A LEAST-COST STRATEGY FOR EVALUATING A BROWNFIELDS REDEVELOPMENT PROJECT SUBJECT TO INDOOR AIR EXPOSURE REGULATIONS

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ABSTRACT

This paper presents a framework for alleviating the risk of exposure during brownfields redevelopment projects by improving the prediction of contaminated indoor air concentrations, and by searching for the optimal balance between increasing site characterization budgets and decreasing contingency measures to cover the risk exposure (and also to quantify and manage the risk). A three-dimensional model *CompFlow Bio* is used to anticipate the intrusion pathways of TCE from a residual source zone into buildings. The result indicates that the geological condition of the site and the heterogeneity in each stratigraphic unit have the most compelling impact on the indoor air concentration of TCE. We develop a methodology by which to price the risk associated with the number of sampling data available from site characterization and long-term monitoring, incorporating hydrogeological as well as financial uncertainties into an insurance premium. As a result, the trade-off between increasing site-investigation budgets and overall cost reductions is optimized.

INTRODUCTION

Brownfields are defined by the U.S. Environmental Protection Agency (US EPA) as "abandoned, idled, or under-used industrial and commercial facilities where expansion or redevelopment is complicated by real or perceived environmental contamination." Brownfields are usually unintended by-products of industrial practices of the last several decades, in which measures were not taken to ensure that industrial operations did not harm the natural environment. In brownfields, there exist known and potential contaminants, such as volatile organic compounds (VOCs) or semi-volatile organic compounds (SVOCs) which over time, may be exposed to the air, potentially threaten public health, and have negative impacts on ecological systems. Redevelopment of such brownfields is beneficial for the environment as well as for communities. It is an efficient, effective, and environmentally friendly way to encourage development using existing infrastructures, services, and resources. Redeveloping brownfields can also generate great economic benefits if appropriate and reasonable methodologies are designed. There are strong environmental, social, and economic grounds to redevelop and utilize brownfields (US EPA, 1999; NRTEE, 2003; UK Environment Agency, 2003).

Since the 1980s, North America and Europe have made moves to foster sustainable redevelopment of brownfields. The United States of America enacted the Liability Act Superfund to reclaim 1,410 heavily contaminated sites, and the National Brownfields Association has estimated that 600,000 brownfield sites exist across the nation (Mueller, 2005). Canada also has paid a great deal of attention to brownfield redevelopment projects (aboutRemediation™, 2012). Policy makers and developers have focused their efforts on transforming brownfields into industrial areas, commercial areas, and residential areas, depending on the characteristics of the community and the site itself. At the same time, brownfield redevelopment projects also harbor great risks, which can impede the decision-making process. Major risks faced during brownfield redevelopment associated with costs include possible cost overruns in cleanup operations (the technologies for remediation of brownfields are summarized by Reddy et al., (1999)), possible liability claims from accidents or contaminant exposure from past spills or spills during the cleanup, and

uncertainty about future community acceptance (Wade VanLandingham et al., 2002). All of these risks mainly arise from imperfect knowledge of the complexity of brownfield sites. Complications include complex geological formations and physical properties of the subsurface, the uncertainty of the source zone, the number and features of existing and potential contaminants, and the unreliability of detecting and contouring of the contaminant plume. As a result, a better understanding of the physics of contaminated soil vapor transport and developing a methodology to evaluate the associated risks are crucial.

