



A stochastic optimization model under modeling uncertainty and parameter certainty for groundwater remediation design: Part II. Model application

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ABSTRACT

A new stochastic optimization model under modeling uncertainty (SOMUM) and parameter certainty is applied to a practical site located in western Canada. Various groundwater remediation strategies under different significance levels are obtained from the SOMUM model. The impact of modeling uncertainty (proxy-simulator residuals) on optimal remediation strategies is compared to that of parameter uncertainty (arising from physical properties). The results show that the increased remediation cost for mitigating modeling-uncertainty impact would be higher than those from models where the coefficient of variance of input parameters approximates to 40%. This provides new evidence that the modeling uncertainty in proxy-simulator residuals can hardly be ignored; there is thus a need of investigating and mitigating the impact of such uncertainties on groundwater remediation design. This work would be helpful for lowering the risk of system failure due to potential environmental-standard violation when determining optimal groundwater remediation strategies.

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1. Introduction

A complete description of a stochastic optimization model under modeling uncertainty and parameter certainty (SOMUM) has been provided in the first companion paper. In this part, a practical petroleum-contaminated site in western Canada will be used as a case study to demonstrate the applicability of the model. To begin, results from modeling calibration and verification, hypothetical tests and optimal design will be presented in detail. The optimization results obtained from the SOMUM model will then be compared to those from: (a) stochastic optimization models accounting for physical-property (or parameter) uncertainty (SOMUP) [1,2] and (b) a deterministic optimization model (DOM) under certainty (i.e. no uncertainty is addressed) [3]. Through the comparison, the impacts of modeling and parameter uncertainties on optimal design strategies can be investigated. The implicit in the modeling effort will also be discussed.

The site is located approximately 20 km north of the Town of Kindersley in Canada and has been in operation since the late 1950s. The previous characterization results indicated that it has complex heterogeneous and anisotropic hydrogeological conditions and the soils can be categorized into clay till, silty clay, and sandy soil (Figure S1 in the supplementary material). Due to oil leak-

age, petroleum hydrocarbons were detected in the subsurface. The major contamination sources included a gas plant on the west side of the site (S1), a disposal pit formerly located in the northeast quadrant of the site (S2), and a recirculating pump close to S1 (S3). In 2000, dual phase vacuum extraction was used in the first stage; this practice was found to successfully remove the petroleum hydrocarbons existing as NAPL (nonaqueous phase liquid) and air phases. However, the groundwater samples taken from the site indicated that the BTEX (benzene, toluene, ethyl-benzene and xylenes) concentrations still violate the environmental standards issued by the CCME [4] and SERM [5].

Thus, a pump-and-treat system was recommended in the second remediation stage, mainly for controlling the transport of contaminated groundwater, preventing uninterrupted expansion of contamination zones, and decreasing the dissolved contaminant concentrations [7]. The remediation durations were assumed to be 5, 10, 15 and 20 years. This selection was mainly based on the remediation cost and timeframe, compared to other techniques such as natural attenuation. In situ bioremediation was not considered either, due to the extremely low temperature in the long winter. To support optimal design of the pump-and-treat system, a three-dimensional multiphase multi-component simulator was used to predict the fate and transport of BTEX in the groundwater.

The detail of the simulator description has been shown in the first companion paper. The simulation area was considered as a three-dimensional heterogeneous domain, with an area of 270 m × 225 m and a depth of 10 m (Figure S2 in the supplement-

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tary material). Vertically, the domain was divided into four layers, which were 1, 2, 3 and 4 m, respectively. Horizontally, each layer was discretized into 54×45 grid blocks, with each one being dimensions of 5 and 5 m in x, y directions, respectively. The total number of grids was thus 9720 ($54 \times 45 \times 4$). In the simulation, non-flow boundary conditions were assigned on the top and at the bottom of the simulation domain, forming a steady groundwater flow from northeast to southwest.

2. Simulator validation

The identified parameters input to the simulator were classified into three types: hydrologic parameters, hydrocarbon source parameters, and control parameters. Site hydrologic parameters, including hydrologic properties (e.g., water dynamic viscosity, water density, water surface tension, average recharge rate, water saturation, residual water saturation) and porous medium properties (e.g., hydraulic conductivity in three dimensions, ratio of horizontal to vertical hydraulic conductivity, porosity, bulk density, surface ground elevation, groundwater elevation, groundwater gradient and direction, longitudinal dispersivity, transverse dispersivity and vertical dispersivity); hydrocarbon source parameters, including hydrocarbon phase properties (e.g., NAPL density, NAPL dynamic viscosity, hydrocarbon solubility, aquifer residual NAPL saturation, vadose zone residual NAPL saturation, soil/water partition coefficients and NAPL surface tension), dissolved constituent properties (e.g., initial concentrations of contaminants in saturated zone, NAPL/water partition coefficient, constituent solubility and contaminants' half-life constants in aquifer) and hydrocarbon release information (e.g., NAPL flux, beginning time, ending time, and NAPL volume released). Additionally, some control parameters were determined since the numerical method for solving the simulator was based on finite difference methods with some non-linear processes. The control parameters included simulation time horizon, allowable time increment, time interval to write effluent concentrations, number of time steps and iterations, termination constraints, domain types and definitions, flow or transport simulation selection control, connection and communication between property data and numerical grids, etc.

