Asian Journal of
Science, Technology, Engineering, and Art

e-ISSN : 3025-4507
p-ISSN : 3025-5287
Index : Harvard, Boston, Sydney University, Dimensions, Lens, Scilit, Semantic, Google, etc

https://doi.org/10.58578/AJSTEA.v1i2.1934

LEAD AND ZINC GROUNDWATER CONTAMINANT TRANSPORT MODELLING USING MT3DMS IN XAYSOMBOUN PROVINCE, LAO PDR

Phoummixay Siharath[1], Somchay Vilaychaleun[2], Khampasith Thammathevo[3], Chankhachone Sonemanivong[4], Soulyphan Kannitha[5], Bounmy Phommakone[6], Keoduangchai Keokhamphui[7], Guillermo III Quesada Tabios[8]

[1,2,3,4,5,7]National University of Laos, Laos
[6]United Nations Development Programme, Laos
[8]University of the Philippines Diliman, Quezon City, Philippines
phoummixay2011@gmail.com; somchay.v@fe-nuol.edu.la

Article Info:

Submitted:	Revised:	Accepted:	Published:
Sep 20, 2023	Oct 10, 2023	Oct 15, 2023	Oct 20, 2023

Abstract

Contaminant transport modelling is commonly applied in the Groundwater Modelling System (GMS). Modular Three-Dimensional Multispecies Transport (MT3DMS) package is one of other packages, developed by the U.S. Geological Survey, this research presents the employing of the M3TDMS package as excellent tools to establish the 3D conceptual model of contaminant transport modeling, simulate and predict the multispecies of Lead and zinc substances which transport in the groundwater, there are 15 boreholes that were observed and monitored, the results of the contaminant transport modeling was found the Lead(Pb) contaminant transport with initial concentrations of 3.96 mg/l at borehole MB48 as point source, the concentration reduced to 0.1 mg/l, after 3,650 days simulation. The initial zinc (Zn) concentration of 0.886 mg/l at borehole CV04 decreases to 0.023 mg/l after 3,650 days simulation.

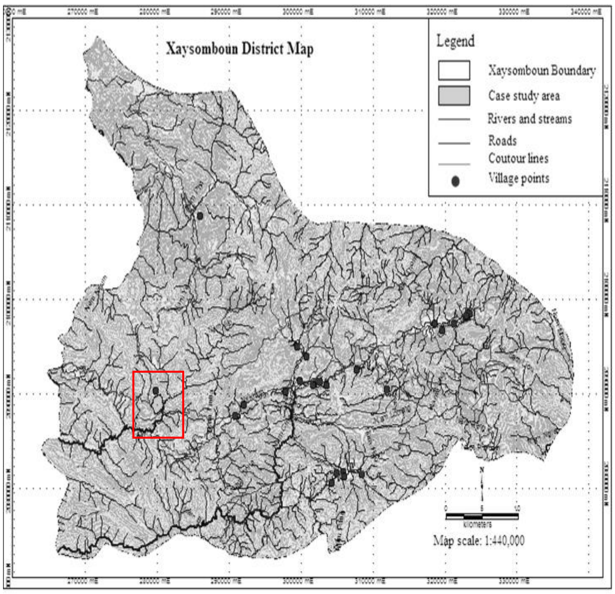
Keywords: Groundwater, Modelling, MT3DMS, Lead (Pb), Zinc (Zn)

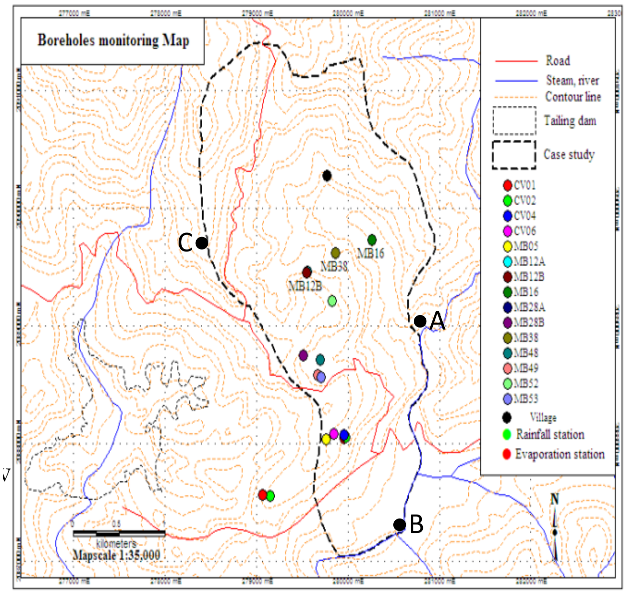
Introduction

The MT3DMS is a Modular Three-Dimensional Multispecies Transport Model for modeling of advection, dispersion, and chemical reactions of contaminants in groundwater systems (Arlen W. Harbaugh, et al.,2000, Phoummixay Siharath, et al.,2022), the package of the MT3DS is usually established and employed the integration of advection and diffusion for contaminant transport modelling, it is able to work and play with chemical reaction of multi-substances with many types of external sink and source in the groundwater system (Gerrit Jousma, 2008, Chunmiao Zheng , 1999). Besides that, the MT3DMS is applied and modelled with the mixed Eulerian - Lagrangian approaches, that called Partial Differential Equation (PDE) numerical methods to deal with the 3-dimensional advective, dispersive and reactive equations in the groundwater contaminant transport modelling. Moreover, the MT3DMS has been established and applied the Finite Difference Methods (FDM) in with any block centered flow model as well as MODLFOW (C.Zheng, 1990, Randall J. LeVeque, 2005).

The Study Area

The study area is a central of Laos and far from Vientiane Capital approximately 120 km, according to the characteristic the physical terrain, it is extremely mountainous area (Chankhachone Sonemanivong, et al.,2023), the province has established since 13 December, 2013 (Lao Statistics Bureau, 2015), that connects to four provinces from the North to the South. Therefore, the highest mountain is called Phu Bia (Soneteng Buaxaiya, et al, 2021, Phu Bia Mining Annual review, 2009). From geographic terrain, the Mountain has altitude of 2,820 meters and the lowest is 240m of mean sea level (NIER,2022, Geography department, 2010). There are approximately 693.3 hectares or 6.933 square kilometers within the boundary surface area of the study area; it has operated the Sepon mines in the Savannakhet Province since 2003 under Australian company (Yuji Nishikawa et al., 2006), the area has been implemented and mined on copper and gold mines since 2008. Therefore, there are 15 groundwater quality monitoring points as indicates in Figure.1 and 2 for the research.





Mathematical Model

M3TDMS package consists of contaminant transport modeling, which obviously applied the 2 or 3-dimensional of advanced mathematical equation to elaborate from physical to mathematical model (Jacob Bear , Alexander H.-D. Cheng, 2010) , the PDE will be employed in the movement of advection, diffusion in the groundwater contaminant transport modelling (Gerald W. Recktenwald, 2011).

