12th International Environmental Specialty Conference
12ième conférence internationale spécialisée sur le génie de l'environnement

Edmonton, Alberta
June 6-9, 2012 / *6 au 9 juin 2012*

Uncertainty Analysis of AN AQUIVALENCE-BASED Fate and Transport Model using a Hybrid Fuzzy-Probabilistic Approach

Getnet D. Betrie[1], Rehan Sadiq[1], Kevin A. Morin[2], Solomon Tesfamariam[1]
[1]Okanagan School of Engineering, University of British Columbia, Kelowna, BC, Canada
[2]Minesite Drainage Assessment Group, Vancouver, BC, Canada

Abstract: Fate and transport models have extensively been used to predict distribution of toxic substances in the multi-media environment. In mining industry, predictive models are commonly used to evaluate performance of mitigation measures and estimate remediation costs during different phases of a mine lifecycle. These models are often used in deterministic form; however the probabilistic analysis through Monte Carlo analysis simulations is also popular to describe parameter uncertainties. In pre-mine phase, where data and information that characterize a mine site are scarce, some parameters of fate and transport models can be best described as random and can subjectively be defined as fuzzy variable. This paper presents a fuzzy-probabilistic approach to propagate parameters uncertainties throughout the modeling process. An aquivalence-based fate and transport model was developed for a mine site. This model was integrated with fuzzy-probabilistic algorithm to predict the distribution of copper concentrations in soil and groundwater. The prediction results showed the distribution of copper concentrations in groundwater, the associated prediction uncertainties and sources of uncertainty.

1. Introduction

Mining industry plays a paramount role in economy and overall employment of Canadian (NRCan 2011). However, this industry produces vast amount of solid waste, which may contain sulphidic materials. The exposure of sulphidic materials to water and oxygen can result in acid mine drainage (AMD) that release toxic substances and cause damage to the environment and human health (Morin and Hutt 1997). To prevent the negative impacts and to lower remediation costs, proactive detection and resolution of contaminant concerns from mine sites are of high importance (Price 2009). This proactive detection is often undertaken through pre-mining prediction of future drainage quality of mined materials.

Fate and transport models are one of the predictive modeling tools that help to estimate the maximum contaminant concentrations in different media (e.g., soil, water, sediment, etc.). Predictions of models are often used to plan mitigation measures and estimate the costs of future remediation of sites to reduce the damage to environment and human health. Thus a reliable and accurate prediction of the drainage quality from mine wastes is required for appropriate decision making (Price 2009).

Predictive models, however, have inherent uncertainties such as structural, parameter and input data uncertainties (Walker et al. 2003; Matott et al. 2009). Model structure uncertainty is the conceptual uncertainty that arises due to the imperfect knowledge and simplified descriptions of mine site processes as compared to reality. Parameter uncertainty is the uncertainty related to parameter values that arises because of lack of site characterizing data due to financial and time constraints. Input data uncertainty is the uncertainty related to system data that drive the model (e.g., weather data and waste rocks reactive surface areas).

Parameter and input data uncertainties may originate from randomness due to natural variability resulting from heterogeneity or stochasticity and/or imprecision due to lack of information resulting from systematic measurement error or expert opinions (Baudrit and Dubois 2003). The uncertainties related to randomness and imperfect knowledge referred as stochastic/aleatory uncertainty and epistemic uncertainty, respectively (Walker et al. 2003). The aleatory uncertainty is non-reducible, whereas epistemic uncertainty is reducible by more studies such as more research and data collection (Refsgaard et al. 2007). These inherent uncertainties of modeling are rarely stated or recognized in mining industry (Maest et al. 2005) or simply treated as stochastic uncertainty and addressed using probabilistic approach.

In pre-mine phase, where data and information that characterize a mine site are scarce, some parameters of fate and transport models can be best described as random variables and some can subjectively be defined as fuzzy variables. In cases where model parameters are presented by random and fuzzy variables, two separate methods must be used to propagate the uncertainties (Fearson and Ginzburg 1996). However, most researchers represent the parameters of fate and transport model through probabilistic distribution functions (Sadiq et al. 2003; Luo and Yang 2006) or deterministic values (Mackay et al. 1983, 1989 and 1994). In this paper, hybrid fuzzy-probabilistic approach that considers randomness and imprecision is presented to propagate input parameters uncertainties of aquivalence-based fate and transport model. The remainder of this paper organized as follows: in the next section, the development of an aquivalence-based fate and transport model for a mine site, fuzzy-probabilistic approach and input parameters are presented. The results and conclusion are discussed in the last sections.

