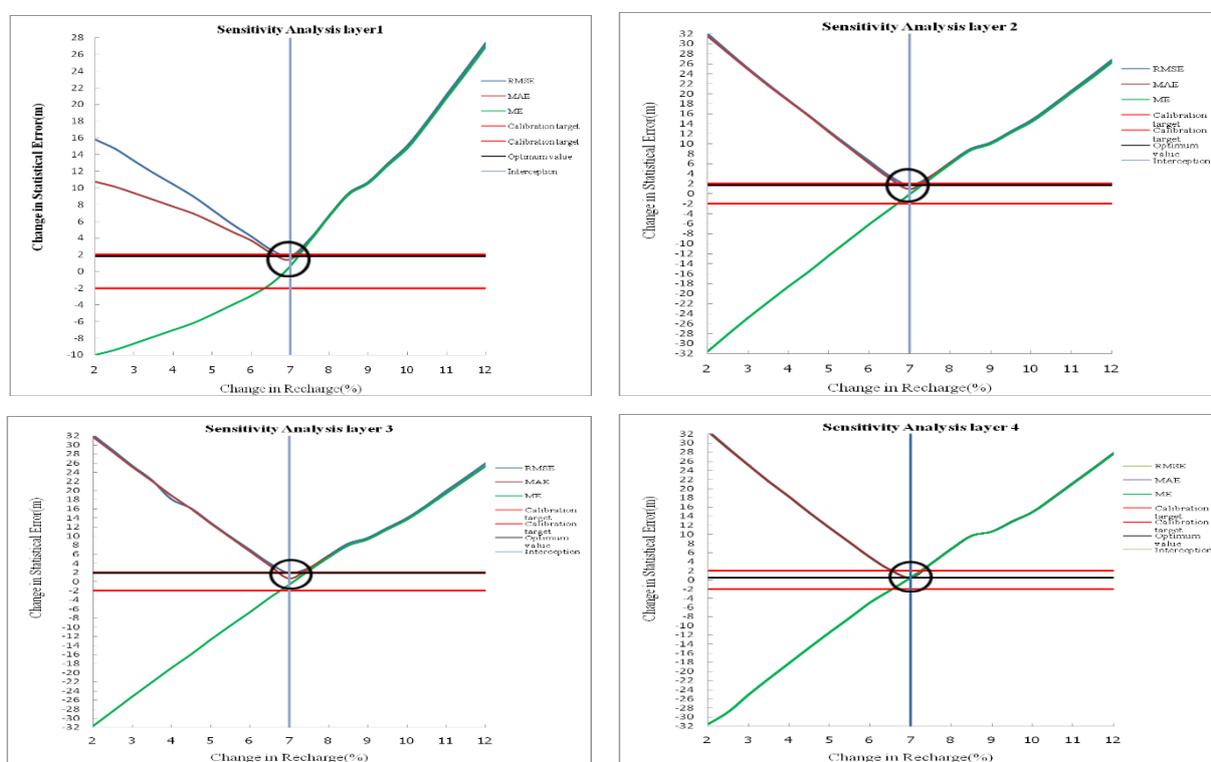


Figure.6. Recharge calibration in the model

Fig.6 has illustrated the variation of statistical error when adjusting percentage and volume of recharge between 2% to 12%. Therefore, the optimum values are inside the black circles as shown between red straight lines of every scenario.

Horizontal hydraulic conductivity and horizontal anisotropy values is adjusted when recharges are fixed and optimum values inside the black circles or Table.1 shows summary of input parameters when recharge is fixed.

4. Results and Discussion

Groundwater balance is a part of groundwater modeling, due to inflow and out flow need to be calculated based on the conceptual model. Therefore, groundwater balance is $-0.0023 \text{ m}^3/\text{d}$ and percent discrepancy is $0.00007 \text{ m}^3/\text{d}$, recharge rate has adjusted from 2% to 12% from annual rainfall and it is found 7% is reasonable recharge which infiltrate through fracture and faults of the aquifer structure to groundwater modeling as shown in Fig.7.

