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GROUNDWATER FLOW AND MULTI-COMPONENT REACTIVE TRANSPORT SIMULATION OF ACID MINE DRAINAGE AT A FORMER MINE SITE

*Rabindra Neupane[1] and Bithin Datta[1]

[1] College of Science and Engineering, James Cook University, Townsville, QLD, Australia

*Corresponding Author, Received: 22 July. 2020, Revised: 15 Aug. 2020, Accepted: 26 Sept. 2020

ABSTRACT: Contamination of groundwater resources due to Acid Mine Drainage (AMD) is one of the severest environmental problems. Understanding complex geochemical processes responsible for the generation of AMD within the mine waste deposits is imperative for effective management and remediation of contaminated mine sites. A multi-component reactive transport simulation is developed based on PHT3D to simulate the geochemical evolution of AMD at the Rum Jungle Mine site that has undergone a long history of groundwater contamination. The reactive transport simulation utilized hydraulic head distribution obtained from MODFLOW based calibrated flow model. Geochemical processes considered for the reactive simulation were conceptualized based on previous geochemical characterization and the contaminant of concerns were limited to copper, iron, manganese, aluminum, zinc, and pyrite minerals considering their environmental significance. The simulation results showed that the simulated plume followed mobility pattern dominated by oxidation of sulfide minerals resulting in AMD and subsequent escalation in the concentration of dissolved metals. Simulated and observed concentration for different reactive species appeared to be in a similar range implying reasonable approximation of the physical system. The detailed calibration of reactive transport simulation is restrained by uncertainties associated with aquifer heterogeneity, sparsity in available information, and inaccurate understanding of the geochemical processes.

Keywords: Groundwater flow, Reactive transport simulation, Geochemical processes, Acid Mine Drainage, Contaminated Mine site

1. INTRODUCTION

Groundwater resources are highly stressed globally under the combined effect of population growth, global climate change, and other anthropogenic alterations leading to widespread problems of over-exploitation and contamination. Acid Mine Drainage (AMD) emanating from reactive tailings and waste rock dumps (WRDs) is considered as a severe environmental phenomenon that critically contaminates groundwater. AMD is produced due to oxidation of sulfide minerals and is characterized by an accelerated drop in pH, and elevated concentration of sulfates and other heavy metals [1]. Evidence from the past mining activities manifests that untreated AMD is capable of imposing abiding ramifications to the ecosystem and environment [2]. The physical and mineralogical composition of the mine waste, as well as the AMD pathways in the system, dictates the extent of the damages. More importantly, AMD is a persistent source of contamination that has the potential to contaminate groundwater for several years even after the cessation of mining operations.

Well-developed groundwater flow and transport simulation is the pre-requisite for the development of effective management and remediation strategies. The simulation of geochemically reactive processes responsible for the generation and transport of AMD is an active field of research in hydrogeology. With the recent advances, several sophisticated numerical models had been developed to investigate the mobility of multi-component reactive contaminants within mine waste deposits. MINTRAN [3], PYROX [4], MIN3P [5], POLYMIN [6], and HYDROGEOCHEM [7] are some of the modelling codes that had been successfully implemented for multi-component reactive transport simulation of field scale contaminated mines. PHT3D [8] is a relatively new three-dimensional multi-component reactive transport simulation code that combines the advantage of well-established modular flow and transport simulators MODFLOW/MT3DMS with extremely versatile capabilities of geochemical modelling code PHREEQC-2 [9]. In this study, a multi-component reactive transport model is developed to simulate the generation and mobility of AMD within the mine waste deposit at former Rum Jungle mine site in Australia that has a long history of groundwater contamination. The simulation is based on PHT3D code which is preferred because of its proficiency in handling a wide range of equilibrium and kinetically controlled reactive processes including aqueous complexation, mineral precipitation, and ion exchange reactions that are typical for a mine site [10].

The groundwater flow model is calibrated against limited observed head data and the simulated geochemical plume is compared against the observed plumes to establish the effectiveness of the simulation code. The study implies that PHT3D simulation is capable of evaluating the geochemical evolution of AMD and therefore provides a reasonable approximation of the physical system and processes. The predictive accuracy of the simulation can be enhanced as more site-specific information about the aquifer heterogeneity, hydrogeological data, and complex geochemical composition and processes of the site become available**.**

2. STUDY AREA DESCRIPTION

The Rum Jungle mine is a contaminated mine site located approximately 64km south of Darwin, near Batchelor in Northern Territory, among the headwaters of East Finniss River in Australia. Recognized as one of Australia's first major Uranium mine, the Rum Jungle mining project yielded approximately 3500 tons of Uranium and 20,000 tons of copper, during its operation. The site was characterized with tropical savannah-like climate and vegetation, has high year-round temperatures (average 28° C) with an average rainfall of 1390mm, and consisted of relatively lower relief with elevations ranging from 60m AHD to 100m AHD.