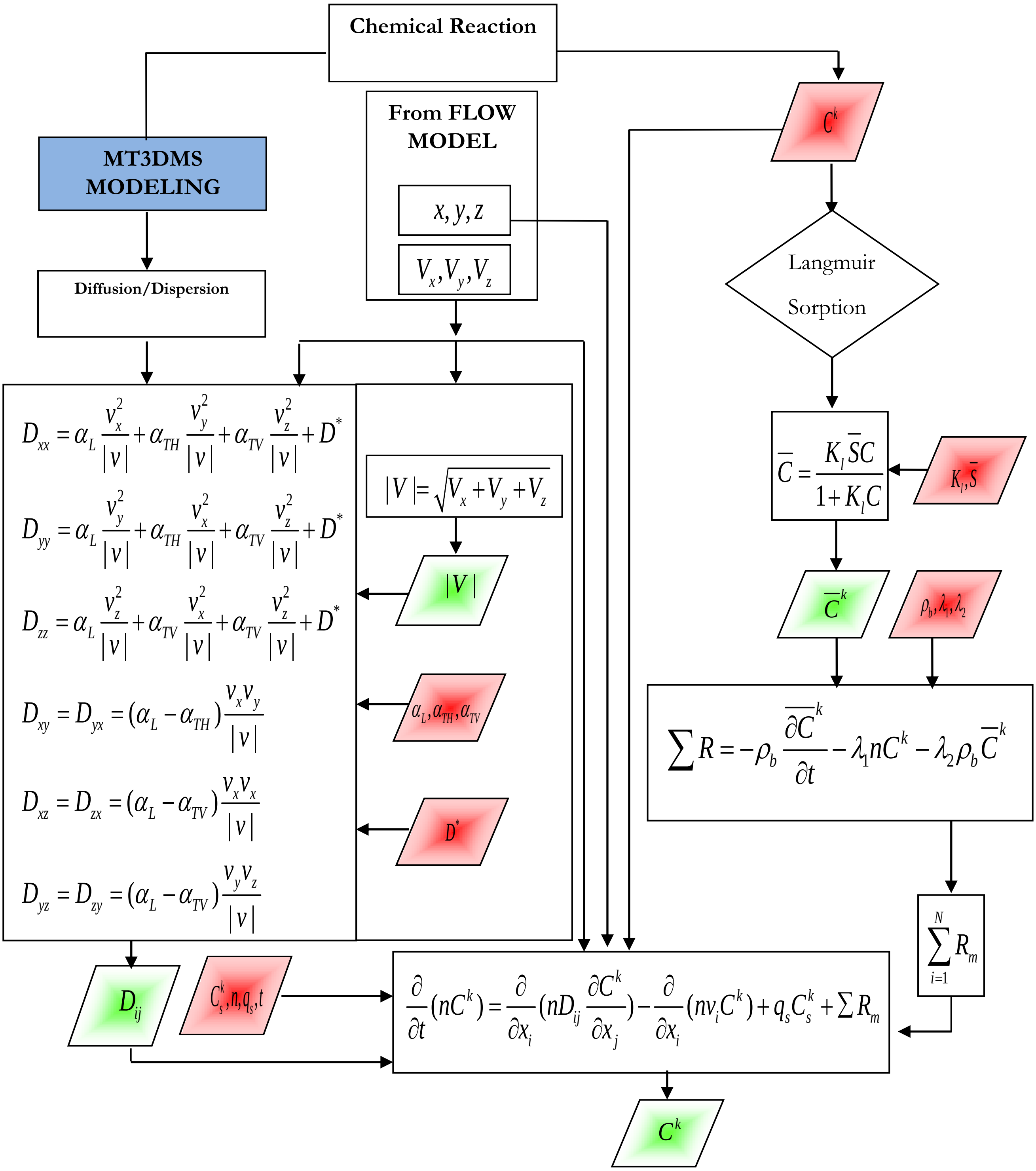


Figure.3. MT3DMS Model Diagram

Initial Condition

Most of the models were employed numerical method to simulate the groundwater modelling, Therefore, prior to dealing with and finding the precise results, initial condition is required to identify to support the groundwater modeling, the governing equation shows as below:

$$C(x, y, z, t) = c_0(x, y, z) \text{ on } \Omega, t = 0 \qquad \text{(a)}$$

Where: $c_0(x, y, z)$: Known concentration distribution.

Ω:Denotes the entire model domain.

Boundary Condition

Boundary condition also plays important role for contaminant transport modeling to model the chemical substances in groundwater modelling. Additionally, there are three types of boundary conditions to apply in contaminant transport modeling (MT3DMS) (Siharath phoummixay and Guillermo III Quesada Tabios,2020, Philip B. , et al., 1994) such as:

Dirichlet: the concentration is specified along the boundary for the entire duration of the simulation

$$C(x, y, z, t) = c(x, y, z, t) \text{, on } \Gamma_1,\ t \geq 0 \qquad \text{(b)}$$

Where: the specified concentration boundary,

Specified concentration along. The specified concentration may be set to vary with time.

Neumann: the concentration gradient is specified across the boundary.

$$\theta D_{ij}\left(\frac{\partial C}{\partial x_j}\right) = f_i(x, y, z, t), \text{ on } \Gamma_2, t \geq 0 \qquad \text{(c)}$$

Where: Known function representing the dispersive flux normal to the boundary, a special case is a no dispersive mass flux boundary where $f_i(x, y, z, t) = 0$

Cauchy: The Cauchy boundary condition, both concentration value and concentration gradient are specified.

$$\theta D_{ij}(\frac{\partial C}{\partial x_j}) - q_i C = g_i(x,y,z,t), \text{ on } \Gamma_3, t \geq 0 \quad \text{(d)}$$

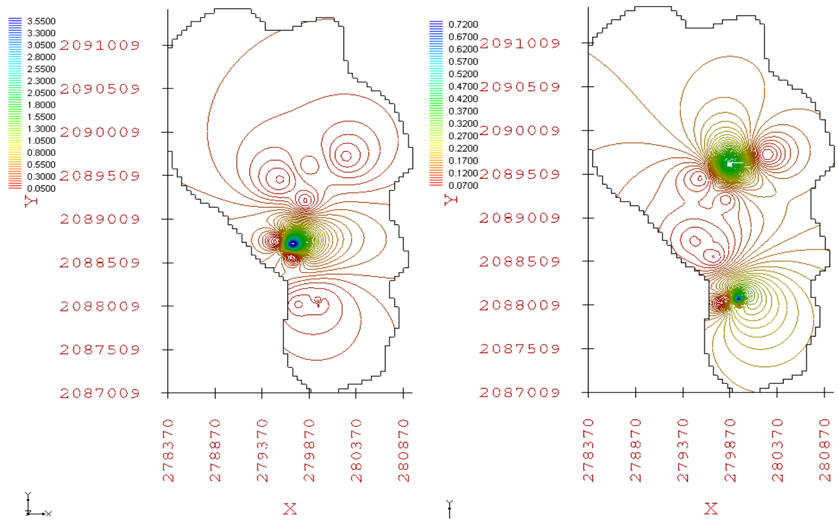


Figure 4. Boundary condition of Lead and zinc substances.

Table.1. Groundwater quality monitoring in domain area

Hole_ID	X	Y	Z	Pb (mg/l)	Zn (mg/l)
MB38	279862.4	2089621	630.807	0.2749	0.4600
MB48	279695.7	2088716	631.854	3.9628	0.0900
MB49	279664.7	2088585	631.591	0.0540	0.0700
MB52	279825	2089219	631	0.0449	0.0944
MB53	279705.6	2088562	630.207	0.0398	0.0700
MB16	280261.6	2089732	630	0.0386	0.0725
MB28A	279510.1	2088748	640.73	0.0323	0.0700
MB28B	279514.3	2088754	639.706	0.0335	0.0850
MB12A	279554	2089464	640.866	0.0323	0.0775
MB12B	279544.7	2089454	641.797	0.0561	0.082
CV01	279960	2088047	615.797	0.0661	0.0724
CV02	279970.7	2088055	616.27	0.0524	0.0724
CV04	279958.2	2088072	615.349	0.3099	0.8863
CV06	279847.5	2088082	614.341	0.0786	0.1106
MB05	279760.6	2088032	625.353	0.0863	0.0649

Calibration Method

The calibration model was iterated and repeated by trials and errors values, the models were run until the results come up with the fitness and acceptable observed and simulated concentration (Paul K.M. van der Heijde,1992). Eventually, the model shows the final outcomes of each scenario of the contaminant transport modelling (Sandown Mark et al, 2011) the equations are showed as below:

Root Mean Squared Error

(e)

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}[(h_{ob} - h_{si})_i]^2}{n}} \quad (8)$$

Where:

RMSE: Root Mean Squared Error m

h_{ob}: Observed concentration from actual site m

h_{si}: Simulated concentration from model m

n: Number of observed well of groundwater

i: Order of observed groundwater numbers

The calibration target perspective indicates how to obtimimze between the observed and simulated values. To have appropriate value in the calibration model, the model iterates to minimize the error value and also to repeat trails and errors values until the model is run completely and successfully and matched with the calibrated target (Jacques.W. Delleur,2006, Sami L.R. Shaheen,2007).