Soil vapor VOC intrusion pathways into buildings have been commonly studied using analytical models, numerical modeling, and field studies. A discrepancy between field measurements and analytical solutions is often seen. The influence of the geometry of houses on the soil vapor distribution is often ignored. Yu et al. (2009) simulated the TCE soil vapor intrusion into a single house using *CompFlow Bio* in two dimensions. They examined the roles that a number of uncertainties—heterogeneity, the pressure difference between indoor and outdoor, source-zone location, aperture of the crack in the foundation slab, depth of the foundation slab, capillary fringe thickness, and infiltration rate—might play in determining the indoor air concentration of TCE. The largest remaining uncertainties result from the inherent complexity of the geology, heterogeneity, which was responsible for deflecting the groundwater plume upward towards the capillary fringe, diffusing across the capillary fringe, and then migrating into the basement. This work intends to use the three-dimensional *CompFlow Bio* model to simulate the fate and transport of soil vapor into multiple residential houses. We focus more on the significance of the geological conditions, the geometry of house locations, and the heterogeneity influencing the indoor air concentration distribution of TCE. Attenuation factors in different scenarios are calculated in contrast with those using the model by Johnson and Ettinger (1991).

Developers want to keep project overhead as low as possible, but characterizing site geology and probing for contaminants are necessary and costly. What is the most cost-effective way to conduct site characterization? To answer this question, different concentration and permeability sampling schemes are set up. The heterogeneous permeability fields are constructed using a conditional stochastic approach, generating a high-resolution aquifer analog based on permeability measurements. The geostatistical program *S-GEMS* (Stanford geostatistical earth modeling software) is utilized for this purpose. Once we have concentration measurements, an optimal estimator Kalman filter can be used to deduce a minimum error estimate to improve model prediction. Zhang and Pinder (2005) applied this algorithm to determine the least-cost design of groundwater quality monitoring networks.

How can one optimize the trade-off between increasing site-investigation budgets and overall cost reductions? First of all, the cost of risks, combining both hydrogeological and financial risks, is defined using a modified actuarial approach. The risk-cost-benefit analysis is then conducted according to the Massmann and Freeze (1987) strategy, of which the objective function is the sum of the project risk, cost, and benefit, to maximize profits by adjusting the number of data. The financial factors, which in most cases follow a Geometric Brownian Motion, (e.g., the discount rate, U.S. house price index), are estimated using financial models, and their importance is weighed compared with the hydrogeological factors (mentioned above) contributing to uncertainties in the decision-making process.

SIMULATING THE FATE AND TRANSPORT OF SOIL VAPOUR TCE

The numerical simulator *CompFlow Bio* is applied to the soil-vapor-intrusion problem in this case. It is a fully coupled, multiphase, multicomponent model capable of simulating groundwater flow and solute transport with variable water saturation in the subsurface. It involves advective and diffusive transport of TCE in water, oil, and gas phases under scenarios with different geological and hydrogeological conditions, (e.g., heterogeneity, the capillary fringe thickness, the existence of low permeable

soil and the distance of houses offsetting the TCE plume).

Conceptual Model

The hypothesis of this model is that a brownfield site has been remediated and residential buildings have been built, but a residual TCE source exists below the water table in the subsurface. The problem is as illustrated in Figure 1. The source of TCE, which is located upstream of residential houses, can either dissolve into the ambient groundwater or volatilize into the ambient soil gas. It continues to migrate along with groundwater flow, diffuse across the capillary fringe, and is subsequently transported towards the foundation slab of a structure located below grade, due to the vacuum pressure in the basement.

The computational model domain for the base scenario is depicted in Figure 2 and Figure 3 without the clay layer. Six houses are constructed on the domain with seven monitoring wells in the front, and the central houses are aligned with the source zone. The houses are depressurized, with the pressure difference from the ambient atmosphere pressure 10 *Pa*. The aquifer is heterogeneous. The permeability field is created stochastically with the same statistics (mean, variance and correlation lengths) as the Borden field site (see Figure 4). Five scenarios are set up for investigating the sensitivities of the different influential factors.

1) Base scenario;
2) Base scenario under recharge condition with recharge rate of 20 cm/yr;
3) Base scenario with a layer of clay permeability 10^{-15} m^2 and the thickness 2 m situated beneath the houses;
4) The same as case (3) but under recharge conditions;
5) The vadose zone is 7 m thicker than the one in the base scenario.