In validating the simulator, the data of 2001 and 2002 were used for calibrating the simulator, and those of 2003 were used for verification. Our results indicated that the errors between predicted and observed benzene concentrations ranged from -13.8 to $248.9 \mu\text{g/L}$; the mean absolute error was $72.78 \mu\text{g/L}$ and the mean relative error was 30.02%. The errors for toluene concentrations varied from -2.4 to $22.8 \mu\text{g/L}$, with their mean absolute and relative errors being $5.72 \mu\text{g/L}$ and 79.01%, respectively. The mean absolute errors for ethyl-benzene and xylenes were 4.2 and $17.28 \mu\text{g/L}$, respectively; the mean relative errors for the two species were 16.68% and 11.26%, respectively. This demonstrated the developed simulator could be used in the remediation design as the error levels were generally acceptable.

3. Results analysis

Simulation results showed that the peak concentration of benzene, toluene, ethyl-benzene and xylenes would be respectively 6376.5, 852.3, 2304.2 and $418.4 \mu\text{g/L}$ 10 years later, if no remediation action was undertaken [6]; these would be a number of times higher than the environmental standards. The contamination would become increasingly serious with the spreading of BTEX in the groundwater. Thus, the pump-and-treat system was recommended, with the durations assumed to be 5, 10, 15 and 20 years. Many factors (including contaminant concentrations of the injected and extracted water, pumping rates, well number, well location, etc) can influence the optimal remediation strategies. This

study only chose pumping rates as decision variables (i.e. explanatory variables). If more factors need to be addressed, they can be introduced into the inputs of proxy simulators which need to be re-generated.

Two injection and four extraction wells were determined as remediation wells from various alternatives (Figure S2 of the supplementary material) as they were located around the contaminant sources and can be operated rather conveniently. In terms of the local technical and hydrogeological conditions, pumping rates at these wells would not be higher than $100 \text{ m}^3/\text{d}$. The system also included eight monitoring wells. Note that, the explanatory variables were normalized in the range 0 and 1 by dividing their values by 100, and natural logarithms of simulated benzene concentrations at the monitoring wells were considered as response variables. This treatment would be effective in decreasing computational errors.

According to EEP [6], layers 2–4 would be located in the saturated zone, while layer 1 would be situated in the unsaturated zone. Since the most serious plume was mainly observed in layer 2, the optimal design only targeted at this layer. Moreover, only a single species (i.e. benzene) was considered in the case study. This simplification was based on the findings that (a) the concentrations of toluene, ethyl-benzene, and xylenes would become lower than the respective environmental standards once the benzene concentration satisfied the standard (determined to be 0.5 mg/L in this design); (b) benzene generally has higher toxicity than the other three contaminants [5].

The proxy simulators were generated via stepwise response surface analysis (SRSA) based on 250 statistical samples obtained from various runs of the simulator. Because a total of eight monitoring wells were used as checking points and 4 types of remediation periods (i.e. 5, 10, 15 and 20 years) were considered, a total of 32 proxy simulators were created; each one represented the contamination concentration at one monitoring well for one type of remediation period. Figs. 1 and 2 present the histograms of residuals generated by the proxy simulators for wells BH110 and BH109. Since most of the figures have approximately symmetrical shapes, the normality of the residuals could be straightforwardly assumed. Although not shown for the residuals generated from other proxy simulators, their histograms also revealed that the normality assumption could be given.

Both JB -test and L -test were performed to verify the normality of residuals. Fig. 3 presents the calculated JB -statistic values. As shown in Fig. 3(a), the average JB -statistic value is 1.61, with the maximum and minimum values being 8.15 and 0.01. Given a significance level of 0.05, most of the statistic values are lower than the critical one (5.99). The only exception occurs at well BH110 where the JB -statistic is about 8.15; however it is lower than the critical value (9.20) given the significance level of $\alpha = 0.01$. Similar results can also be observed from Fig. 3(b)–(d). Therefore, it is judged the normality hypothesis can hardly be rejected since all JB -statistic values are lower than or very near the critical ones given a significance level of 0.01. Fig. 4 shows the L -statistic values for residuals under normality hypothesis. Except for wells BH105, BH107 and BH116 in Fig. 4(b) and well BH116 in Fig. 4(c) and (d), the statistic values of all others are lower than the critical value when the significance level is 0.05. However, when the significance level equals 0.01, the L -statistic values of all wells are lower than the critical value, indicating the normality hypothesis for the residuals of the proxy simulators can also be accepted according to the L -test given a significance level of 0.01.

Fig. 5 gives the estimated lower and upper bounds of the residuals under a 95% confidence level, when remediation durations are 5, 10, 15 and 20 years, respectively. It is indicated that the averaged lower and upper bounds of the mean residuals at the eight wells range from -0.21 to 0.22. This shows the assumed zero