2.1 Environmental Mismanagement

Environmental ramifications evident during the initial mining operation may have been largely disregarded considering the perceived importance of the project [11]. Mining activities combined with inefficient tailings management practices resulted in the direct release of significant volumes of acids and metalliferous drainage to the surface and subsurface water resources collectively known as Acid Mine Drainage (AMD). The ongoing environmental problem at the site instigated major rehabilitation plans aiming to reduce metal loading to surface water and limit the generation of AMD. AMD and metal leaching from waste rock dumps continue to contaminate water resources posing significant threats to the environment and the ecosystem [12].

Groundwater remains the least investigated component despite substantial evidence suggesting ongoing pollution of the subsurface environment. The current understanding is limited to a simplified conceptual model based on sparse site-specific information. There exist significant uncertainties regarding the aquifer heterogeneity, groundwater flow pathways, and geological controls on the flow, characterization of the contamination sources, and spatial extent of the groundwater contamination. However, some preliminary modelling efforts have been carried out for the site. For instance, [13] developed groundwater flow and transport models to simulate the historic and current condition focusing on non-reactive transport processes. Incorporating complex geochemical processes prevalent at the site [14] developed a multi-component reactive transport simulation based on finite element simulation code, HYDROGEOCHEM. The study was preliminary in nature as the simulation was primarily based on the sparse hydrogeological and geochemical data available at that time. Some more information had been released ever since, allowing better calibration of the flow model. Besides, geochemical characterization carried at the site facilitated a better understanding of the geochemical processes and mineralogical composition to achieve significant improvements over the previous simulations.

2.2 Site Layout

Flooded open pits, backfilled pits, Waste Rock Dumps (WRDs) and partially-mined Browns oxide pits are the main features of Rum Jungle mine site. Main, Intermediate, and Dysons WRDs stored the waste rock removed during mining operations. Among other major features are East Finniss Diversion Channel (EDFC), Copper Extraction Pad Area, and Old Tailings Dam area which received tailings during initial mining operations.

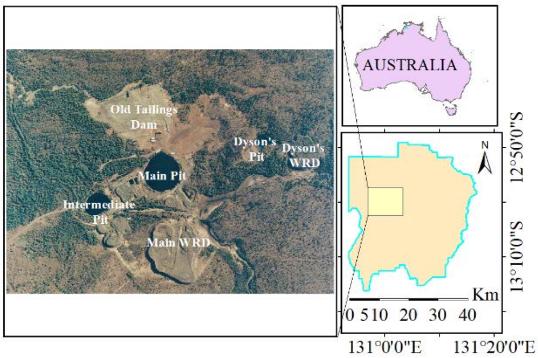

Fig.1 Location map: Rum Jungle Mine Site

3. METHODOLOGY

The study was completed in three stages. In the first stage, a three-dimensional numerical flow model, representing the complex groundwater flow system is developed using the finite-difference flow modelling code MODLFOW. Thus developed numerical model was calibrated against the observed head and other available parameters. In the final stage, the flow fields obtained from the calibrated flow models was used as underlying flow-field for the development of the complex multi-component reactive transport model using PHT3D code.

3.1 Governing Equation of Flow and Transport

Groundwater flow is simulated by combining Darcy's law and the continuity equation. The general differential equation representing three-dimensional transient groundwater flow through the continuous heterogeneous medium under anisotropic condition can be represented as [15]:

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)=S_s\frac{\partial h}{\partial t}-q_s \quad (1)$$

K_x, K_y, K_z are the hydraulic conductivities (LT^{-1}) along x, y and z axes respectively, h = potentiometric head (L), S_s= specific storage of the porous medium(L^{-1}), q_s = volumetric inflow rate per unit volume from sources and sinks (T^{-1}).