2. Methodology

2.1 Aquivalence-based fate & transport model

Mackay (1991) has developed an approach for the estimation of chemical distributions in multimedia based on the complexity of transport and transformation processes. Mackay (1991) defined four primary compartments, namely, air, water, soil and sediments. This model uses aquivalence (A, mol/m^3) as the controlling variable instead of using concentration (mol/m^3). A linear relationship existing between these quantities (i.e., $C = A \cdot Z'$). The Z' is the aquivalence capacity, which depends on the characteristics of the chemical, the medium, and temperature. The aquivalence value of water (Z'_W) is actually defined as 1.0 and the values for other media are obtained by multiplying Z'_W by partition coefficients of particular medium. Rates of diverse processes (mol/h), ranging from wet and dry deposition from the atmosphere to the chemical transformation to re-suspension of bottom sediments, can be expressed as the product of an aquivalence and a transport or transformation parameter or D value (mol/Pa.h). There are three types of D values:

- for chemical transport by advection flow D is expressed as GZ', where G is a mass phase flow rate (m^3/h),
- for chemical transport by diffusion, D is given as UAZ', where U is a mass transfer coefficient (MTC) (m/h), and A is area (m^2), and
- D for chemical transformation is equal to VkZ', where V is the compartment volume (m^3), and k is a first order rate constant (h^{-1}).

In this study, a steady-state aquivalence based model is developed to simulate fate of heavy metals in soil and water media from a hypothetical mine site. The mine system consists of tailings, soil layer and an aquifer. It was assumed that the tailings are sources of copper metal emission (E_S) into soil. Intermedia transport, water-to-soil and soil-to-water mass flow through diffusion and advection were considered. The diffusion of copper from water to soil (D_{WS}) and soil to water (D_{SW}) are calculated based on mass transport coefficient. The advection through soil (D_{AS}) and groundwater (D_{AW}) values, which are the transport of copper through pore water of soil and groundwater, are calculated based on infiltration and groundwater flow rates, respectively. An algorithm for calculating the metal concentration in soil and water is presented in Table 1.

Table 1: Algorithm for computing Cu concentrations in soil and water

Steps	Parameters and Equations
Define physico-chemical properties of pollutants.	K_d (Partitioning with soil)
Define multimedia physical properties.	Length (l), Width (w), depths of groundwater and soil (d_{gw} and d_s), densities etc.
Define flow rates or advection velocities in soil-water system. Similarly reaction rates can be determined from half lives ($H_{1/2}$) or kinetic coefficients (k) in water and sediments.	G_{gw}, G_s (flow rates) $k = 0.693/H_{1/2}$ for first order kinetic Practically half-lives are very long, so no reaction loss is expected
Calculate the aquivalence capacity (Z') of all compartments.	$Z'_w = 1$, $Z'_s = Z'_w K_d$
Calculate the advection D-values.	Reaction $D_{RW} \approx 0$ and $D_{RS} \approx 0$ Advection $D_{AW} = Z'_w G_{gw}$ and $D_{AS} = Z'_S G_S$
Calculate the diffusion D-values Z'_W and Z'_S are aquivalence capacities of water and soil, respectively. A is the area of soil-groundwater interface.	$D_{SW} = AU_{11} Z'_S$ and $D_{WS} = A U_{11} Z'_W$ U_{11} = mass transfer coefficient (MTC) by (Mackay et al. 1996)
Define pollutant loads by direct emissions in soil (E_S) C_{cu} and MW are copper emissions and molecular weight	$E_S = \frac{C_{Cu} \times G_S}{MW}$
Calculate aquivalence (A_i). A_W and A_S, the aquivalence of water and soil	$A_W = \frac{E_S}{D_{WS} - D_{AW}}$ and $A_S = \frac{E_S D_{AW}}{(D_{WS} - D_{AW}) \times (D_{AS} + D_{SW})}$
Calculate concentrations (mg/L) in multimedia. MW = molecular weight (Cu =63.55)	$C_W = MW \times Z'_W \times A_W$ (groundwater) $C_S = MW \times Z'_S \times A_S$ (soil)