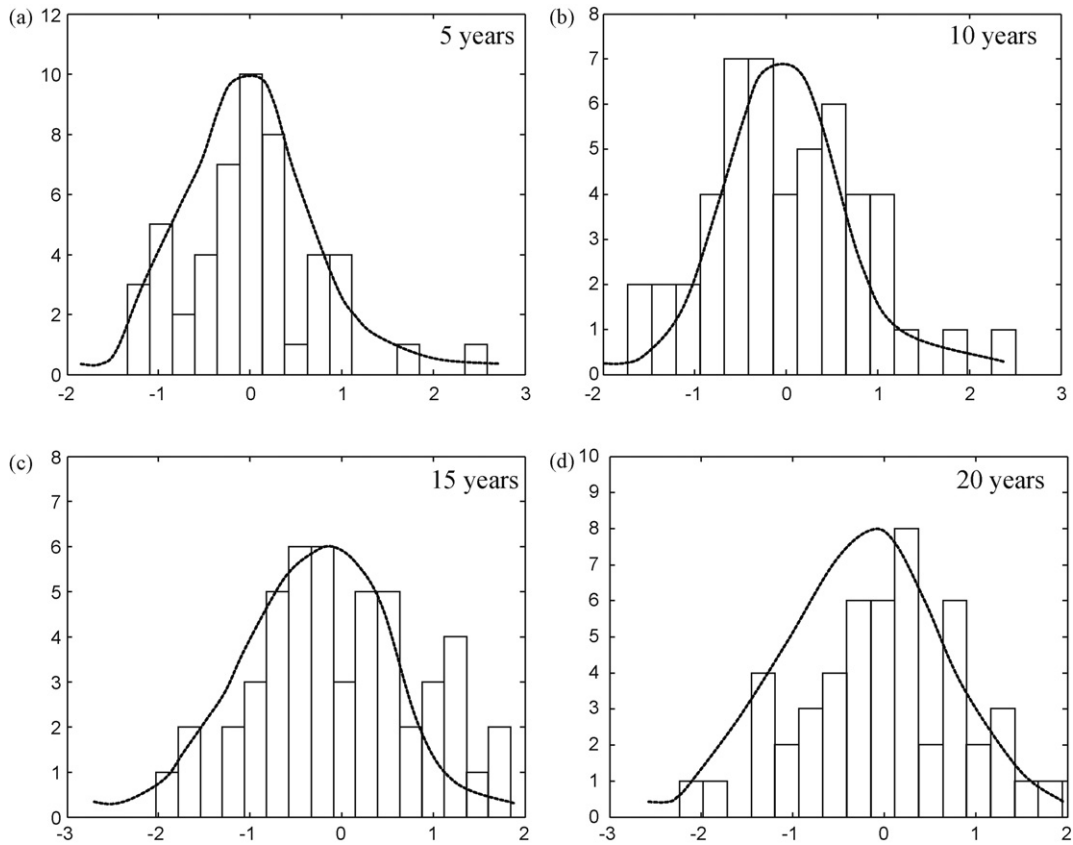


Fig. 1. Statistic histograms for proxy-simulator residuals at well BH110 (the horizontal axis represents the estimated error, and the vertical axis represents the frequency falling between the corresponding range). (a) 5 years, (b) 10 years, (c) 15 years, and (d) 20 years.

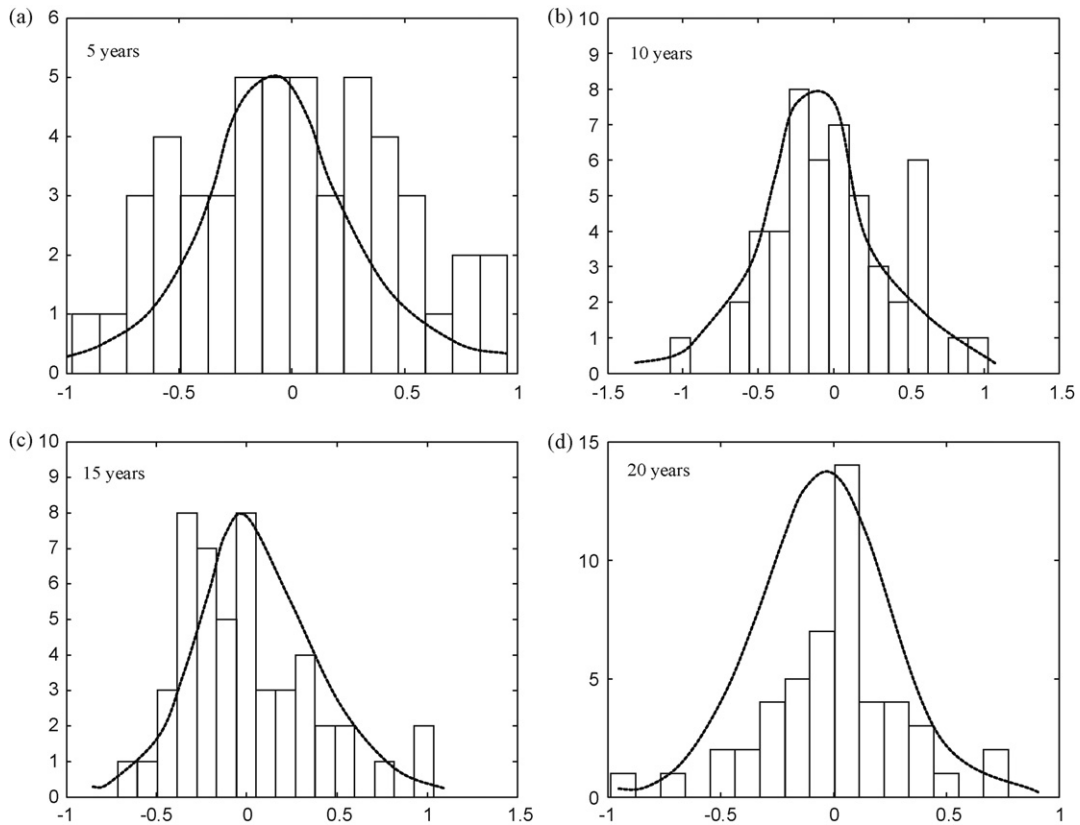


Fig. 2. Statistic histograms for proxy-simulator residuals at well BH109 (the horizontal axis represents the estimated error, and the vertical axis represents the frequency falling between the corresponding range). (a) 5 years, (b) 10 years, (c) 15 years, and (d) 20 years.

