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Design of Groundwater Remediation Systems under Stepwise Quadratic Response Surface Analysis

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Abstract. Solving groundwater remediation optimization problems based on numerical simulators which would usually bring high computational cost to the decision-makers. In order to overcome this problem, a surrogate-based approach is proposed, where a parametric statistical method (SQRSA) is used to create a series of surrogates that provide a direct and rapid response bridge between remediation strategies and remediation performance. SQRSA has the advantages of (i) automotive selection of potential explanatory variables (e.g., the pumping rates at various remediation wells), (ii) providing a flexible manner for examining the linear, interactive, and quadratic effects of operating conditions on the naphthalene levels, and (iii)alleviating the computational efforts in optimization processes.

Keywords: groundwater remediation, optimization, numerical simulators, surrogates

1. Introduction

In China, there are a lot of sites that have been polluted by petroleum hydrocarbons because of the leakages from underground storage tanks and pipelines. These may pose significant threats to the underlying groundwater and the health of the neighboring communities [1].In recent years, a large number of remediation methods have been applied to remove the groundwater contaminants [2].A problem associated with these remediation actions is the deficiency in understanding processes controlling the fate of contaminants may lead to a large inflation of expenses [3].

Over the past decades, various simulation-based groundwater management models were undertaken to improve remediation efficiency [4-5].Due to the difficulties in alleviating the high computational cost and amounts of data requirement in stochastic analysis, a series of effective surrogates were applied to replace the complex simulation equations. Although the above efforts were useful for increasing computational efficiency, the conventional regression surrogates can hardly select the variables automatically.

Stepwise quadratic response surface analysis (SQRSA) is proposed. It is a useful technique for tackling these concerns, since it supports automatic selection of models in cases where a large number of potential explanatory variables exist and no prior knowledge on which to base the surrogate selection, and it can be used to capture the relationships between contaminant concentrations and system operation patterns perfectly.

2. Methodology

2.1 Stimulation Model

BIOPLUME III is a two-dimensional, finite difference model for simulating the biodegradation of hydrocarbons in ground water. The model simulates both the aerobic and anaerobic biodegradation processes in addition to advection, dispersion, sorption, and ion exchange. The mass transport equations are operated to

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forecast the spatial variation of contaminant concentration. For this case, the aquifer is homogeneous and isotropic, where oxygen is used as an electron acceptor. The general equations are as follows：

$$\frac{\partial(bH)}{\partial t}=\frac{1}{R_h}\left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial H}{\partial x_j}\right)-\frac{\partial(bHV_i)}{\partial x_i}\right]-\frac{H'W}{n}-\frac{Q}{n}\delta\left(x-x^{(r)}\right)H \tag{1}$$

$$\frac{\partial Pb}{\partial t}=\left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial P}{\partial x_j}\right)-\frac{\partial(bPV_i)}{\partial x_i}\right]-\frac{P'W}{n} \tag{2}$$

$$\Delta H_{so}=\frac{P}{F_o},\qquad P=0\qquad if\qquad H>\frac{P}{F_o} \tag{3}$$

$$\Delta P_{os}=HF_o,\qquad H=0\qquad if\qquad P>HF_o \tag{4}$$

where H is the concentration of hydrocarbon; H' is the concentration of hydrocarbon in source or sink fluid; P is the concentration of oxygen; P' is the concentration of oxygen in source or sink fluid; Q is the pumping rate; $x^{(r)}$ is the coordinates of the well; ΔH_{SO} is the loss of the contaminant concentration due to aerobic biodegradation; ΔP_{OS} is the concentration loss of the electron acceptor; F_O is the stoichiometric ratio for oxygen.

2.2 Stepwise quadratic response surface analysis

Stepwise quadratic response surface analysis (SQRSA) is used to quantitatively describe the relationship between response variables and explanatory variables. The least squared fitting is a general means of determining coefficients of the surrogate. C_k is the expected contaminant concentration of kth monitoring well after remediation. C_k can be regarded as a polynomial function of a set of explanatory variables (q_1, q_2,…, q_n),which represents the injection/extraction rates. The surrogate can be formulated as follows:

$$C_k=a_{0,k}+\sum_{i=1}^{n}a_{i,k}q_i+\sum_{i=1}^{n}\sum_{j=1}^{n}a_{ij,k}q_iq_j\,(i\neq j)+\sum_{i=1}^{n}a_{ij,k}q_i^2+e_k \tag{5}$$

