A Study of Various Approaches for Groundwater Contaminant Transport Modeling.

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Abstract

The objective of present study is to review the significant works carried out in the multifaceted field of groundwater contamination. Contaminants can be descripted in a broad category from physical groundwater quality parameters to emerging heavy metals and toxic substances. Multi-directional transport of these contaminants can be mathematically modeled with the help of various groundwater modeling programming codes such as, MODFLOW, MT3DMS, RT3D, FEMWATER, MODPATH, SEAM3D etc. The computational models that are simulated to represent graphically the fate of transport require authentication from field observations. Soft computational modeling is preferred by experts to optimize a combination of remediation processes to overcome such complex phenomena that is groundwater contaminant transport study.

Key-words: Groundwater, Contaminants, Transport, Modeling, GMS, GIS

I. **Introduction:** Initializing a research work in the field of groundwater contamination and transport modeling, one should have a basic knowledge of different hydrological and contaminant phenomena. The aim of this review is to bring up sufficient information about contaminant hydrology in one's hand.

Conceptual Model Concept:

The first step in developing the groundwater model is the construction of a conceptual model of the hydro-geologic system for the study area using regional and site-specific hydro-geologic and climatic information as derived from the field observations. (He, 2004) The conceptual model is generally developed as a multi-dimensional groundwater flow system with a uniform regional infiltration and anisotropic aquifer characteristics. The aquifer water levels and surrounding surface water bodies connected with the aquifer are also conceptualized.

1. **Groundwater:** Water after infiltration, gets stored between rock fractures in the subsurface zone is described as groundwater. Impervious or semi pervious bed rock strata that holds groundwater is called an aquifer system generally consisting silt, clay, rock-minerals, granite, gneiss, marbles, etc. Occurrence and movement of groundwater is controlled by rock formations of varied composition and structure and range in age from Archean to Recent. (Tiwari, 2015-2016)
   Over exploitation of groundwater mainly for domestic and agricultural and in some cases industrial purposes has been leading towards its vulnerability to contamination.(Suhag, 2016) Groundwater potential and its vulnerability can be understood by the hydro-geo-chemical processes that take place in subsurface environment.

2. **Contamination and Pollution:** Groundwater contamination, as per WHO usage (UNESCO, 1992) is: Introduction into water of any substance in undesirable concentration not normally present in water, e.g. microorganisms, chemicals, waste or sewage, which renders the water unfit for its intended use'.
   The term groundwater pollution is defined in the International glossary of hydrology (UNESCO, 1992) as: 'Addition of substances which impair the suitability of water for a considered purpose'. (Zaporozec, 2002)

   Generally, physical groundwater quality parameters including Nitrate(NO_3^{2+}), Fluoride(F^-), Iron(Fe), Arsenic(As) Lithium(Li), etc. are observed in water. Their presence in more than the permissible limits prescribed for drinking water by Bureau Indian Standard. The Other contaminants include bacteria, phosphates and heavy metals which are a result of human activities including domestic sewage, agricultural practices and industrial effluents. (Suhag, 2016)

   Table: Geogenic Contaminants and their presence in India

Contaminant	No. of States affected	No. of District affected
Nitrate(NO_3^{2+})	21	387
Fluoride(F^-)	20	276
Iron(Fe)	24	297
Arsenic(As)	10	68

   (Source: Central Ground Water Board, PRS (Suhag, 2016))

   The sources of contamination include pollution by landfills, septic tanks, leaky underground gas tanks, and from overuse of fertilizers and pesticides. It has been pointed out that nearly 60% of all districts in the country have issues related to either availability of ground water, or quality of ground water. (Suhag, 2016)

3. **Contaminant Transport Study:** Important stages involved in the development of a transport model explained by (Anderson Mary, 1992) are Conceptual model design, Development of physical/mathematical model, Model calibration, Sensitivity analysis and Future prediction.

Conceptualised contamination transport models can specifically simulate the origin of contaminant and its release in the subsurface medium. (Morrison, 2014) These models require a significant database useful as input parameters since they attend to site-specific conditions which are widely used by experts.

The complex phenomenon of transport of contaminant is governed by a few physico-chemical and biological processes such as advection-dispersion, diffusion, capillarity, etc. In advection process, the contaminants are transported at an average rate equal to the seepage velocity by the flowing fluid in response to a hydraulic gradient. (Mohamed, 2018)

Diffusion process is molecular-based where the transport takes place from high to low molecular concentration. It is governed by the continuous change in various parameters such as thermal gradient and pressure gradient. The dispersion process is associated with the spreading nature of fluid particles that are at one time close together tend to move apart due to variations in the velocity and movement in the porous medium of the fluid. (Mohamed, 2018)

II. Various Approaches for the study of Contaminant Transport Modeling

1. Groundwater Modeling System Modules

GMS is a multi-directional modelling system that involves groundwater flow and various contaminant transport models with a graphical user interface for analysis often applied to solve and predict in-situ solute transport scenarios. FEMWATER is a useful tool while solving density-governed and salinity intrusion contaminant problems.

