A GIS-based modeling system for petroleum waste management

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Abstract With an urgent need for effective management of petroleum-contaminated sites, a GIS-aided simulation (GISSIM) system is presented in this study. The GISSIM contains two components: an advanced 3D numerical model and a geographical information system (GIS), which are integrated within a general framework. The modeling component undertakes simulation for the fate of contaminants in subsurface unsaturated and saturated zones. The GIS component is used in three areas throughout the system development and implementation process: (i) managing spatial and non-spatial databases; (ii) linking inputs, model, and outputs; and (iii) providing an interface between the GISSIM and its users. The developed system is applied to a North American case study. Concentrations of benzene, toluene, and xylenes in groundwater under a petroleum-contaminated site are dynamically simulated. Reasonable outputs have been obtained and presented graphically. They provide quantitative and scientific bases for further assessment of site-contamination impacts and risks, as well as decisions on practical remediation actions.
Keywords Contamination; decision-support; GIS; groundwater; numerical simulation; petroleum waste; soil

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Introduction

Problems of contaminant leakage and spill from pipelines and storage tanks in petroleum industries have been paid significant attention in the past decades (Dowd, 1984; Newton, 1991). The number of underground storage tanks for petroleum products in the North America was estimated to be between 1.5 and 2 millions (Predpall *et al.*, 1984). Tejada (1984) reported that as many as 23% of the tanks leak. Soil and groundwater in thousands of sites have been contaminated by petroleum derived contaminants. Therefore, in-depth analysis on impacts associated with the exposed chemicals is desired for effective environmental management.

To evaluate the impacts, it is important to gain an insight into the fate of contaminants underground. This requires effective models to simulate a variety of processes in soil and groundwater. In fact, the fate of leaked petroleum products (i.e. nonaqueous phase liquids, NAPLs) in the subsurface is related to a number of physical, chemical, and biological processes. Upon release to the environment, NAPLs will migrate downward under the force of gravity. When significant amounts of NAPLs are released, they will transport downward until they encounter a physical barrier or are affected by buoyancy forces near the groundwater table. Once the capillary is reached, NAPLs may move laterally as a continuous, free phase layer along the upper boundary of the water-saturated zone due to gravity and capillary forces. The convection, dispersion, diffusion, adsorption, volatilization, and biodegradation may govern transport of a variety of petroleum-derived chemicals in the groundwater system. Previously, a number of studies have been undertaken for simulating the fate of NAPLs in soil and groundwater. For example, Abriola and Pinder (1985a, b) proposed a comprehensive approach to simulate simultaneous transport of a chemical contaminant in three physical forms: as a non-aqueous phase, as a solute component of a water phase, and as a mobile fraction of a gas phase. Kaluarachchi and Parker (1989) formulated a finite element model for simulating multi-phase flow of organic contaminants. Katyal *et al.* (1991) used a two-dimensional finite element program to simulate multi-phase and multi-component transport of NAPLs in subsurface with an assumption of first order decay. In general, most of the resent modeling efforts were based on multi-phase, multi-component analyses, such as MOVER, BIOF&T, and UTCHEM (Katyal, 1997; Freeze *et al.*, 1995), which can effectively reflect complexities in subsurface systems. However, extensive applications of the developed models to practical problems were limited due to the ineffectiveness in presentation and management of their inputs/outputs and the lack of dynamic and interactive systems for depicting the related spatial information graphically.

Fortunately, important progress has been made during the last decade with regard to geographical information systems (GIS) for dealing with spatial data and presenting them graphically (Matttikall, 1994; Hiscock *et al.*, 1995; Wilkinson, 1996). Especially, GIS can be used to represent the landscape by means of locationally referenced data describing the character and shape of geographic features. It has been widely used in environmental modeling and risk assessment. For example, Schenk *et al.* (1993) studied the integration of a three-dimensional groundwater model with a multi-dimensional GIS system. Batelaan *et al.* (1993) incorporated a groundwater model within a GIS system. However, most of the previous studies were limited within the scope of interactive and visual representation of modeling results (Bober *et al.* 1996; Stein *et al.* 1995). Very few of them could reach the level of producing user-friendly software packages (Ehlers *et al.*, 1989; Lovertt *et al.*, 1997).

This research is to provide an extended integration for the subsurface modeling and GIS application, emphasizing the following objectives.

