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Uncertainty and the Johnson-Ettinger Model for Vapor Intrusion Calculations

by

James W. Weaver
Ecosystems Research Division
National Exposure Research Laboratory
Athens, Georgia 30605

Fred D. Tillman
National Research Council
National Exposure Research Laboratory
Athens, Georgia 30605

U.S. Environmental Protection Agency
Office of Research and Development
Washington, DC 20460

14750

Notice

The U.S. Environmental Protection Agency through its Office of Research and Development funded and managed the research described here. It has been subject to the Agency's peer and administrative review and has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

Vapor intrusion is a complex problem where EPA is continuing to develop policies and guidance. This document presents the results of ORD-sponsored research and neither states EPA policy nor requirements for assessment and clean up. The latest EPA policies and requirements should be obtained from the EPA Office of Solid Waste and Emergency Response.

Abstract

The Johnson-Ettinger Model is widely used for assessing the impacts of contaminated vapors on residential air quality. Typical use of this model relies on a suite of estimated data, with few site-specific measurements. Software was developed to provide the public with automated uncertainty analysis applied to the model. (See http://www.epa.gov/athens/onsite.) An uncertainty analysis was performed on the model, that accounted for synergistic effects among variable model parameters. This analysis showed that a simple "one-at-a time" parameter uncertainty analysis provides a rough guide for the uncertainty generated by individual parameters and allowed their ranking. The one-at-a-time analysis, however, underestimated the uncertainty in the model results when all or groups of parameters were assumed to be uncertain. An apparent increase in simulated cancer risk caused by the uncertainty introduced from the input parameters was as much as 1285%. The model response to the input parameters showed that for the example studied, there was a positive skew in the model response to parameter variation.

Foreword

The National Exposure Research Laboratory's Ecosystems Research Division (ERD) in Athens, Georgia, conducts research on organic and inorganic chemicals, greenhouse gas biogeochemical cycles, and land use perturbations that create direct and indirect, chemical and non-chemical stresses, exposures, and potential risks to humans and ecosystems. ERD develops, tests, applies and provides technical support for exposure and ecosystem response models used for assessing and managing risks to humans and ecosystems, within a watershed / regional context.

The Regulatory Support Branch (RSB) conducts problem-driven and applied research, develops technology tools, and provides technical support to customer Program and Regional Offices, States, Municipalities, and Tribes. Models are distributed and supported via the EPA Center for Exposure Assessment Modeling (CEAM) and through access to Internet tools (http://www.epa.gov/athens/onsite).

Intrusion of contaminated vapors into buildings ("vapor intrusion") can provide a significant pathway for exposure to hazardous contaminants. Assessment of this problem is difficult because of limitations of sampling methodologies, contamination in external ambient air, internal sources and sinks of contaminants and, as discussed in this report, uncertainty in model application. The work described in this report is intended to set the stage for more widespread application of uncertainty analysis in site assessment, and to provide readily-available tools to streamline the required calculation. To meet this goal, three tools that are direct results of this work are available at http://www.epa.gov/athens/onsite.

Eric J. Weber, Ph. D.
Director, Ecosystems Research Division
Athens, Georgia

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Acronyms and Abbreviations

EPA	Environmental Protection Agency
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
JEM	Johnson-Ettinger Model
MDP	Model Development Platform
OAT	One at a time
OSWER	Office of Solid Waste and Emergency Response
RCRA	Resource Conservation and Recovery Act

1 Introduction

Vapors originating from subsurface contamination might migrate into residences and cause an immediate threat, or if at lower, less detectable levels, a chronic health risk. EPA concern over this problem resulted in the publication of a draft guidance for assessing risks (US EPA, 2002) at Superfund[1] and Resource Conservation and Recovery Act (RCRA) corrective action sites[2]. The draft guidance, and that of some State Agencies, uses the Johnson-Ettinger Model (JEM) (Johnson and Ettinger, 1991) as the basis for screening decisions at sites. A companion document (Tillman and Weaver, 2005) describes these issues in more detail. Generally though, the JEM is used under conditions of few measured or calibrated site-specific data. Where indoor air sampling is not undertaken, there is consequently no opportunity for calibration of the model results to site conditions nor corroboration by site-specific indoor air concentrations.

Consequently, there is a need for clear understanding of the uncertainties associated with this model. Uncertainties exist in several arenas, including:

1. *Model:* Does the conceptual basis of the model adequately represent the field site? Is there sufficient knowledge to make this determination?
2. *Parameters:* Do the choices of parameter values adequately represent the field phenomena?

The work reported in this document addresses the second of these questions. Parameter uncertainty is addressed because of the simplified nature and widespread acceptance of the JEM. Given that the model is used frequently, its usage could be improved by, first, understanding its uncertainties and, second, by providing the community with a readily-available version that provided an automated uncertainty analysis. Uncertainty analysis in general was recommended in the US EPA, User's Guide for Evaluating Subsurface Vapor Intrusion into Buildings, where it is stated that:

> "Because of the paucity of empirical data available for either bench-scale or field-scale verification of the accuracy of these models, as well as for other vapor intrusion models, the user is advised to consider the variation in input parameters and to explore and quantify the impacts of assumptions on the uncertainty of model results. At a minimum, a range of results should be generated based on variation of the most sensitive model parameters" (US EPA, 2004).

This work does, in fact, address the ranges of sensitive parameters, but goes a necessary step beyond to address the synergistic effects of simultaneous variation of multiple model parameters on the JEM output.

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[1] Formally known as the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)

[2] Leaking underground storage tank (LUST) sites were specifically excluded from coverage by the guidance document.

Johnson (2002) addressed the sensitivity and range of input studies in a detailed study of JEM parameters and their variation (Johnson, 2002). Johnson's analysis focused on variation of parameters taken one-at-a-time. His work also (Johnson, 2002, Appendix A) was presented in terms of three dimensionless parameters that encapsulate all the inputs to the original model. Although this provides a concise means to present results, a fairly high degree of sophistication is needed for relating the results to the primary input parameters. For these reasons, a software package was developed to perform an automated uncertainty analysis using the primary inputs to the model. This software provides options to perform the calculations on the original model formulation (Johnson and Ettinger, 1991) and for some of the EPA additions (US EPA, 2004). Generally, this work provides an alternate means of evaluating uncertainty in the model and is complimentary to the prior work by Johnson (2002).

2 Background on the Johnson-Ettinger Model (JEM)

JEM results are often given in terms of the "alpha" parameter (α) that is defined by

$$\alpha = C_B / C_s$$

where C_B is the concentration in the building and C_S is the concentration in the in the source. For the following model results, the source can be treated as the soil gas below the building or, as included in the EPA OSWER version of JEM, from the capillary fringe. Both options are included in the software described below for consistency with both approaches.

The JEM α is computed from

$$\alpha = \frac{A \exp(B)}{\exp(B) + A + \frac{A}{C}[\exp(B) - 1]}$$

where the dimensionless quantity A is given by:

$$A = \frac{D_T^{eff} A_B}{Q_B L_T}$$

where D_T^{eff} is the effective diffusion coefficient of the contaminant in soil [L^2/T], A_B is the subsurface foundation area [L^2], Q_B is the volumetric flow rate of air in the building [L^3/T] and L_T is the distance from contamination to the bottom of foundation [L]. The air flow rate in the building, Q_B, is broken down into the building volume [L^3], V_B, and the air exchange rate [T^{-1}], E_B.

The dimensionless quantity B is given by

$$B = \frac{Q_s L_C}{D_C^{eff} N A_B}$$

where Q_S is the soil gas flow rate into the building [L^3/T], L_C is the thickness of the foundation [L], D_C^{eff} is the effective diffusion coefficient for the contaminant in the crack [L^2/T], and N is the crack ratio [dimensionless]. The crack ratio is defined by

$$N = {A_C}/{A_B}$$

where A_C is the area of the crack [L^2]. OSWER (US EPA, 2004) relates the crack ratio to building properties by

$$N = \frac{4\, W_C \sqrt{A_B}}{A_B}$$

where W_C is the width of the crack [L]. Johnson and Ettinger (1991) use the assumption that the floor/wall cracks and openings are filled with dust and dirt characterized by a density, porosity and moisture content similar to that of the underlying soil to justify equating D_T^{eff} and D_C^{eff}.

The diffusion coefficient is estimated from the Millington-Quirk relationship

$$D_T^{eff} = D_A \frac{\theta_A^{3\frac{1}{3}}}{\eta^2} + \frac{D_w}{H} \frac{\theta_W^{3\frac{1}{3}}}{\eta^2} \qquad D_T^{eff} = D_A \frac{\theta_A^{3\frac{1}{3}}}{\eta^2} + \frac{D_W}{H} \frac{\theta_W^{3\frac{1}{3}}}{\eta^2}$$

where D_A is the air phase diffusion coefficient [L^2/T], θ_A is the air-filled porosity [L^3/L^3], η is the porosity [L^3/L^3], D_W is the water phase diffusion coefficient [L^2/T], θ_W is the water content [L^3/L^3], and H is the Henry's Law Coefficient [unitless] (See US EPA, 2004). A depth-weighted average diffusion coefficient is used to average-out the effects of layering in the vadose zone (Johnson and Ettinger, 1991).