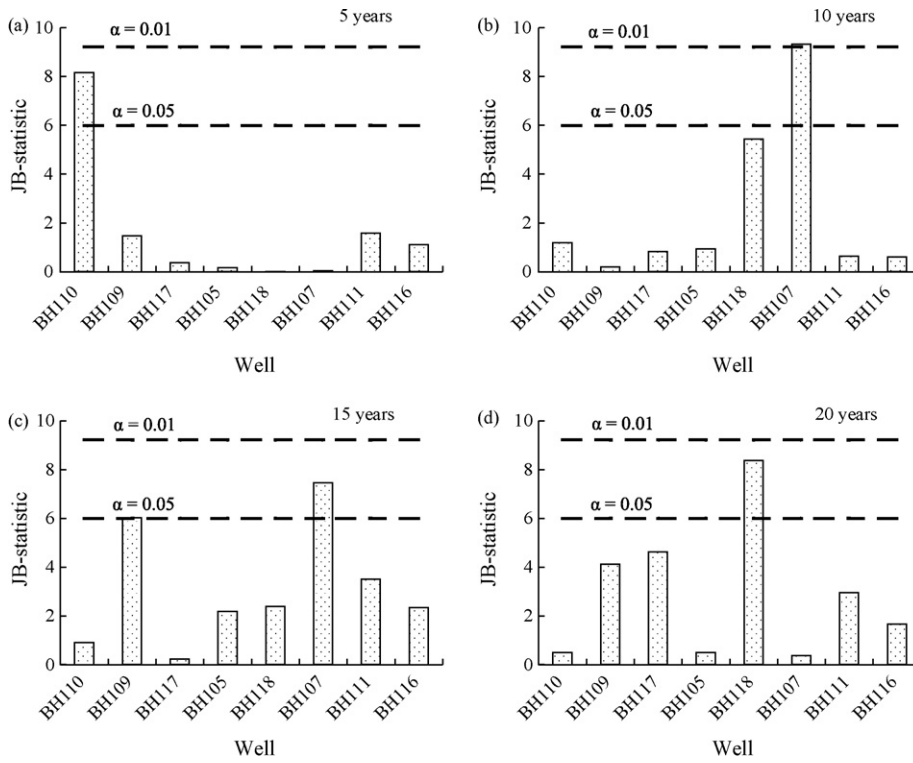


Fig. 3. The Jarque–Bera test results. (a) 5 years, (b) 10 years, (c) 15 years, and (d) 20 years.

mean for all residuals completely falls into the ranges constituted by the lower and upper bounds. Thus, the zero-mean assumption can be accepted under a 95% confidence level. The t -test is also performed to verify the hypothesis that $H_0: \mu_{0k} = 0, \sigma_k^2$ unspecified, against $H_1: \mu_{0k} \neq 0, \sigma_k^2$ unspecified, where μ_{0k} and σ_k^2 are

expected value and variance of the residual generated by the proxy simulator for well k . As shown in Fig. 5(a), the averaged t -statistic value is 0.05, with the largest and smallest values being 0.40 and -4.72×10^{-4} , respectively. Similar results can also be observed in Fig. 5(b)–(d). In comparison, given a significance level of 0.05, the

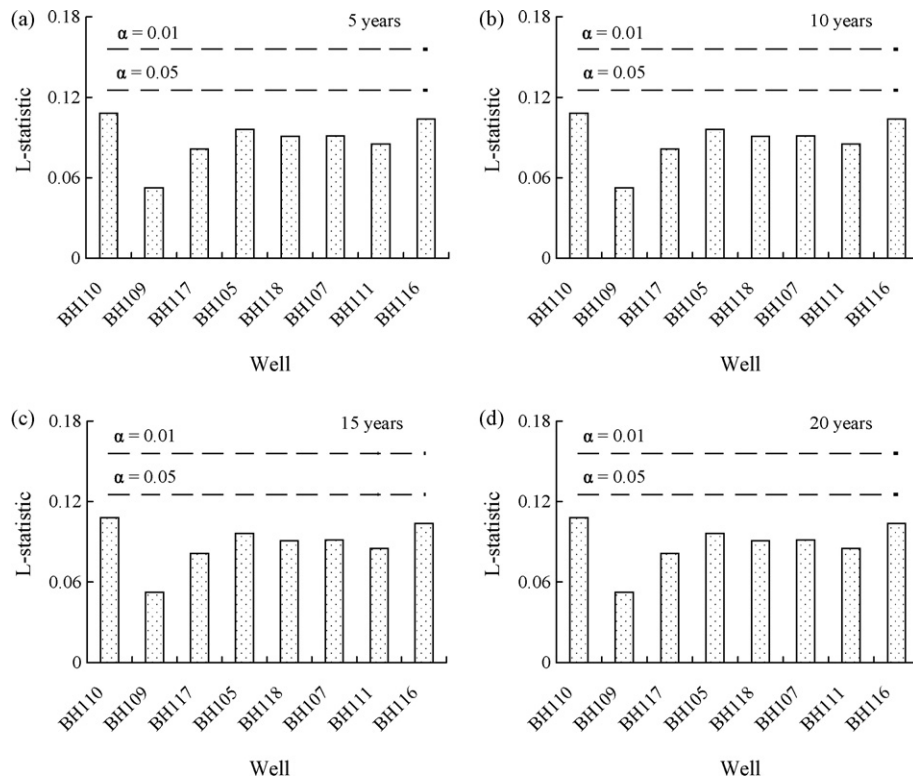


Fig. 4. The Lilliefors test results. (a) 5 years, (b) 10 years, (c) 15 years, and (d) 20 years.