2.2 Fuzzy-probabilistic approach for uncertainty modeling

Fuzzy-probabilistic is hybrid of fuzzy arithmetic and Monte Carlo (MC) analysis. This approach has been used to propagate parameter uncertainties in risk analysis (Guyonnet et al. 2003; Kentel and Aral 2004). The hybrid fuzzy-probabilistic approach is an integration of fuzzy arithmetic at each α-cut and Monte Carlo algorithm. The aquivalence fate model is written in terms of fuzzy arithmetic operation (Ross 2004). This model is integrated with the fuzzy-probabilistic algorithm to compute the contaminant concentrations in groundwater. The fuzzy-probabilistic algorithm is presented as follows:

i. Select a value of α and compute min and max values. This provides fuzz numbers $A_1, \ldots A_m$.

ii. Generate n random number and sample n pdf's. This provides random variables $B_1,\ldots,B_n$.
iii. Run the model for fuzzy-random parameters combination (A_1, $B_1,\ldots,B_n$).
iv. Repeat step ii-iii for A_2-A_m.
v. Generate fuzzy outputs from CDFs at a selected level of probability.

2.3 Model input parameters

The input parameters (i.e., physico-chemical characteristics of pollutant and the multimedia environment) of the fate and transport model are provided in Table 2. Clay till thickness (d_S) of 8 m and groundwater elevation (d_{GW}) of 712 m at hypothetical mine site were used. The clay till overlies an aquifer that is considered as homogenous and well mixed. The aquifer has a length and width of 1245 m. It is assumed that infiltration through the clay till (G_S) is gravity driven and it transports the copper concentrations to groundwater. The soil-water mass transport coefficient (U_{11}) is obtained from MacKay (1996). The concentration in the tailings is equal to the pollutant's aqueous solubility and it migrates vertically through the clay till by advection and diffusion. The mass flux at the clay-aquifer interface mixes homogenously over a given aquifer thickness. The pollutant also migrates from the aquifer to the surrounding lake by advection flow (G_{gw}). Table 2 also shows the probabilistic or possiblistic distribution of input parameters together with their values. The probabilistic distributions of the random parameter are determined by fitting the concentrations of copper data obtained from Morin et al. (2010) using @Risk Software (Palisade 2005) and from literature for partitioning coefficient of copper (Allison and Allison 2005). The triangular distribution type of the fuzzy parameters is subjectively selected and their values are obtained from literature (Morwijk 1993). The developed integrated model was used to simulate transport of copper concentrations into the soil and groundwater.

Table 2: Input parameters of an aquivalence-based fate model

Parameter	Symbol	Units	Variable Type	Value/Distribution/Fuzzy number
Molecular weight	MW	g/mol	constant	63.6
Half-lives in water	$H_{1/2}$-water	h	constant	1E+40
Half-lives in soil	$H_{1/2}$-soil	h	constant	1E+40
Aquivalence capacity	Z'_w		constant	1
Width	w	m	constant	1245
Length	l	m	constant	1245
Thickness of groundwater	d_{gw}	m	constant	712
Thickness of soil	d_s	m	constant	8
Soil-water mass transport	U_{11}	m/h	constant	1.0E-05
Density of solids	ρ_s	kg/m^3	fuzzy	triangular: (2600,2740,2800)

Advection of soil	G_s	m^3/hr	fuzzy	triangular: (2,10,18)
Advection of groundwater	G_{gw}	m^3/hr	fuzzy	triangular: (0.01,0.3,0.6)
Partition coefficient of Cu	log K_d	l/kg	random	lognormal~(2.5,0.6)
Copper concentration	C_{Cu}	mg/l	random	lognormal~(8.9,1.56)