The dimensionless quantity C is given by

$$C = \frac{Q_s}{Q_B}$$

The indoor air concentration, C_B itself is given by

$$C_B = \alpha_{SG}\ C_{SG}$$

for a soil gas source, and

$$C_B = \alpha_{GW}\ C_{GW}\ H$$

for a ground water source. The coefficients α_{SG} and α_{GW} are the attenuation factors calculated for soil gas or ground water sources, respectively. The differences between these two are described in Section 6.

Taking this a step further for carcinogenic compounds at a specified cancer risk, the allowable building concentration, $C_{B\text{-}A}$, can be calculated from:

$$C_{B-A} = \frac{TR\ AT}{URF\ EF\ ED}$$

where TR is the target risk level [unitless], AT is the averaging time [T], URF is the inhalation unit risk factor $[M/L^3]^{-1}$, EF is the exposure frequency [T/T], and ED is the exposure duration [T] (based on US EPA, 2001).

3 Models and Modeling

Subsurface transport models are based on a mathematical statement of conservation of mass. Ancillary relationships are needed to estimate fluxes that are used in the mass conservation equation. Inputs to these models provide the means to quantify the relationships for specific site conditions and are called the parameters of the model. Other inputs represent the forcing functions that represent the boundary and initial conditions. Generally the forcing function represents the input of contaminants into the system, while the model parameters represent the transport properties of the media.

All models are based on simplification and approximation. Models designed for the same problem can be based on vastly different assumptions. These assumptions can and do introduce limitations. Understanding of general types of models and their common assumptions and the way that a specific model of interest was developed is critical for choosing, applying and evaluating model usage. Without this knowledge model selection, usage and interpretation are at best uninformed and there is a very weak basis for critical evaluation of model results.

An important division between types of models is that between analytical and numerical models. Analytical solutions are based on mathematical functions that are or have the potential to be exact solutions of the transport equation. Analytical solutions of the transport equation

- cannot simulate heterogeneous formations,
- require the assumption of one-dimensional flow,
- only represent uniform flow,
- includes transport by advection in the direction of flow only, and
- do not allow representation of irregular boundaries.

Numerical models are based on approximations that that are formulated over necessarily small parts of the simulation domain. The two most common numerical methods are finite difference and finite element, both of which require a grid to be placed over the domain. This provides a way to identify these models—if there is a gridded domain then the model is most likely to be a numerical model; otherwise the model is analytical.

Requirements for application of models are described in detail by Anderson and Woessner (1992) and Zheng and Bennett (1995) and are echoed by the US EPA, Committee on Regulatory Environmental Modeling (Pascual et al., 2003). These and similar guidelines have been proposed and described in many other publications. The material that follows matches the common threads of these proposals: Use of models requires development of a conceptual model of site conditions followed by selection of a model that matches those conditions. The location and types of boundary conditions must be chosen and parameterized. Parameter values must be assigned based on site conditions. These are either taken from site-specific measurement, literature values or other estimates. Site data, which for contamination problems, includes concentrations,

are used to test the model predictions. Input parameters and forcing function values can be adjusted to match site data. That this is a legitimate activity follows from: imprecision in measurement of input parameters, spatial variability in media properties that do not allow measurement of properties at all points, inability to measure all parameters because of technical, programmatic or cost limitations. A calibrated model has essentially been forced to match a set of field data. By taking this process one set further, the calibrated model is tested against a data set that was not used in calibration. The model has then been demonstrated to match existing data and in the best case, match a data set which was not used in calibration. Iteration may be required for further adjustment of parameters. At the end of this process, uncertainty in model results has been reduced to the minimum level possible (See Pascual et al., 2003, page 11).

Model applications which are not subjected to the process described above have an inherently higher level of uncertainty in their results. Without site specific measurement of model outputs (i.e., concentrations), it is not possible to assure that a model represents subsurface conditions. In cases where few parameters are measured and outputs are not measured, the uncertainty in results shall be high. In these cases, a single set of parameters can not provide a certain result. Although average parameter values may be used in a simulation, the model results which also appear as a single set of values, do not convey any information on the degree of certainty in the results. It may be possible in some cases to define generic best or worst case parameter sets that could be run singly and represent the best or worst case results. These are not necessarily identifiable in advance, but must be established by evaluating the model behavior.

As a summary, the U.S EPA, Committee on Regulatory Environmental Models recommended a set of best practices that included:

- peer review of models,
- assessment of data quality,
- corroboration of model results with data,
- sensitivity analysis, and
- uncertainty analyses.

4 Uncertainty Calculations

Johnson and Ettinger state in their original paper (Johnson and Ettinger, 1991):

> "Here we [...] formulate a heuristic model for predicting the intrusion rate of contaminant vapors into buildings through foundations... This model can be used as a risk assessment screening-level tool; it can be used to identify sites, or contaminant levels, for which contaminant exposures through a vapor inhalation pathway may cause adverse health effects. It can also be used as a tool to help identify sites where more detailed numerical simulations or field sampling are appropriate."

To achieve these goals the model must be appropriate for the site and building conditions and be properly parameterized. This work focused on the impacts of parameterization, specifically considering how the model behaves when inputs are uncertain. Inputs are surely uncertain when

1. model inputs are not measured on a site-specific basis,
2. spatial variability is not considered. and
3. model results are not corroborated against measurements.

Oreskes (2003) presented a framework for understanding the scientific usage of models, and stated that:

> "Models can never fully specify the systems that they descried, and therefore are always subject to uncertainties that we cannot fully specify".

To begin to specify uncertainty, the JEM was re-implemented in a Java package called the Model Development Platform (MDP) (Weaver, 2004). This software allows the JEM to be run directly from the Internet and is available at the web address: http://www.epa.gov/athens/onsite.

The approach taken to assessing uncertainty was to assume that some simple parameters of the model should be known to a sufficient degree of accuracy to be input as constants. The presumed constant parameters of the JEM are the building length and width, foundation thickness, depth of the bottom of the foundation below grade, and chemical of interest. Several parameters are use to estimate the temperature-dependent Henry's constant of the chemical of interest. These parameters are also all treated as constants and are embedded within the software.

All other parameters of the model are assumed to be uncertain with a known range of possible values. For this analysis, the range of values were presumed to be known, but not statistical distributions of the parameters. The desire was to apply a screening approach that could account for multiple parameter uncertainty, without introducing more uncertain quantities such as statistical distributions of parameters. Thus

the range of each parameter was estimated by determining a low and high value. The model was run for every possible combination of the high and low values. From the results, the highest and lowest values of α, A, B, and C are determined. This procedure contains two implicit assumptions. First, that each parameter is uniformly distributed and as a result, equally probable. Second, that the extreme values of the model result occurs from parameters set to the limits of their ranges. In all cases tested, the extremes were found to occur at these endpoints. Correlation between parameters is neglected on the presumption that the parameter values vary only over a small range where each combination is possible regardless of correlations among them. The results, then, should be interpreted as giving the *plausible* range of output, given the ranges of the inputs. Each result is assumed to be equally probable and the intent is to define the best and worst case outputs. Further details on the background for this approach are given in the Appendix.

For nominally more precise and more powerful uncertainty analyses (like Monte Carlo simulation), statistical distributions and correlations are required. It is instructive to note that the Monte Carlo method was developed for the inherently random simulation associated with radioactive decay (Metropolis and Ulam, 1949). In examples cited by Metropolis and Ulam, the probabilities are easily assigned (i.e., the direction a an emitted neutron takes after nuclear fission). For other problems, such as the JEM for subsurface vapor transport, the probabilities are difficult to assign on a problem-specific basis, and particularly where site assessment protocols call for limited data collection. Thus the desire in this work was to provide a screening analysis that accounted for the uncertainties and synergies among parameters.

The uncertain parameters of the JEM were assumed to include the temperature, some building parameters and all soil parameters. Specifically the latter two were the:

- enclosed space mixing height,
- floor-wall crack width,
- indoor air to subsurface pressure differential,
- air exchange rate,
- hydraulic conductivity,
- vadose zone thickness,
- porosity,
- residual water content,
- effective water saturation,
- parameter "m" of the van Genuchten model,
- mean particle diameter, and
- soil gas flow rate.

The options of running the original JEM or a modified version influence the number of parameters (Table 1) treated as being uncertain. If the capillary fringe is excluded (original JEM) then the mean particle diameter is not used. If the soil gas flow rate is used (original JEM), then the hydraulic conductivity and pressure differential are not used. If definitive values can be assigned for the potentially uncertain parameters, the software allows a single value to be used. This, in turn, reduces the number of simulations by a factor of two for each parameter set to a fixed value.

An alternative to this approach would be to vary each parameter individually, requiring at most 26 runs of the model (two runs per parameter listed above). As will be shown, this simple "one at a time" (OAT) analysis underestimates the uncertainty in the output. OAT underestimates uncertainty when there are synergistic effects or interactions among parameters (see Campolongo et al., 2000). The form of the JEM indicates that there are interactions among parameters because they occur as multipliers or divisors of each other. Most notably are the three dimensionless parameters (A, B, and C) formed from combinations of basic inputs.

Table 1 Required number of simulations for four types of simulation.

Simulation Type	Calculated Soil Gas Flow Rate	Parameters		Maximum Number of Simulations
		Always Fixed	Potentially Variable	
Soil Gas to Indoor Air	y	4	11	2048
	n	4	9	512
Capillary Fringe to Indoor Air	y	4	12	4096
	n	4	11	2048

Table 2 Parameters used with ground water or soil gas sources and calculated or entered soil gas flow rate.