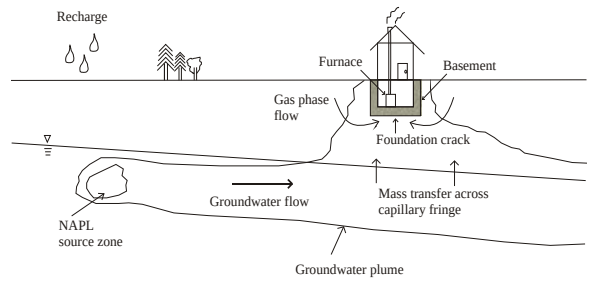

Figure 1. Conceptual model

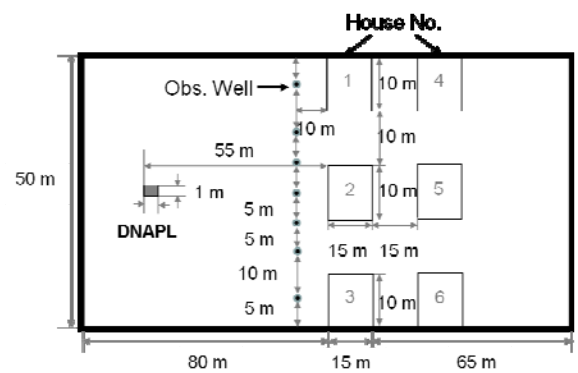

Figure 2. The plan view of the model domain for the base scenario

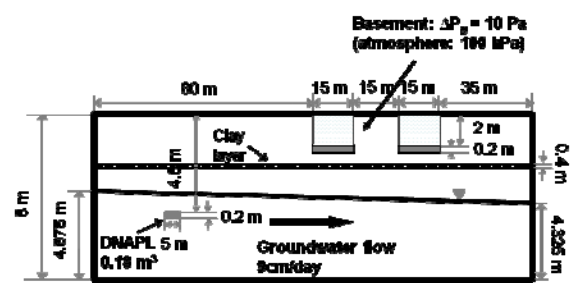

Figure 3. A 2D cross-sectional view of the model domain for Scenario 3 with a clay layer

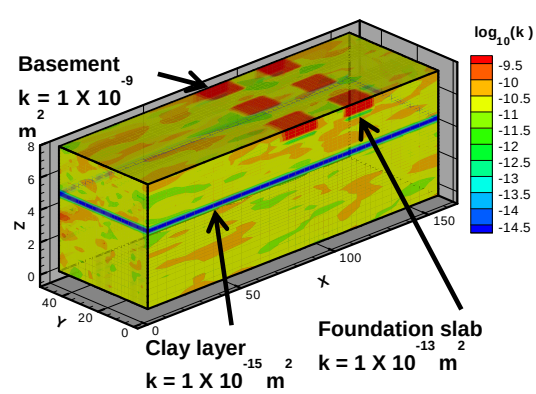

Figure 4. 3D plot of the heterogeneous permeability field with a clay layer

Model Results

The results in Figure 5 for Scenarios 1, 2, and 5 show that the TCE plume travels longitudinally along the groundwater flow direction for some distance, and then transfers across the capillary fringe into the vadose zone. The plume is quite narrow because the transverse migration of the plume is primarily driven by the concentration gradient and heterogeneity. When the vacuum pressure is applied, the central houses directly above the groundwater plume have the highest indoor air concentration of TCE. The TCE concentrations in the lateral houses vary, which results from heterogeneity, i.e., the structure of the permeability field. If a low-permeability soil layer is located below the foundation slab, when it is saturated with water, it behaves as a barrier and prevents the soil vapor from migrating upwards into the basement. The thicker vadose zone alters the offset between the source zone and center of the foundation slab, allowing more mass transfer of vapor TCE into the houses. The indoor air concentration of TCE calculated for the five scenarios is illustrated in Figure 6. It indicates that the geological clay unit and the recharge condition play important roles in vapor TCE transport.

