CSCE Annual Conference
Growing with youth – Croître avec les jeunes

Laval (Greater Montreal)
June 12 - 15, 2019

CONTAMINANT TRANSPORT MODELING FOR RISK ASSESMENT

Jamil, S.[1,4]
[1] University of Regina, Canada
[4] sjo988@uregina.ca

Abstract: Groundwater is an important source of drinkable water; especially in a country like Canada where a large percentage of municipalities drinking water is supplied by groundwater resources. However, the contamination of groundwater is increasing ever more with time. Contaminant transport refers to the spreading of the contaminants from the source of contamination to the drinking water supplies. Nevertheless, the groundwater contaminant transport modelling is a rarity as part of the risk assessment process. Detailed calculations, in-depth scientific and technical knowledge is required in addition to understanding of complex hydrogeological settings. The development of commercial softwares has reduced the time and effort to predict the groundwater transport mechanism with the varying hydrogeological conditions. Nevertheless, it remains imperative to understand the mathematical relations and definitions with respect to the constant and variable input parameters to accurately predict the groundwater transport models. This research is an attempt to *(A) gather the numerical equations typically used for modeling the contaminant concentration and transportation within the groundwater system. (B) Outline a workflow example for computer based modelling using GMS software using the MODFLOW and MT3DMS simulation models.*

1 INTRODUCTION

Groundwater is an important natural resource, useful for different purposes; drinking, irrigation, and industrial processes (Nampak et al., 2014). Globally the 69.1% supply of drinking water is from fresh water sources while the 30.9% of drinking water is sourced from ground reservoirs. Historically the groundwater is becoming ever more exposed to contamination. Specially in countries like Canada where about 30.3% of municipalities the drinking water is supplied by groundwater resources. In addition to posing a widespread threat to the water quality, these contaminants have a strong toxic and harmful effect on the ecosystem and the human health (Langwaldt and Puhakka, 2000; Aral, 2010).

Environmental risk assessment helps analyse, consider and then develop a framework for the “risks to human health, welfare and ecosystems that are the result of adverse developmental impacts on the natural environment.” (Beer & Ziolkowski, 1995). Risk assessment and transport modelling of groundwater contamination is an effective way to evaluate the impact of contamination and protect the subsurface resources. Typically applied to evaluate the extent of migration of contaminants from an existing pollution source such as contamination plume from a spill or a source of contamination as a waste disposal facility.

The modelling process of contaminant transport is a mean to design remedial strategies and accurately predict contaminant concentrations to facilitate site remediation and water quality improvement decisions. Addressing these impacts on the groundwater can incur significant social and economic costs (Lahoz et al., 2011). Mathematical models for contaminant transport in the subsurface such as conventional numerical methods are the most widely used techniques (Ren and Zheng, 1999). Fetter et. al. has defined contaminant mass transport as the transport of solutes dissolved in groundwater by the advection, diffusion and dispersion methods (Fetter et al., 1998).

The purpose of this research is to (1) briefly overview the process and concepts around the contaminant transport modelling. Numerous authors have used presented solution to estimate the concentration of the contaminants from the source along with the groundwater flow over a finite distance and time. The most commonly used equations are presented in the sections below.; (2) use GMS software to simulate different contaminant models to graphically represent the contaminant transport phenomenon. The software uses the MODFLOW and MT3DMS simulators to model the groundwater flow. An academic license was used for this research along with the dataset as permitted by the GMS team.

2 RISK ASSESSMENT

A human health risk assessment consists of four primary elements: (1) data collection and evaluation; (2) an exposure assessment; (3) a toxicity assessment; and (4) risk characterization (U.S. Environmental Protection Agency 1989). Identification of the contaminant; evaluating the concentrations; and examining the characteristics of the and the environmental settings that may affect the fate, transport, and persistence of the contaminants.

To identify the factors affecting the fate, transport, and persistence of the contaminants, a qualitative risk assessment is conducted. The objectives of the qualitative risk assessment are to (1) determine the locations of potential contaminant sources; (2) identify and assess the potential exposure pathways; and (3) evaluate the likelihood of potential impacts with the contaminants (Cushman & Ball, 2000). In practice, a qualitative risk assessment may involve a walk through survey, corresponding with regulatory officials, reviewing available public databases and reviewing the regional topography, geology and hydrogeology.