3. Results and discussion

The prediction of Cu concentrations in groundwater is presented in Figure 1. It depicts cumulative distribution functions of copper concentrations in groundwater at α-cut 0, 0.5, and 1. The vertical shape of the lower bound distributions at α-cut 0, and 0.5 indicate these results lack randomness and approach fuzziness. Whereas, the distributions shape of α-cut 1 and upper bound of α-cut 0 and 0.5 indicate these distributions have both fuzziness and randomness. The horizontal distance between the lower and upper bounds shows the uncertainty due to imprecision. The lower and upper bounds of α-cut 0 provide a probability level of a given concentration value occurs. For example, the probability of Cu concentration less than 4 mg/l in the groundwater is 60% as shown in Figure 1.

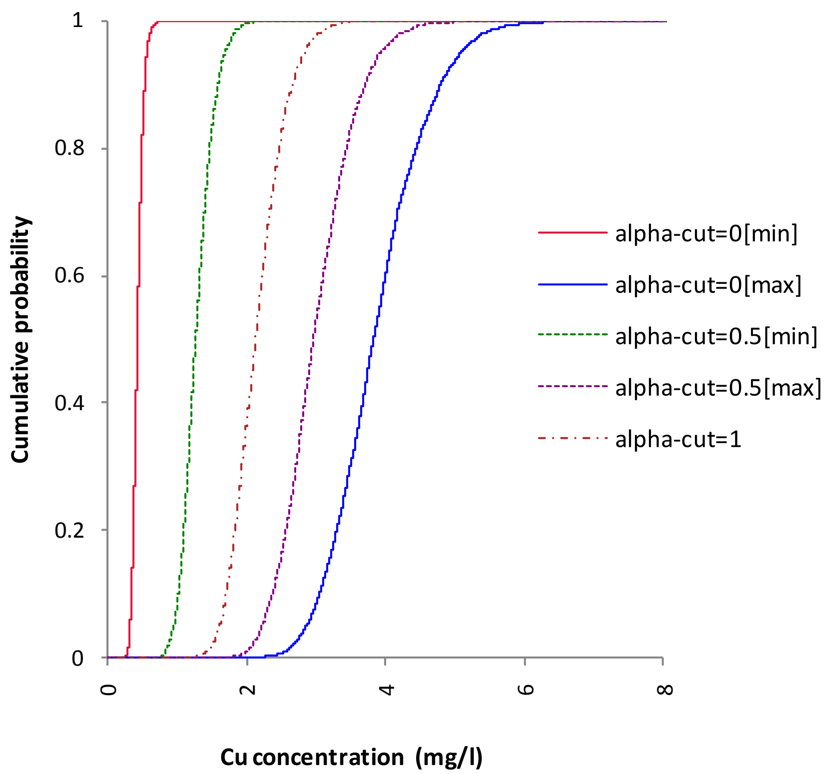

Figure 1: Prediction of Cu concentrations in groundwater

The prediction of Cu concentrations in soil is presented in Figure 2. It shows that lower bound distributions of α-cut 0 and 0.5 are vertical and coincided. This shows that the prediction uncertainties lack randomness and approach fuzziness. Whereas the distributions of α-cut 1 and the upper bound distributions of α-cut 0 and 0.5 show the prediction uncertainties have randomness than fuzziness. For example, there is 60% probability that the Cu concentration in the soil is less than 1.09 x 10^{-7} mg/kg.