- To develop a GIS-based simulation (GISSIM) system for petroleum waste management. This system will contain an advanced 3D numerical model for simulating the fate of contaminants in soil and groundwater, as well as a data management system based on GIS for supporting the simulation process and presenting the modeling inputs and outputs graphically.
- To apply the developed system to a North American case study. Concentrations of benzene, toluene, and xylenes in groundwater under a petroleum-contaminated site will be dynamically simulated. The modeling database will be interactively handled by GIS. Thus, impacts of the contamination in different time stages under a variety of remediation scenarios will be predicted.

The GIS-based simulation (GISSIM) system

Multi-component transport model

One of the key components in the GISSIM system is a multi-component transport model. It can be used for simulating the transport and biodegradation of multiple contaminants in the subsurface under various site conditions and remediation scenarios. The general equation can be formulated as follows (van Genuchten and Wierenga 1976):

$$\partial(\theta_m C_{wm})/\partial t + \partial(\theta_{im} C_{wim})/\partial t + \partial(f \rho P_{wm})/\partial \mathrm{t} + \partial[(1-f)\rho P_{wim}]/\partial t$$
$$= \partial\,(\theta_m D_{ij}\,\partial C_{wm}/\partial \mathrm{x}_j)/\partial x_i - \partial(q_i C_{wm})/\partial x_i - q_s C_{ws} \qquad (1)$$

where C_{wim} is concentration of contaminant w in immobile water [ML^{-3}]; C_{wm} is concentration of contaminant w in mobile water [ML^{-3}]; C_{ws} is concentration of contaminant w in injected fluid [ML^{-3}]; D_{ij} is hydrodynamic dispersion tensor corresponding to a direction defined by i, j [$L^2\,T^{-1}$]; f is fraction of sorption site which is in direct contact with mobile liquid; i, j are the directions in a Cartesian coordinate system; P_{wim} is adsorbed phase concentration of contaminant w in immobile phase [MM^{-1}]; P_{wm} is adsorbed phase concentration of contaminant w in mobile phase [MM^{-1}]; q_i is Darcy velocity in direction i [LT^{-1}]; q_s is volumetric flow rate of fluid injection (or withdrawal) per unit volume of porous medium [$L^3 L^{-3} T^{-1}$]; t is time [T]; x_i, x_j are distances in direction i and j [L], respectively; ρ is soil bulk density [ML^{-3}]; θ_{im} is fraction of soil filled with immobile water; and θ_m is fraction of soil filled with mobile water.

The value of D_{ij} is defined as follows (Bear, 1972):

$$\theta_m D_{ij} = d_L |q| \delta_{ij} + (d_L - d_T)\, q_i q_j / |q| + \theta_m \tau D_c \delta_{ij} \tag{2}$$

where d_L is longitudinal dispersivity [L]; d_T is transverse dispersivity [L]; D_c is molecular diffusion coefficient [$L^2 T^{-1}$]; $|q|$ is absolute value of Darcy velocity [LT^{-1}], $|q| = (|q_i|^2 + |q_j|^2)^{1/2}$; q_j is Darcy velocity in direction j [LT^{-1}]; δ_{ij} is Kronecker delta; and τ is tortuosity.

Using the following continuity equation for water flow:

$$-\partial(q_i)/\partial x_i = \partial(\theta_m)/\partial t - q_s\,, \tag{3}$$

and assuming a linear sorption isotherm ($P_m = K_d C_m$ and $P_{im} = K_d C_{im}$), we can rewrite Eq. (1) as follows:

$$\begin{aligned}&\partial C_{wm}/\partial t\,[\theta_m + f\rho k_d] + \partial C_{wim}/\partial t\,[\theta_{im} + (1-f)\rho k_d]\\ &= \partial(\theta_m D_{ij} \partial C_{wm}/\partial x_j)/\partial x_i - q_i \partial C_{wm}/\partial x_i - q_s(C_{ws} - C_{wm})\end{aligned} \tag{4}$$

The concentrations in mobile and immobile phases have the following relation (Kaluarachchi and Parker, 1990):

$$\partial C_{wim}/\partial t\,[\theta_{im} + (1-f)\rho k_d] = X\,(C_{wm} - C_{wim}) \tag{5}$$

where X is a mass transfer coefficient for diffusive mass exchange between the mobile and immobile phases [T^{-1}].