Additionally, the comparison of the five different scenarios is conducted in terms of the attenuation coefficient (defined as the ratio of the contaminant vapor concentration in buildings to the vapor concentration at the source of contamination) with respect to the Johnson and Ettinger (1991) (J&E) model. The attenuation coefficients calculated by the *CompFlow Bio* are far smaller compared to those under the same conditions using the J&E model (see Table 1).

Since heterogeneity is a primary driving factor in determining soil gas exposure pathways, the Monte Carlo method is adopted, using permeability as the primary uncertainty for the model input, to address this issue. Figure 7 shows the concentration results for different permeability realizations. The differences in indoor air concentration of TCE can reach up to four orders of magnitude in one single house.

Table 1. The attenuation coefficients calculated using both J&E and *CompFlow Bio* (CFB) models

	Scenario	J&E attenuation coefficient $\alpha_{J\&E}$ (x10^{-6}) House No.						CFB attenuation coefficient α_{CFB} (x10^{-6}) House No.					
		1	2	3	4	5	6	1	2	3	4	5	6
1)	Base scenario	3.3	3.4	3.3	2.2	2.3	2.2	9x10^{-5}	0.116	2x10^{-3}	1x10^{-3}	0.167	4x10^{-3}
2)	Infiltration = 20 cm/yr	3.3	3.4	3.3	2.3	2.3	2.2	5x10^{-7}	6x10^{-3}	2x10^{-3}	3x10^{-3}	0.023	8x10^{-3}
3)	Clay – no recharge	3.3	3.4	3.3	2.2	2.3	2.2	1x10^{-4}	0.011	4x10^{-4}	8x10^{-4}	0.031	2x10^{-3}
4)	Clay – with recharge	3.3	3.4	3.3	2.2	2.3	2.2	3x10^{-5}	6x10^{-7}	1x10^{-7}	2x10^{-5}	1x10^{-5}	2x10^{-7}
5)	Thicker vadose zone	3.3	3.4	3.2	2.2	2.3	2.2	3x10^{-5}	0.090	6x10^{-3}	0.010	0.171	0.017

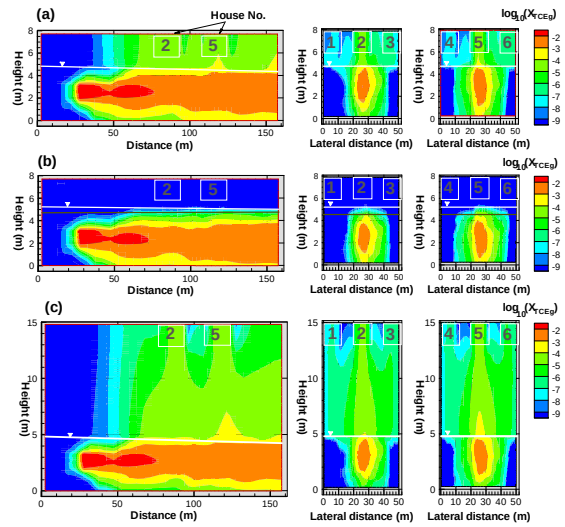

Figure 5. 2D cross-section plots along x- axis and y-axis of mole fraction of TCE in gas phase 1800 days after TCE was injected into the aquifer: (a) Scenario 1, (b) Scenario 4, and (c) Scenario 5

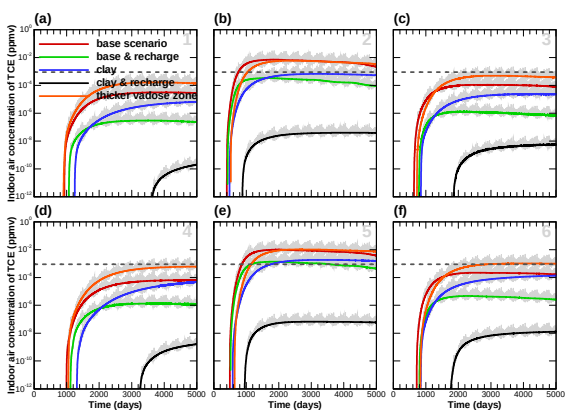

Figure 6. Indoor air concentration of TCE in logarithmic scale with transient air exchange rate limited to wind speed for the five scenarios: (a) house no. 1, (b) house no. 2, (c) house no. 3, (d) house no. 4, (e) house no. 5, and (f) house no. 6
Note: The numbers 1–6 represent the house number from Figure 2. The dashed line represents the regulatory limit for TCE