Parameter	Calculated Soil Gas Flow Rate		Estimated Soil Gas Flow Rate	
	Ground Water Source	Soil Gas Source	Ground Water Source	Soil Gas Source
Hydraulic conductivity	y	y	n	n
Thickness	y	y	y	y
Porosity	y	y	y	y
Residual Water Content	y	y	y	y

Water Content	y	y	y	y
van Genuchten "m"	y	y	y	n
Particle Diameter	y	n	y	n
Soil Gas Flow Rate	n	n	y	y
Mixing Height	y	y	y	y
Floor-wall Crack Width	y	y	y	y
Pressure Differential	y	y	n	n
Temperature	y	y	y	y
Total	12	11	11	9

5 Vapor Intrusion Uncertainty Calculation

The uncertainty calculation is packaged into a Java Applet that runs from the US EPA web site at http://www.epa.gov/athens. The applet is known to run with either the Microsoft Internet Explorer, Netscape Navigator or Firefox web browsers. A java run time environment must be installed and enabled. When visiting the web site, the background (Figure 1) and about screens (Figure 2) give a brief overview of the calculation and contact information for the model.

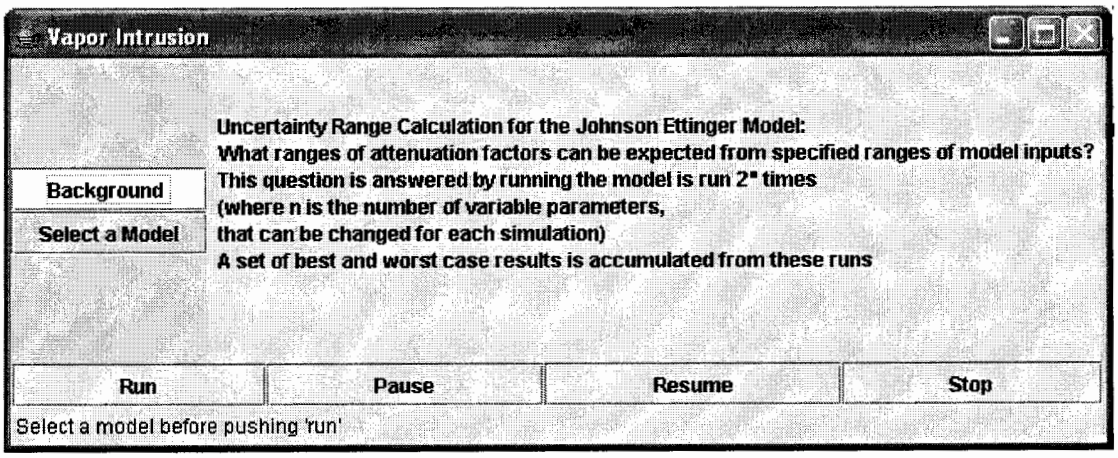

Figure 1 Background screen giving a brief overview of the calculation.

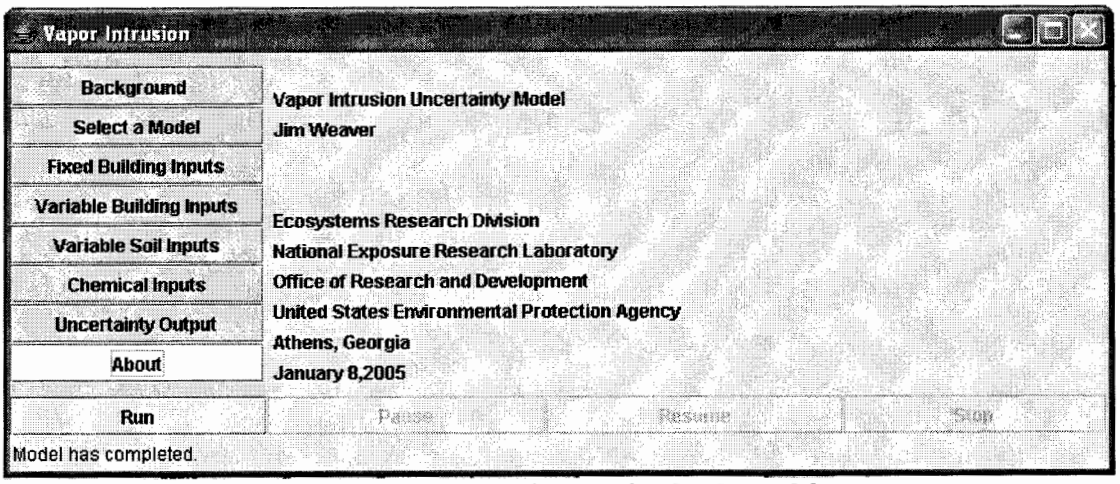

Figure 2 The "about" screen that gives contact information for the model.

The "Select a Model" screen (Figure 3) gives choices for input models. The Java code used to build this model allows for the inclusion of various choices of models. In this case, the main choices only relate to input unit sets. Future development may include alternate model formulations. Once the selection of a model has been made, as shown in Figure 3, the interface is populated with input and output screens appropriate to the choice of model.

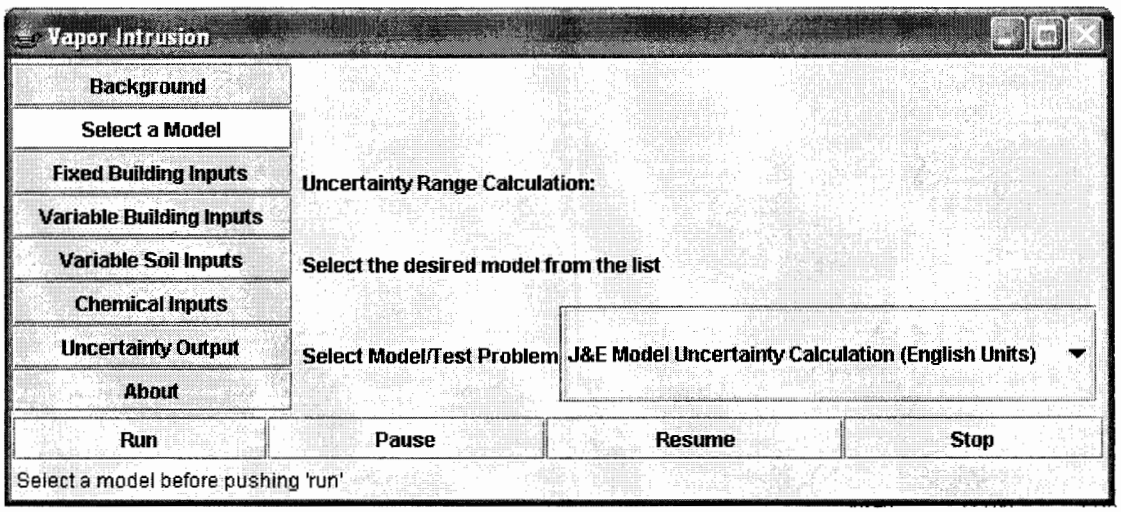

Figure 3 The selection screen allows choices of models. Currently the only choices are among input units.

6 Input Parameters

For the current JEM model there are four input screens for the model. These are shown in Figure 4 through Figure 9.

6.1 Building

The simplest parameters defining the building are assumed not to vary (Figure 4). These include the length [ft] and width [ft] of the building and the foundation thickness [ft]. The foundation may be below grade, as in the case of a basement. Thus this depth [ft] may also be specified.

Building parameters that are harder to specify are treated as potentially uncertain (Figure 5). These are, in order of entry:

- Enclosed space mixing height [ft]
- Floor-wall crack width [mm]
- Indoor air to subsurface pressure differential [g/cm-s^2]
- Air exchange rate [hr $^{-1}$]

For each uncertain parameter a low and high value are entered. These should be chosen to cover the entire likely range of values for the parameter. Where little information exists on parameter values, running the model for a several orders-of-magnitude variation provides a conservative approach for assessing the potential impacts on indoor air quality.

Enclosed space mixing height: The mixing height represents a concept that the contaminated vapors emerge from cracks in the floor/slab of a residence and are then mixed with the ambient air in the building. In order to avoid directly simulating this mixing process, a height is selected to form a zone over which the contaminant vapors are assumed to be distributed uniformly. OSWER selected a mixing height of 2.44 m (8 ft) for one-story slab-on-grade homes and 3.66 m (12 ft) for basement homes. The latter number reflects an assumption that there is some mixing from the basement into an upper story, but limited to less that the full height of the upper story (or the mixing height might be 7.32 m (16 ft)).

Crack ratios were estimated and reported in various publications (Table 3). While all the others presented ranges of one order of magnitude or greater, ASTM 1739-95 presented a only single crack ratio value. Using the parameters for the OSWER-derived example problem presented in Section 7, crack width ranges were calculated. These ranges reflect a variety of assumptions concerning this parameter.

Table 3 Crack ratios, estimated crack thicknesses for the default problem of Section 7.