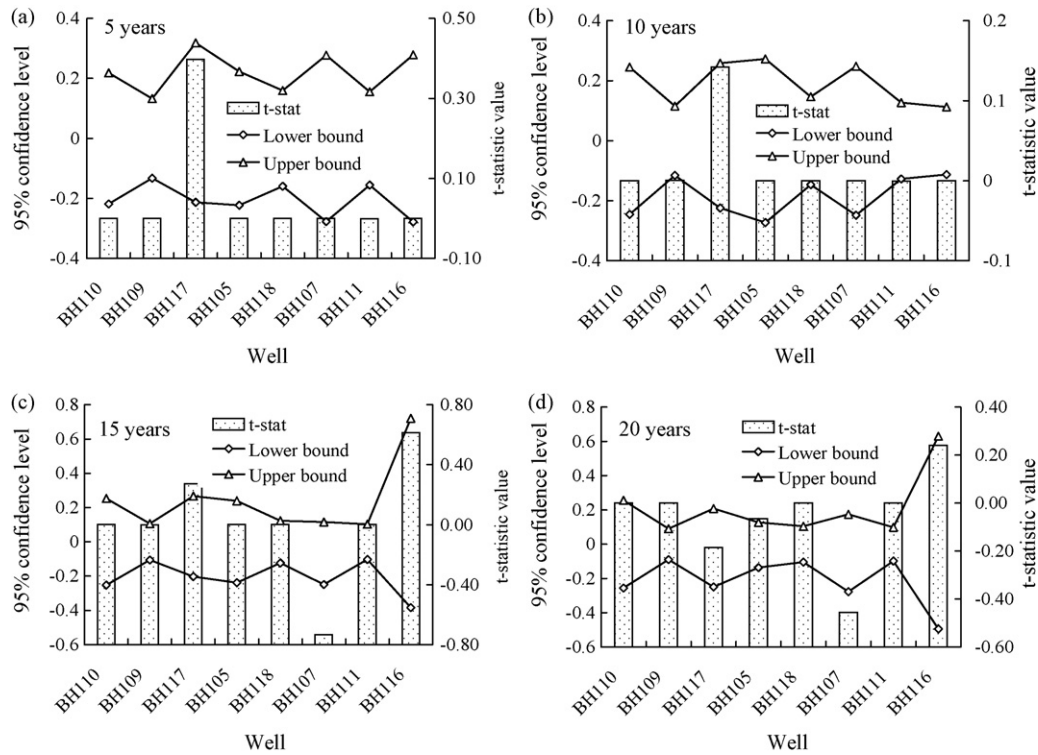


Fig. 5. The *t*-tests results. (a) 5 years, (b) 10 years, (c) 15 years, and (d) 20 years.

value of $t_{0.05/2(50-1)}$ is 2.01, indicating the rejection regions of $[-\infty, -2.01]$ and $[2.01, \infty]$. As all of the *t*-statistic values fall out of these ranges, the null hypothesis (H_0) of $\mu_{0k} = 0$ can hardly be rejected, and accordingly the zero-mean assumption is accepted. Based on this hypothesis, σ_k^2 can be estimated by:

$$\sigma_k^2 = \sum_{u=1}^N \frac{(e_{k,u} - \bar{e}_k)^2}{N} \quad (1)$$

where $e_{k,u}$ is residual of the proxy simulator for well k for sample u ; \bar{e}_k is average of samples $e_{k,u}$; N is number of samples.

Fig. 6 presents the estimated variances under the zero-mean hypothesis, which were introduced to formulate the SOMUM problem. Fig. 7 shows the optimal pumping strategies under the confidence levels of 0.90, 0.95, 0.975 and 0.99. When the remediation period is 5 years (Fig. 7a), wells M3 and M5 would have the highest pumping rates, with an average value equal to or near $100 \text{ m}^3/\text{d}$. This shows that most of the contaminated ground-

water would be extracted from well M5 while most of clean water would be injected into well M3. Wells M1 and M2 would also play roles in remediation, with an average pumping rate of $30.0 \text{ m}^3/\text{d}$ approximately. Wells M4 and M6 would have no contribution to the remediation since no contaminated/clean water would be extracted/injected from/into the wells. When the remediation period is extended to 10 years, the average pumping rates at wells M3 and M5 would reduce by 44.3% and 71.4%, respectively (Fig. 7b); those at wells M1 and M2 would increase by 1.64 and 1.04 times when the confidence level (π) ranges from 0.90 to 0.99. In comparison, the pumping rates at wells M4 and M6 would be 0 and $1.54 \text{ m}^3/\text{d}$, respectively. This shows wells M1, M2, M3 and M5 would have much more significant contribution to groundwater remediation than wells M4 and M6. Over the 15-year period of remediation (Fig. 7c), the average pumping rates would be 47.5, 5.50, 45.2, 0, 1.01 and $2.21 \text{ m}^3/\text{d}$ at the six wells, respectively. Once the remediation period increases to 20 years, only wells M1 and M3 would be active with the rates both being $23.3 \text{ m}^3/\text{d}$ (Fig. 7d), and the other wells would be shut down.

