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Quasi-Monte Carlo based global uncertainty and sensitivity analysis in modeling free product migration and recovery from petroleum-contaminated aquifers

Li He[a,*], Gordon Huang[b], Hongwei Lu[b], Shuo Wang[a], Yi Xu[b]

[a] *MOE Key Laboratory of Regional Energy and Environmental Systems Optimization, Resources and Environmental Research Academy, North China Electric Power University, Beijing 102206, China*
[b] *Chinese Academy for Environmental Planning, Beijing 100012, China*

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ABSTRACT

This paper presents a global uncertainty and sensitivity analysis (GUSA) framework based on global sensitivity analysis (GSA) and generalized likelihood uncertainty estimation (GLUE) methods. Quasi-Monte Carlo (QMC) is employed by GUSA to obtain realizations of uncertain parameters, which are then input to the simulation model for analysis. Compared to GLUE, GUSA can not only evaluate global sensitivity and uncertainty of modeling parameter sets, but also quantify the uncertainty in modeling prediction sets. Moreover, GUSA's another advantage lies in alleviation of computational effort, since those globally-insensitive parameters can be identified and removed from the uncertain-parameter set. GUSA is applied to a practical petroleum-contaminated site in Canada to investigate free product migration and recovery processes under aquifer remediation operations. Results from global sensitivity analysis show that (1) initial free product thickness has the most significant impact on total recovery volume but least impact on residual free product thickness and recovery rate; (2) total recovery volume and recovery rate are sensitive to residual LNAPL phase saturations and soil porosity. Results from uncertainty predictions reveal that the residual thickness would remain high and almost unchanged after about half-year of skimmer-well scheme; the rather high residual thickness (0.73–1.56 m 20 years later) indicates that natural attenuation would not be suitable for the remediation. The largest total recovery volume would be from water pumping, followed by vacuum pumping, and then skimmer. The recovery rates of the three schemes would rapidly decrease after 2 years (less than 0.05 m^3/day), thus short-term remediation is not suggested.

1. Introduction

Nonaqueous phase liquids (NAPLs) are among the most common type of pollutants in soils and groundwater. Their presence can create a hazard to public health and the environment. One of the widely-encountered sources of NAPLs is the spills involving the release of petroleum products such as gasoline, diesel fuel and lubricating and heating oil from underground leaking oil tanks and pipelines. Light NAPLs (LNAPLs), existing as a type of free product in the subsurface, can be recovered through skimmer (i.e., no pumping is implemented), water pumping and vacuum pumping schemes [1–3]. Free product recovery has increasingly received attention in the past years due to its economic and temporal efficiencies [3,4].

Studies have been conducted in modeling migration and recovery of free product (LNAPLs) in unconfined aquifers [3,5,6]. Kaluarachchi and Parker [1] developed a numerical model named ARMOS to simulate free product migration and recovery in unconfined aquifers. Based on the assumption of local vertical equilibrium, the area flow equations for water and hydrocarbon can be derived with reduced dimensionality and nonlinearity. The model was also capable of simulating free phase hydrocarbons under conditions involving hydrocarbon skimming with or without water pumping. Kaluarachchi [3] investigated the effects of subsurface heterogeneity on free-product recovery system designs using a vertically integrated three-phase flow model. Results from a series of hypothetical field-case simulation revealed that the effects were enhanced at relatively low water-pumping rates, and the difference in results produced by homogeneous and heterogeneous simulations was substantial.

Charbeneau et al. [7] proposed two simple models for predicting free product recovery rates using wells and vacuum pumping systems. The models incorporated vertical variations in LNAPL saturation and relative permeability through the use of effective LNAPL-layer values. Compared to ARMOS, the models were rather simple but their applicability was unable to address multiple-well pumping strategies. Li et al. [8] presented the simulation of a dual-phase vacuum extraction process via a finite element multiphase flow model. It was observed that the model was computationally

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* Corresponding author. Tel.: +86 10 61772980; fax: +86 10 61772960.
E-mail address: heliy111@gmail.com (L. He).

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efficient due to the vertical integration of governing equations for water, oil, and gas flow. Yen and Chang [9] used a bioslurping simulation model for predicting three-phase (water, oil, and gas) flow and transport in groundwater and gas phase flow in the unsaturated zone. Through the model, one can gain insight into the recovery and migration of LNAPLs with vacuum enhanced recovery and multispecies (dissolved in groundwater) and gas phases (in unsaturated zone) transport in heterogeneous, anisotropic porous media.

The above mentioned efforts in free product recovery were presented as either analytical equations or two-dimensional numerical models. However, few of the studies considered the impacts of parameter uncertainty on LNAPL migration and recovery processes [3]. Due to inevitable errors in modeling formulation, data observation and parameter estimations, model predictions could depart from the true values considerably [10–15]. Sensitivity analysis is an effective approach for analyzing effects of parameter variations on remediation performance. However, it investigates the impacts by treating the parameters as individual values rather than sets of values [16]. Recently, generalized likelihood uncertainty estimation (GLUE) methods have been widely applied in for calibration and uncertainty estimation of mathematical models [16–26].