Incorporating decay losses λ_{wm} and contaminant loading from a hydrocarbon source to the mobile phase H_w in Eqs (4) and (5), we have (Kaluarachchi and Parker, 1990):

$$\begin{aligned}&\partial C_{wm}/\partial t\,[\theta_m + f\rho k_d] + \partial C_{wim}/\partial t\,[\theta_{im} + (1-f)\rho k_d]\\ &= \partial(q_m D_{ij} \partial C_{wm}/\partial x_j)/\partial x_i - q_i \partial C_{wm}/\partial x_i - q_s(C_{ws} - C_{wm}) - l_{wm} + H_w\end{aligned} \tag{6}$$

$$\partial C_{wim}/\partial t\,[q_{im} + (1-f) r k_d] = X\,(C_{wm} - C_{wim}) - l_{wm} \tag{7}$$

Generally, the above model has the capabilities to model complex heterogeneous and anisotropic hydrogeology. Through this modeling system, concentrations of up to five contaminants in a three dimensional domain can be predicted at a prescribed time horizon. The modeling outputs will provide important bases for decisions of site remediation actions. More detailed formulation and solution processes for the multi-phase and multi-component transport model in porous media were provided by Kaluarachchi and Parker (1990), Katyal (1997), Katyal and Parker (1992), and Chen *et al.* (1998).

GIS system

In general, GIS is used in three areas throughout the system development and implementation process: (i) managing spatial and non-spatial databases; (ii) linking inputs, model, and

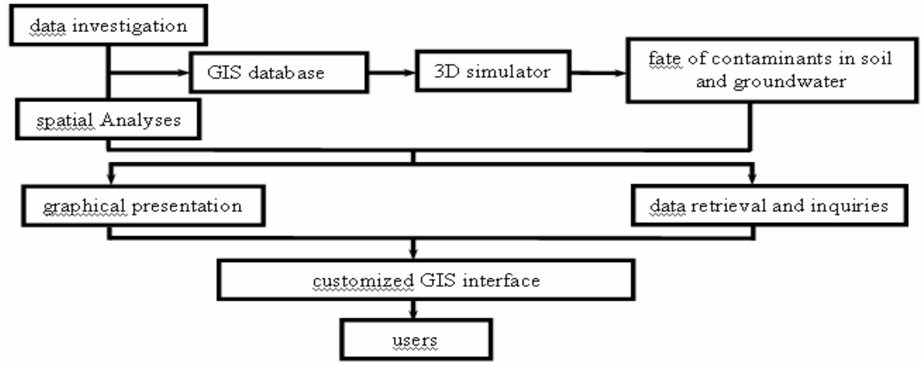

Figure 1 Structure of the GISSIM structure

outputs; and (iii) providing an interface between the GISSIM and its users. The goal is to couple GIS with the model to allow smooth communication between the modeling system and its users. Figure 1 shows the structure of the proposed GISSIM system.

(a) Database management. Generally, spatially referenced physical data for the groundwater model can be divided into two categories, one value per location (or one-for-one), and many values per location (or many-for-one). Data of the one-for-one category can be stored as location attributes attached to a conventional GIS coverage. In this type of database, the location ID is used as a key for data storage and retrieval. Data of the many-for-one category can be stored in separate databases with one file for each attribute at each physical location. In this type of databases, a file name should reflect both the location ID and the name of the physical attribute it stores. In this study, a number of locations are considered, with each of them referring to a group of attribute data. This leads to large amounts of files corresponding to inputs and outputs of the simulation model. To enhance management of these files, a communication channel between Microsoft Access database and GIS-ArcView database is built through Visual Basic programming.

(b) Model interface. This study considers both hydrogeologic characteristics and contaminant features in evaluating the impact of contamination sources on subsurface water quality. GIS is used to access and manipulate a great variety of input data and provide a wide range of analytical functions for preparing modeling inputs. GIS, with its spatial analysis functions, can also connect individual modeling components to form an integrated system. Its interface generates proper input data files automatically for the model, serving as a bridge between the input data and the simulation model. The generated GISSIM system links digital data, model, and computational outputs together. The GISSIM's retrieval and presentation function allows users to retrieve and analyze information on site conditions and modeling results dynamically. A geographic "hot link" is created as a hyper-media function to communicate spatially referenced information into various types of data. For example, a contaminant's concentration at a spatial location can be retrieved through clicking on that location at the screen referring to a subsurface layer. In addition, the model interface connects the simulation results in a graphic display supported by GIS.