(Chen, 1999) in their three-dimensional finite element model through saturated-unsaturated porous media for Florida Superfund site concluded from a combination of FEMWATER, GMS and GIS predicted that the two plumes would not merge together but the main volume would migrate closer to the bay.

a. MODFLOW model input-output for transport model

The characterization of flow systems based on numerical groundwater models is developed to simulate the effects of groundwater potential, recharge and flow directions. In most problems, the computing models used are the USGS 3D finite difference model (Trescott, 1975) and the USGS MODLFOW (McDonald and Harbaugh,1988).

MODFLOW-88 has been restructured to MODFLOW-2000 (Harbaugh et al.,2000) and MODFLOW-2005 (Harbaugh, 2005). The MODFLOW 2005 version includes the simulation of saturated- unsaturated flow process, groundwater simulation-optimization process, irrigation process, density dependent flow process, parameter optimization process and solute transport process. (Zhou, 2011)

b. MT3DMS

MT3DMS is a three dimensional modular-transport model that is used in conjunction with MODFLOW in a two-step Flow and Transport simulations. After the groundwater flow model is calibrated in MODFLOW, the contaminant source locations and contaminant concentration values are input into the model. Then various contamination concentrations submitted in the MT3DMS package to simulate the transport. The advection-dispersion and diffusion chemical reactions are involved in MT3DMS. It is developed by (Chunmiao Zheng, 1990) using Finite Difference Method.

A research for the Wang-Tien landfill site, in south western Taiwan, performed by (Chen C. S., 2016) which explains contaminant transport from their study region to the adjacent Hsu-Hsian Creek which gets polluted and the water available turns unfit for drinking purpose. The results also gave a plume of contaminated groundwater that extends 80 m in length and 20 m in depth north eastward from the landfill site. (Chen C. S., 2016)

c. RT3D

RT3D- Reactive Transport Modeling in 3D with GMS is developed by Battelle Pacific Northwest National Laboratory that uses FDM- Finite Difference Method. It is a modified version of MT3DMS that uses various reactive chemical packages. The simulation of natural dilution and bioremediation can be performed well by RT3D.

SWAT-MODFLOW-RT3D, is an integrated model combining the semi-distributed watershed model SWAT (Soil and Water Assessment Tool) with the groundwater flow model MODFLOW and the solute reactive transport model RT3D for the simulation of nitrate (NO_3) fate and transport in a Sprague River Watershed (4100 km^2) in Oregon. (Wei, 2018) RT3D uses NO_3 concentration of deep percolation water from SWAT and groundwater heads and flows from MODFLOW to simulate spatially varying groundwater NO_3 concentration and NO_3 loading to/from streams, with the latter used by SWAT to route NO_3 mass through the network. (Wei, 2018)

2. GIS Approach

In recent years, a vast number of geographical information based systems have been used to identify regions prone to contamination with the help of various geo analyst and spatio statistical tools. Krigging, IDW method of interpolation and contour methods are used for spatial distribution of contaminants.

An integration of GIS technology and groundwater simulation models was incorporated as a “loose-coupling” tool created by (Gogu, 2001) between the spatial-database scheme and the groundwater numerical model interface GMS for Walloon region, Belgium.

(Menezes, 2009) developed a GIS based Contaminant Transport Model (GIS-CONTRAM) to show the fate of transport in subsurface using Model Builder and Visual Basics (VB) tools from ArcGIS. The CONTRAM model provided reasonable results when verified with Visual MODFLOW.

3. AEM- Analytical Element Model

It is a numerical method developed by (O. Stark, 1989) useful to solve different groundwater flow and contaminant transport governing equations that denotes each aquifer property as an individual element and its influence on the flow direction.

AEM models with high resolution provide much more accurate results than conventional numerical models in large-hydraulic-stress situations that are a part of common remedial systems such as pumping, injection, trench, slurry wall and low permeability barriers. (He, 2004) TWODAN (Fitts, 1997) is a commercially available AEM groundwater model as well as WinTran (J. Rumbaugh, 1995). The flow portion of WinTran is based on the AEM theory, similar to that used in TWODAN; the transport portion of the model is a classic finite-element model. (He, 2004)

4. HYDROSCAPE

HYDROSCAPE is a Matlab based software program compiled as an executable file that uses an analytical solution to the advection–dispersion equation (ADE) to solve solute contaminant transport problems. (Funk, 2017)

It has an easy-to-use interface that produces high-quality outputs, includes a parameter estimator algorithm, and allows the user to upload maps from Google Maps. There also is a provision for custom source region built up (arbitrary user-defined source function/geometry and spatial variations in source concentration).

III. Observation and Conclusion

This review study suggests that any problem related to contaminant transport in groundwater can be solved by selecting a proper numerical/analytical model. Factors such as hydrogeology, type of contaminants, aquifer properties and solute transport process that takes place in one's study region that governs the selection of such proper models.

Different hydro-geo-chemical parameters can change the behavior of a single suitable model thus, adjusting every simulation with observations from field is involved while calibration of a model.

Vast amount of data has to be incorporated while developing a multi-dimensional groundwater model. Use of GMS is preferred over other advanced softwares as it involves major programming codes which are MODFLOW, MT3DMS, PHT3D, FEMWATER, SEAWAT, SEAM3D, etc.

New methodologies can be generated with the integration of GIS and GMS such as Arc Hydro Groundwater executable programming code and GIS CONTRAM. Also the integration of surface and subsurface contamination transport can be achieved with SWAT-MODFLOW-RT3D programming code.

IV. References

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