Characterization of risk associated with with contaminated site can usually be conducted through ERA (Environmental Risk Assessment) and HRA (Health Risk Assessment) guidelines (Carrington and Bolger, 1998). The ERA approach is to compare contaminant concentration with the corresponding groundwater quality guideline and to characterize the risk due to guideline violation. The HRA is to identify the risk of health impact due to chronic intake of contaminant. To quantify human health risks, pollutants are characterized as carcinogens and non-carcinogens. As a result, the concept of HI is applied. The degree of exposure to a chemical is a function of many variables described as follows (USEPA, 1992):

$$\boldsymbol{CDI = CW \cdot IR \cdot EF \cdot ED/(AT \cdot BW)}$$

where *CDI* is the chronic daily intake (mg/kg · d), *CW* is pollutant concentration in groundwater (mg/L), *IR* is human ingestion rate (L/day), *EF* is exposure frequency (days/year), *ED* is average exposure duration (year), *BW* is average body weight (kg), and *AT* is averaging time days). The ERA and HRA may obtain different insights about

3 CONTAMINANT TRANSPORT

The primary physical processes governing contaminant transport in groundwater are advection, diffusion and dispersion. In case of low flow rate, usually diffusion is the dominant process, while advection and dispersion are predominant in high flow rate situations (Rowe 1987, Shackelford 1988, 1989), as indicated in table 1.

The fate and transport of these contaminants in the groundwater is based on the principle of mass conservation. This principle governs the advection-dispersion solution and provides the fundamental equation for the contaminant transport model derivations (McDonald 1988). As per mass conservation principle the in-flux and the out-flux, can be mathematically expressed as:

Flux in – Flux out = $\triangle$Contaminant Concentration

Where, Flux of the contaminant is defined as the total mass of a contaminants passing through a defined cross-sectional area over a period of time (ITRC, 2010). Mathematically, contaminant mass flux is the product of the contaminant concentration in groundwater and the groundwater flux. Thus, contaminant mass flux (J) can be calculated as follows (modified after Bear and Cheng, 2010):

$$J = q_0 \,.\, C = - K \,.\, i \,.\, C$$

where

q_0 = groundwater flux, $L^3/L^2/t$ (e.g., volume/area/d)

K = saturated hydraulic conductivity, L/t, (e.g., m/d)

i = hydraulic gradient, dimensionless (e.g., m/m)

C = contaminant concentration, M/L^3 (e.g., mg/volume)

Table 1. Physical process effecting contaminant transport (modified after national research council)

Process	Definition	Significance
Advection	Mass Transport due to bulk water flow	Most dominant in high flow rate media
Diffusion	Mass spreading due to concentration gradient	Most dominant in low flow rate media
Dispersion	Mass spreading due to heterogeneities and flow fields	Results in greater mass spreading

Groundwater being a complex and fuzzy system with many uncertainties; there are multiple fluxes governing the movement of solute or contaminants. Advective flux (J_{adv}) refers to the movement of contaminant along the flow direction of water and the hydrodynamic flux (J^*) refers to the combined effect of longitudinal and lateral spreading of contaminant. The total flux in any given direction is a sum of advective and hydrodynamic fluxes and is therefore given by (ITRC, 2010) :

$$J_{total} = J_{adv} + J^*$$

$$J_{total} = v_i \,.\, n_e \,.\, C + (- n_e \,.\, D_i \,.\, \partial C/\partial i)$$

$$J^i = v_i \,.\, n_e \,.\, C - n_e \,.\, D_i \,.\, \partial C/\partial i$$

The contaminant transport equations are formulated for a 3-Dimentional and 2 Dimensional solutions, nevertheless, a one dimensional solution is simple and applicable to most of the practical problems. The above equation can be modified for a multi-dimensional model as follow:

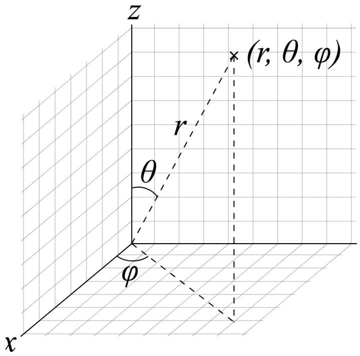

Figure 1: A general co-ordinate system representing the x, y & z co-ordinates modified after Andeggs.