However, GLUE does not consider individual or interactive influences of parameters on predictions. This probably leads to the increase in computational effort since overmuch uncertain parameters need to be considered by GLUE. If global sensitivity analysis (GSA) is performed before GLUE, then those substantially sensitive parameters can be screened out and input to GLUE procedures. Due to the decrease of uncertainty parameters, the required realizations can be reduced. Moreover, GLUE generally employs regular Monte Carlo (MC) sampling with an assumption of uniformly-distributed random parameters, while MC cannot guarantee the sampling data are generated with low discrepancy. This causes slow convergence rate in computation and probably in underestimation of uncertainty predictions due to high possibility of missing part of important parameter values in sampling. Much research has been undertaken in development and application of high-efficient sampling rules such as Latin Hypercube (LH), Markov Chain Monte Carlo (MCMC), adaptive MCMC [26], and quasi-Monte Carlo (QMC). Particularly, QMC has shown its superior advantages over regular MC in generating low-frequency sampling data and high efficiency over LH [27].

Therefore, this paper aims to present a new global uncertainty and sensitivity analysis (GUSA) framework based on GSA and GLUE methods. Through GUSA, not only global sensitivity and uncertainty of input parameters can be evaluated, but also uncertainty in modeling predictions can be quantified. GUSA is applied to a practical petroleum-contaminated site in Canada to investigate free product migration and recovery processes under aquifer remediation schemes.

2. Materials and methods

2.1. Aquifer overview

The aquifer to be investigated is located at the Cantuar site in southwest Saskatchewan, Canada [33]. The existing site characterization results showed that the stratigraphy at the aquifer consisted of native silt and silty clay extending from surface to between approximately 7.6 m and 12.5 m depth. Underlying silty clay was clay matrix till extending to between 9.4 m and 15.2 m depth. Sand was encountered with or underlying the clay matrix till between approximately 9.4 m and 15.2 m depth. Silty clay and sand underlying the top soil were over majority of the aquifer. Clay/till underlay the sand over the majority of the site, and extended to the maximum exploration depth of 14.0 m. Groundwater table was measured between approximately 4.8 m and 13.2 m below ground surface, predominantly located in the clay tills. The groundwater flow direction was from southeast toward northwest with a gradient of approximately 0.1 m/m.

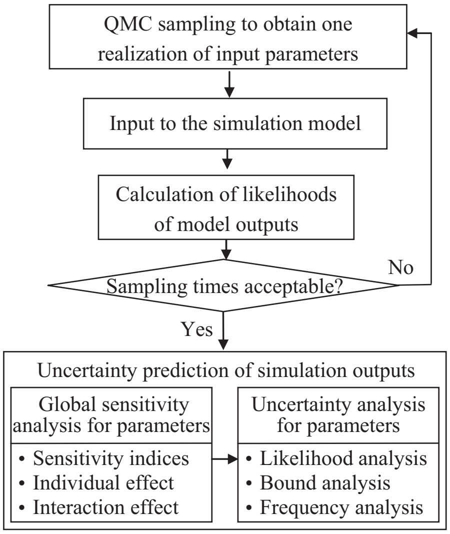

Fig. 1. Flowchart of QMC-based GUSA.

Free phase hydrocarbons (i.e., free product) have infiltrated through fractures near an underground storage tank ever buried into the subsurface. The hydrocarbons migrated along saturated fissures in the clay vertically toward the groundwater table, and finally piled up at the groundwater surface. Fig. S3 in the Supplementary data shows the monitoring well locations and estimated contamination plume of the aquifer. During the 25-April-2000 monitoring program, free product was detected in monitoring wells BH101 (725 mm), BH103 (1773 mm), BH105 (545 mm), BH106 (201 mm), BH108 (176 mm), BH110 (398 mm), BH111 (250 mm), BH201 (453 mm), BH202 (192 mm) and BH401 (262 mm) located across the site. Fig. S4 in the Supplementary data presents the free product thickness on 25th May, 2000 at the site, which indicated that the peak free phase hydrocarbon thickness was approximately in the range of 1.8–2.5 m. The GUSA framework was applied to this aquifer to evaluate performance of three potential aquifer remediation schemes. Note that this section, only residual free product thickness, total recovery volume and recovery rate were examined at well BH401 under three 20-year remediation schemes: skimmer, water pumping (1 m^3/hr), and vacuum pumping (−4 m water column).

2.2. Global uncertainty and sensitivity analysis

The QMC-based GUSA framework is shown in Fig. 1. In terms of the figure, a mathematical simulation model is selected for capturing the free product migration and recovery processes in an unconfined aquifer. The model can be used to predict the free product migration and recovery processes under pumping-based remediation schemes. The following gives the volume balance equations for water, NAPL and air phases in the unsaturated and saturated zones [2,3,28]:

$$\frac{\partial V_{\mathrm{w}}}{\partial t} = \frac{\partial}{\partial x_i}\left(T_{\mathrm{w}ij}\frac{\partial Z_{\mathrm{aw}}}{\partial x_j}\right) + R_{\mathrm{w}}\delta(x_i - x_i^*)\delta(x_j - x_j^*) \tag{1}$$

$$\frac{\partial V_{\mathrm{o}}}{\partial t} = \frac{\partial}{\partial x_i}\left(T_{\mathrm{o}ij}\frac{\partial Z_{\mathrm{ao}}}{\partial x_j}\right) + R_{\mathrm{o}}\delta(x_i - x_i^*)\delta(x_j - x_j^*) \tag{2}$$