It can also be observed from Fig. 7 that a long remediation period corresponds to a low total pumping rate. This is because high volumes of contaminants need to be extracted to lower the benzene concentrations when the duration is short. This would further enhance the injection rates to maintain a stable hydraulic gradient of the aquifer. The increases in both extraction and injection rates would thus cause the growth of pumping rates for shorter-duration remediation than for longer ones. The effect of π levels on remediation strategies can also be observed from Fig. 7. For example, when π rises from 0.90 to 0.99 (5-year period of remediation), the total pumping rate would increase by 17.6%; it would be enhanced by 2.08, 1.42 and 0.55 times respectively for the 10, 15 and 20 years of pumping, when π varies from 0.95 to 0.99. This demonstrates that an increased π level would lead to the growth of total pumping rate, implying an enhanced remediation cost would be afforded.

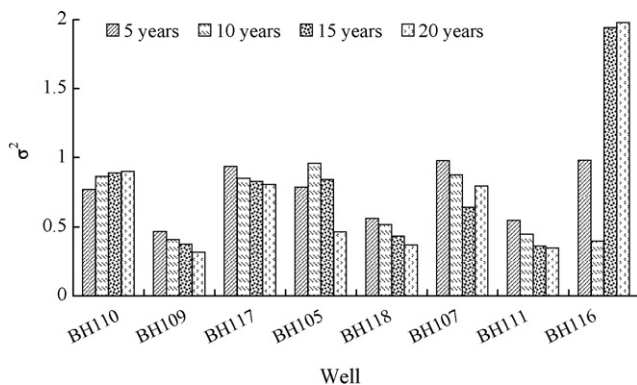


Fig. 6. Estimated variances of the proxy-simulator residuals.

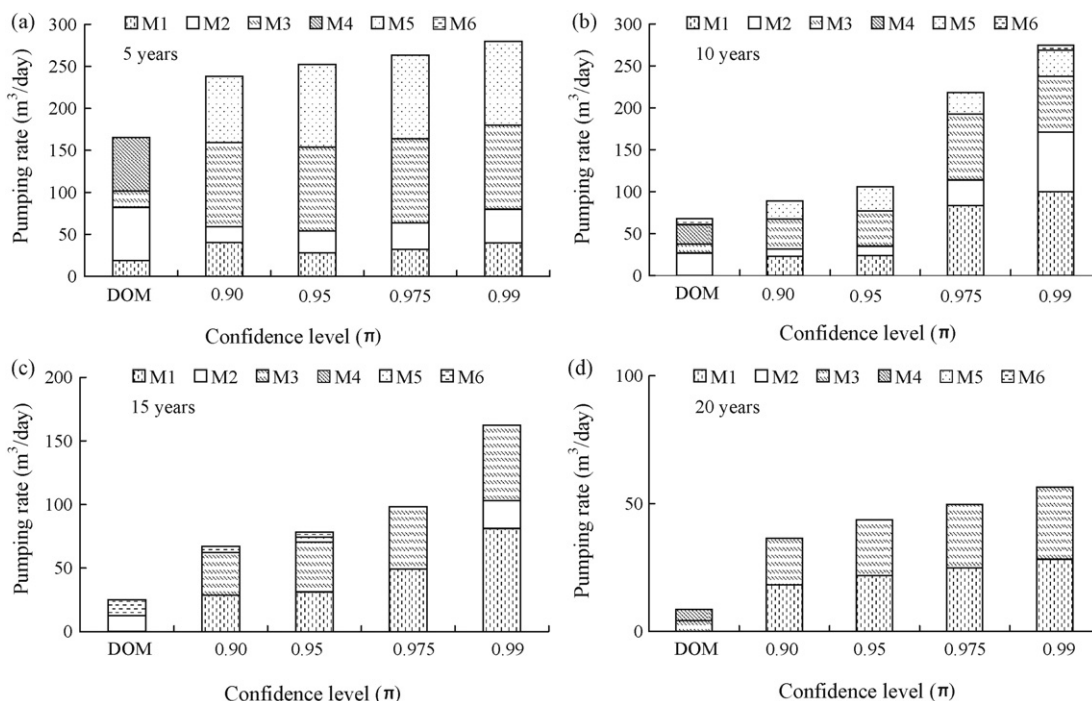


Fig. 7. Optimal remediation strategies. (a) 5 years, (b) 10 years, (c) 15 years, and (d) 20 years.