where $a_{0,k}$ is an intercept term of surrogate k; $\sum_{i=1}^{n}a_{i,k}q_i$ are linear terms of surrogate k; $\sum_{i=1}^{n}\sum_{j=1}^{n}a_{ij,k}q_iq_j\,(i\neq j)$ are interaction terms of surrogate k; $\sum_{i=1}^{n}a_{ij,k}q_i^2$ are quadratic terms of surrogate k; e_k is the error of surrogate k; n is the number of explanatory variables. As the responses can be multiple, they can be described as follows:

$$C=AQ+E \tag{6}$$

$$C=\left[C_1,C_2,...,C_k\right]^T \tag{7}$$

$$A=\begin{bmatrix} a_{0,1} & a_{i,1} & ... & a_{ij,1} & ... & a_{ii,1} & ... \\ a_{0,2} & a_{i,2} & ... & a_{ij,2} & ... & a_{ii,2} & ... \\ & ... & & ... & & ... & \\ & ... & & ... & & ... & \\ a_{0,k} & a_{i,k} & ... & a_{ij,k} & ... & a_{ii,k} & ... \end{bmatrix} \tag{8}$$

$$Q=\left[1,Q_i,...,Q_iQ_j,...,Q_i^2...\right]^T \tag{9}$$

$$E=\left[e_1,e_2,...,e_k\right]^T \tag{10}$$

where C is the response vector; Q is the explanatory vector; A is the coefficient matrix; E is the error vector; K is the number of responses; and superscript T means the transpose of the matrix. SQRSA is an effective technique, as it supports automatic selection of models in cases where there are a lot of potential explanatory variables and there is no anterior knowledge on which to base surrogate selection. It can also be used to perfectly capture the relationships between contaminant concentrations and operating conditions.

3. Case study

The developed model is applied to a petroleum-contaminated aquifer located in a power plant of Anhui province. The constituent of interest is naphthalene in this study, which has seriously affected the surrounding environmental quality and human health. The underground storage pool is at the up gradient location of the site where the naphthalene concentration (approximate 80 mg/L) in groundwater is higher than the regulated environmental guideline (1mg/L). Thus, soil and groundwater contamination at this site may pose environmental risks and health impacts on the surrounding communities. Remediation actions are desired to clean up the contaminated groundwater.

In the simulation domain, a total of 2 injections, 4 extractions, and 4 monitoring wells are selected in the plume. Thus, a pump-and-treat system is established in this site, mainly for controlling the transport of contaminated groundwater.Fig.1 shows the simulation domain and the location of each wells.

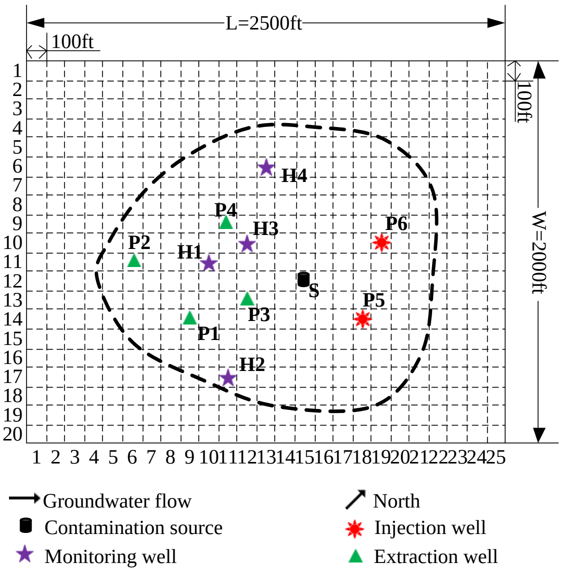

Fig.1: Simulation domain and well location.

The extraction rates (q_1, q_2, q_3 and q_4) in extraction wells P1, P2, P3 and P4 and the injection rates (q_5 and q_6) in injection wells P5 and P6 are selected as control variables to produce a series of operation scenarios. The naphthalene concentrations in monitoring wells are simulated during a 3-year remediation period under each operation condition. Fig. 2 shows the results of expected naphthalene concentrations of wells H1, H2, H3 and H4 under various operation scenarios. It shows that different results are generated under different scenarios. Thus, it is necessary to acknowledge the relationship between system operation patterns and contaminant concentrations, such that the trade-off between system cost and remediation efficiency can be analyzed.