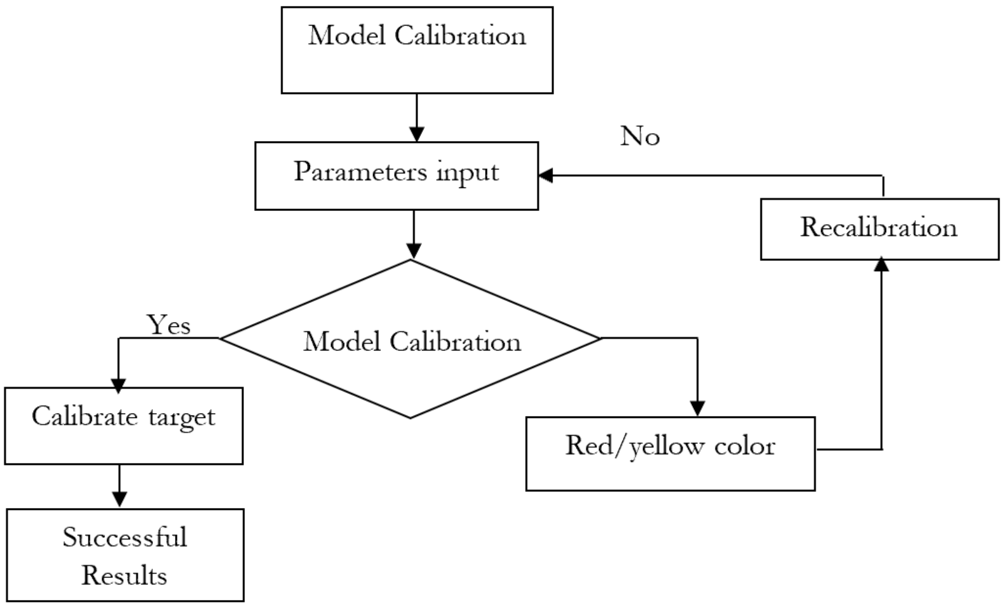


Figure.5. Calibration target perspective

Results and Discussion

Lead and Zinc Findings

The zinc contaminant transport was referred to the groundwater quality that collected from 15 boreholes monitoring. Therefore, the concentration data was processed and employed to the MT3DMS model, it illustrates Lead monitoring at borehole CV04 with highest. An initial concentration of 0.88 mg/l, the final calibration was completely conducted and Figure 4 presents the scatter plot of observed and simulated Lead and zinc concentration.

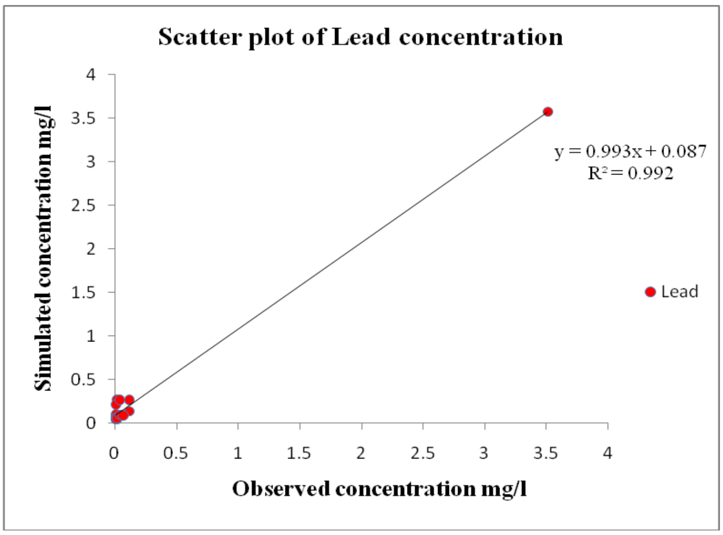


Figure 6. Lead scatter plot (observed and simulated concentration).

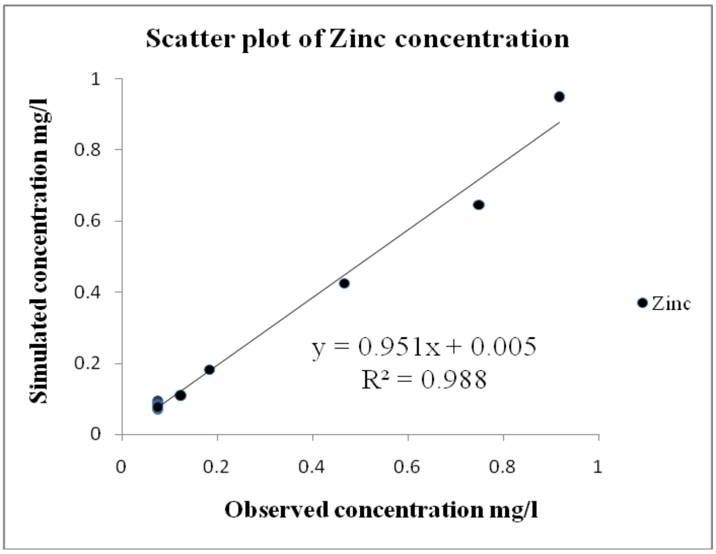


Figure 7. Zinc scatter plot (observed and simulated concentration).

To compare the chemical substance pollutants in the study such as Lead and zinc transport models, there was 3.961 mg/g of Lead substance that indicates the highest concentration at borehole MB48(point source) in the domain site as initial value of concentration, therefore, the Lead concentration is higher than the groundwater standard. The relationship between observed and simulated concentrations calibrated completely as presented in Figure 4 and 5. Additionally, Figure 8 and 9 illustrate on the Lead concentration contour in every year (10 years) and they dispersed and advected slowly from point source to Nam Mo River.

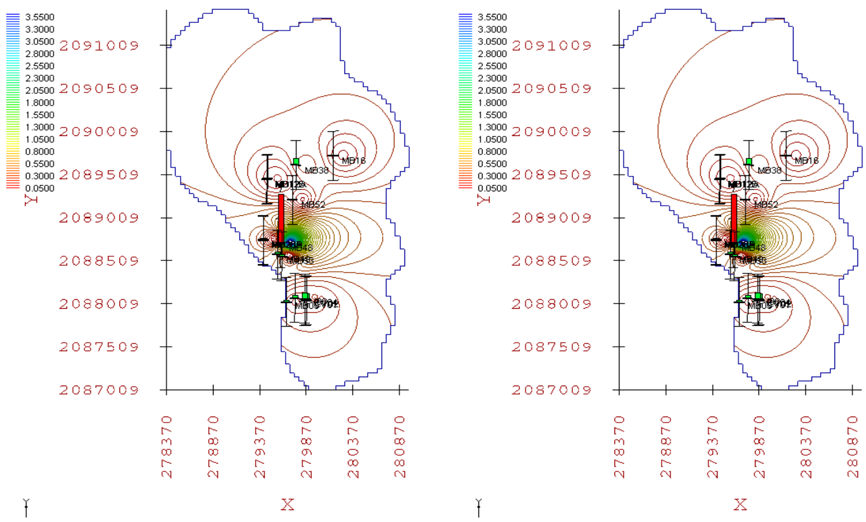


Figure 8. Lead contaminant transport modeling when calibrated (layer 1and 2), (a).