Publication	Crack ratio		Crack width (mm) for conditions of Section 7		Comment
	Minimum	Maximum	Minimum	Maximum	
Nazaroff (1992), Revzan et al. (1991) Nazaroff et al. (1985)	0.0001	0.001	0.25	2.5	Back-calculated from measured soil gas flow rates into buildings
Figley and Snodgrass (1992)	--	--	Hairline	5	Most measured cracks < 1 mm
ASTM E1739-95	0.01	0.01	25	25	Default
VOLASOIL	0.000001	0.0001	0.0025	0.25	"Good" and "bad" foundations, respectively
Johnson and Ettinger (1991)	0.001	0.01	2.5	25	Illustrative values

OSWER selected a default *building air exchange* rate of 0.25 hr^{-1}, based on a data set that included 2844 homes divided by season and geographic region (U.S. EPA, 2004). A value near the lower end (lesser air exchange) for the composite data was selected (0.25 hr^{-1} versus 0.21 hr^{-1}), given the range of 0.21 hr^{-1} to 1.48 hr^{-1}. Other work referenced by OSWER suggests bounds of 0.1 hr^{-1} to 2 hr^{-1}.

If the value of a potentially variable parameter can be fixed to a single value, then the software accommodates this possibility. Entering the *same* value as both the low and high values fixes the value and eliminates it as an uncertain parameter. The number of simulations is reduced by a factor of 2 for each such fixed parameter.

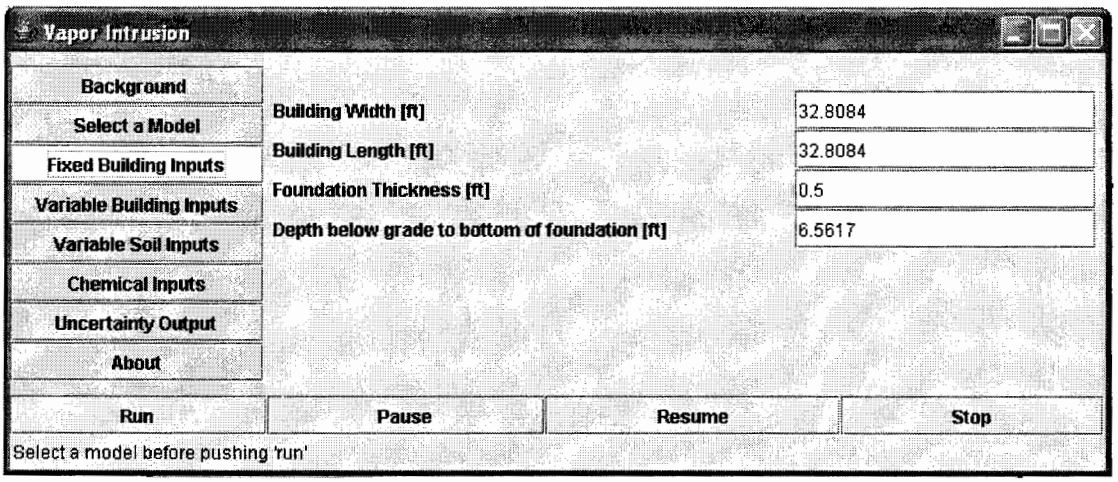

Figure 4 The input screen for entering fixed building parameters.

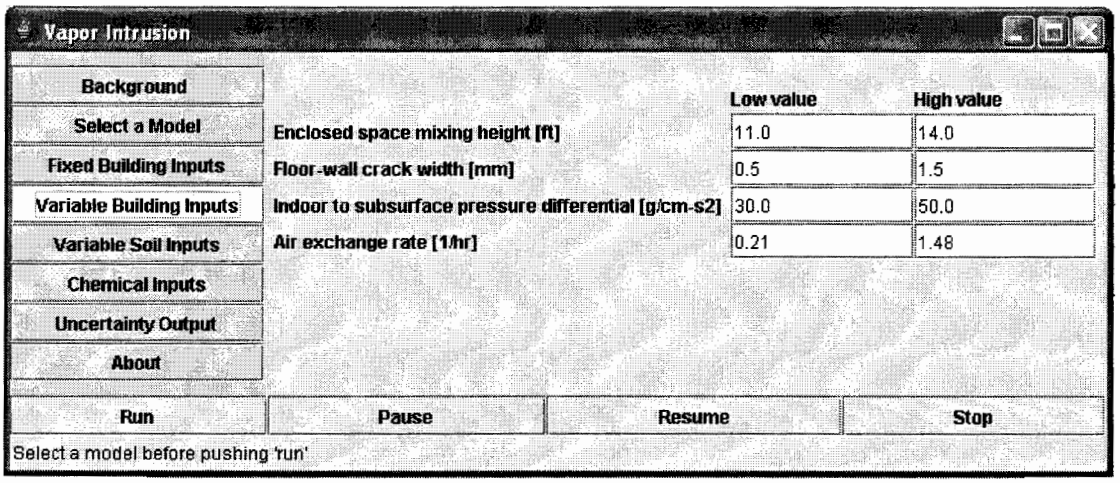

Figure 5 The building input screen for entering building parameters that will be considered variable.

6.2 Soil

Because of limited measurement at field sites, imprecision in measurement techniques and spatial variability, all soil parameters are presumed to be uncertain (Figure 6). The soil parameters include the:

- hydraulic conductivity [cm/s],
- thickness (depth to water table) [ft],
- porosity [dimensionless],
- residual moisture content [dimensionless],
- effective saturation [dimensionless],
- van Genuchten model parameter "m", and
- mean particle diameter in the capillary fringe[cm].

Two questions are given the user concerning the capillary fringe and the soil gas flow rate. These are discussed separately below.

6.2.1 Soil Properties (Hydraulic Conductivity, porosity, residual moisture content, van Genuchten model "m")

The van Genuchten (1980) model represents the soil capillary pressure curve by a function given by

$$\frac{\theta_w - \theta_{wr}}{\theta_m - \theta_{wr}} = \left(\frac{1}{1 + (a\,h)^n} \right)^m$$

where θ_w is the water content, θ_{wr} is the residual water content, θ_m is the saturated water content, and a [1/L], n, and m are fitting parameters. Further, the saturated moisture content, θ_m, is usually taken as the porosity and m is set equal to the quantity 1 – 1/n for mathematical convenience. Data are fit to the van Genuchten model for determining appropriate values of a, θ_{wr}, θ_m, and m.

Tabulations of soil properties have been made from agricultural soils (e.g., Carsel and Parrish, 1988) that show that there is a great deal of variability associated with each Soil Conservation Service (SCS) soil type. Even though a sandy soil, for example, may underly a building, there are many types of sand that differ in their hydraulic behavior. Additionally, because soils are typically heterogeneous, the capillary properties of soils can vary greatly at one site. Therefore, because capillary pressure curves are typically not measured at vapor intrusion sites, the selection of capillary properties by SCS soil class names does not assure that representative values are used in simulation. A range of possible values for each SCS soil type are given in Table 4, Table 5, and Table 6.

Table 4 Saturated and residual water contents from the Carsel and Parrish (1988) soil parameter data set.

Soil Type	Saturated Water Content (θ_m)			Residual Water Content (θ_{wr})		
	Sample size	mean	Standard deviation	Sample size	mean	Standard deviation
Clay	400	0.38	0.09	353	0.068	0.034
Clay Loam	364	0.41	0.09	363	0.095	0.010
Loam	735	0.43	0.10	735	0.078	0.013
Loamy Sand	315	0.41	0.09	315	0.057	0.015
Silt	82	0.46	0.11	82	0.034	0.010
Silt Loam	1093	0.45	0.08	1093	0.067	0.015
Silty Clay	374	0.36	0.07	371	0.070	0.023
Silty Clay Loam	641	0.43	0.06	641	0.089	0.009
Sand	246	0.43	0.06	246	0.045	0.010
Sandy Clay	46	0.38	0.05	46	0.100	0.013
Sandy Clay Loam	214	0.39	0.07	214	0.100	0.006
Sandy Loam	1183	0.41	0.09	1183	0.065	0.017

Table 5 n and alpha parameters of the van Genuchten model from the Carsel and Parrish (1988) soil parameter data set.

Soil Type	van Genuchten n			van Genuchten a (m^{-1})		
	Sample size	mean	Standard deviation	Sample size	mean	Standard deviation
Clay	400	1.09	0.09	400	0.80	1.2
Clay Loam	364	1.31	0.09	363	1.9	1.5
Loam	735	1.56	0.11	735	3.6	2.1
Loamy Sand	315	2.28	0.27	315	12.4	4.3
Silt	82	1.37	0.05	82	1.6	0.7
Silt Loam	1093	1.41	0.12	1093	2.0	1.2
Silty Clay	374	1.09	0.06	126	0.5	0.50
Silty Clay Loam	641	1.23	0.06	641	1.0	0.60
Sand	246	2.68	0.29	246	14.5	2.9
Sandy Clay	46	1.23	0.10	46	2.7	1.7
Sandy Clay Loam	214	1.48	0.13	214	5.9	3.8
Sandy Loam	1183	1.89	0.17	1183	7.5	3.7

Table 6 Hydraulic conductivity from the Carsel and Parrish (1988) soil parameter data set.