3 Dimensional Solution; *For a homogeneous medium where Dx , Dy and Dz do not vary in space and in general Dx ≠ Dy ≠ Dz; in addition to steady and uniform velocity.*

$$\partial C/\partial t = [D_x (\partial^2 C/\partial x^2) + D_y (\partial^2 C/\partial y^2) + D_z (\partial^2 C/\partial z^2)] - [v_x (\partial C/\partial x) + v_y (\partial C/\partial y) + v_z (\partial C/\partial z)]$$

2 Dimensional Solution; When the direction of flow is parallel to the x-axis

By Andeggs - Own work, Public Domain, https://commons.wikimedia.org/w/index.php?curid=7478049

$$\partial C/\partial t = [D_i (\partial^2 C/\partial x^2) + D_j (\partial^2 C/\partial y^2)] - [v_x (\partial C/\partial x)]$$

1 Dimensional Solution; In case of homogenous and isotropic porous medium;

$$\partial C/\partial t = [D_x (\partial^2 C/\partial x^2)] - [v_x (\partial C/\partial x)]$$

where

C = Concentration of the contaminant species M/L^3 (e.g., mg/volume)
t = time d (days)
v = velocity of ground water in *i* direction m/d (e.g., meter/day)
D = distance covered by contaminant in *i* direction m (e.g., meters)

4 WORKFLOW

The workflow is created in GMS software package using the MODFLOW & MT3DMS simulation. MODFLOW is a computer code that solves the groundwater flow equation, the U.S. Geological Survey modular finite-difference flow model while MT3DMS (Modular Transport, 3-Dimensional, Multi-Species model) is a modular three-dimensional transport model for the simulation of advection, dispersion, and chemical reactions of dissolved constituents in groundwater systems (Zheng, 1990). The software license and the data used was an academic copy for research purposes only, kindly offered by the GMS Aquaveo team. This simulation approach is used to model advanced transport for the contaminants.

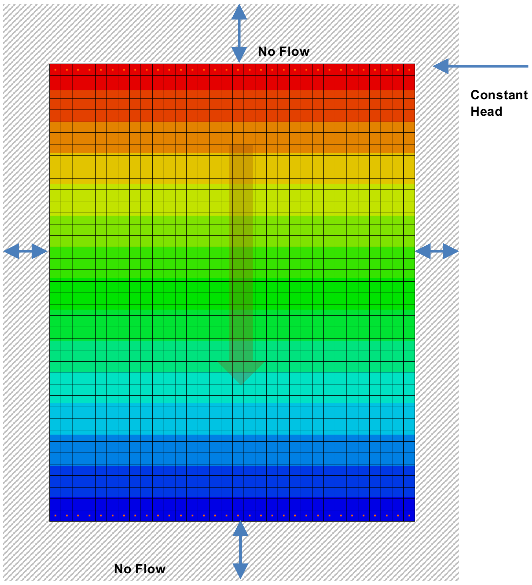

Figure 2: Two Dimensional grid with a North-South flow and no flow boundaries using constant head values.

4.1 Advective Flow

The advection term of the transport equation, describes the transport of contaminants at the same velocity as the groundwater. On a field scale-level the advection term dominates over the other terms (Zheng et. al., 1999).

An *advective flow* simulation is modelled using a simple one-dimensional field with North-South flow orientation, maintaining constant heads, no-flow and no mass flux boundaries as shown in figure 2. A contaminant tracer is simulated for a period of 365 days and a maximum of 12 times steps to model the contaminant movement per 30 days' period.

A tracer of 500 mg/L value was used as source of contamination. Using the advection package the MT3DMS simulation was run to model the contaminant transport from source along the flow of groundwater over a period of 365 days, representing the advective transport and change in contaminant concentration as shown in figure 3.