The screenshot shows a software window titled 'Flow Budget' with two tabs: 'Cells' and 'Zones'. The 'Zones' tab is active, showing a dropdown menu for 'Zone' set to 'All zones' and an unchecked checkbox for 'Use all timesteps'. The main area contains a table with two columns: 'Budget Term' and 'Flow (m³/d)'. The table is divided into sections for 'IN:', 'OUT:', and 'SUMMARY:'. The 'IN - OUT' and 'Percent Discrepancy' values in the 'SUMMARY' section are circled in red.

Budget Term	Flow (m ³ /d)
IN:	
Constant heads	787.63353800774
Recharge	2464.8280441761
Total IN	3252.4615821838
OUT:	
Constant heads	3252.463909626
Recharge	0.0
Total OUT	3252.463909626
SUMMARY:	
IN - OUT	-0.002327442169
Percent Discrepancy	0.0000715594054
Flow Budget for Zone 1	
IN:	
Constant heads	787.63353800774
Recharge	2464.8280441761
Total IN	3252.4615821838
OUT:	
Constant heads	3252.463909626
Recharge	0.0
Total OUT	3252.463909626
SUMMARY:	
IN - OUT	-0.002327442169
Percent Discrepancy	0.0000715594054

Figure.7. Groundwater budget for steady state in study area.

Hydraulic conductivities are depended on material property. Based on boreholes geological data, study site consists of limestone, schist, redbed siltstone and braccia. Hence, it is very hard work to achieve correct hydraulic conductivities of individual material. Eventually, it found appropriate values as following: Horizontal hydraulic conductivities of limestone, schist, redbed siltstone and braccia are 0.1 m/d, 0.36 m/d, 0.19 m/d and 0.01 m/d, respectively, and horizontal anisotropy of limestone, schist, redbed siltstone and braccia are 1 m/d, 12 m/d, 0.3 m/d 0.01 m/ respectively, the model is defined vertical anisotropy (kh/kv) of each material is 10 m/d as shown in Table.1.

Table.1. Summary of input parameters to groundwater model

ID	Aquifer	Kh	Hori_anisotropy	Kh/Kv
1	Limestone	0.1	1	10
2	Schist	0.36	12	10
3	Redbed	0.19	0.3	10
7	Braccia	0.001	0.01	10

The results achieved determinations of coefficient (R^2) of individual layer in steady state, in order to determine confidence of observed and simulated hydraulic head. It needs to know this value to illustrate the confidence of the model. Therefore, as shown in Fig.8 and Table 2, coefficient of determination of first, second, third and fourth layer are 0.963, 0.96, 0.959 and 1, respectively

Table.2. Summary of Statistical error

Layer	ME	MAE	RMSE	R^2
Layer1	0.633	1.415	1.84	0.963
Layer2	-0.108	0.935	1.767	0.96
Layer3	-0.67	1.125	1.953	0.959
Layer4	0.574	0.574	0.574	1

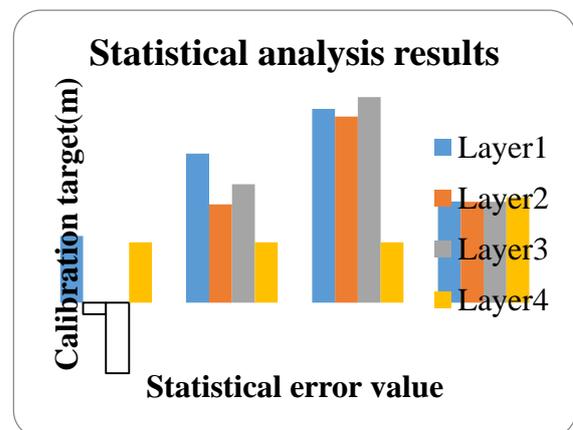
**Figure.8.** Statistical analysis results