Soil Type	Hydraulic Conductivity (m/d)		
	Sample size	mean	Standard deviation
Clay	114	0.048	0.10
Clay Loam	345	0.062	0.17
Loam	735	0.25	0.44
Loamy Sand	315	3.5	2.7
Silt	88	0.060	0.079
Silt Loam	1093	0.11	0.30
Silty Clay	126	0.0048	0.026
Silty Clay Loam	592	0.017	0.046
Sand	246	7.1	3.7
Sandy Clay	46	0.029	0.067
Sandy Clay Loam	214	0.31	0.66
Sandy Loam	1183	1.1	1.4

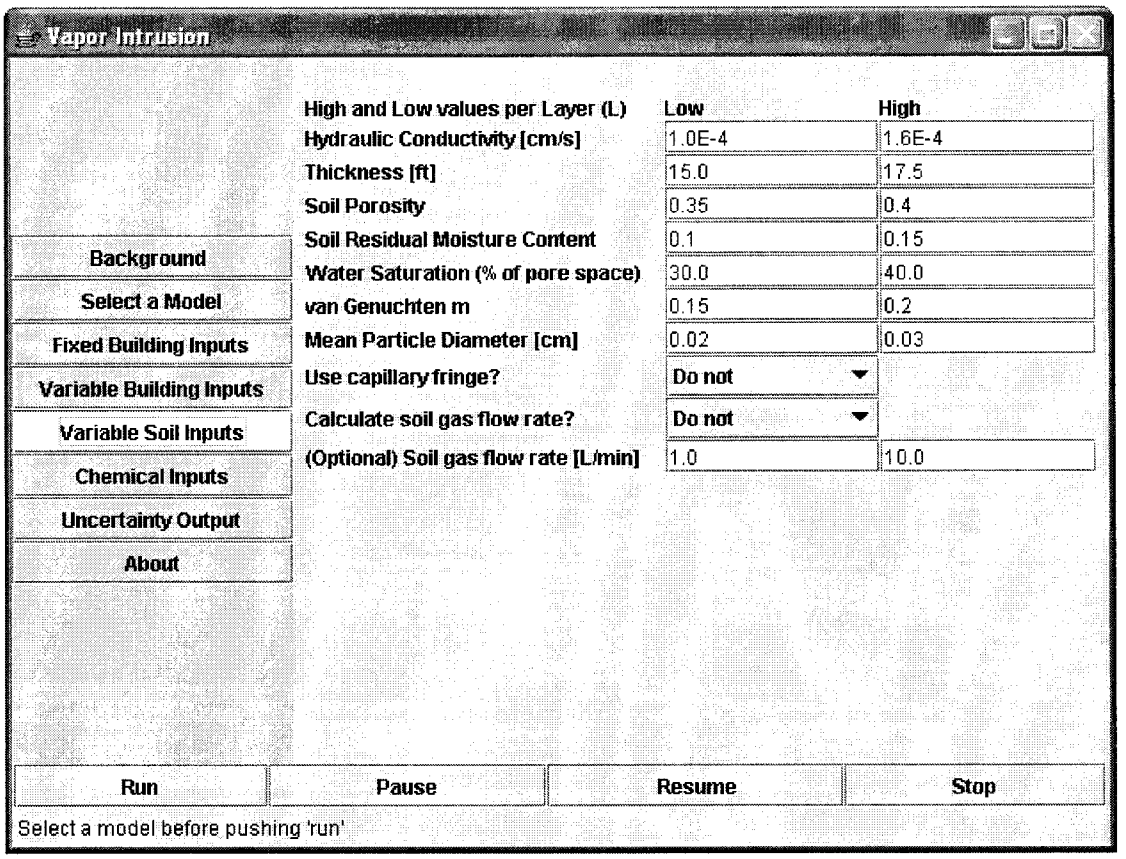

Figure 6 Variable soil inputs that consist of low and high values of each parameter and two choices: to include capilary fringe or not; and to use a calculated gas flow rate or values that are directly input on this screen.

6.2.2 Capillary Fringe

The original JEM model assumed that the source of indoor air contamination was the soil gas. OSWER extended the original model to include a calculation of partitioning across a simplified representation of the capillary fringe. The capillary fringe is simplified as a zone of uniform water content, extending a certain distance above the water table. The capillary fringe water content is determined from

$$\theta_{cz} = \theta_{cz-R} + \frac{\eta_{cz} - \theta_{cz-R}}{2^m}$$

where θ_{cz} is the water content of the capillary zone, $\theta_{cz\text{-}R}$ is the residual water content of the capillary zone η_{cz} is the porosity of the capillary zone and m is the van Genuchten model parameter "m" of the capillary zone. The capillary zone height [cm], h_{cz}, is determined from the mean particle diameter using the empirical function:

$$h_{cz} = \frac{0.15}{0.2\,\phi}$$

where φ is the mean particle diameter of the capillary zone [cm] (US EPA, 2004).

Using the capillary fringe in the computation assumes that contaminated ground water is the source of indoor air contamination. The choice between these two options is shown in Figure 7, that shows an example where the capillary fringe calculation is not used.

Use capillary fringe?	Do not

Figure 7 Option for use of capillary fringe. Here the capillary fringe calculation will not be included since the problem is assumed to be a soil gas/indoor air problem.

6.2.3 Calculated Soil Gas Flow Rate

The soil gas flow rate can be entered directly in liters per minute on the last line of input. When this input is intended to be used, the soil gas flow rate is not calculated (i.e., the selection "Do Not" is made). This option is shown in Figure 8 where the soil gas flow rate, is not to be calculated and that the range of simulated values will be 1 L/min to 10 L/min.

Calculate soil gas flow rate?	Do not	
(Optional) Soil gas flow rate [L/min]	1.0	10.0

Figure 8 Options for calculating the soil gas flow rate. Here the soil gas flow rate will not be calculated and the range of values will be 1 L/min to 10 L/min.

The OSWER default value of 5 L/min was based upon the assumption that coarse grained soils/backfill underlying a house control the entry of vapors. Flows may be much lower under other circumstances as the OSWER range of 1 L/min to 10 L/min was determined for coarse-grained soils only.

6.3 Chemical

Chemical properties are assigned in the model by picking the chemical name. From this, the model selects the air and water phase diffusion coefficients and the temperature-adjusted Henry's law coefficient. The temperature can be treated as a variable parameter (Figure 9).

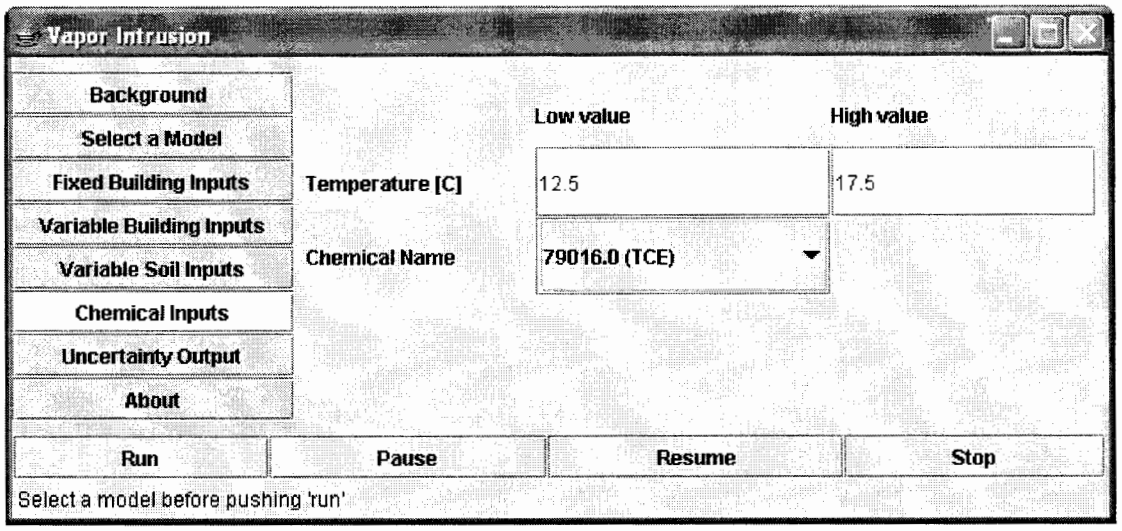

Figure 9 The chemical input screen allows selection of the chemical and the temperature range.

6.4 Output

The model output is given as the minimum and maximum values of several outputs of the model (Figure 10). Each row of output gives an extreme value of an output along with the corresponding values of the other outputs (here, A, B, and C). For example reading across the first row of results (Figure 11), the smallest value of alpha (1.59E-5) corresponds to A of 1.909E-5, B of 2047.0, and C of 9.501E-5.

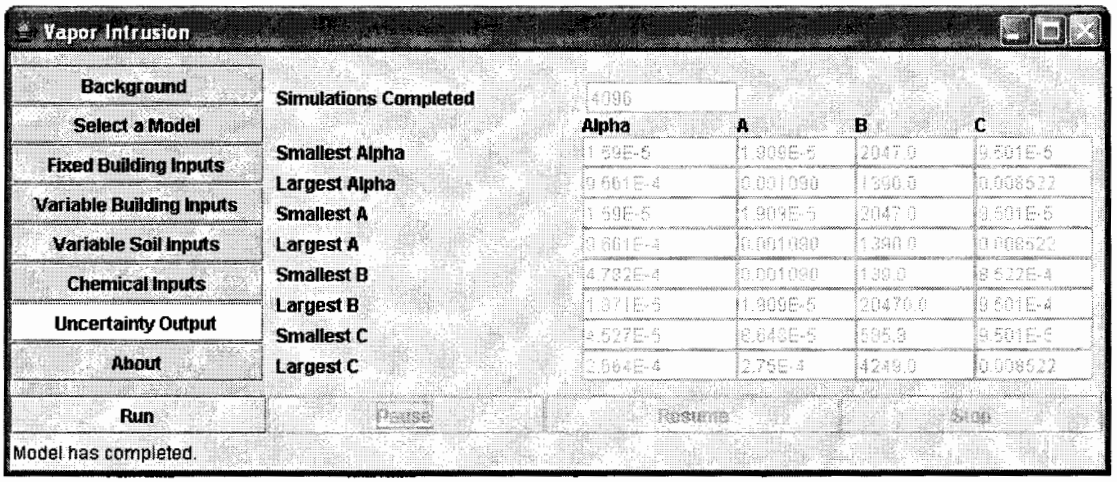

Figure 10 Uncertainty Output after 4096 simulations.