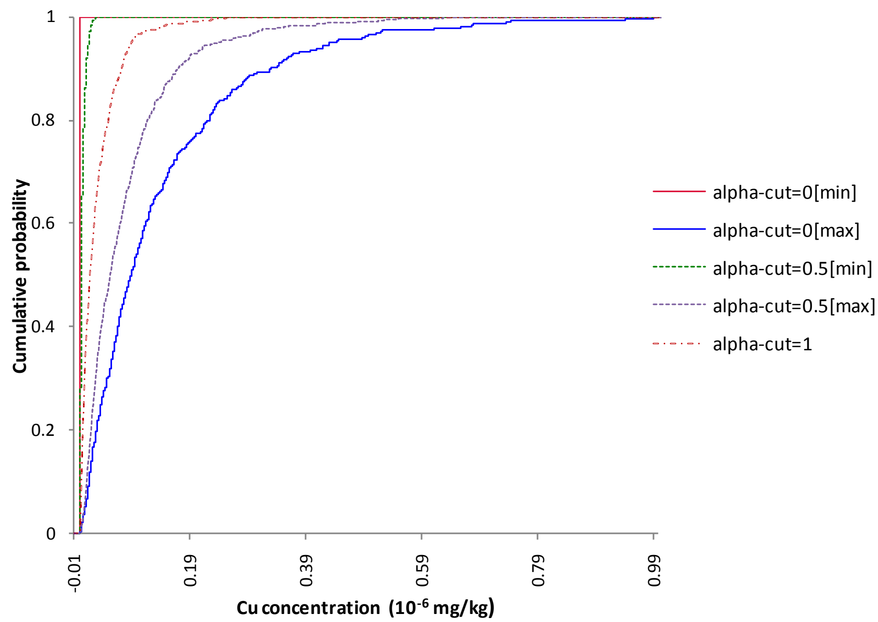

Figure 2: Prediction of Cu concentrations in soil

The membership functions of Cu concentrations in groundwater at 50th, 75th and 95th fractiles are presented in Figure 3. The supports (i.e., membership at zero) of a fuzzy number show that the possible ranges of Cu concentration in groundwater at a given fractile. The Cu concentration value at membership equal to one (i.e., the full membership) shows the most likely values Cu concentration in the groundwater. For 95th fractile, the lower and upper bound range of Cu concentrations in groundwater is 0.56 to 5.07 mg/l, respectively. The values outside of this range are not a member of fuzzy number at 95th fractile. The most likely value of Cu concentration in groundwater at 95th fractile is around 1.93 mg/l as shown in Figure 3. The support of a fuzzy number provides a range of uncertainty. In Figures 3, the supports of membership (i.e., uncertainty band) increase as the fractile level increase from 50th to 95th.

The membership functions of Cu concentrations in soil at 50th, 75th and 95th fractiles are presented in Figure 4. The uncertainties (i.e., supports of membership) increase as the fractile level increase from 50th to 95th fractiles. For the 50th and 95th fractiles, the uncertainty bands increased from 0.0 - 8.17×10^{-8} to 2.93×10^{-10} – 4.72×10^{-7} mg/kg. For these fractiles, the most likely values increased from 1.65×10^{-8} to 9.87×10^{-8} mg/kg, respectively.

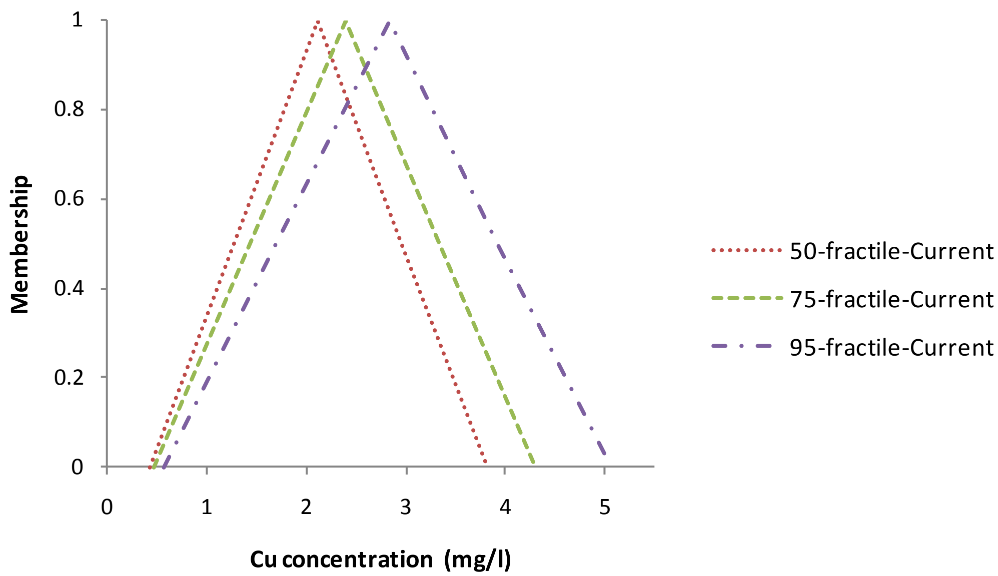

Figure 3: Membership functions of Cu concentrations in groundwater at 50th, 75th and 95th fractiles