Table.3. Summary of observed, computed head and residual in GMS 6.5

Borehole Name	Observed Head	Layer1		Layer2	
		Computed Head	Residual	Computed Head	Residual
MB38	628.45	628.61	0.16	628.85	0.40
MB48	628.82	629.35	0.53	628.85	0.034
MB49	627.5	629.36	1.86	627.71	0.21
MB52	628	628.42	0.428	628.55	0.51
MB53	626	626.96	0.96	626.64	0.64
MB16	623.5	619.97	-3.53 ¹	624.20	0.70
MB28A	631.59	631.93	0.34	631.86	0.27
MB28B	631.07	631.88	0.80	631.75	0.67
MB12A	633.5	632.274	-1.24	633.06	-0.43
MB12B	633.82	632.70	-1.1	633.16	-0.65
CV01	609.122	610.4	1.28	610.32	1.20
CV02	609.118	611.27	2.15 ²	610.53	1.42
CV04	611.368	612.30	0.94	611.48	0.11
CV06	613.5	614.76	1.26	613.13	-0.36
MB05	617.5	622.09	4.59 ³	611.11	-6.38 ⁴

¹ Fair calibration of MB16,layer1² Fair calibration of CV02,layer1³ Poor calibration of MB05,layer1⁴ Poor calibration of MB05, layer2

Borehole Name	Observed Head	Layer3		Layer4	
		Computed Head	Residual	Computed Head	Residual
MB38	628.45	628.96	0.51	629.03	0.58
MB48	628.82	627.35	-1.46		
MB49	627.5	625.87	-1.62		
MB52	628	628.60	0.60		
MB53	626	625.45	-0.54		
MB16	623.5	624.08	0.58	624.06	0.56
MB28A	631.59	631.69	0.105		
MB28B	631.07	631.51	0.43		
MB12A	633.5	633.16	-0.33		
MB12B	633.82	633.20	-0.61		
CV01	609.122	609.61	0.49		
CV02	609.118	609.79	0.67		
CV04	611.368	610.64	-0.72		
CV06	613.5	612.2	-1.25		
MB05	617.5	610.59	-6.90 ⁵		