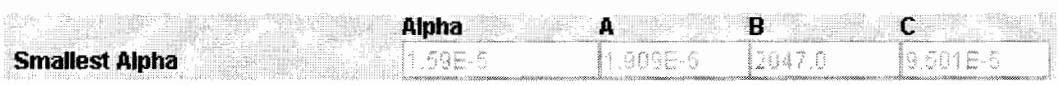

Figure 11 Example from the output screen that shows the results for the smallest alpha value (1.59E-5). The corresponding values of A, B and C are given in the last three columns.

7 Sample Simulations

A set of simulations were performed to study variation in the JEM model results given reasonable ranges of input values (Table 7 and Table 8). The values in Table 8 were drawn from the OSWER document (US EPA, 2004) and use the ranges of values either explicitly reported or set to an amount of variation equal to +/- 25% of the OSWER default value. For this example, the contaminant was trichloroethene in a sandy loam soil, and its source was the soil gas. The soil gas flow rate was not calculated from the soil parameters, but rather input directly.

Table 7 Fixed parameters for the example simulation.

Fixed Parameter	Value
Building Width	32 ft
Building Length	32 ft
Foundation Thickness	0.32 ft
Depth to Contamination	6.15 ft
Chemical	trichloroethene

Table 8 OSWER defaults, ranges and sources of variability for example simulation.

Parameter	Variability Source	Values		
		Low	OSWER default	High
Mixing height [ft]	OSWER range	8	12	16
Floor-wall crack width [mm]	OSWER range	0.5	1	5
Air exchange rate [hr^{-1}]	OSWER range	0.1	0.25	1.5
Depth below grade [ft]	+/- 25%	22.1	29.5	36.9
Porosity	+/- 25%	0.29	0.387	0.484
Residual moisture content	+/- 25%	0.029	0.039	0.049
Moisture content	OSWER range	0.039	0.103	0.17
Soil gas flow rate [L/min]	OSWER range	1	5	10
Temperature [C]	+/- 25%	11.25	15.0	18.75

A baseline simulation using the fixed parameter values and the OSWER defaults (Table 7 and Table 8) generated an α value of 6.48×10^{-4}. To compare results from various

simulations, this baseline attenuation coefficient was used to calculate indoor air and soil gas concentrations assuming 1 x 10^{-6} excess cancer risk level. The corresponding soil gas concentration was 34.16 $\mu g/m^3$ and the associated indoor air concentration was 0.0221 $\mu g/m^3$. All subsequent results from the model were presented in terms of increased (or decreased) cancer risk relative to this base case.

From the calculated soil gas concentration of 34.16 $\mu g/m^3$, the increase/decrease in risk was calculated for various scenarios corresponding to differing levels of parameter uncertainty. The first experiment evaluated the risk associated with one-at-a-time uncertainty due to individual parameters of the model. These results are presented as items A through I in Figure 12 and Table 10, and show how the calculated risk changes by considering uncertainty in various input parameters. The risk can decrease below the default-parameter case (column 3 of Table 10) when a "best case" parameter set is encountered. Alternately, the risk may increase when a "worst case" is encountered (column 4 of Table 10). These results indicate that there can be an apparent risk that is due to an increase in parameter uncertainty. Reducing parameter uncertainty reduces this apparent risk. Generally, the results also showed skewed results toward increased risk, even though most parameter ranges were balanced about the defaults (Table 8). Figure 12 shows that there is an insignificant to modest increase in risk due to increasing the single parameters over their default values. Some parameters caused no increase in risk at all (floor-wall crack width and temperature). Of the single parameter simulations, only the air-exchange rate caused an increase in risk above 100%.

When taken in groups, however, synergies among related sets of parameters become evident (Figure 12 and Table 11). Subsurface and building properties were taken as two independent groups for evaluation. The subsurface was further divided into two sets for simulation. First were the soil properties: porosity, residual water content and water content. Their variation as a group produced an increased cancer risk of 117.9% (row J of Table 11), more than that produced by any single member of this group. The second of the subsurface parameter sets included these same soil parameters, but added depth to the contamination and soil gas flow rate. The risk increased by 262.3% over the baseline scenario (row K of Table 11). From the single parameter results, it is seen that changing each of these parameters produced modest increases in risk. Taken together, however, the increase in risk was higher. The next group contained the building parameters: mixing height, floor-wall crack width, and air exchange rate. Individually these parameters increased risk by 50.1%, 0.0% and 150.0%, respectively. Varying these parameters together the increase over the default risk was 274.9% (row L of Table 11). Omitting the floor-wall crack width resulted in the same 274.9% increase in risk, so the impact of this parameter was not amplified by its inclusion in the group.

Parameters that were judged as being the least-known were also grouped together. Most of these (excepting the floor-wall crack width) produced increases in risk on their own. Together the uncertainty in these parameters increased the risk by 941.6% (row M of Table 11). When all uncertain parameters were included in the calculation the increased risk was 1258.4% (row N of Table 11).

Table 9 Risk parameters for the uncertainty calculation.

Risk Parameter	Value
Averaging Time, AT	70 yr
Inhalation Unit Risk Factor, URF	0.00011 $(\mu g/m^3)^{-1}$
Exposure Frequency, EF	350 d/yr
Exposure Duration, ED	30 yr
Source Concentration	34.16 $\mu g/m^3$

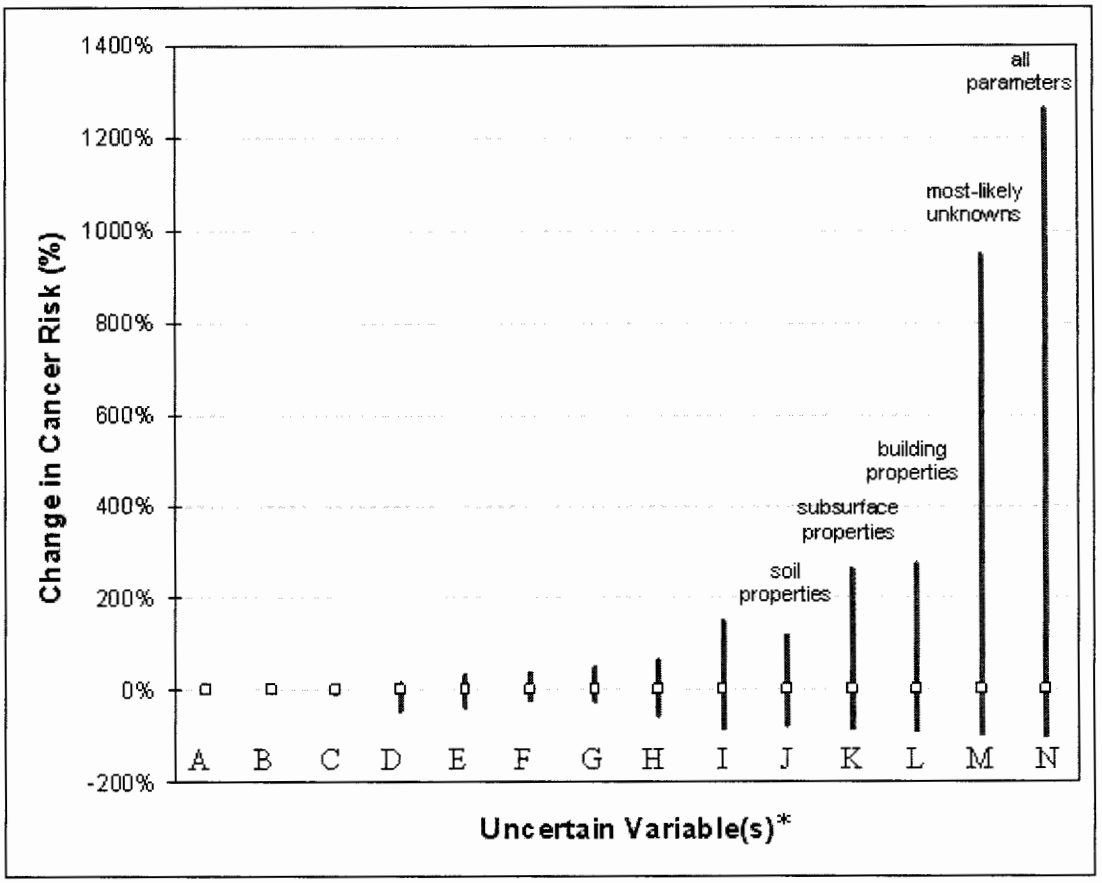

Figure 12 Results from uncertainty analysis using OSWER default as the baseline case and +/- 25% parameter ranges.