4. Models comparison

To compare the impact of modeling uncertainty on remediation strategies to that of physical-property uncertainty, five scenarios were designed which were S1, S2, S3, S4, and S5 (Table 1). Optimal solutions under scenarios 2 and 3 were solved in terms of the following procedures: to begin, the Mont-Carlo technique was used to run the simulator, generating 250 statistical samples based on the provided stochastic parameters (shown in Table 1); the inputs of samples were pumping rates at remediation wells and the outputs were probabilities of benzene concentrations at monitoring wells satisfying the environmental standard. The samples were employed by the SRSA tool to create proxy simulators. The proxy simulators were then input to model (2) to replace the initial Mont-Carlo-based simulator, formulating the following conventional SOMUP problem:

$$\text{Minimize } TR = \sum_{i=1}^{I+J} q_i \quad (2a)$$

$$\text{s.t. } 0 \leq q_i \leq q_{i,\max} \quad \text{for all } i = I+1, I+2, \dots, I+J \quad (2b)$$

$$\sum_{i=1}^I q_i = \sum_{i=I+1}^{I+J} q_i \quad (2c)$$

$$\Pr\{c_k^p(q_1, q_1, \dots, q_{I+J}) \leq MCL\} \geq \pi \quad \text{for all } k = 1, 2, \dots, K \quad (2d)$$

Table 1
Scenarios designed for comparison of uncertainty impacts.

Scenario	Residual		Porosity		Permeability		Uncertainty	Uncertainty sources	Model
	DT	CV	DT	CV	DT	CV			
S1	–	–	–	–	–	–	–	–	DOM
S2	Log-normal	Calculated by Eq. (1)	–	–	–	–	Modeling uncertainty	Proxy simulator residuals	SOMUM
S3	–	–	Normal	10%	Log-normal	10%	Parameter uncertainty	Physical property	SOMUP
S4	–	–	Normal	20%	Log-normal	20%	Parameter uncertainty	Physical property	SOMUP
S5	–	–	Normal	40%	Log-normal	40%	Parameter uncertainty	Physical property	SOMUP

Note: CV denotes coefficient of variance, which is defined as ratio of standard deviation to mean value; DT denotes distribution; – means uncertainty is not considered.

where TR is total pumping rate for all injection/extraction wells; I and J are numbers of injection and extraction wells, respectively; q_1 to q_I are decision variables, indicating the pumping rate at injection wells 1 to I , respectively; q_{I+1} to q_{I+J} are decision variables, indicating the pumping rate at extraction wells $I+1$ to $I+J$, respectively; $q_{i,\max}$ is maximum pumping rate for the i th well; \Pr represents the probability of constraint satisfaction; c_k^p is contaminant concentration predicted by the proxy simulators for well k ; MCL is maximum contaminant level which is determined in terms of the given environmental standard; π is confidence level. Model (2) can be solved through optimization solvers like Lingo as it is a quadratic programming problem.

Fig. 8 shows the comparison of optimization results for the remediation periods of 5 and 15 years. As shown in Fig. 8(a), the total pumping rate would be $165 \text{ m}^3/\text{d}$ when neither modeling uncertainty nor parameter uncertainty is considered (in scenario S1). However, when modeling uncertainty is addressed in scenario S2, the total pumping rate would be increased by 43.9%. In comparison, if only parameter uncertainty is accounted for, the total pumping rate would be increased by 7.78%, 23.1%, and 56.5% in scenarios S3, S4, and S5, respectively. If assuming the remediation cost is proportional to the total pump rate, then this implies the increased remediation cost for mitigating the modeling-uncertainty impact would be no less than that for mitigating the parameter-uncertainty impact. This is extremely significant when the coefficient of variance (CV) is not larger than 40%. The increased

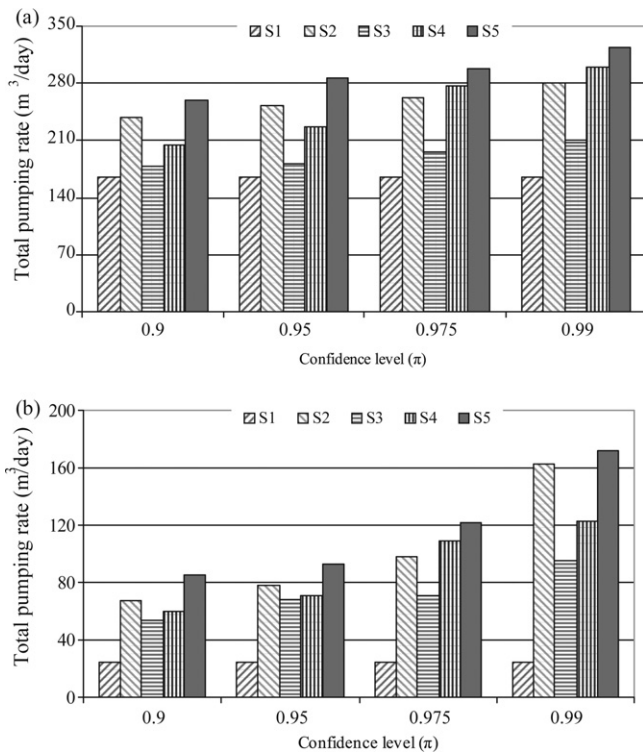


Fig. 8. Comparison of optimization results under scenarios S1–S5 for a remediation period of (a) 5 years and (b) 15 years.

cost in scenario S2 would be less than that in scenario S5, suggesting parameter uncertainty has the most significant impact on remediation cost, while modeling uncertainty is the second most significant. Fig. 8(b) also illustrates the increased remediation cost for mitigating modeling-uncertainty impact would be higher than that in the scenarios with the CVs being lower than 40%.

