

ESTIMATING EXPOSURE AND UNCERTAINTY FOR VOLATILE CONTAMINANTS IN DRINKING WATER

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Estimating Exposure and Uncertainty for Volatile Contaminants in Drinking Water

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(ABSTRACT)

The EPA recently completed a major study to evaluate exposure and risk associated with a primary contaminant, radon and its progeny in drinking water (EPA, 1995). This work resulted in the development of a Monte Carlo Simulation model written in the programming language C. The model developed by the EPA has been used to estimate the cancer fatality risk from radon in water for exposed populations served by community ground water supplies, and to provide a quantitative analysis of the uncertainty associated with the calculations (EPA, 1995).

This research is a continuation of the study conducted by the EPA. In this project, a Monte Carlo computer model will be developed to evaluate the risk associated with exposure to volatile compounds in drinking water. The model will be based on a computer program (developed previously by the EPA) for estimating the risks associated with exposure to radon in drinking water. The model will be re-implemented in the form of a computer program written in C. The analysis for radon will be extended to include the entire range of contaminants found in drinking water supplies. The initial focus of the project has been on extending the analysis to cover the ingestion exposure pathway for volatile compounds, but ultimately the risk via ingestion and dermal sorption will also be evaluated.

The integrated model can estimate the risks associated with various levels of contaminants in drinking water and should prove valuable in establishing Maximum Contaminant Levels (MCLs) for the entire range of contaminants found in water supplies and generated in water treatment and distribution systems.

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1. INTRODUCTION AND OBJECTIVES

INTRODUCTION

The potential for the volatilization of contaminants from drinking water to indoor air was first identified by Prichard and Gesell (1981) in the context of radon. Those authors reported typical radon transfer efficiencies (the fraction released) for several types of household water use including showers, baths, toilets, and dishwashers. A subsequent study by Hess et al. (1982) showed a strong correlation between concentrations of radon in air and in household water supplies, further verifying this exposure pathway. A detailed review of the potential for drinking water to serve as a source of airborne radon was provided by Nazaroff et al. (1987).

Attention was subsequently focused on the release of volatile organic compounds from drinking water (Andelman, 1985a and 1985b). In the ensuing years Andelman and co-workers carried out several additional experimental and field studies further elucidating this exposure route, the results of which have been summarized in a detailed review by Andelman (1990). A number of studies have also been conducted by other research workers. Research carried out in showers included detailed experimental studies by Hodgson et al. (1988), Jo et al. (1990a, 1990b), McKone and Knezovich (1991), Tancrede et al. (1992), Giardino et al. (1992) and Giardino and Andelman (1996), as well as a field study by Stern and Andrews (1989). The work of Jo et al. (1990a, 1990b) also considered dermal sorption while the study of Giardino et al. (1992) focused on the role of the drop-size distribution generated by the shower head. Related theoretical assessments were made by McKone (1987), Little (1992), and Wilkes et al. (1992, 1996). Volatilization from showers has been studied most extensively, primarily because it has been shown to represent the most significant contributor of the various water use scenarios (McKone, 1987). More recently, however, experimental research has been reported on washing machines (Shepherd et al. 1994) and kitchen sinks (Howard and Corsi 1995).

The EPA has recently completed a major study to evaluate the risks associated with exposure to radon in drinking water (EPA, 1995). This work led to the development of a Monte Carlo computer model written in the programming language C. Two versions of the radon exposure model were implemented; a simple one-compartment model as well as a three-compartment model based on that developed by McKone (1987). These models have been used to estimate the cancer fatality risk from radon in water for exposed populations served by community ground water supplies, and to provide a quantitative analysis of the uncertainty

associated with the calculations (EPA, 1995). However, public health agencies frequently get inquiries as to the safe level of other drinking water contaminants. These include compounds that can cause population exposure via ingestion, inhalation, and dermal sorption. There is now a need to extend the analysis for radon to include the entire range of contaminants found in drinking water supplies. The initial focus will be on extending the analysis to cover the ingestion exposure pathway for volatile compounds, but ultimately the risk via ingestion and dermal sorption will also be evaluated.

The previously developed model was based on an estimated transfer efficiency (essentially the fraction released while the water is being used) and used radon as a benchmark volatile compound. That approach is acceptable provided radon is the only contaminant being examined. However, when estimating inhalation exposure to a range of volatile compounds, the transfer efficiency becomes a function of the volatility of the particular compound (expressed by the Henry's Law constant), especially for those compounds of low volatility. If this is not correctly accounted for, the predicted inhalation exposure will be substantially over-estimated (Little, 1992).

It will be possible to use the fully developed model to estimate the risks associated with various levels of contaminants in drinking water. The model should prove valuable in establishing Maximum Contaminant Levels (MCLs) for the entire range of contaminants found in water supplies and generated in water treatment and distribution systems. It should also be useful, in conjunction with appropriate economic models or analyses, for evaluating the costs associated with achieving the desired MCLs.