Table 10 Single Parameters used for One-At-A-Time (OAT) uncertainty assessment of the example problem.

Code	Parameter Groups	Parameters	Change in Risk Given Uncertainty in Results	
			Decreased Risk	Increased Risk
A	Single	Floor-Wall Crack Width	0.0%	0.0%
B	Single	Temperature	0.0%	0.0%
C	Single	Soil Residual Water Content	-7.6%	7.8%
D	Single	Soil Gas Flow Rate	-44.1%	11.0%
E	Single	Porosity	-34.9%	33.1%
F	Single	Sample Depth	-20.5%	34.7%
G	Single	Mixing Height	-25.0%	50.1%
H	Single	Water Content	-53.8%	65.2%
I	Single	Air Exchange Rate	-83.3%	150.0%

Table 11 Parameter groups for synergistic uncertainty analysis.

Code	Parameter Groups	Parameters	Change in Risk Given Uncertainty in Results	
			Decreased Risk	Increased Risk
J	Soil Properties	Porosity Residual Water Content Water Content	-74.7%	117.9%
K	Subsurface Properties	Sample Depth Porosity Residual Water Content Water Content Soil Gas Flow Rate	-83.2%	262.3%
L	Building Properties	Mixing Height Floor-Wall Crack Width Air Exchange Rate	-87.5%	274.9
M	Least-known Parameters	Mixing Height Floor-Wall Crack Width Air Exchange Rate Porosity Residual Water Content Water Content Soil Gas Flow Rate	-97.4%	941.6%
N	All Parameters	Building Mixing Height Floor-Wall Crack Width Air Exchange Rate Sample Depth Porosity Residual Water Content Water Content Soil Gas Flow Rate Temperature	-97.9%	1258.4%

Most of the ranges presented in Figure 12 are skewed toward increased risk. Examination of the parameter ranges (Table 8), however, shows that most of the parameter ranges were symmetric about the default value. Thus, the input ranges do not suffice to explain the skew of the results. Figure 13 shows the numerator, denominator and value of the JEM α as a function of the air exchange rate. The highest α, and therefore highest apparent risk, occurred for the lowest value of the air exchange rate (0.1 hr^{-1}). This value is proportionately higher than the lower apparent risk at the high end of the air exchange rate range (1.5 hr^{-1}). Thus, the results are skewed toward higher apparent risk. When the JEM α is deconstructed into its numerator and denominator, it is clear that the denominator is insensitive to air exchange rate and that the pattern in the α values is due to the numerator.

The numerator of the JEM α contains the term:

$$A \exp(B)$$

where

$$A \propto \frac{1}{Q_B} = \frac{1}{E_B V_B}$$

and B does not depend on the air exchange rate. Since the A term is inversely proportional to the air exchange rate, E_B, the steep drop in the JEM α and its numerator result from hyperbolic function behavior evident in both the formula and the Figure 13 results.

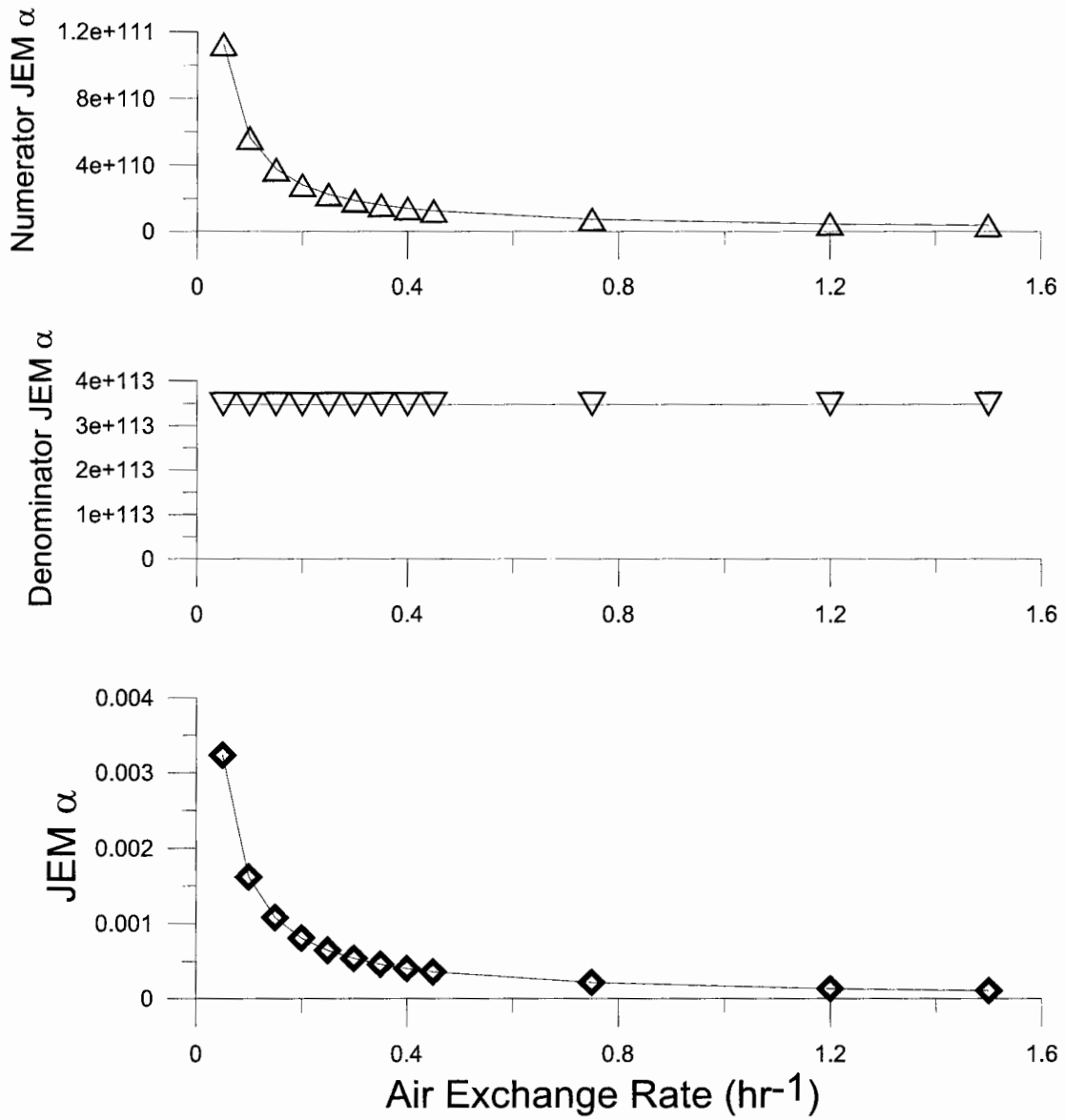

Figure 13 The numerator, denominator and calculated JEM alpha as function of the air exchange rate.

Table 12 The impact of variation in air exchange rate on results.

Air Exchange Rate (hr^{-1})	JEM α	Single Parameter Change in Apparent Risk
0.1	1.62×10^{-3}	+150.0%
0.25 (default value)	6.28×10^{-4}	0.0%
1.5	1.08×10^{-4}	-83.3%

The response of the JEM to reduced uncertainty ranges was evaluated by running sets of simulations where all parameters were assumed uncertain, but where the ranges were reduced from one simulation to the next. The response of the model was expressed as a function of normalized inputs. Input variability was expressed by

$$x' = \sum \frac{\Delta x}{x_d}$$

where Δx is the range of input values and x_d is the default or median value. Similarly, the results were represented by

$$y' = \frac{\Delta y}{y_d}$$

where Δy is the range of outputs (here JEM α) and y_d is value produced by the simulation using the default or median values.[3] Figure 14 shows the response of the model to variation in the uncertainty in each of the model inputs. The sample problem presented in this section is plotted to the far right hand side of the figure (x' of 16). Beginning with the sample problem, the variability in each parameter was reduced by a fixed percentage until the there is no variability left. At this point, all parameters are certain as there is no range in either input or output. The plot shows that as the uncertainty in the model inputs increases, there is a proportionately greater increase in the uncertainty in the output (α).

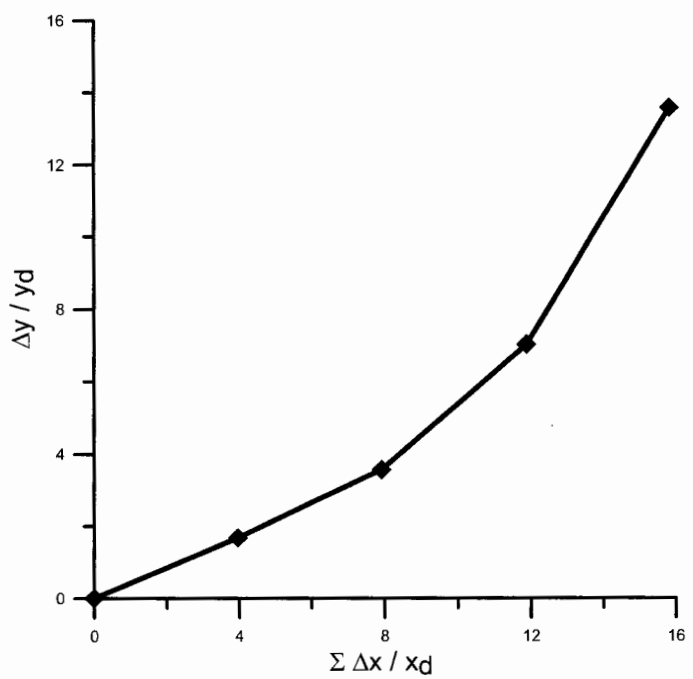

Figure 14 Response of the model to reduction in uncertainty in all inputs.