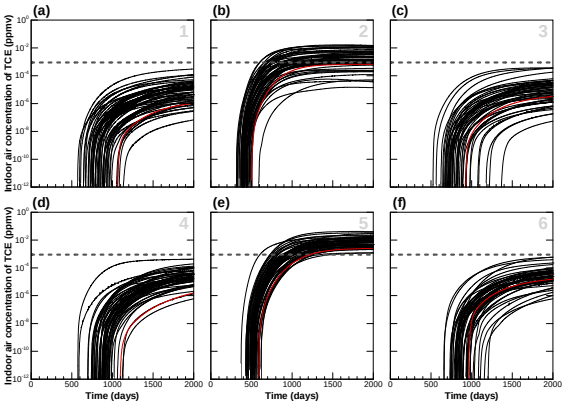

Figure 7. Indoor air concentration of TCE in logarithmic scale with the air exchange rate 0.5/hr for 50 unconditioned random permeability realizations: (a) house no. 1, (b) house no. 2, (c) house no. 3, (d) house no. 4, (e) house no. 5, and (f) house no. 6
Note: The numbers 1–6 represent the house numbers from Figure 2. The dashed line represents the regulatory limit. The red line represents the hypothetical real world result

DATA-WORTH ASSESSMENT

Kalman filtering (KF) is a technique to describe how a system would respond after processing measurements to achieve an optimal estimation. It is, in essence, a recursive solution to a least-squares problem. In this work, KF is applied to estimate and predict the indoor air concentration in multiple houses, with prior knowledge and statistical information on state variables obtained from the *CompFlow Bio* model.

Methodology

The strategy to assess the data-worth issue here is to choose one of the randomly generated permeability realizations to be reality, and to extract the permeability data from 1 to 7 boreholes in front of the houses as the sampling data. The next step is to use the statistics and the correlation of the sampling data, to apply the kriging technique to reconstruct the permeability field of the entire domain, and then to employ a sequential Gaussian simulation to create multiple realizations (shown in Figure 8). 1, 3, 5, and 7 boreholes of data (labelled as 1K, 3K, 5K, and 7K) are taken respectively for the inspection, and an extreme case with 80 boreholes of data (80 K) is also considered. Every permeability realization is used as a numerical model input to estimate the indoor air concentration of TCE at six houses and five observation wells at 100-day intervals over 2000 days. Sequentially, the space-time TCE concentration covariance matrix is constructed for the 11 locations. Concentration samples are taken from 2, 4, and 7 locations (taken as 2C, 4C, and 7C) out of 11, and then KF is used to update the concentration estimation by minimizing the error covariance matrix. The concentration sample in house no. 2 is always included.

The purpose of this method is not only to examine the data-worth issue for this application, but also to use sparse data to infer whether one of the houses located adjacent to house no. 2 has indoor air problems subject to the condition that house no. 2 is monitored and has problems; adjacent houses are not monitored, but developers assume liability if a problem occurs. After filtering, the expected value and the standard deviation of the TCE concentration in adjacent houses can be calculated.