⁵ Poor calibration of MB05,layer3

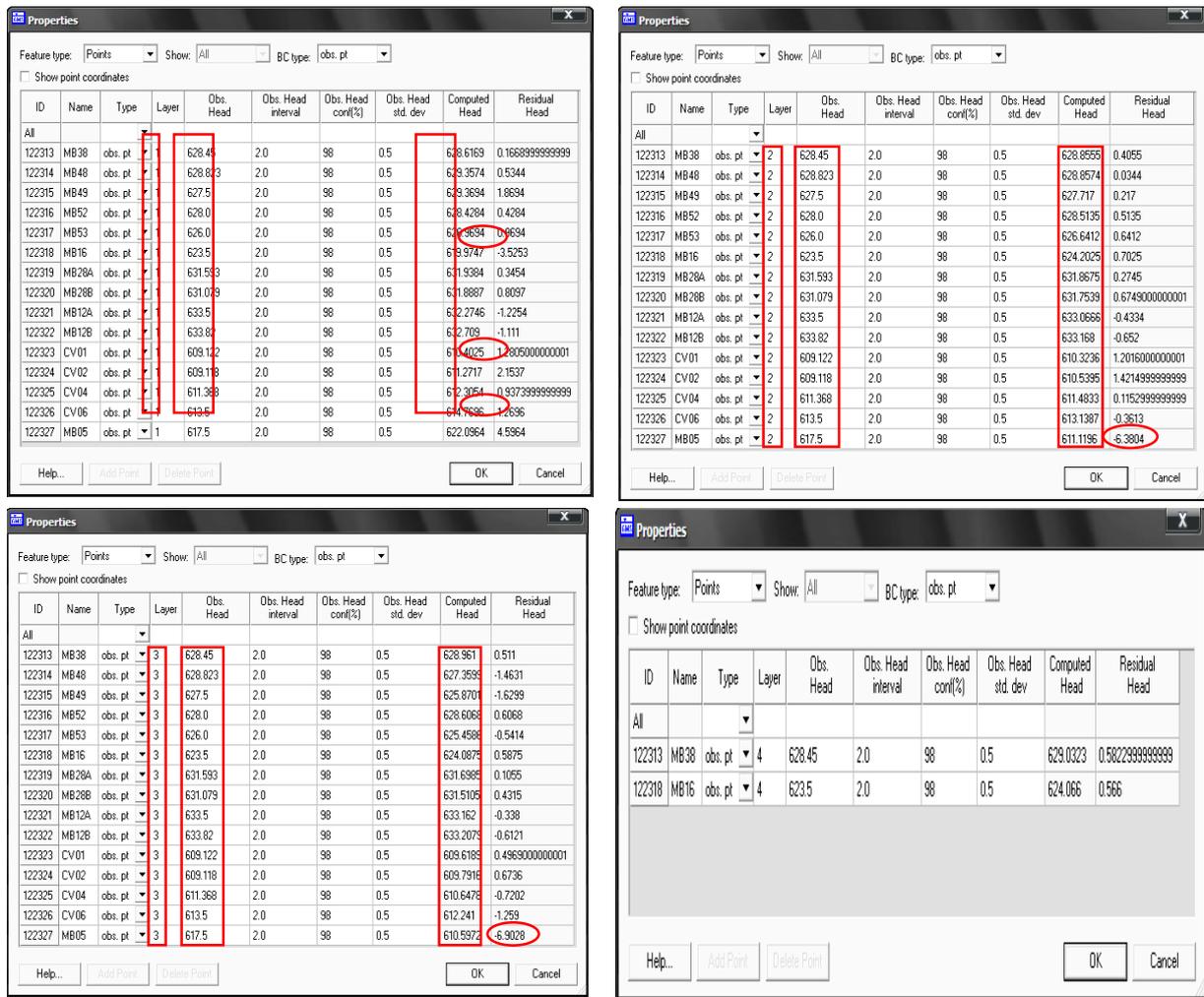


Figure.9. Attribute table generation of observed and computed head layer 1, 2, 3 and 4

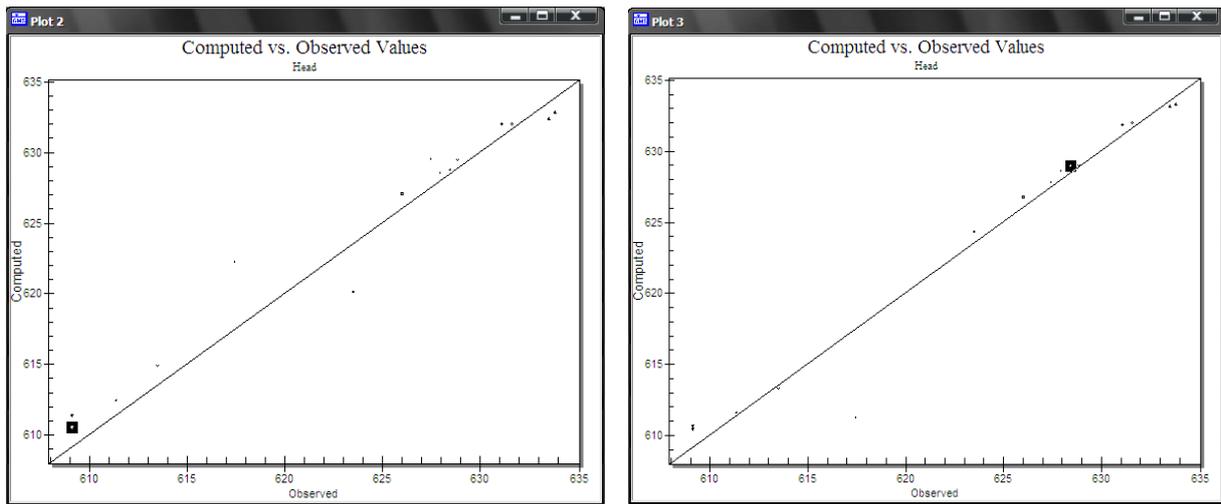


Figure.10.Scatter plot of coefficient of determination (hydraulic head layer1 and 2)