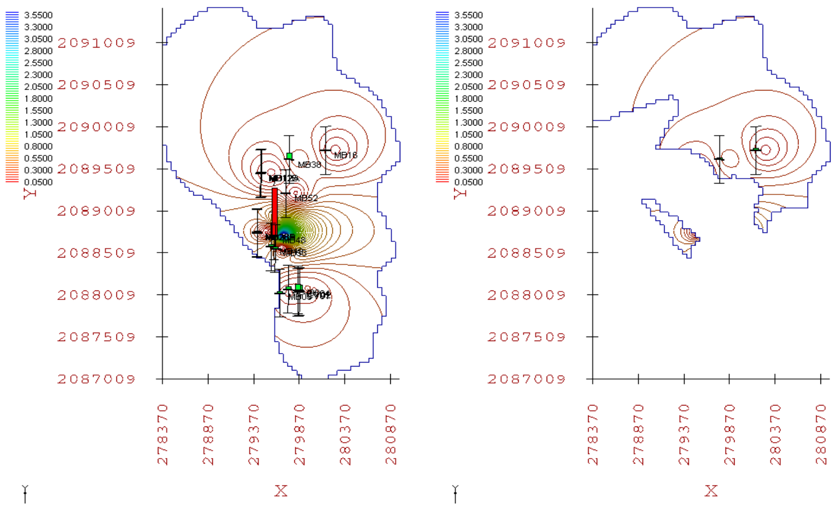


Figure 8. Lead contaminant transport modeling when calibrated (layer 3 and 4), (b).

0 years 1 years 2 years

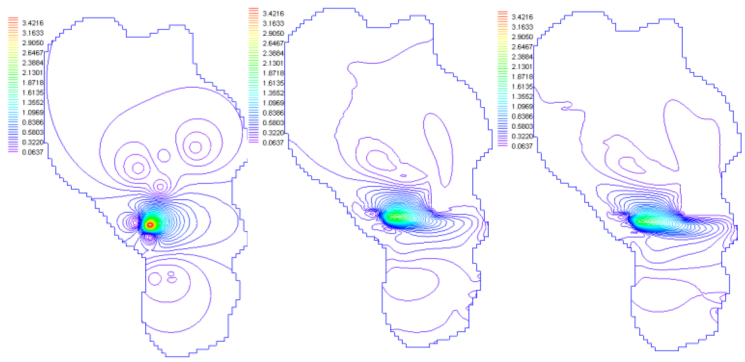


Figure 9. Lead continuous transport modeling (0-3 years simulation), (a)

3 years 4 years 5 years

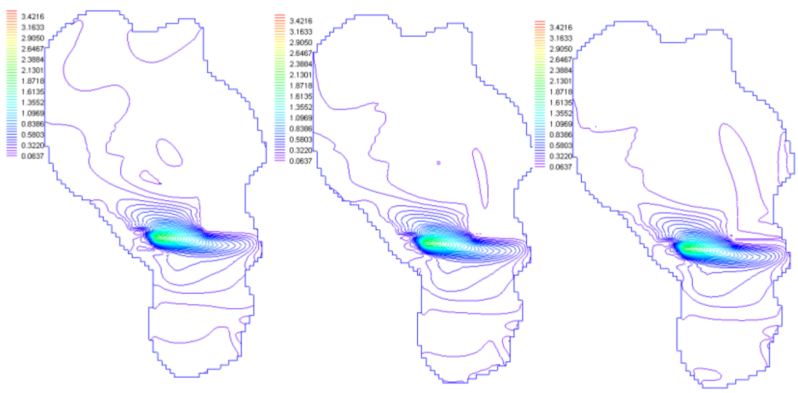


Figure 9. Lead continuous transport modeling (4-5 years simulation), (b)

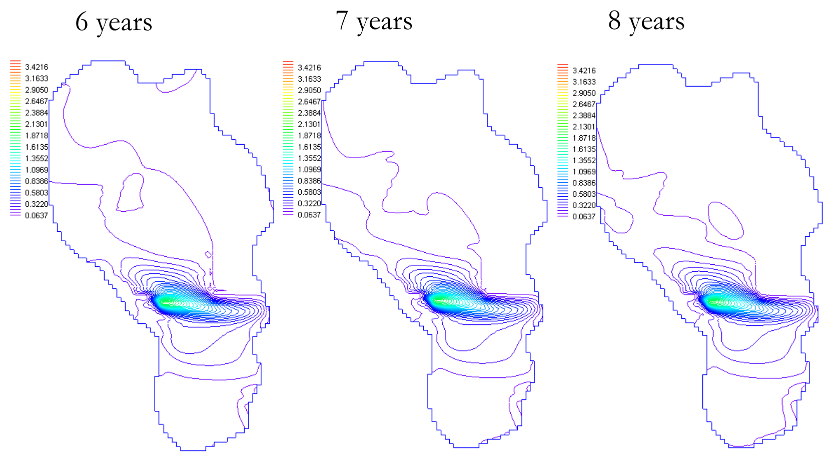


Figure 9. Lead continuous transport modeling (6-8 years simulation), (c).

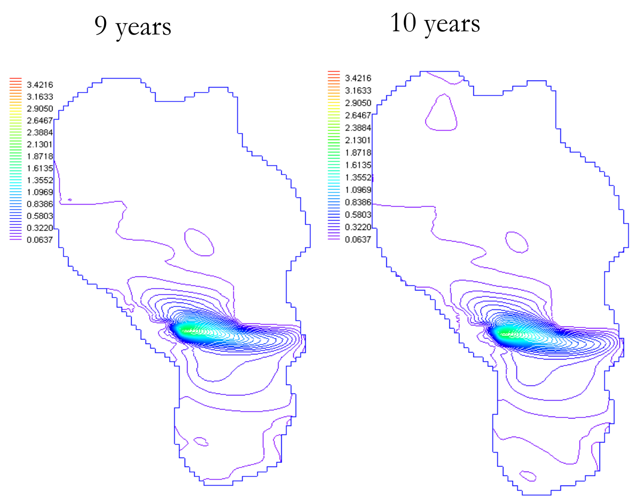


Figure 9. Lead continuous transport modeling (9-10 years simulation), (d).

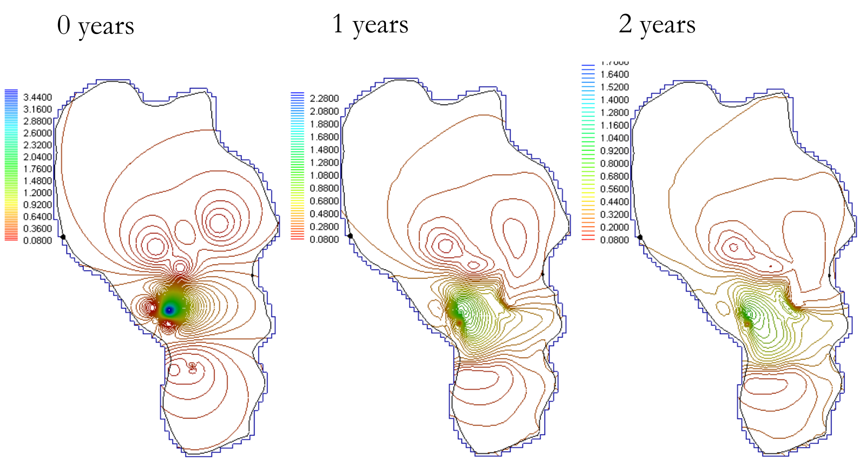


Figure 10. Lead instantaneous transport modeling (0-2 years simulation), (a).