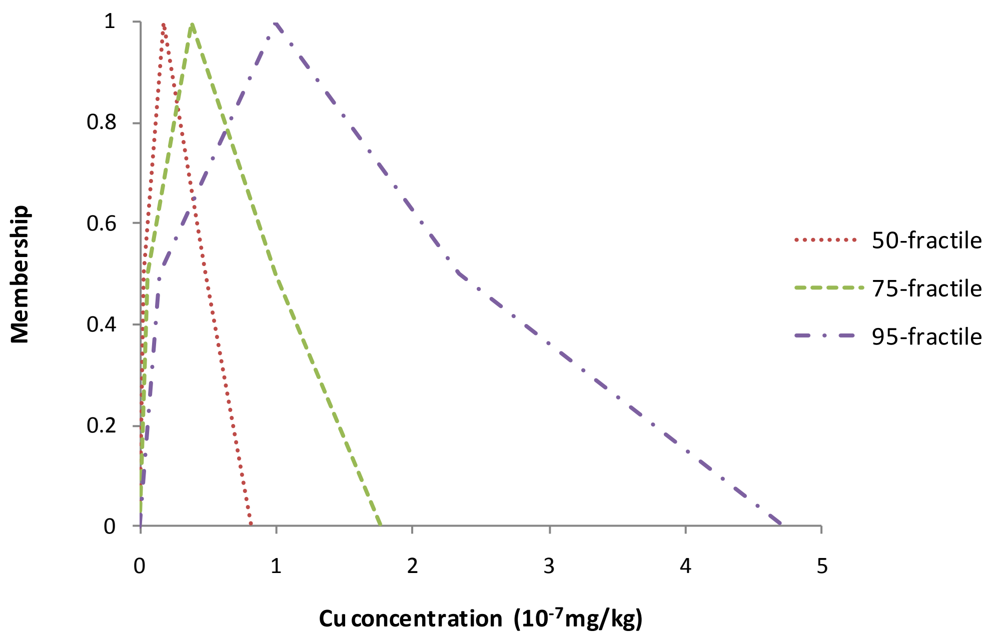

Figure 4: Possibility distribution of Cu concentrations in soil at 50th, 75th and 95th fractiles

4. Conclusions

In this study, aquivalence-based fate and transport model was developed to simulate distributions of heavy metals in a mine site environment. This fate model is integrated with fuzzy-probabilistic algorithm to propagate input parameter uncertainties that arise due to randomness and lacks of information. The fuzzy-probabilistic algorithm is developed by combining fuzzy arithmetic with Monte Carlos algorithm. The results of these simulations showed that the distribution of copper concentrations in soil and groundwater in term of cumulative distribution functions (CDFs) and possibility distributions. The CDFs results show the magnitude of the prediction uncertainties, confidence level and indicate sources of input uncertainties (i.e., randomness or imprecision). The information on sources of uncertainties will help modelers and decision makers to determine needs for further research and data collection activities to reduce parameter uncertainty. However, this approach does not provide reasonable results in case a model has complex equations (e.g., subtraction operation in a denominator) and repeated use of a fuzzy number in equations.

Acknowledgments

We would like to thank Minesite Drainage Assessment Group (MDAG) for providing valuable data. Moreover, the financial supports from second and third authors through their NSERC-DG programs are also appreciated.

References

Allison, J.D. and Allison, T.L. 2005. Partition coefficients for metals in surface water, soil and waste. U.S. Environmental Protection Agency, Washington DC, EPA/600/R-05/074, USA.

Baudrit, C. and Dubois, D. 2003. Joint propagation and exploitation of probabilistic and possibilistic information in risk assessment. *Journal of LATEX Class Files,* 1 (11):1-13.

Fearson, S., Ginzburg, L.R., 1996. Different methods are needed to propagate ignorance and variability. *Reliability Engineering and Systems Safety,* 54: 133–144.