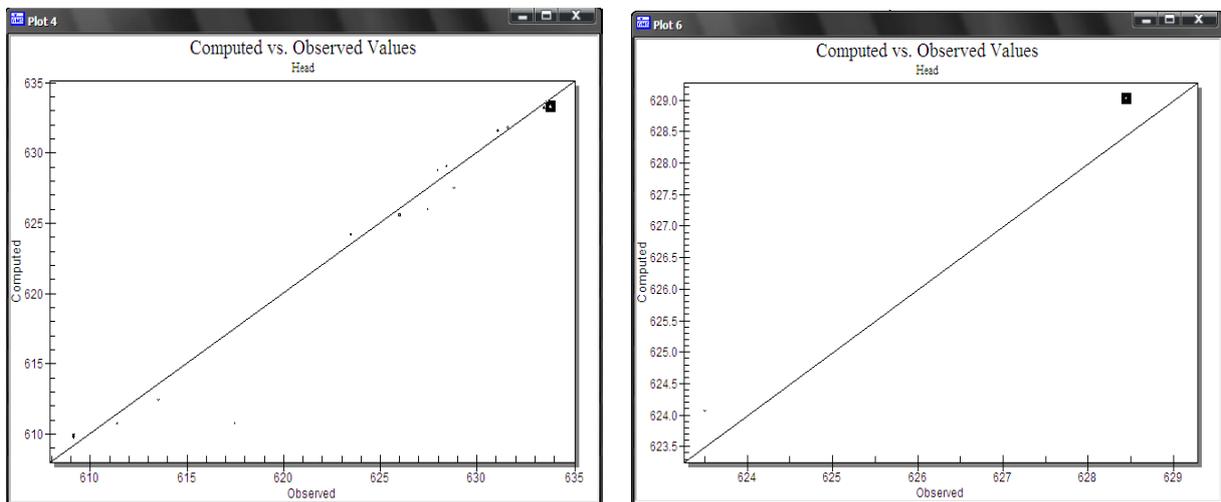


Figure.11.Scatter plot of coefficient of determination (hydraulic head layer3 and 4)