[3] y' could, of course, be generalized to include more than one output by including a summation.

Conversely, the uncertainty in the model output could be reduced one parameter at a time by reducing input parameter uncertainty. The one-at-a-time uncertainty analysis results presented in Table 10, indicate that individually, the air exchange rate, water content, mixing height, source depth, and porosity have the greatest impact on the model output uncertainty. Of these increasing the air exchange rate increased risk by the most, 150%, when treated as the only uncertain parameter. Eliminating its uncertainty while still acknowledging uncertainty in all other parameters, reduced the apparent increased cancer risk from 1258.4% to 443.4% (Figure 15 and Table 13). Fixing the value of each parameters in turn reduced the apparent increased cancer risk due to uncertainty in model inputs to 20.6%.

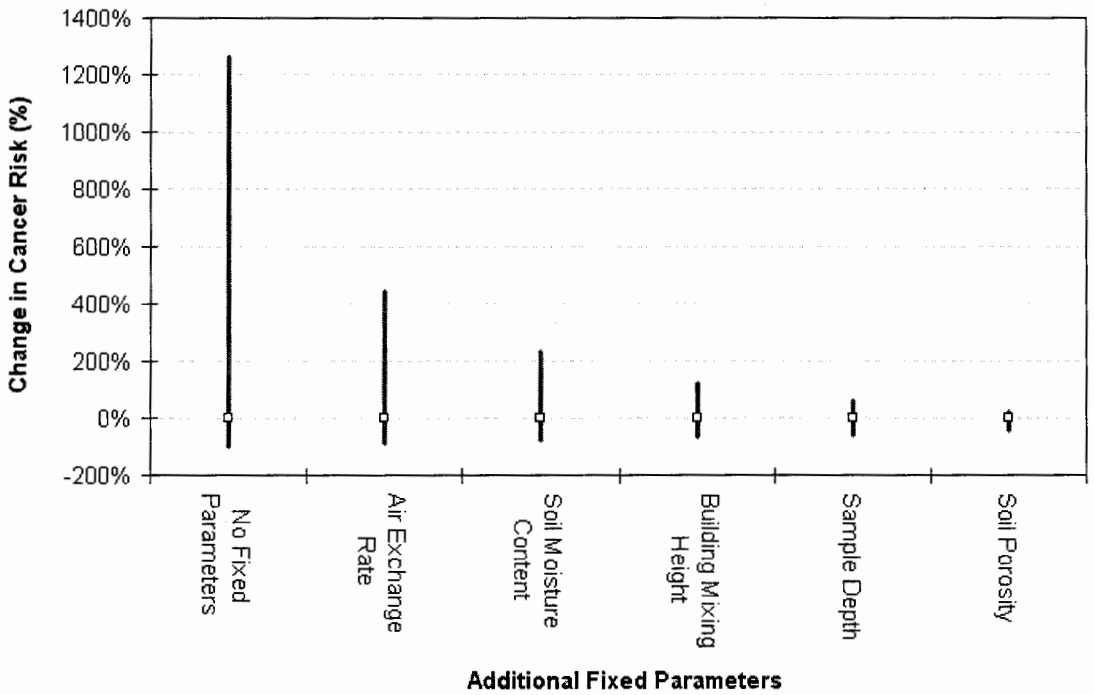

Figure 15 Reduction in model uncertainty by fixing one parameter at a time.

Table 13 Changes in apparent risk due to sequential fixing of uncertain parameters.

Additional Fixed Parameter	Cancer Risk			Change in Risk Given Uncertainty in Results	
	Low	OSWER Default Case	High	Decrease	Increase
None	2.1×10^{-8}	1.0×10^{-6}	1.6×10^{-5}	-97.9%	1258.4%
Air Exchange Rate	1.3×10^{-7}	1.0×10^{-6}	5.4×10^{-6}	-87.4%	443.4%
Water Content	2.5×10^{-7}	1.0×10^{-6}	3.4×10^{-6}	-75.1%	235.1%
Mixing Height	3.3×10^{-7}	1.0×10^{-6}	2.2×10^{-6}	-66.8%	123.4%
Source Depth	4.0×10^{-7}	1.0×10^{-6}	1.6×10^{-6}	-60.3%	63.2%
Porosity	5.3×10^{-7}	1.0×10^{-6}	1.2×10^{-6}	-46.6%	20.6%

8 Conclusions

Many of the input parameters of the Johnson and Ettinger model have significant associated degrees of uncertainty, particularly when the model is used in a generic sense where parameters are not measured on a site-specific basis nor calibrated to measured indoor air concentrations.

OAT Results: One-at-a-time (OAT) uncertainty analysis, as would be typically performed due to the difficulties of evaluating all possibilities, gives a rough guide to the model output uncertainty associated with any single parameter. A ranking can be made from OAT results of the uncertainties associated with each parameter. The response of the model to variation in parameters is, however, nonlinear and varies over its range of values (illustrated by Figure 13). The example problem showed that the model was insensitive to the floor-wall crack width and the temperature. Conversely the air exchange rate was the single most sensitive input parameter of the model.

Synergistic Effects: When many or all parameters of the model are considered uncertain, synergistic effects create greater uncertainty in the model results than when only one parameter is varied. The example given showed an increase in cancer risk of almost 1300% over the default case. Uncertainty in the input parameters generates apparent cancer risk that is due only to the parameter uncertainty. That is, the additional risk is not due to any "real" factor operating in the field. Varying some of these estimates by fairly modest amounts caused the estimated risk to increase (or decrease) by a dramatic amount.

The JEM equation is nonlinear and its response to parameter variation is decidedly nonlinear also. Accounting for input parameter uncertainties resulted in apparent cancer risks that were usually skewed toward increased risks. In the case of the air exchange, rate this behavior was shown to be due to the model equation structure itself: the denominator is insensitive, while the numerator was inversely proportional to this parameter. This alone generated the increased apparent cancer risk in the model results.

Use of the JEM in screening of sites for vapor intrusion should account for input parameter uncertainty. Simulation using default parameters, generally picked at the midpoint of their possible ranges, does not correctly represent the possible model outputs. Standard approaches for application of models as presented in Section 3, indicate that a necessary step in model application is calibration of results to field data. In situations where the model is not calibrated to measured indoor air data, and subsequently demonstrated to have predictive capability, the input parameters cannot be assured to represent the properties of the flow system. By performing an uncertainty analysis, as presented here, a range of potential outputs is revealed to the decision maker. An informed choice can then be made concerning the risks simulated by the model.

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9 Appendix

The uncertainty analysis for the Johnson and Ettinger (JEM) model was performed using a subset of the model input parameters that were presumed uncertain. These parameters were described by their range only. This approach was based on two assumptions. First is that the parameters were uniformly distributed. For many of the parameters very little data exist on their values, so that distributions and correlations are similarly unknown. The second assumption is that the extremes (maximum and minimum) of the simulations occur at the endpoints. This was likely to be the case as the α function is composed of exponentials. The result was shown empirically when simulations with intermediate parameter values always showed their extremes to lie at the endpoints of the parameter ranges. Further, this observation agrees with figures presented in Johnson (2002) over a range of A, B and C values.

The A, B, and C variables encapsulate the basic JEM input parameters into three dimensionless groups. These dimensionless groups could possibly form the basis for an uncertainty analysis. Such an analysis would require far fewer simulations (8 versus 512 or more, see Table 1) because there would be only three variable parameters.

Use of the dimensionless parameters has the promise of allowing simple definition of generic worst cases. If one could be assured that the extreme values of model output always occurred with extreme values of the inputs (A, B, and C), then case-specific uncertainty analysis is unnecessary. Because of linkages between the parameters, however, a consistent choice of the minimum and maximum of A and B can not be made. Table 14 shows the required maximum or minimum values of the basic parameter values required to give maximum A, B and C values. Two inconsistencies exist for selecting the maximum parameters:

- maximizing A requires maximum A_B; maximum B requires minimum A_B
- maximizing A requires maximum D_T^{eff}; maximum B requires minimum D_C^{eff}

The converses apply for selecting the minimums of A and B. In all cases the dependencies are somewhat arbitrary and could be broken if the area of the crack was made independent of the foundation area, and if the diffusion coefficients were not arbitrarily set equal to each other. At some level the parameters would necessarily remain linked: the area of the cracks cannot approach the area of the foundation, and some basic parameter values (i.e., the air and water phase diffusion coefficients) are the same for either subsurface or crack diffusion coefficients. Relaxing these assumptions to the maximum allowable, would enable the search for extreme values of the JEM, using the using the maximum and minimum of the parameter values given in Table 14.

Table 14 Relationships between basic input parameters and the maximum values of the dimensionless groups A, B, and C. (The minimum values of these parameters occur with the opposite choices of the basic input parameters.)

Maximum value of the dimensionless parameter:	***occurs with* maximum value of:**	***and* Minimum value of:**
A	D_T^{eff} A_B	Q_B L_T
B	Q_S L_C	D_C^{eff} η A_B
C	Q_S	Q_B