Guyonnet, D., Bourgine, B., Dubois, D., Fargier, H., Côme, B., and Chilès, J.-P. 2003. Hybrid approach for addressing uncertainty in risk assessments. *Journal of Environmental Engineering*, 129 (1): 68–78.

Kentel, E., and Aral, M.M. 2004. Probabilistic-fuzzy health risk modeling. *Stochastic Environmental Research and Risk Assessment*, 18: 324-338.

Luo, Y. and Yang, X. 2007. A multimedia environmental model of chemical distribution: Fate, transport, and uncertainty analysis. *Chemosphere*, 66: 1396-1407.

Mackay, D., Joy, M. and Paterson, S. 1983. A Quantitative Water, Air, Sediment Interaction (QWASI) Fugacity Model for Describing the Fate of Chemicals in Lakes. *Chemosphere*, 12:277-291.

Mackay, D., and Diamond, M. 1989. Application of the QWASI (Quantitative Water Air Sediment Interaction) Fugacity Model to the Dynamics of Organic and Inorganic Chemicals in Lakes. *Chemosphere*, 18: 1343-1365.

Mackay, D. 1991. *Multimedia Environmental Models: The Fugacity Approach*. Lewis Publishers. Chelsea, MI, USA.

Mackay, D., Sang, S., Vlahos, P., Gobas, F., Diamond, M. and Dolan, D. 1994. A Rate Constant Model of Chemical Dynamics in Lake Ecosystem: PCBs in Lake Ontario. *Journal Great Lakes Research*, 20(4): 625-642.

Mackay, D., Di Guardo, A., Paterson, S., and Cowan, C. E. 1996. Evaluating the environmental fate of a variety of types of chemicals using the EQC model. *Environmental Toxicology and Chemistry* 15 (9): 1627-1637.

Maest, A. S., Kuipers, J. R., Travers, C. L., and Atkins, D. A., 2005. *Predicting water quality at hardrock mines: methods and models, uncertainty and state-of-the-Art*. Kuipers & Associate and Buka Environmental.

Morin, K. A. & Hutt. N. M. 1997. *Environmental Geochemistry of Minesite Drainage: Practical Theory and Case Studies*. MDAG Publishing, Vancouver, BC. Canada.

Morwijk Enterprises Ltd. 1993. Bell 92 Closure Plan, Support Document D, Hydrogeology. Dated April 23, 1993.

Morin, K.A., Hutt, N.M. and Aziz M.L. 2010. Thirty-One Years of Monitoring Minesite-Drainage Chemistry, During Operation and After Closure: The Bell Minesite, British Columbia, Canada. http://www.mdag.com/case_studies/MDAG-com_Case_Study_33-31_Years_of_Minesite-Drainage_Chemistry_at_Bell Minesite.pdf

Natural Resource Canada 2011. Important facts on Canada's natural resources, http://www.nrcan.gc.ca/statistics-facts/minerals/902#sec1, access date: 2011/08/11

Price, W. A. 2009. *Prediction Manual of Drainage Chemistry from Sulphidic Geologic Materials*. Canadian Mine Environment Neutral Drainage (MEND), Report 1.20.1.

Refsgaard, J.C., van der Sluijs, J.P., Højberg, A.L. and Vanrolleghem, P.A. 2007. Uncertainty in the environmental modelling process–A framework and guidance. *Environmental Modelling and Software*. 22(11): 1543-1556.

Sadiq, R., Husain, T., Veitch, B., and Bose, N. 2003. Distribution of arsenic and copper in sediment pore water: an ecological risk assessment case study for offshore drilling waste discharges. *Risk Analysis*, 23: 1309-1321.

Ross, T. 2004. *Fuzzy logic with engineering applications*. John Wiley & Sons, New York, NY, USA.

Walker, W.E., Harremoës, P., Rotmans, J., van der Sluijs, J.P., van Asselt, M.B.A., Janssen, P. and Krayer von Krauss, M.P. 2003. Defining uncertainty: a conceptual basis for uncertainty management in model-based decision support. *Integrated Assessment*, 4(1): 5-17.