The transport of a conservative solute is governed by the combined effect of advection, diffusion, and hydrodynamic dispersion and can be represented by the advection-dispersion equation as [16]:

$$\frac{\partial(\theta C)}{\partial t}=\frac{\partial}{\partial x_i}\left(\theta D_{i,j}\frac{\partial C}{\partial x_i}\right)-\frac{\partial}{\partial x_j}(q_i C)+q_s C_s \quad (2)$$

C = Concentration of pollutant dissolved in groundwater (ML^{-3}), θ= Porosity of the porous medium (Dimensionless), t= time (T), x= Distance along the Cartesian axes (L), q_i= Seepage or linear pore velocity (ML^{-1}) , $D_{i,j}$ = Hydrodynamic dispersion coefficient (L^2T^{-1}) , q_s = volumetric inflow rate per unit volume from sources and sinks (T^{-1}), C_s= Concentration of the source or sink (ML^{-3})

Complex geochemical processes were incorporated by adding a chemical source/sink term capable of addressing a wide range of equilibrium and kinetically controlled reactive transport processes [16]:

$$\frac{\partial(\theta C)}{\partial t}=\frac{\partial}{\partial x_i}\left(\theta D_{i,j}\frac{\partial C}{\partial x_i}\right)-\frac{\partial}{\partial x_j}(q_i C)+q_s C_s+\sum_{n=1}^{N}R_n \quad (3)$$

$\sum_{n=1}^{N} R_n$ =chemical sink/Source term representing the rate of change in solute mass of particular species due to N chemical reactions.

3.2 Model Conceptualization

The groundwater model conceptualization includes identifying main features and hydrogeological processes influencing groundwater flow and transport processes at the site. The conceptual model was primarily developed from hydro-geological information available from geophysical investigations, borehole logs from monitoring bores, pumping tests, groundwater level time trends, and groundwater quality data as reported in [13].

3.2.1 Geology

Rum Jungle mine site is situated at the triangular area of the Rum Jungle Mine field. Rum Jungle complex and meta-sedimentary rock of Mount Partridge Group are two major lithological units at Rum Jungle Mine site. Rum Jungle Complex is predominated with granites that occur southeast of Giant's Reef fault and had undergone in situ lateralization. Mount Partridge Group is locally overlain by hematite quartzite breccia and consisted of Carter formation, Geolsec Formation, Coomalie Dolostone, and Whites Formation. Carter formation primarily comprised of course to medium-grained siliciclastics whereas Coomalie Dolostones consist of dolomite with minor chert lenses. The Whites formation that hosted most of the Uranium and Ploymetallic mineralization, consists of graphite, serictic, chloritic, and calcareous slate-phyllite-schist. While the stratigraphic succession had been preserved, entire rocks of Mount Partridge Group had been folded, faulted, and metamorphosed to greenschist facies [13].

3.2.2 Hydrogeology

Groundwater flow and transport process are facilitated by shallow residual soils derived from local bedrock and underlying moderately to slightly weathered fractured bedrock. The network of groundwater monitoring bores suggested aquifer are predominantly unconfined although some pumping test suggested semiconfined condition. Groundwater is generally observed less than 12m below ground surface and is strongly influenced by rainfall suggesting active recharge. Groundwater flow in shallow aquifer is controlled by primary permeability of unconsolidated overburden soils, while secondary permeability (faults /fractures /karstic features) govern flows in the deeper aquifer units.

3.2.3 Mineralogy

Geochemical site characterization performed at the site suggested that primary mineralogy at the site is dominated by minerals of sulfide, silicate, and aluminosilicate. Sulfide minerals were the most abundant minerals and were mostly present in the form of pyrite in almost all WRDs. Following pyrite were the smaller amount of Muscovite, Chlorite, Kaolinite, Magnesite, Gypsum, and Dolomite that remained dispersed throughout different WRDs. Jarosite was present as the only acid-storing secondary minerals [13].

3.3 Numerical Model

The simulation of groundwater flow was performed using modular three-dimensional flow modelling code, MODFLOW, which is capable of simulating a variety of boundary conditions, and complex hydrogeological system [17]. The reactive transport simulation was performed using PHT3D code. The numerical model was developed based on the simplifying assumption that the aquifer system can be sub-divided into hydro-stratigraphic units and can be represented as a single model layer with representative hydraulic properties.