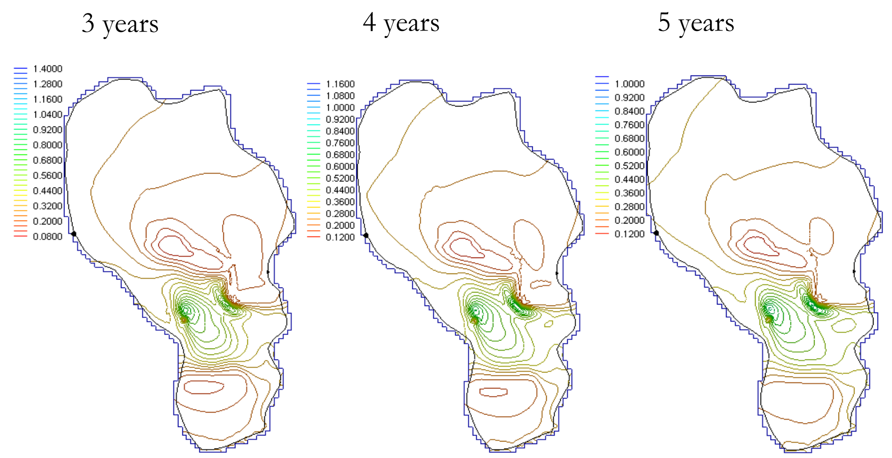


Figure 10. Lead instantaneous transport modeling (3-5 years simulation), (b).

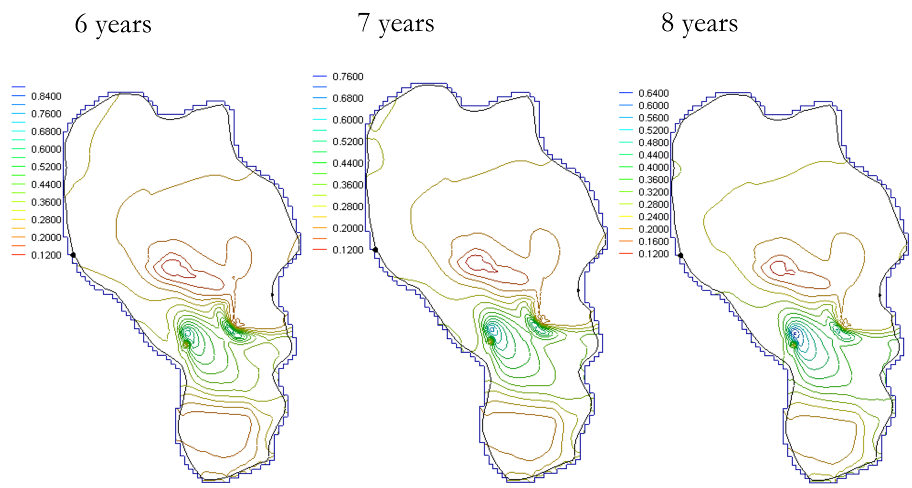


Figure 10. Lead instantaneous transport modeling (6-8 years simulation), (c).

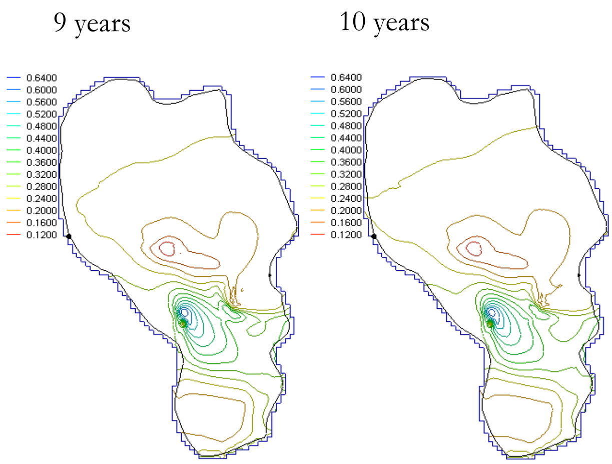


Figure 10. Lead instantaneous transport modeling (9-10 years simulation), (d).

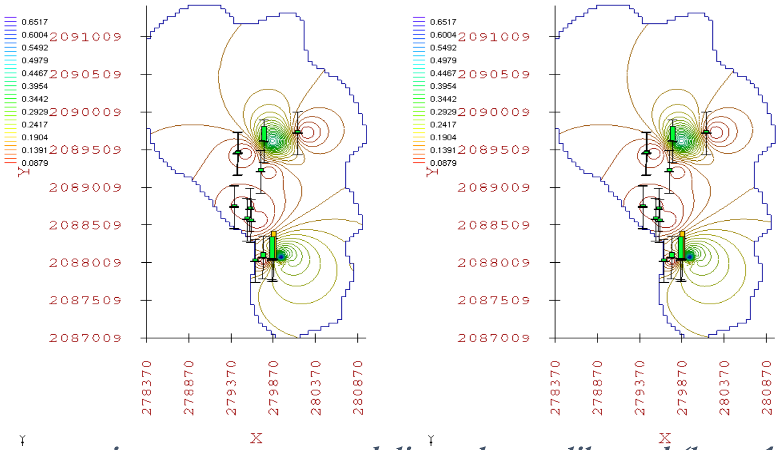


Figure 11. Zinc contaminant transport modeling when calibrated (layer 1and 2), (a).

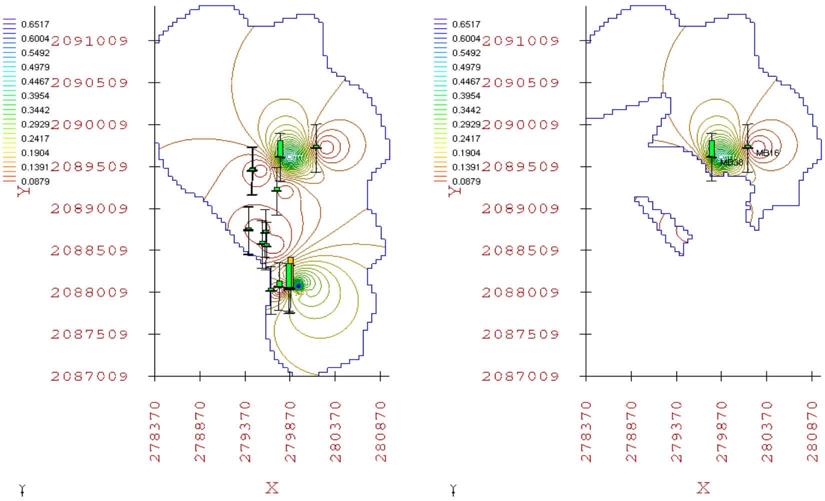


Figure 11. Zinc contaminant transport modeling when calibrated (layer 3 and 4), (b).

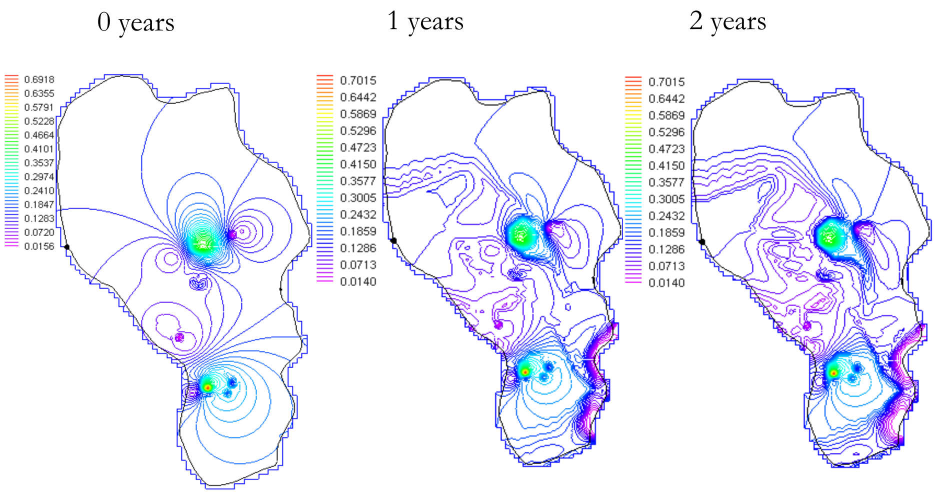


Figure 12. Zinc continuous transport modeling (0-2 years simulation), (a).