(c) User interface. This component provides a two-way communication between the system and its users. On one hand, the system user may interactively delineate an area of concern, identify contamination sources to be considered, add additional data, or specify a particular planning objective. On the other hand, the system explains to the user about each

step in the modeling process and displays results from running the simulation model. The system provides its user an evaluation of the quality of data, accuracy of the result, and level of uncertainty. If the user is not satisfied with the results from available data, the system can recommend to its user what data are needed to improve the modeling performance. The user interface makes the implementation of the GISSIM a robust and user-friendly process. Data display is the final stage in the modeling process, which is concerned with the communication of essentially geographic information to the user. The most powerful medium for this communication is the graphic image, usually in the form of maps, charts, or tables. ArcView, a geographical data browsing system, is used for displaying modeling results. The software allows users to create their own views of geographical data. Users may use basic ArcView statistical and spatial query functions to selectively output information. The Avenue scripting language, as part of the ArcView product, is used to create a user interface. Distribution of pollutant concentrations in the subsurface at a prescribed time can thus be displayed dynamically through contours and 3D surfaces within the GISSIM system.

Case study

Overview of the study system

The study site is located in western Canada (Figure 2). It was operated as a natural gas processing plant from the mid 1960s to the early 1990s. The plant was utilized to remove naphtha condensate from the natural gas stream prior to transport to a regional transmission line. Throughout the history of the site, the condenstate was disposed of in three perforated underground storage tanks (USTs) (Figure 3), which then leaked into soil and finally to groundwater following seepage. Two contaminant concentrated zones were formed in the subsurface capillary fringe (at the interface between unsaturated and saturated zones).

The site is bounded in all directions by agricultural land. There are several farmer residences located within 1.5 km radius of the site all with domestic water withdrawal wells. In recent years, agricultural land in the southeast has been used for livestock husbandry (for cows and horses). Groundwater was encountered between 5 and 10 m below surface. The