3.3.1 Model Discretization

The model domain was spatially discretized into three-dimensional grids of uniform cell dimensions 30m*30m. Vertically, the entire model domain was discretized into 5 distinct layers extending from a maximum of 102m AHD to a minimum of -40m AHD. Surface topography obtained from the Digital elevation map was used to define ground elevation. Layer 1 had a thickness of 15m which represented unconsolidated units comprising of laterite, saprolite, alluvium, and other waste materials. Layers 2, 3, and 4 represented partially weathered and fractured bedrocks with a thickness of 10m, 30m, and 10m respectively whereas layer 5 typically represented deeper highly impermeable bedrocks. The hydro-stratigraphic units forming the aquifers were assumed to be heterogeneous and anisotropic. The spatial heterogeneity of each layer was represented by dividing the domain into different zones with their respective hydrogeological parameters.

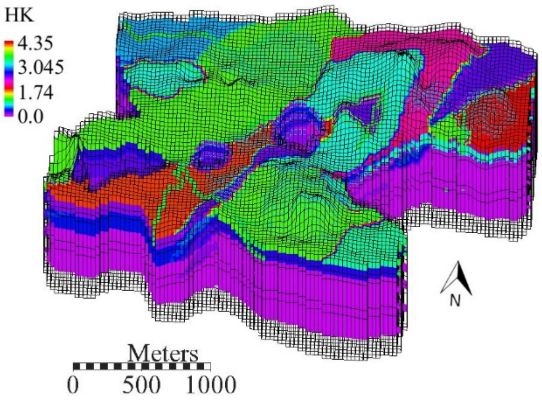

Fig.2 Three-dimensional Model domain with zones of Hydraulic Conductivity

3.3.2 Model Boundary conditions

The model boundary was delineated following natural topography, with topographic highs representing recharge areas and topographic lows representing discharge areas. The water table forms the upper boundary of the numerical model. The water level in East Branch of Finniss was assumed invariant with time and was represented as constant head boundaries. Model cells surrounding flooded main and intermediate pits ware considered as time-variant constant head boundaries and were assigned geodetic elevations of water levels in the pits. Depending upon the relative elevations of groundwater table and geodetic elevation of flooded open pits, they can be considered either source or sinks to groundwater systems. Remaining perimeter boundaries are considered as no-flow boundaries with negligible cross-boundary flows. In absence of other sources of recharge, incident rainfall and surface water bodies are only external sources of recharge into the system. Recharge from infiltration of precipitation was simulated using the recharge package and represent as a fixed percentage of incident precipitation applied only in the topmost layer. Relatively shallow creeks and surface drainage features such as Fitch Creek, Wandering Creek, and Old Tailings Creek were represented as drains and were characterized by their geodetic elevations and drain conductance. Aquifer properties such as horizontal conductivities, specific yield, specific yields, and effective porosity were initially obtained from the previous hydrogeological investigation report [13] and were subjected to further calibration. The final flow and transport parameters used for the simulation are shown in table 1.

3.3.3 Steady-State and Transient State

Major hydrogeological conditions essentially remained unchanged since mine closure and the groundwater system is assumed to have been approaching a steady-state condition. Therefore, a simplified steady-state flow model was developed to simulate hydraulic head using long term annual average precipitation of 1484mm/year. Model parameters and boundary conditions were specified as discussed earlier except time-variant constant head-boundaries at pits are replaced with their average geodetic water levels elevations. To achieve faster convergence, layer top elevation was applied as initial hydraulic heads for the steady-state model.

To simulate the response of dynamic stresses and impact of storage parameters, the transient model was developed. Although perimeter boundary conditions remained unchanged, time-varying hydrogeological stresses such as long-term rainfall values and time-varying constant head boundaries were implemented based on the conceptual model. Storage parameters were applied based on previously calibrated groundwater model for the site developed by RGC [13].

The choice of initial condition significantly influences the model performance of the transient model. Initial heads for transient simulation was obtained using two different scenarios. In the first scenario, observed head values were interpolated throughout the model domain using an inverse distance weighted method that was then utilized as initial heads. In the second scenario, hydraulic head distribution obtained from the steady-state model was utilized as the initial head. The model exhibits better convergence when initialized using steady-state model simulated hydraulic heads.