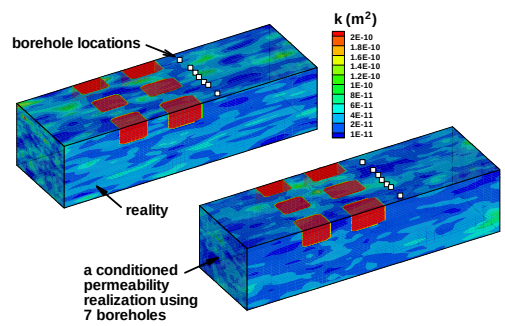

Figure 8. An example of a randomly generated permeability field realization conditioned on the 7 boreholes data

KF Results

Combinations of different numbers of permeability data and concentration data are made in order to get a good estimation of reality. The representative four cases (1K, 2C; 1K, 4C; 7K, 4C; and 7K, 7C) are chosen for illustration in Figure 9.

Increasing the number of permeability samples can give a better estimation of the expected value of the TCE concentration in comparison with reality; increasing the number of concen-

tration samples may reduce the variance in the TCE concentration, so that the uncertainty in prediction may be reduced.

The probability of failure is the likelihood that indoor air concentration of TCE exceeds a regulatory level. It is defined as the total number of Monte Carlo realizations in which the failure occurs, divided by the total number of realizations. The probability is calculated for house no. 1, 3, 4, 5, and 6 at each monitoring interval; the result is shown in Figure 10.

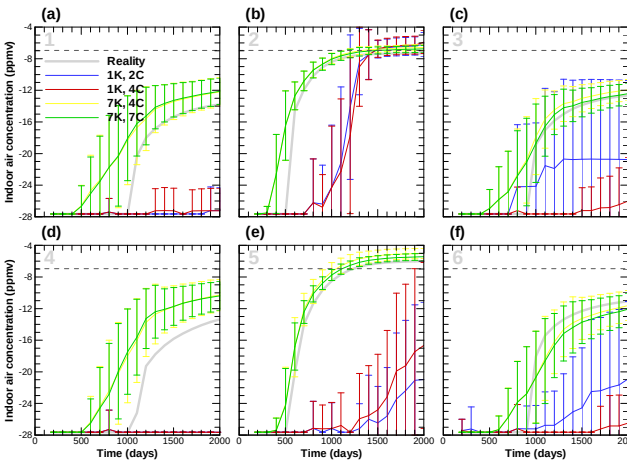

Figure 9. Updated indoor concentration of TCE in logarithmic scale using a Kalman filter: a) house no. 1, b) house no. 2, c) house no. 3, d) house no. 4, e) house no. 5, and f) house no. 6
Note: The number 1 – 6 represents the house number from Figure 2. The dash line represents the regulatory limit. The red line represents the hypothetical real world result

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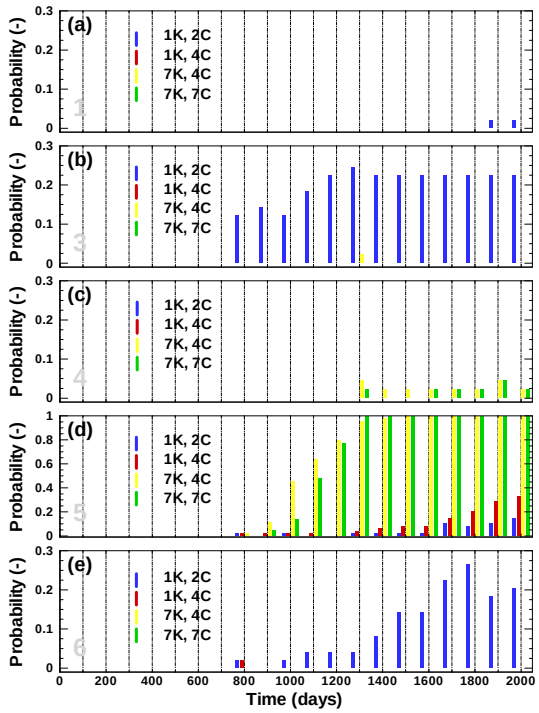

Figure 10. The probability of failure at each 100 days monitoring intervals for four cases: (a) house no. 1, (b) house no. 3, (c) house no. 4, (d) house no. 5, and (e) house no. 6
Note: The numbers 1–6 represent the house number from Figure 2