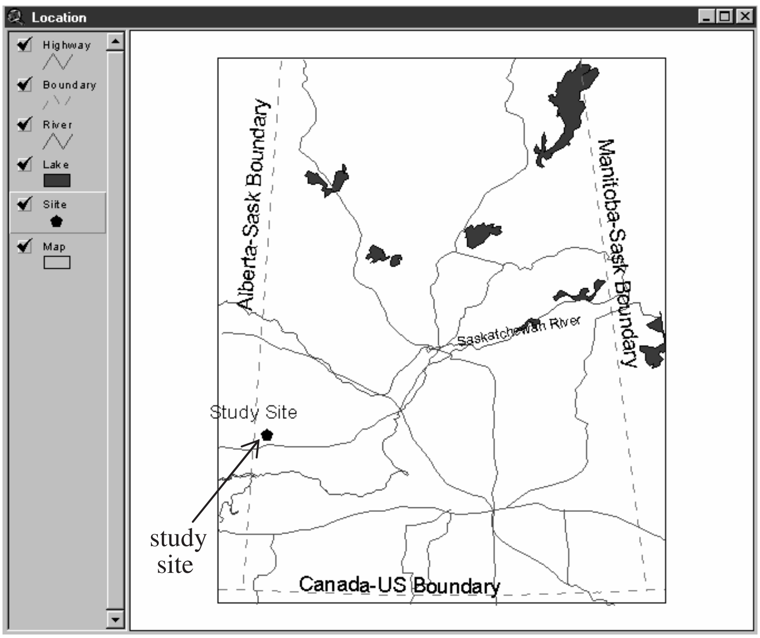

Figure 2 The study site

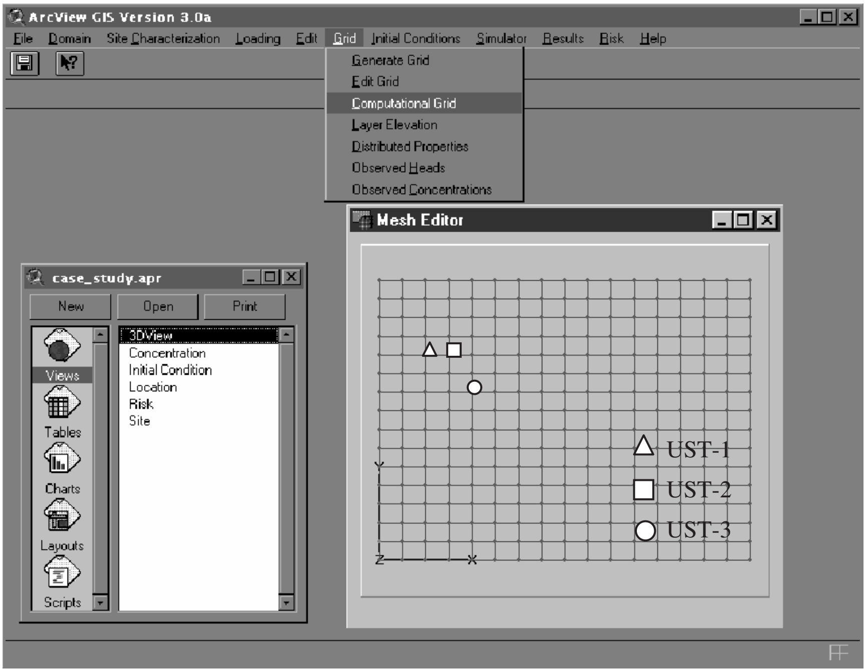

Figure 3 The GISSIM system

general groundwater flow direction is towards the south, with the gradient of the water table being slightly from northeast to southwest. The groundwater table is predominately located within a clay-till soil layer.

The site conditions and modeling outputs can be conveniently represented through the developed GISSIM system. For instance, facilities and emission sources on the site can be presented graphically through the GIS. The observed and predicted contaminant concentrations, as well as information on the groundwater table, can be displayed based on two-dimensional contour lines or three-dimensional surfaces. The stratigraphy in subsurface can be revealed through provision of soil distributions at different elevations and cross sections. In addition, many modeling parameters at a spatial location, such as hydraulic conductivity, soil density, water saturation level, and air pressure, are grouped into a many-for-one data category in the GIS. The above information can be retrieved by clicking the related features (point, lines, and polygons) in the GISSIM system.

GISSIM modeling process

The GISSIM modeling process involves the following four steps:

Step 1: *Digitization and GIS database development*

This step is to provide a database of pollution-related parameters at the site. It contains a variety of data related to on-site hydrological and geological conditions, soil types, source distributions, contamination levels, and surrounding environmental features (e.g. residential zones, river, and lakes). The database is useful for further modeling study. The information sources include existing maps, digital data, and site investigation reports.

Step 2: *Grid system development*

The multi-component transport model is implemented through a computational grid system. Normally, two-dimensional grid systems can be directly generated through the GIS. Since this study requires a three-dimensional (3D) mesh, an external mesh editor is launched to create and edit 3D finite element meshes. This editor allows generation of irregular quadrilateral meshes in two or three dimensions, as well as analysis of soil and groundwater properties in the study domain (Figure 3).

Step 3: *Simulation modeling*
The multi-component transport simulator can be launched through the proposed event-driven interface. After the modeling inputs are prepared through the GIS database, the simulator can be used for predicting the fate of benzene, toluene and xylenes (BTXs) in the aquifer.

Step 4: *Results representation*
The simulation outputs are first transformed into an acceptable format for the GIS. They can be presented in several ways, such as statistical chart, contour lines, and 3D surfaces. Figure 4 presents the simulation results through contour lines.

Results

After the model is well calibrated and verified, it can then be used for dynamically simulating the fate of contaminants under a number of remediation scenarios. Figure 4 shows distributions of benzene, toluene and xylene concentrations 10 years later when no remediation action is undertaken. It is indicated that the peak benzene concentration will still be 7.40 mg/L 10 years later, which is higher than the regulated 1.90 mg/L in the local Non-Potable Groundwater Quality Guidelines. This peak occurs at about 30 m west of UST-2 and 30 m northeast of UST-3. The results also demonstrate that, due to the large