Table 1 Flow and Transport Model Parameters

Aquifer parameter	Value
Length in X direction	3866.8 (m)
Length of Y direction	2567.1(m)
Number of layers	5
Hydraulic conductivity (Kh)	(m/d)
Layer 1	0.5-4.2
Layer 2	0.12-0.859
Layer 3	0.00864-0.432
Layer 4	0.00864-0.12
Layer 5	0.0043-0.0086
Kh/Kv	10
Effective porosity	
Layer 1	0.2
Layer 2-5	0.01
Specific Storage	2.00E-06 (1/m)
Specific Yield	
Layer 1	0.05
Layer 2-5	0.005
Longitudinal dispersivity (αL)	10 (m/d)
Transverse dispersivity (αT)	0.1 (m/d)
Vertical dispersivity (αV)	0.01(m/d)
Average Rainfall	1484(mm/year)
Recharge rate	9.0-35.0 (%)

3.3.4 Reactive Transport Simulation

Significant volumes of mining waste generated during mining operations contain highly reactive mineral assemblages including reactive sulfides which is the primary source of AMD. In the absence of acid-neutralizing minerals, accelerated oxidation of sulfide minerals results in the formation of AMD within the tailings and WRDs. Site-specific geochemical characterization report suggested the presence of significant volumes of residual sulfides at all mine waste deposits and was therefore considered as potential sources of AMD. Contaminants of concern were limited to the oxidation reaction of pyrite and suite of metals such as copper, iron, manganese, aluminium, and Zinc considering their higher concentration as well as their perceived environmental significance. The current understanding of geochemical processes is based on generalized assumption and could be better represented as more site-specific information regarding mineralogical composition, migration pathways, spatial concentration, and oxidation kinetics becomes available. The typical chemical reactions considered for reactive simulation is shown in table 2.

Table 2 Typical chemical reactions considered for multi-component reactive transport simulation [9]

Chemical Reactions	Reaction constant
Equilibrium Reactions	
Al+3 + H2O = AlOH+2 + H+	-5.0
Al+3 + 2 H2O = Al (OH)2+ + 2 H+	-10.1
Al+3 + 3 H2O = Al (OH)3 + 3 H+	-16.9
Al+3 + 4 H2O = Al (OH)4- + 4 H+	-22.7
Al+3 + SO4-2 = AlSO4+	3.5
Al+3 + 2SO4-2 = Al (SO4)2-	5.0
Al+3 + HSO4- = AlHSO4+2	0.46
Cu+2 + H2O = CuOH+ + H+	-8.0
Cu+2 + 2 H2O = Cu (OH)2 + 2 H+	-13.86
Cu+2 + 3 H2O = Cu (OH)3- + 3 H+	-26.9
Cu+2 + 4 H2O = Cu (OH)4-2 + 4 H+	-39.6
Cu+2 + SO4-2 = CuSO4	2.31
Fe+2 + H2O = FeOH+ + H+	-9.5
Fe+2 + SO4-2 = FeSO4	2.25
Fe+2 + HSO4- = FeHSO4+	1.08
Fe+3 + H2O = FeOH+2 + H+	-2.19
Fe+3 + 2 H2O = Fe (OH)2+ + 2 H+	-5.67
Fe+3 + 3 H2O = Fe (OH)3 + 3 H+	-12.56
Fe+3 + 4 H2O = Fe (OH)4- + 4 H+	-21.6
2 Fe+3+2H2O = Fe2(OH)2+4 + 2H+	-2.95
3Fe+3+ 4H2O = Fe3(OH)4+5 + 4H+	-6.3
Fe+3 + SO4-2 = FeSO4+	4.04
Fe+3 + HSO4- = FeHSO4+2	2.48
Fe+3 + 2 SO4-2 = Fe (SO4)2-	5.38
Mn+2 + H2O = MnOH+ + H+	-10.59
Mn+2 + SO4-2 = MnSO4	2.25
Zn+2 + H2O = ZnOH+ + H+	-8.96
Zn+2 + 2 H2O = Zn (OH)2 + 2 H+	-16.9
Zn+2 + 3 H2O = Zn (OH)3- + 3 H+	-28.4
Zn+2 + 4 H2O = Zn (OH)4-2 + 4 H+	-41.2
Zn+2 + SO4-2 = ZnSO4	2.37
Zn+2 + 2SO4-2 = Zn (SO4)2-2	3.28
Equilibrium minerals	
FeS2 + 2 H+ + 2 e- = Fe+2 + 2 HS-	-18.479

Hydraulic head distribution obtained from MODFLOW simulation was utilized as the underlying flow field for reactive transport simulation. Reactive simulation incorporated advection, dispersion, diffusion, and chemical reaction to the extent possible. Perimeter boundaries represented barriers to reactive transport processes whereas models cells representing WRDs and flooded open pits were represented as areas of specified concentration. All the potential sources were assigned their respective concentration in terms of moles/litres as per the requirement of transport simulation code. In the absence of accurate site-specific source characterization, this was a reasonable approximation. Geochemical reactions within the waste deposits are assumed to proceed sufficiently fast and therefore simulated assuming geochemical equilibrium which is a simplifying assumption. The reaction network for reactive simulation consisted of 6 equilibrium aqueous components (Fe, Al, Cu, Mn, Zn & pH), and equilibrium mineral reaction of pyrite.