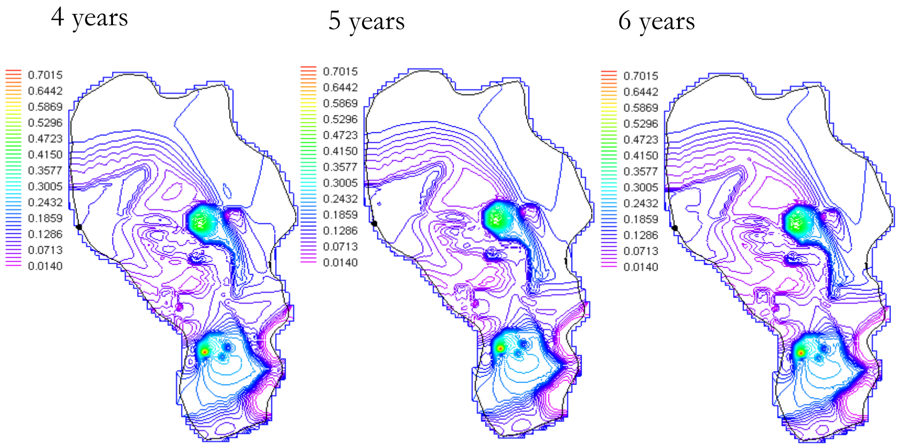


Figure 12. Zinc continuous transport modeling (4-6 years simulation), (b)

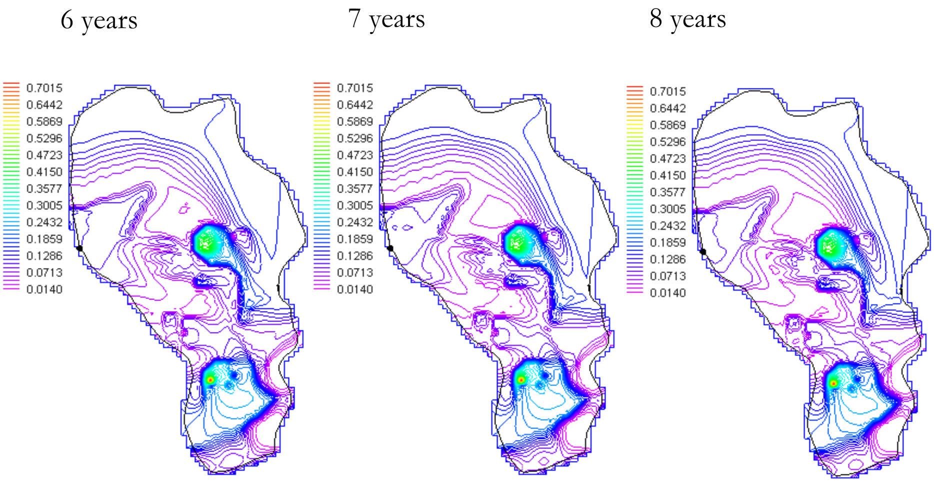


Figure 12. Zinc continuous transport modeling (6-8 years simulation), (c).

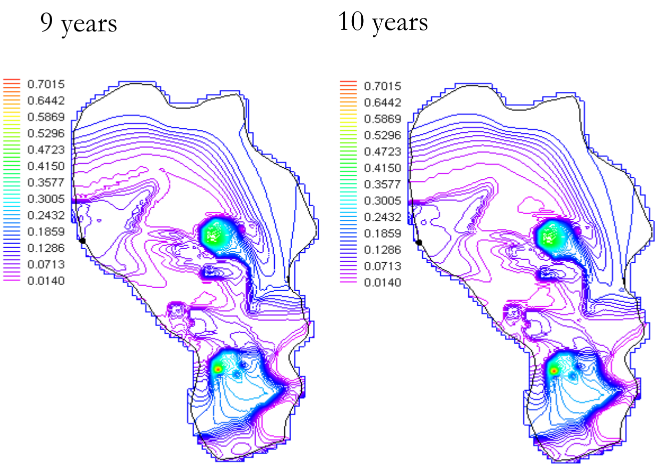


Figure 12. Zinc continuous transport modeling (9-10 years simulation), (d).

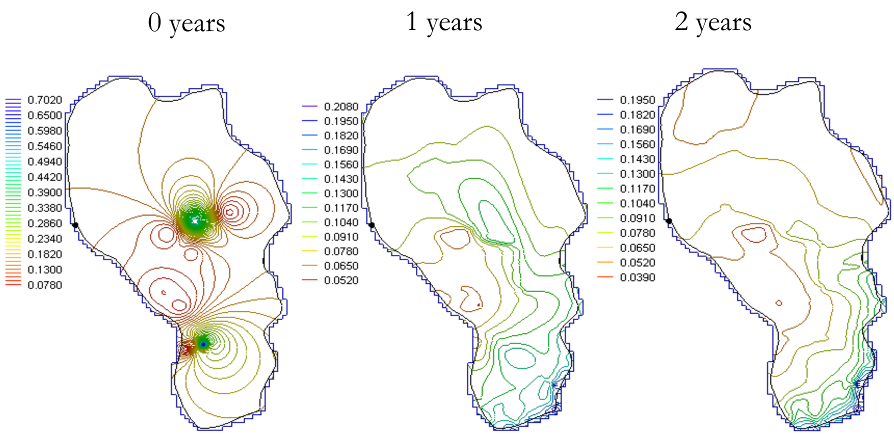


Figure 13. Zinc instantaneous transport modeling (0-2 years simulation), (a).

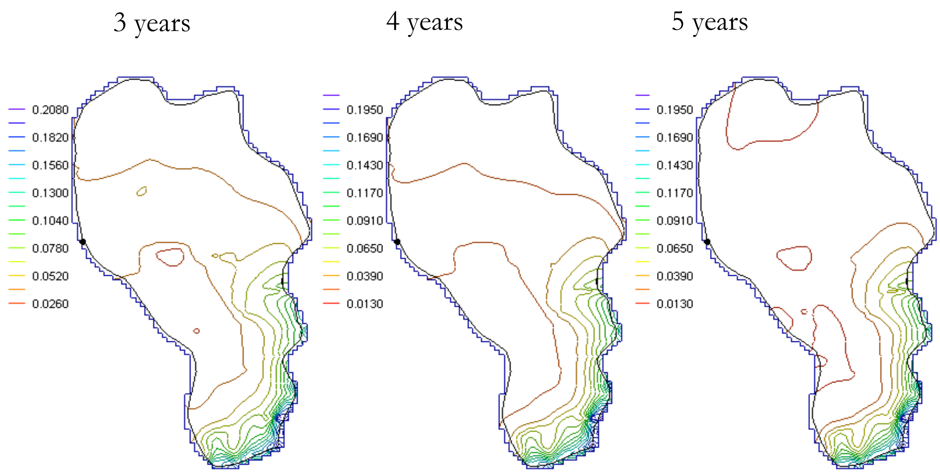


Figure 13. Zinc instantaneous transport modeling (3-5 years simulation), (b)

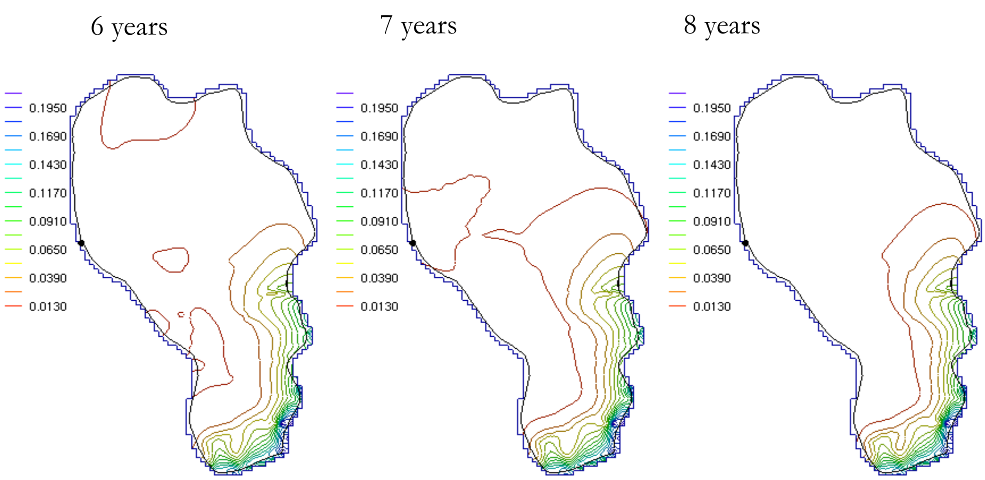


Figure 13. Zinc instantaneous transport modeling (6-8 years simulation), (c).