LEAST-COST OPTIMIZATION

As mentioned above, after the brownfield site is cleaned up, there is still a chance that the residential houses will be affected unexpectedly by contaminated soil vapor. If it happens, the cost is essentially described as the probability of failure times the cost of failure, with an additional safety loading term to compensate against the associated hydrological and financial uncertainties. The probability of failure can be obtained from the last section (above), and the cost of failure is contributed by the house price as well as the uncertainty of the financial market. The safety loading term reflects the level of risk aversion and is usually defined as the variance or standard deviation in the cost of risk. The total cost concerned for the redevelopment is the sum of the cost of risk and the cost of data. In order to determine the least cost among the numerous cases listed earlier, the objective function is herein proposed in Equation 1 and 2.

$$Obj = E[H] + A[H] + \sum_{i=1}^{N} (n_C w_C + n_K w_K) \exp\left\{\int_{t_0}^{t_i} \pi_t \, dt\right\} \exp\{-d_i t_i\}\} \quad (1)$$

and $H(t_0) = \sum_{i=1}^{m} H_i(t_0)$ (2)

where H is the present value of the sum of the basic risk capital in each future period $(t_{i-1}, t_i]$; $E[H]$ is the expected value of losses from repossessing houses in each future period $(t_{i-1}, t_i]$; $A[H]$ is the uncertainty in predicting future repossession expenditures due to imperfect knowledge of hydrogeology and financial market; n_C is the number of sample locations for soil gas concentration; n_K is the number of wells extracting permeability; w_C is the unit cost for each sample concentration, w_K is the cost of taking one borehole permeability measurement, π_t is the inflation rate at time t and d_i is the discount rate at time t_i.

Suppose that every house is sold at $200,000, and that the central two houses have been repurchased since a potential soil vapor TCE exposure risk is considered. If the indoor air concentration of TCE in lateral houses exceeds the regulatory limit, it assumes that developers have the liability for repurchasing the house, and when the house is resold, it will lose 20% of its original value. For developers, the maximum liability would be when all the lateral houses are repossessed and they can never sell them again, which is $800,000. The expected value of H, the safety loading term, the cost of data and the total cost-risk are shown in Figure 11, with numerous permeability and concentration sampling schemes.

If more permeability data are available prior to the model prediction and more concentration data are applied for data assimilation, there is a lower expected value of risk, due to the fact that the lateral houses in reality have no risk of exceeding the regulatory limit. Such a situtation also means a lower safety loading reserve for contingency. The cases with 5 and 7 wells of permeability data show this pattern, while the case with only 1 well of permeability data shows some oscillations and therefore should not be used for this demonstration. On the other hand, with more data, the operational cost increases. Consequently, there must be an optimal solution in which the cost-effectiveness is achieved. In Figure 11(d), seven wells of permeability data with four of concentration data gives us the minimum cost; seven wells of permeability data with seven of concentration data can be an alternative solution.

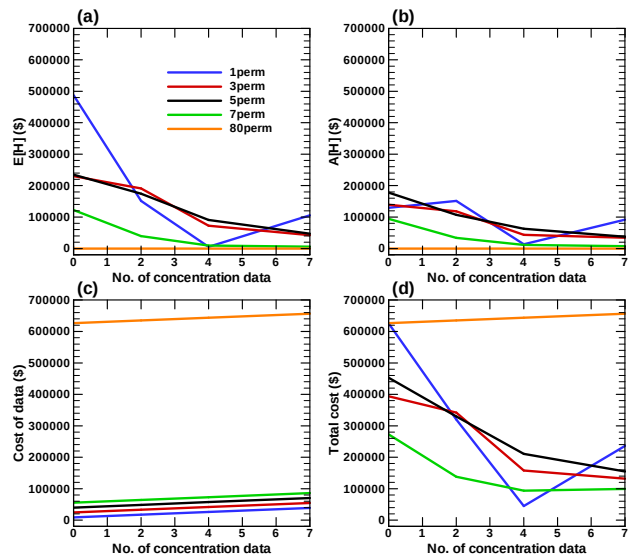

Figure 11. The variability of the related costs with different number of permeability and concentration data: (a) the expected value of the cost of risk, (b) the safety loading term on the cost of risk, (c) the cost of data, and (d) the overall cost