Initially, reactive transport simulation was executed for 26years (1985-2011) considering idealized scenarios having initial concentration value close to zero across the model domain. The simulation was executed again for 4 years (2011-2015) using concentration distribution simulated for 2011 as initial concentration. Although directly specifying field measured concentration would be more pragmatic [16], insignificant details about the initial concentration limited applicability of this approach.

4. RESULTS AND DISCUSSION

4.1 Calibration and validation of the Flow Model

The model was calibrated using a manual trial and error history matching approach. Aquifer properties and model boundary conditions were iteratively adjusted within a realistic limit and new zones were introduced whenever required until a reasonable match was obtained between the simulated and observed head. Hydraulic conductivities, recharge rates, and model boundary conditions are some parameters that were calibrated. Observed hydraulic head values obtained from 17 different monitoring locations for 4 years monitoring period was divided into calibration and validation dataset. Head values for March 2011 were utilized for steady-state calibration, whereas hydraulic heads for March 2012 and March 2013 were used for transient calibration. The performance of the calibrated model was evaluated based on standard statistical measures. The calibration target was set to be within $\pm 1m$ of observed hydraulic heads with a confidence level of 95%.

4.1.1 Steady-State Calibration

The calibrated steady-state model had a Mean Absolute Error of 0.70m, Root Mean Square Error (RMSE) of 0.80m, Nash–Sutcliffe Efficiency (NSE) of 0.89, Normalized Root Mean square Error (NRMSE) of 1.3% and R-Squared value of 0.92. The Steady-state calibrated model provided approximate distribution of hydraulic conductivity, recharge zones, and model boundary conditions.

4.1.2 Transient calibration and validation

Aquifer parameters and model boundary approximated from the steady-state calibrated model were subjected to further calibration. The transient simulation was executed for 731 days between March 2011 and March 2013. Transient calibration was undertaken to calibrate storage parameters and refine aquifer parameters and model boundary conditions until a satisfactory match was obtained between simulated and observed heads. Other key model parameters were adopted from previously reported groundwater models. The simulation was validated by executing the final calibrated model in predictive mode, and comparing model predicted head value with observed head values for March 2015 that was deliberately excluded from the calibration dataset. Calibration performance measures as shown in Table 3 and scatter plots of simulated vs observed heads as shown in Fig.3 demonstrate a good degree of correspondence between simulated and observed head values.

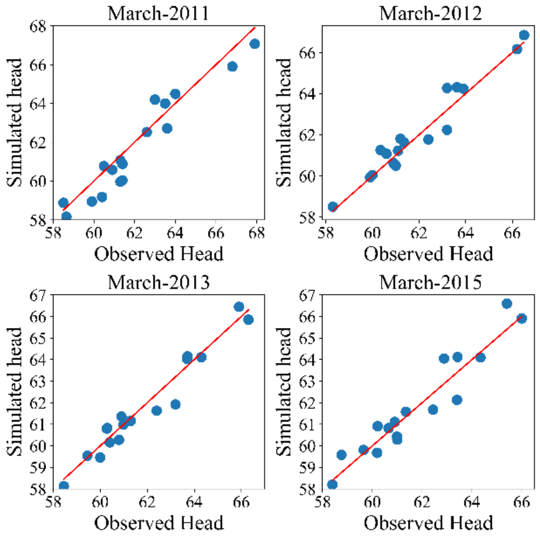

Fig.3 Simulated vs observed head for steady and transient state condition

Table 3 Calibration and Validation Statistics

Statistical Measures	Calibration 2012	2013	Validation 2015
MAE (m)	0.515	0.481	0.57
RMSE	0.663	0.59	0.69
NRMSE (%)	1.073	0.955	1.17
NSE	0.91	0.932	0.9
R^2 Value	0.924	0.933	0.908

Limited model sensitivity analysis inferred that the model is highly sensitive to hydraulic conductivity, recharge rates, and model boundary conditions. In contrast, storage parameters showed lesser sensitivities to model output.