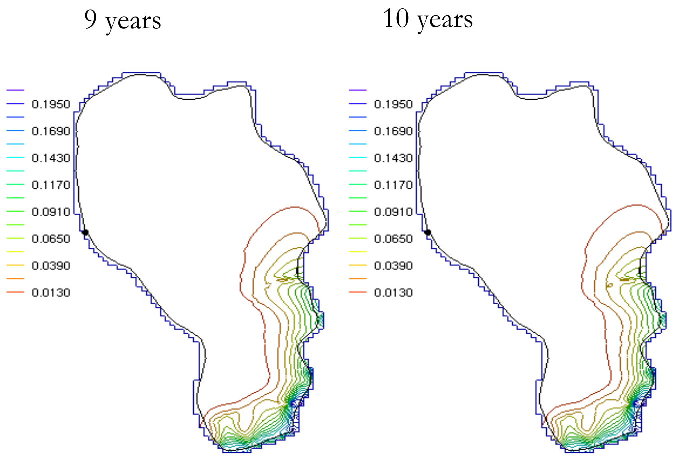


Figure 13. Zinc instantaneous transport modeling (9-10 years simulation), (d).

Figure 6 and 7 present the observed and simulated concentration of Lead and zinc to compare how confidence of the model which indicates in Figure4, consequently, an average model is significantly possible to trust when R^2 are 0.992 and 0.988, respectively.

Figure 8 and 11 show concentration contour of Lead and zinc which generated from MT3DMS in different scenario layers from layer 1 to layer 4 with showing simulated concentration in green, yellow and red color, the green color was well calibrated, yellow color were acceptable but red color was poorly calibrated.

At MB48, as point source of chemical substance concentration reduced, the simulation time increases, thereby given an initial concentration of Lead and zinc at 3.96 mg/l and 0.88 mg/l, respectively at simulate time 0, and the respective substance slightly decreases to 0.1 mg/l and 0.023 mg/l at simulation time 3,650 days.

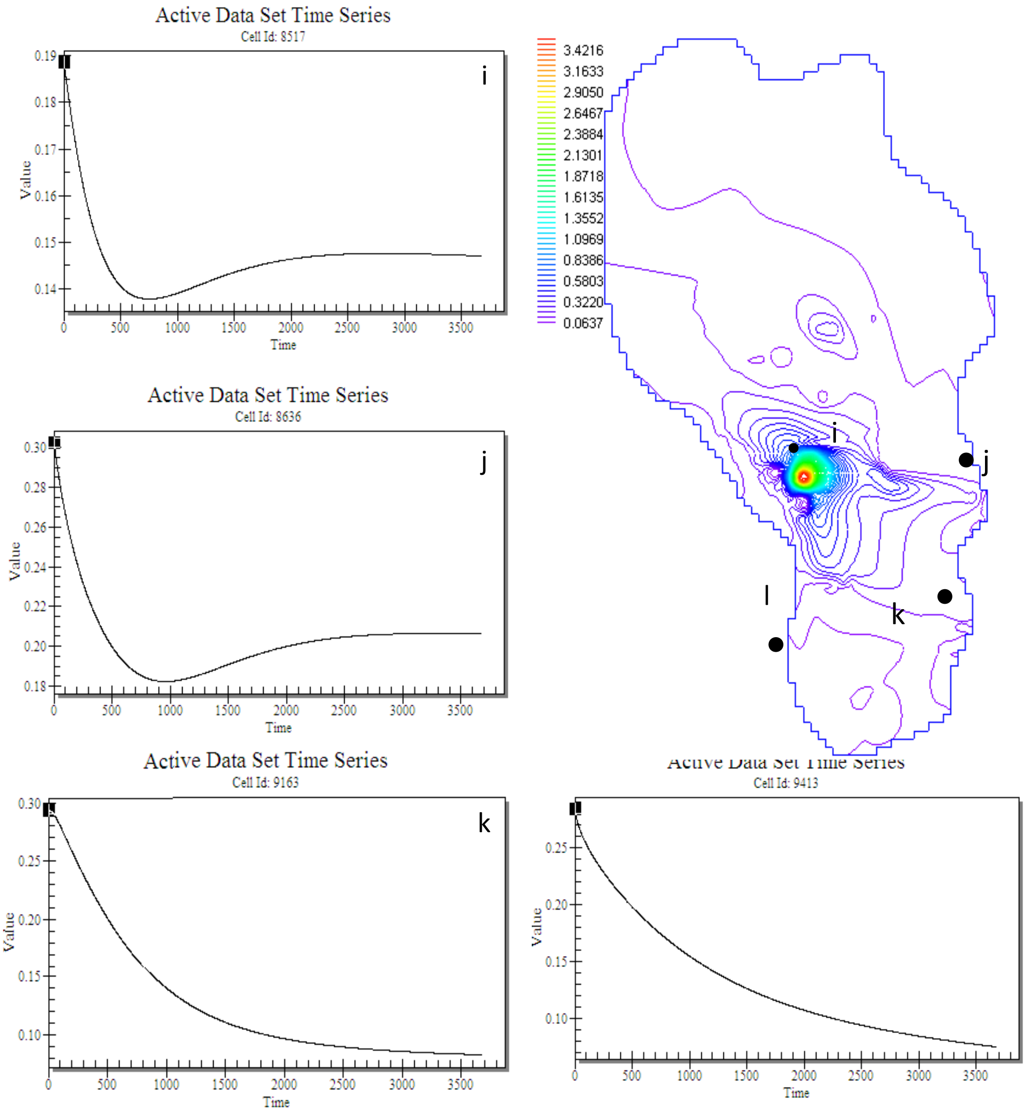


Figure.14. Investigation of lead continuous time pollutant transport modeling.

The Lead contaminant transport modeling illustrated the concentration movement and dispersion from the point sources to Nam MO River which is nearby Nam MO Village as depicted in Figure14. With regarded points j, k and l along the Nam MO River and point i is in the middle of point source and Nam MO River on the model. Figure14(i-j) indicated, the concentrations reduce gradually then after 3 years increase to 0.156 mg/l and 0.21 mg/l, respectively. Figure 14 illustrated; lead concentration decreases gradually at simulation time 3,650 days.