4.2 Dispersive Flow

Dispersion in porous media refers to the spreading of contaminants over a greater region than would be predicted solely from the average groundwater velocity vectors (Anderson 1979 and 1984). Dispersion in porous media refers to the spreading of contaminants over a greater region than would be predicted solely from the average groundwater velocity vectors (Anderson 1979 and 1984).

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The dispersive flow simulation is modelled using a 3-dimensional grid with flow and mass flux boundaries. The groundwater flow direction is oriented from north to south based on an injection well and the two pumping wells.

The source of contamination is generated from an injection well with a pumping rate to 150 Qft^3/day for a period of 365 days. Using 12 time steps the simulation was modelled for the flow of contaminant from the source towards the pumping wells as shown in figure 4. The flow simulated for dispersive and advective flow shows the concentration of contaminants spreading and reducing over time and distance as per the colored regions.

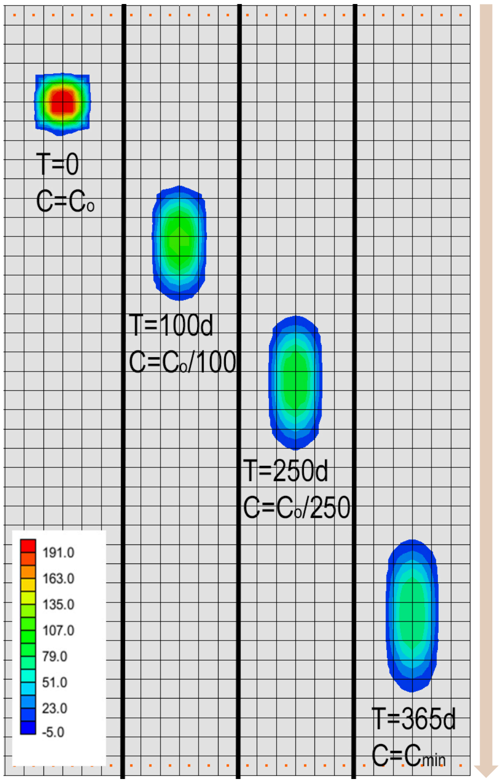

Figure 3: Advective transport of contaminant away from the source along the groundwater flow direction. The green arrow represents the direction of groundwater flow.

5 CONCLUSION

Contaminated soil and groundwater remediation and risk assessment has grown and evolved in attempts to improve the decontamination. Modeling of the contaminant in the groundwater, whether from a potential release or from a latent risk can help assess and quantify the contaminant and the associated hazards.

GMS has proven to be a useful and efficient tool and although a satisfactory modelling can be achieved in order to predict the contaminant spreading, a lot of data is required to quantitatively validate the model, in addition extensive knowledge of the groundwater hydrogeology, contaminant type and the properties of the soil.

Nevertheless, the results obtained from the models remain an effective method to estimate and predict the movement of contaminants and their concentrations, and can serve as a preventive measure in improving the overall drinking water quality.

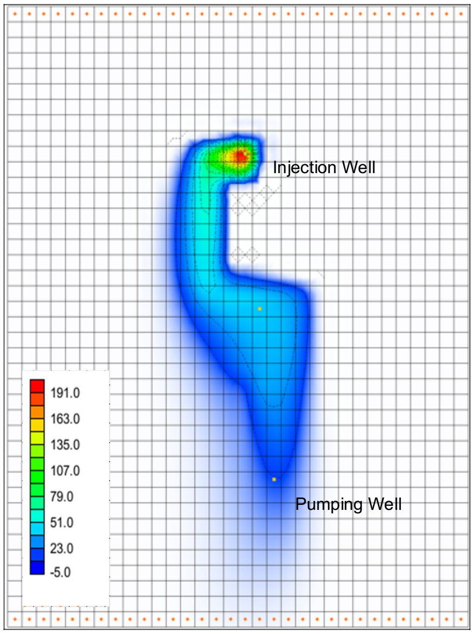

Figure 4: Dispersive transport of contaminant from the source (injection well) along the groundwater flow direction to the pumping wells.

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