4.2 Reactive Simulation Results

The result of reactive simulation indicated the progressive evolution of acidic conditions as plume advances. Aqueous contamination plume seems to follow a mobility pattern dominated by sulfide oxidation, governed by oxygen diffusion rate and water. The rapid oxidation of reactive sulfides during the initial simulation period results in the release of a considerable amount of sulfates as a direct oxidation product. This accelerates a decrease in pH and subsequent generation of acid and metalliferous drainage as shown in Fig.4. However, with gradual depletion in reactive pyrite, contamination plume attains a relatively stable configuration resulting in a slug-like movement of plume along the direction of flow.

The simulation result suggests the presence of a high concentration of dissolved SO4 (sulfate) which is associated with sulfide toxicity. Sulfates are released as the direct oxidation product of sulfide minerals and are transported conservatively in the absence of carbonate minerals. In contrast, the plume of Iron seems retarded compared to Sulfates resulting in the lower concentration of dissolved iron. This behavior of Iron is well supported by the fact that, under acidic conditions, Iron undergoes a reduction reaction with sulfates and forms precipitates of amorphous iron Sulfides [18].

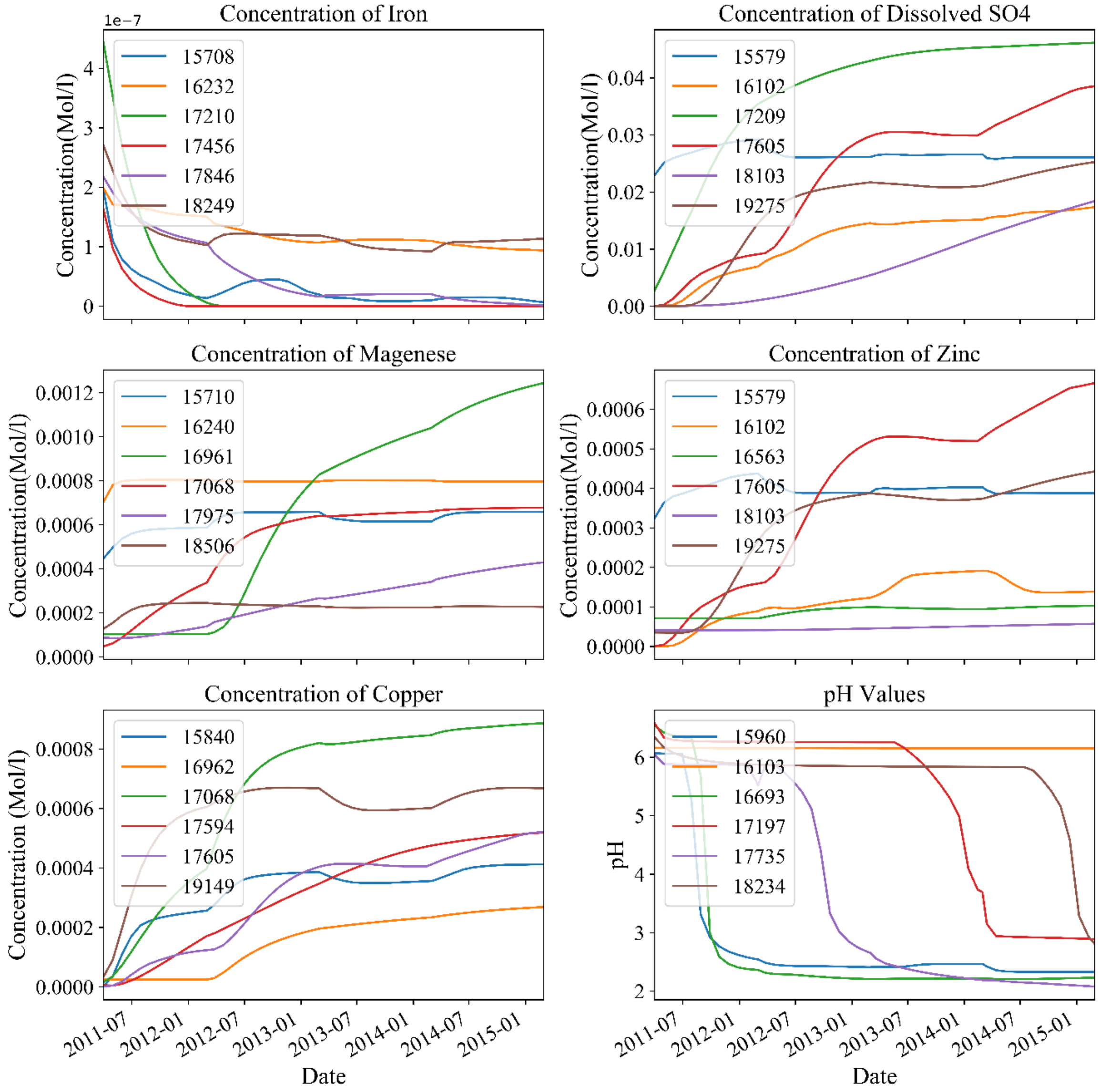

Fig.4 Simulated concentration of different reactive species at 6 selected model cells

Other reactive metals considered for simulation (Al, Mn, Cu, and Zn) shows a similar trend. Observed concentration plume suggests that under acidic conditions, the concentration of dissolved metals are significantly elevated and transported downgradient from the source as the simulation proceeds in time. The concentration of metals is controlled by the oxidation-reduction reactions of sulfides minerals prevalent at the site. Areas within the approximate vicinity of intermediate WRDs demonstrated the highest available concentrations of dissolved metals. This is consistent with the conceptual model as they were conceptualized as areas with the highest acid generating potential. For analytical purposes, 6 different model cells within the proximity of the WRDs were selected and the concentration of different dissolved species was compared. Fig.4 demonstrates the overall trend of different reactive species considered for the study.

Detailed calibration of the reactive solute transport model was constrained due to the sparsity of available concentration measurements that appear to be highly inconsistent across different temporal domains. The performance of the reactive transport simulated was therefore evaluated by comparing the simulated concentration with limited concentration measurements from a few monitoring locations. Simulated and observed concentrations appear to be in a similar range implying that simulation is capable of incorporating important geochemical processes at site and provides a reasonable approximation of the physical system, although not exact.