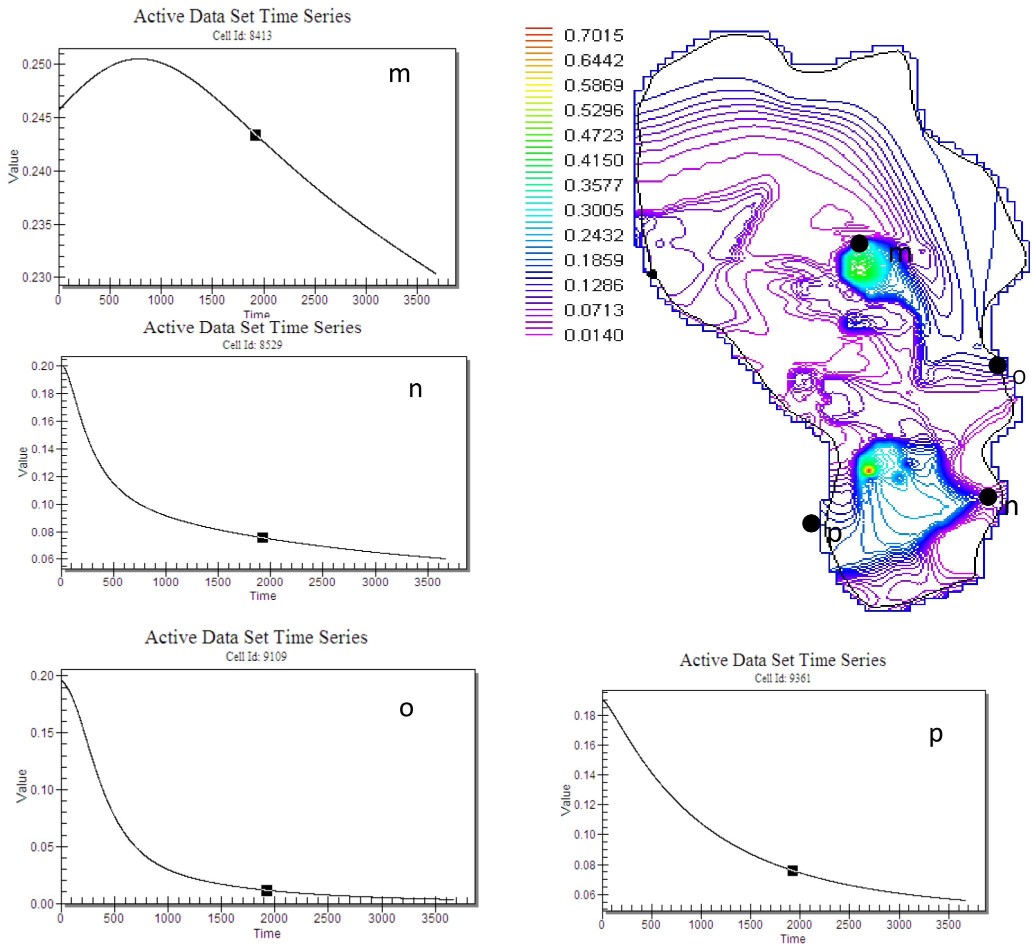


Figure.15. Investigation of zinc continuous time pollutant transport modeling.

At interesting points n, o and p along Nam MO River and point m is nearby point source on the model. Figure m illustrates pollutant concentrations increase gradually from time 0 to 2.5 years, thereafter, the pollutant concentration diminishes from 0.25 to 0.23 mg/l. Figure 15(n–p) shows pollutant concentration decreases gradually at simulation time 10 years. Zinc contaminant transport modeling illustrated the pollutant concentration movement and dispersion from the point sources to Nam MO River which is nearby Nam MO Village as depicted in Figure15.

Conclusion

The MT3DMS packages were employed to simulate the contaminant transport modeling and also prediction, therefore, the models found that Lead concentration as point source at borehole MB48, with instantaneous-time pollutant concentration of 3.96 mg/l, it was very light minimally diminished to 0.1 mg/l, after 10 years simulation. Meanwhile, at borehole CV04, the zinc concentration was 0.88 mg/l as initial concentrations, it was deliberated as point source and concentration reduced to 0.023 mg/l, afterwards the 10 years modelling.

The highest concentration point is the point source at borehole MB48 as the Lead continuous-time. Moreover, the zinc continuous-time pollutant obviously indicates the highest concentration at CV04 considering as the point source of the pollutant, with simulation time 10 years in order to predict the concentration.

There are also existing other observed points moved and dispersed slightly from the observed sources to southeast in the 10 years simulation time as predicted in the groundwater of the contaminant transport modelling.

According to the findings of Lead and zinc contaminant transport modeling, most of the pollutants are contaminated and transported through aquifer (Limestone, Schist, Redbed and Breccia from the top to bottom layer, finally, it links to Nam MO River. Therefore, to prevent and protect the water-ecological system and health that would be hazarded due to the nearby local communities that uses the groundwater as prioritized water source, the groundwater should be pumped to remediate and treat them, before transporting to the groundwater environment to Nam MO river, a pumping systems should be installed to pump and treat contaminant groundwater before transporting to the groundwater environment, to protect living things from hazard due to surrounding communities using groundwater as main source of water.

Acknowledgements

The authors would like to acknowledge AUN/SEED-Net, JICA program for being very kind financial support which enabled to gather relevant data for this study and also Phu Bia Mining to assist and provided data-information to our team during data collection and site visit.

References

Arlen W. Harbaugh, Edward R. Banta, Mary C. Hill and Michael G. McDonald. (2000). MODFLOW-2000, the U.S. Geological survey modular, groundwater model- user guide to modularization concepts and the groundwater flow process.

Chunmiao Zheng, and P. Patrick Wang. (1999). MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection,Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems. http://www.geology.wisc.edu/~andy/g727/mt3dmanual.pdf.

C.Zheng. (1990). A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems, pp.1-1.

Chankhachone Sonemanivong, Phoummixay Siharath, Somchay Vilaychaleun, Khampasith Thammathevo, Biswadip Basu Mallik, Khanti Phanthavong,2023, Reservoir Enlargement and Energy Production Comparison of Dry, Normal and Wet Year at Nam Sana1 Hydro Power Plant Kasy District, Vientiane Province, DOI: **https://doi.org/10.55927/ajns.v2i2.4039**

Gerrit Jousma, 2008, Guideline on: Groundwater monitoring for general reference purposes.

Geography department. (2010). Geographical map in Laos.

Gerald W. Recktenwald. (2011). Finite-Difference Approximations to the Heat Equation

Jacob Bear , Alexander H.-D. Cheng,2010, Modeling Groundwater Flow and Contaminant Transport.

Jacques.W. Delleur. (2006). The handbook of groundwater engineering, second edition, pp 2-10.

Lao Statistics Bureau, 2015, The 4th Population and Housing Census (PHC), the result of populations and housing census, https://lao.unfpa.org/sites/default/files/pub-pdf/PHC-ENG-FNAL-WEB_0.pdf,pp 24.

Randall J. LeVeque ,2005, Finite Difference Methods for Differential Equations.

Siharath, Phoummixay, Sonemanivong, Chankhachone, Thammathevo, Khampasith, Vilaychaleun, Somchay, Mallik, Biswadip Basu, Khounpaserth, Phouphavanh, Sanvilay, Vilakone, Phommixay, Souliphone, 2022, Arsenic and Copper Contaminant Transport Modelling In Xaysomboun Province, LAO PDR, **DOI:** https://doi.org/10.15864/jmscm.4302

Soneteng Buaxaiya, Chittana Phompila, Kaisone Phengsopha, Bakham Chanthavong, Kethsa Nanthavongduangsy, Sithong Thongmanivong, Himlal Baral, 2021, Assessment of Potential Ecotourism Site in Xaisomboun, Central Laos,DOI: 10.4236/jssm.2021.146043

Phu Bia Mining (2009). Growth by discovery and development in Lao PDR, Annual Review 2009.

Philip B.Bediet,Hanadi S. Rifai, Charles J. Newell .(1994). Groundwater contaminant transport and remediation, pp 302-303.

Paul K.M. van der Heijde,1992, Ground-Water Modeling Issues in Groundwater Modeling Issues in Ground-Water De ater Development: elopement: Model Calibration and Verification

Siharath phoummixay and Guillermo III Quesada Tabios ,2020, Applied Finite Difference method for groundwater flow modeling in Xaysomboun Province, Lao PDR, **DOI:** https://doi.org/10.15864/jmscm.2101

Sandow Mark Yidana.(2010).Groundwater flow modeling and particle tracking for chemical transport in the southern Voltaian aquifers. pp. 709-721.

Sami L.R. Shaheen. (2007). Nitrate Pollution and Groundwater Modeling of Wastewater Plant in Rafah Area, Gaza Strip, Palestine.

The National Institute of Economic Research (NIER), Center for Socio-Economic Science and Policy Research (CSPR), 2022, Strategic Environment Assessment on Green Growth Strategy.

Yuji Nishikawa. (2006). Sector plan for sustainable development of the mining sector in the Lao PDR. MINDECO, pp. 7.