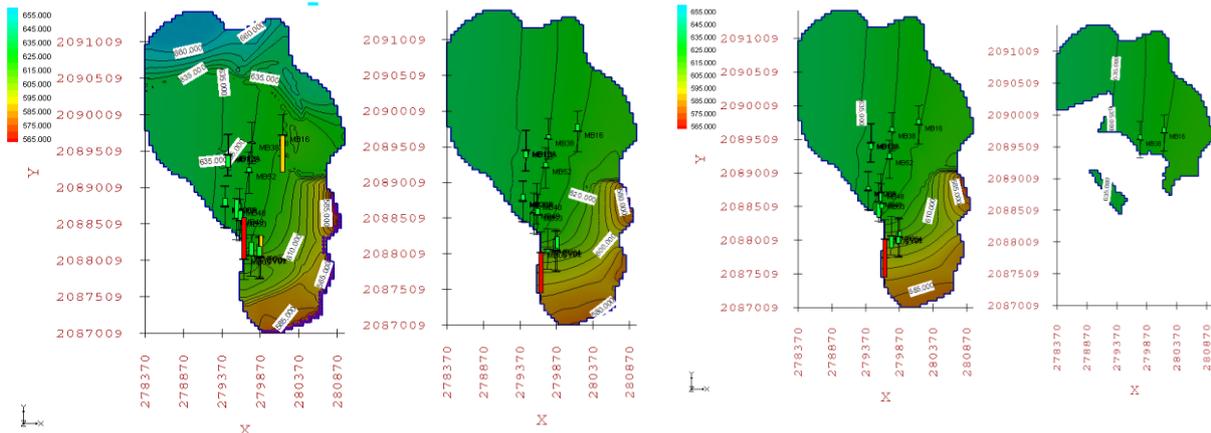


Figure.12.hydraulic head from layer1 to 4 after calibrated

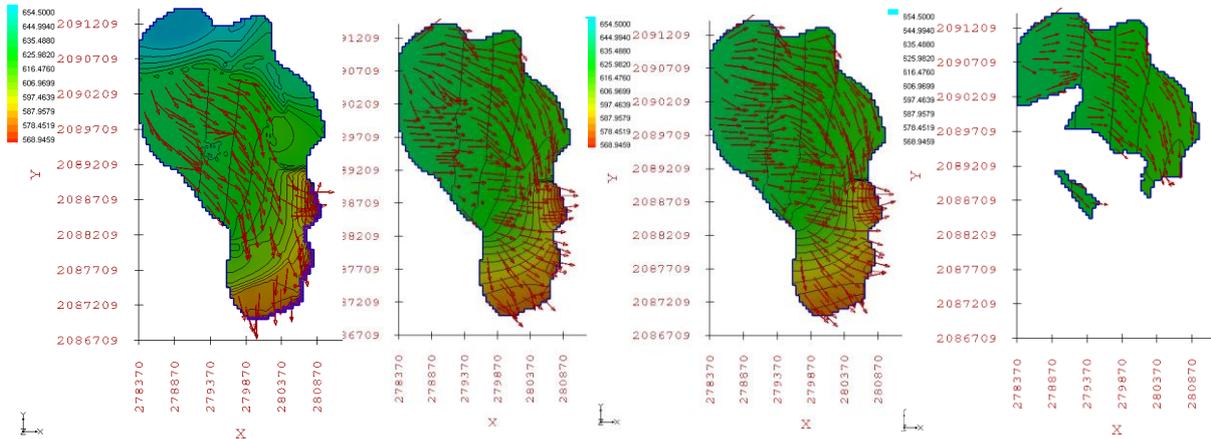


Figure.13. Groundwater flow direction from layer1 to 4

Fig. 10 and 11 have scattered plot of observed head and computed head in order to compare how confidence of the model. Therefore, in average model is significantly possible to trust when considering R^2 according to Table.2.

Fig.12. has shown hydraulic head contour which generated from GMS 6.5 in different scenario layers from layer 1 to 4 with showing computed hydraulic head in green, yellow and red color, the green color are well calibrated, yellow color are acceptable but red color are poor calibrated, indicated in Table.3, Then, Fig.13 has illustrated flow direction of groundwater in the model of each layer, so that flow direction is going to the Nam MO River which lies on the boundary.

5. Conclusions.

The grid system of the groundwater model covered an area of 2650 m and 4450 m with grid

Cells of size 50 m x 50 m and thickness of 247.8 m is represented in four layers with thickness of each layer by 1.2 m to 78.9 m (top layer), 1.5 m to 59.6 m (first lower layer), 2 m to 47.3 m (second lower layer) and 7.8 m to 37.6 m (bottom layer), respectively.

Calibration model and sensitivity analysis of groundwater modeling, it is an essential of the study in order to come up with the agreement between observed and computed hydraulic head values with trials and errors values to solve the problem, this study has focused on calibration of input parameters such as: recharge, horizontal hydraulic conductivity and horizontal anisotropy, the models come up with reasonable result of each scenario. The root mean square error of steady state of layer 1 to 4 for calibrated outputs are 1.840 m, 1.767 m, 1.963 m and 0.574 m which are within the error tolerance of ± 2 m of hydraulic heads, respectively. Groundwater balance is a part of groundwater modeling, due to inflow and out flow need to be calculated based on the conceptual model. Therefore, groundwater balance is $-0.0023 \text{ m}^3/\text{d}$ and percent discrepancy is $0.00007 \text{ m}^3/\text{d}$. recharge rate has adjusted from 2% to 12% from annual Rainfall and it is found 7% is reasonable recharge which infiltrates through fracture and faults of the aquifer structure to groundwater modeling.

Finally, coefficient of determination (R^2) of individual layer are depicted Table.2, in order to determine confidence of observed and simulated head. It needs to know this value to illustrate the confidence of the model. Thus, coefficient of determination of first, second, third and fourth layer are 0.963, 0.96, 0.959 and 1, respectively, then, groundwater direction moves from north to south east that means it flows from sources to NamMo river.

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