CONCLUSIONS

On the basis of the above results, the following conclusions may be drawn:

- First, the geological condition of an aquifer is one of the most important factors controlling the fate and transport of TCE from a source zone below the water table into houses. When a low-permeability layer saturated with water is located beneath the foundation slab, it prevents the soil gas TCE pathways from moving upwards. If a thicker vadose zone exists, it makes the mass

transfer across the capillary fringe more difficult, and the soil gas is more likely to diffuse away from the houses.

- Heterogeneity in the permeability of the aquifer causes the TCE plume to be deflected upward towards the houses. The impact of heterogeneous porosity will be investigated in future research.
- By using the spatial and temporal sampling data, and dynamically updating the sampling strategy, the model result is greatly improved. The more data that the Kalman filter utilizes for assembling the concentration correlation, the more accurate the estimations are.
- The cost of risk is defined in the same way that actuaries calculate the insurance premium, with an additional term —a safety loading term—to compensate for hydrogeological and financial uncertainties.
- An optimal solution, with the minimum cost of a brownfield redevelopment project for different numbers of permeability data and concentration data, can be obtained by a risk-cost-benefit analysis.

ACKNOWLEDGMENT

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REFERENCES

aboutRemediation™, Brownfields redevelopment toolbox™. Available at http://www.aboutremediation.com/Toolbox/Introduction.asp (accessed April 2012).

Johnson, P.C. and Ettinger, R.A., Heuristic model for prediction the intrusion rate of contaminant vapors into buildings, *Environ. Sci. Technol*., 25: 1445-1452, 1991.

Massmann, J. and Freeze, R.A., Groundwater contamination from water management sites: The interaction between risk-based engineering design and regulatory policy: 1. Methodology, *Water Resources Research*, 23(2): 351-367, 1987.

Mueller, G. R., Brownfields capital - unlocking value in environmental redevelopment, *Journal of Real Estate Portfolio Management, 11*(1), 81-92, 2005.

National Round Table on the Environment and the Economy (NRTEE) Canada, Cleaning up the Past, Building the Future: A National Brownfield Redevelopment Strategy for Canada, 2003. Available at http://nrtee-trnee.ca/wp-content/uploads/2011/06/brownfield-redevelopment-strategy-eng.pdf (accessed February 2012).

Reddy, K. R., Adams, J. A. and Richardson, C., Potential technologies for remediation of brownfields, *Practice Periodical of Hazardous, Toxic, and Radioactive Waste Management*, *3*(2), 19821, 1999.

UK Environment Agency, Brownfield Land Redevelopment: Position Statement. May 2003. Available at http://www.environment-Agency.gov.uk/static/documents/Research/brownfield_land_908146.pdf (accessed February 2012).

United States Environmental Protection Agency (US EPA), A sustainable brownfields model framework. January 1999. Publication Number: EPA-500-R-99-001.

Wade VanLandingham, H., The stormstown group and Meyer, P. B., Public strategies for cost-effective community brownfield redevelopment. Southeast Regional Environmental Finance Center, EPA Region 4, University of Louisville, 2002. Available at http://cepm.louisville.edu/Pubs_WPapers/practiceguides/PG1.pdf.

Yu, S., Unger, A.J.A. and Parker, B., Simulating the fate and transport of TCE from groundwater to indoor air, *Journal of Contaminant Hydrology*, 107(3-4): 140-161, 2009.

Zhang, Y. and Pinder, G.F., Least cost design of groundwater quality monitoring networks, *Water Resources Research*, 41: W08412, doi:10.1029/2005WR003936, 2005.