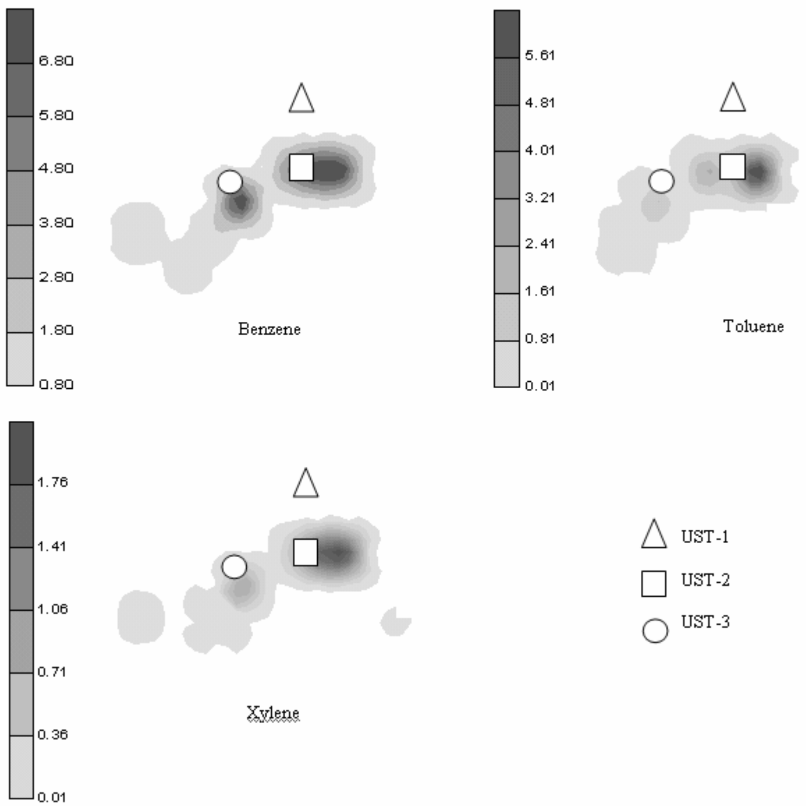

Figure 4 GISSIM modeling results

contamination area and the specific stratigraphic and hydraulic characteristics of the site, BTX in the unsaturated zone will be continuously released to groundwater if no remediation action is undertaken. It is thus not recommended that the on-site groundwater be used for irrigation or drinking water supply even 10 years later under this scenario.

The peak toluene concentration 10 years later will be 6.46 mg/L, which is still higher than the regulated 5.90 mg/L. In comparison, the peak xylenes concentration (2.41 mg/L) is lower than the regulated 5.60 mg/L. If a remediation action with 60% efficiency is undertaken, all pollution problems at the site will be completely resolved 10 years later. In detail, the peak concentrations of benzene, toluene, and xylenes 10 years later will be 1.49, 2.10, and 0.46 mg/L, respectively, which are lower than the regulated values.

Through the GISSIM, the observed and simulated site contamination conditions can be expressed as a set of many-for-one data series where both location-ID and time-series ID are used for identifying information at different temporal and spatial units. Thus, an insight into the fate of contaminants underground can be obtained through provision of the GIS database, the graphical presentation of spatial information, the data retrieval system, and the inherent spatial analysis functions. In detail, questions related to spatial extent of contaminated zones, level of contamination, and temporal variation of pollutant concentrations can be effectively answered through interactions with the GISSIM's user-friendly interfaces.

Conclusions

A GIS-based simulation (GISSIM) system is proposed for petroleum waste management. It contains an advanced 3D numerical model for simulating the fate of contaminants in soil and groundwater, as well as a data management system based on GIS for supporting the simulation process and presenting spatially referenced and time-series information graphically. Through incorporation of GIS within the modeling framework, an object-oriented simulation environment with an open software architecture is provided.

The developed system is applied to a North American case study. Concentrations of benzene, toluene, and xylenes in groundwater under a petroleum-contaminated site are dynamically simulated. Conditions of the contamination in different time stages under a variety of remediation scenarios are predicted. Reasonable results have been obtained and graphically presented. Generally, it is indicated that benzene is the most important contaminant at the site. If no remediation action is undertaken, serious benzene contamination problem will still exist at the site even 10 years later.

Implications of the modeling outputs have been analyzed based on the local Guidelines for Non-potable Groundwater Quality. They provide quantitative and scientific bases for further assessment of site-contamination impacts and risks, as well as decisions on practical remediation actions.

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