This evidence implies that the impact of modeling uncertainty on groundwater remediation design can hardly be ignored. Although part of the previous studies suggested that the introduced proxy simulators have achieved satisfactory approximation performance, ignoring the impact of modeling uncertainty may cause the increase in the risk of system failure due to potential environmental-standard violation. This finding could be particularly favored by system designers who are willing to spend additional money to lower the potential risk of systems failure. Unfortunately, most of the previous studies focused on addressing parameter uncertainty rather than accounting for modeling uncertainty. This new evidence could stimulate more future efforts to be undertaken focusing on investigation and mitigation of modeling-uncertainty impact on remediation design.

Figs. 7 and 8 also indicate that the optimal total pumping rates obtained from DOM would be lower than those from SOMUM. This occurs because that more contaminated groundwater should be extracted to mitigate the effects of modeling uncertainty. Correspondingly, more clean water should be injected to satisfy the environmental constraint. The increased requirement for extraction and injection would thus lead to the rise of total pumping rate. It seems that the SOMUM strategies are rather conservative compared to the DOM ones, due to the need of mitigating modeling uncertainty. However, in practice, inaccurate proxy-simulator forms, missing variables, biased parameters and sampling errors can frequently lead to deviations of outputs, inducing the originally “optimal” solutions to be no more optimal. As the exclusion of this uncertainty from the optimization formulation would lead to a risk of system failure, SOMUM (as a rather robust formulation) would be

much preferred due to its adaptability to accommodate uncertainty in proxy simulators. Nonetheless, this design would lead to the increase of remediation cost along with the growth of total pumping rate. Therefore, there is a trade-off between system-failure risk and remediation cost. This trade-off issue may be addressed using multi-objective or goal programming techniques. In addition, multicriteria decision analysis can also be employed to evaluate the performance of each of remediation strategies identified through the above techniques.

5. Discussion and conclusions

The hypothesis test results indicate that the assumptions for the residuals of proxy simulators can be accepted statistically. However, this does not imply that they are also acceptable under other conditions. When the model is extended to other sites, therefore, the assumptions should be re-tested based on simulation results reflecting the flow and transport of contaminants in new aquifers. If the normality test fails, non-normal (e.g., uniform and gamma) distributions may be assumed and tested for the residuals. Moreover, the proposed SOMUM model can be extended to systems where other learning algorithms are used, such as artificial neural networks [8,9], robust regression [10], regression tree [11], support vector regression [12], and stepwise cluster analysis [2,13]. However, the testing results may vary with the learning algorithms, statistical samples and normality testing methods. Therefore, care should be taken when the model is applied to other studies.

The logarithms of residuals were assumed normally distributed and then verified through Lilliefors and Jarque–Bera tests. The Lilliefors test, based on the Kolmogorov–Smirnov test, was proposed to test the hypothesis that the data come from normally distributed residuals, whose expected values and variances were not specified. However, it could be relatively weak since a large number of data are required to reject the normality hypothesis [14]. Therefore, the Jarque–Bera test, as a more sensitive manner based on classical measures of skewness and kurtosis, was also conducted to test the normality of residuals. The testing results show that most of the residuals are lower than the respective critical values under the significance level of 0.01, indicating that the normality hypothesis can hardly be rejected. Meanwhile, the *t*-test was used to determine whether or not the residuals have zero means. It is found that the zero-mean assumption for all residuals of the proxy simulators could be accepted.

The optimal remediation strategies were determined by solving the SOMUM problem under four scenarios representing different remediation periods. It is found that a long remediation period would generate a low total pumping rate, while an enhanced level would raise the total pumping rate; the peak benzene concentrations would be lower to satisfy the environmental standard.

The solutions were also compared to those obtained from the conventional SOMUP and DOM models. Although the SOMUM strategies were not as cost-effective as the DOM and part of SOMUP strategies, SOMUM could be preferred due to its good adaptability to negligible uncertainty in proxy simulators. To summarize, SOMUM has the advantages of (1) providing mean-variance analysis for the response variables (contaminant concentrations), (2) mitigating the effects of the uncertainty in proxy-model residuals on optimal remediation strategies, (3) offering quantitative information (i.e. confidence level of optimal remediation strategies) to system designers, and (4) reducing the computational cost in optimization processes.

This study only addressed the impact of modeling uncertainty associated with proxy-simulator residuals. However, parameter uncertainty may also affect optimal remediation strategies [15,16]. Future studies would be undertaken to mitigate both effects by improving the proposed SOMUM model. Dual response surface

optimization could be effective in solving this problem. Its basic idea is to create two sets of proxy simulators, respectively predicting the mean values and deviations of model outputs. The prediction results can then be simultaneously input into the optimization model, by regulating that: the mean values of predicted contaminant concentrations are less than the environmental standard; the deviations stemming from the original simulator are lowered to an acceptable level.

The remediation duration is rather long, probably lasting over 10 years. However, the remediation strategies identified through this model were based on an assumption that the hydrogeological parameters will not be subjected to the effect of variability or changes in climatic conditions. For example, the intrinsic permeability was assumed not to vary with the change of ambient or groundwater temperature. However, no evidence in this study has shown whether this assumption would introduce significant modeling errors. Thus, a future research subject is to take into account the climatic variability and/or changes in the remediation design.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at [doi:10.1016/j.jhazmat.2009.11.061](https://doi.org/10.1016/j.jhazmat.2009.11.061).

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