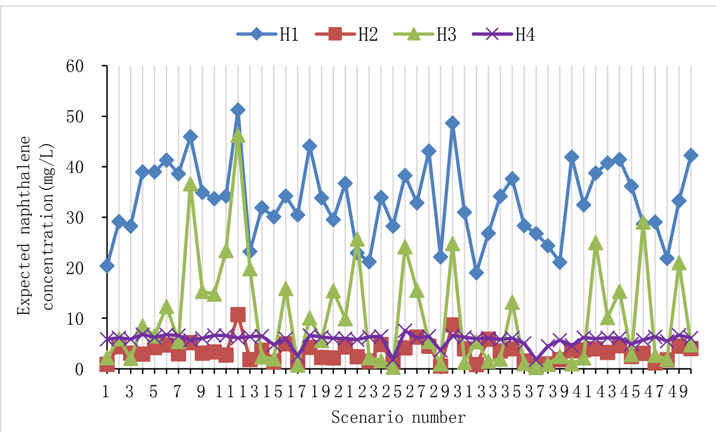

Fig.2: Expected naphthalene concentrations under 50 operation scenarios (3 years).

In order to make the surrogates achieve a perfect performance, the explanatory variables are normalized by dividing them by 97.2(the unit ft^3/s is converted to m^3/h), natural logarithms of the simulated naphthalene concentrations under each scenario are considered as response vectors to avoid scaling problems. Therefore, 4 surrogates with each one targeting on a monitoring well are established. The surrogates contain intercept, linear, interactive, and/or quadratic terms, varying with the locations of the wells and the pumping durations.

Fig. 3 presents the comparison of the results from the mean value of naphthalene concentrations from numerical simulation and regression analysis under various operation scenarios. It is indicated that the regression models can generally reflect the variation of naphthalene concentration under different operation scenarios. The peak values in four monitoring wells can be well caught as well. These results indicate that the generated surrogates can be used for approximating the simulation model with acceptable error levels.

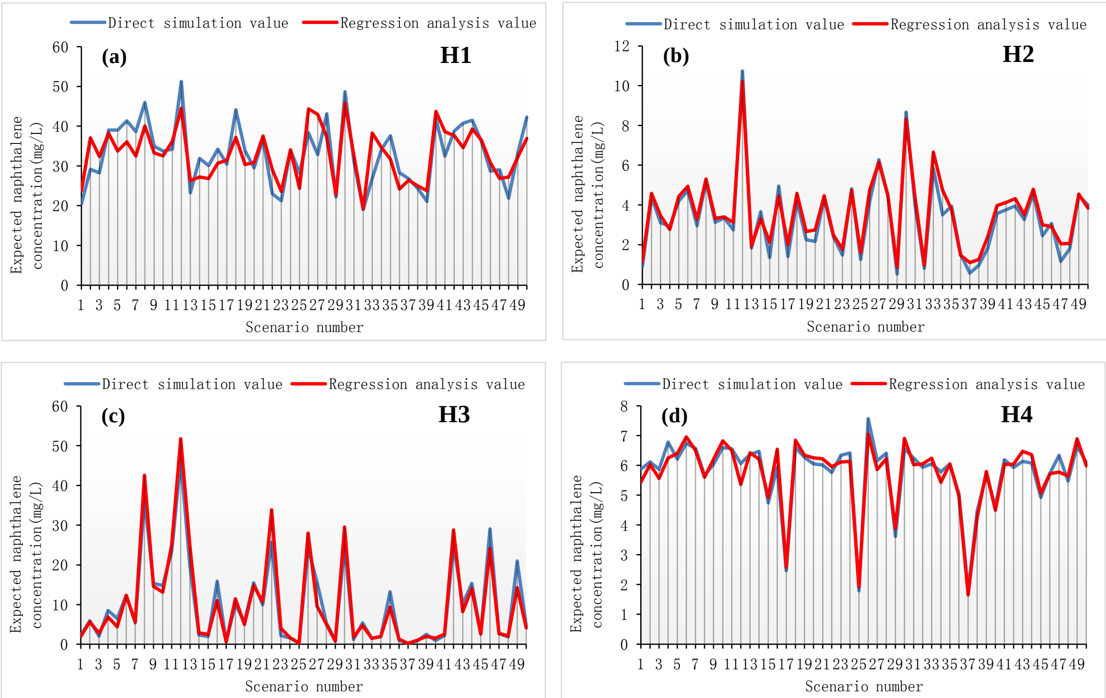

Fig.3: Direct simulation versus regression analysis in naphthalene concentrations.

4. Conclusion

The simulation process employed a set of surrogates that provide a direct and rapid response bridge between remediation strategies (i.e. pumping rates) and remediation performance (i.e. contaminant concentrations) via SQRSA. This bridge is effective in mitigating the computational efforts in optimization processes. SQRSA has the advantage of (i) supporting automatic selection of models in the cases where a large number of potential explanatory variables exist and no prior knowledge on which to base the surrogate selection, (ii) examining the effects of each linear, interactive, or quadratic term on response variables separately and (iii) alleviating the computational efforts in optimization processes.

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