Reactive transport simulation, incorporating complex geochemical processes provides valuable information regarding the fate and transport of acid and metalliferous drainage imparting meaningful insights for the remedial design. In the absence of adequate field-based measurement to characterize the pollution sources, the developed simulation can be easily incorporated within the linked simulation-optimization framework for the characterization of unknown reactive contaminant sources which is usually the most important step in the effective remediation and management of contaminated aquifer. Furthermore, the developed methodology could be applied for the physical simulation of complex multi-component reactive transport processes at more than 50,000 similar field-scale abandoned mine sites located across Australia [19] to devise effective management strategies.

5. CONCLUSION

Three-dimensional groundwater flow and multi-component reactive transport simulation were developed for a former contaminated mine site. The flow simulation was developed considering heterogeneous, anisotropic conditions and was calibrated against hydraulic head obtained from monitoring wells. Hydraulic head distribution obtained from the calibrated simulation was utilized as an underlying flow field for the reactive transport simulation to simulate the response of different physical and geochemical processes at the site. Geochemical processes responsible for the generation and mobility of AMD were the major focus of study. A relatively new and extremely versatile multi-component reactive transport simulation code PHT3D was used for reactive simulation. Simulation results demonstrated that contaminant plume followed the mobility pattern dominated by oxidation of sulfide minerals, resulting in the subsequent generation of AMD and elevated concentration of dissolved metals within the mine waste deposits. Similar values of simulated and observed concentration of different reactive species at limited monitoring locations suggested reasonable approximation of the physical system and justified the suitability of PHT3D in simulating geochemical processes. Detailed more rigorous calibration of the reactive simulation was not attempted because of inherent uncertainties related to aquifer heterogeneities, simplifying assumptions, complex mineralogical composition, uncertain geochemical processes, and data availability limitations. To recapitulate, the study established the feasibility of applying the relatively new multi-component reactive transport simulator, PHT3D, for simulating the fate and transport of the AMD for a complex contaminated mine site. This is the main focus of this study. The insights obtained from the simulation results enhanced the current understanding of the geochemical system at the site, and understanding of the pathways of contaminant transport. These results are useful for better evaluation of potential remediation measures, by incorporating the simulation within a decision support framework.

6. ACKNOWLEDGEMENT

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