OBJECTIVES

In this project, a Monte Carlo computer model will be developed to evaluate the risk associated with exposure to volatile compounds in drinking water. The model will be based on a computer program (developed previously by the EPA) for estimating the risks associated with exposure to radon in drinking water. Specific objectives are to:

- Examine and re-assemble the exposure model previously developed by the EPA;
- Re-implement the model in the form of a computer program written in C;
- Verify the computer program for accuracy by;

- developing an analytical solution to the three-compartment model and comparing numerical output from the program with the analytical solutions,
 - checking the exposure calculations by comparing the output from the computer program to a spreadsheet calculation,
 - comparing the inversion of the probability distribution functions in the computer program against standard spreadsheet functions.
- Compare exposure and risk estimates obtained with new program with those obtained previously by the EPA;
 - Extend the theoretical basis of the inhalation exposure model to include the full range of VOCs;
 - Evaluate effect of varying volatility on inhalation exposure.

At the completion of this project, a computer model will be available that can be used to estimate the risks and associated uncertainties of exposure through inhalation to both radon and the full range of volatile compounds found in drinking water. The computer model will be developed in such a way as to facilitate the possible expansion to include estimation of the risks associated with exposure to contaminants in drinking water via ingestion and dermal sorption. The significance of the overall project is that it will:

- provide research workers and public health officials with a tool to estimate the risks arising through exposure to radon as well as the full range of volatile contaminants in drinking water;
- enable the uncertainties associated with the risk estimates to be quantified;
- base the prediction of the rate of transfer of volatile compounds from drinking water to indoor air on fundamental mass-transfer principles;
- facilitate further refinements to the risk estimation procedure by allowing easy incorporation of additional data as it becomes available;
- lay the foundation for extending the model to include the risks associated with exposure to contaminants in drinking water via ingestion and dermal sorption.

2. LITERATURE REVIEW

Drinking water contaminants

Potable water is in essence defined as "water free from disease-causing organisms, and free from minerals and organic substances that may produce adverse physiological effects and aesthetically pleasing with respect to turbidity, color, taste and odor" (U.S. Drinking Water Regulations, 1997). In the past, water treatment plants have been more concerned with the treatment of biological contaminants in drinking water. Biological contaminants constitute a majority of the regulated contaminants in the Drinking Water Regulations (1997). However, there is now a growing awareness that a wide range of chemicals can occur in the home environment and cause a continuous though low-level human exposure (Andelman, 1985 a).

Field studies conducted by Andelman (1985 a) in small households indicated that indoor air concentrations of trichloroethylene (TCE) could be substantial when TCE-contaminated water was used for domestic purposes. Tancrede et al. (1992) found tap water to be a potential source of VOCs including chloroform (CHCl_3), carbon tetrachloride (CCl_4), trichloroethylene (TCE) and tetrachloroethylene (TTCE). They presented a method to analyze simultaneously several VOCs in the shower. Lindstrom and Pleil (1996) also found VOCs in a large number of public water supplies serving community households with drinking water. Chlorine disinfection processes used to treat the water in such supplies produced chloroform and other trihalomethanes. Hence, a need to identify and consider volatile chemical contaminants in drinking water in the development of regulations was realized which could limit the possible adverse health impacts from the use of contaminated potable water (Andelman, 1985 a).

Exposure and Risk Assessment

Traditionally, regulation and concern about exposures to potentially toxic chemicals and other constituents of potable water supplies have focused on the ingestion pathway. However, research has shown that inhalation exposures resulting from volatilization of VOCs during other water uses, such as showering, can lead to overall doses as large as or larger than those which occur from drinking the water (Andelman, 1990; Wilkes et al., 1992). Andelman (1990) suggested that it might be prudent to consider these routes in evaluating total exposure. He also felt that additional research might be required to quantify these other exposure routes more

accurately. Foster and Chrostowski (1987) developed models for estimating exposure through the inhalation and dermal sorption pathways.

Studies conducted by Jo et al. (1990 a) revealed that skin absorption could be a significant pathway to exposure since the entire body is exposed to chemical contaminants and organic compounds that are volatilized from water while showering. Calculations of dermal sorption during showering based on limited data on the permeability of chloroform through the skin indicated that dermal exposure should account for between 10% and 25% of the dose from inhalation exposure. (Jo et al., 1990 a). The authors showed that the risk associated with a single shower (through inhalation and dermal adsorption) may be as much as 10 times the risk estimated from daily ingestion of tap water.

Wilkes et al. (1992) showed that the physical characteristics of volatilization and indoor pollutant transport, as well as human activity and locations of sources are essential elements of an indoor air quality model. The authors recognized the important characteristics of the physical environment that must be considered to be the contaminant generation and chemistry and the transport kinetics. They also proposed that the model include characteristics of the persons being modeled, namely the water-use activities that lead to exposure, the location of the occupants and their exposure characteristics (ex. breathing rates). By correlating these physical and personal aspects, Wilkes et al. estimated the subject's inhalation exposures from pollutant emissions and ambient air concentrations.

Georgopoulos et al. (1997) formulated a conceptual and theoretical framework for integration of environmental fate and transport models with mechanistic models of physiological pharmacokinetics and models of population dynamics. The framework developed by the authors could be used to study total exposure and biologically effective dose and would improve the quality and consistency of the exposure assessment process (Georgopoulos et al., 1997).

Risk has been defined as the probability of incurring a particular class of disease(s) caused by the environmental agent(s) under consideration (Bogen and Spear, 1987). Bogen and Spear (1997) classified risk as "individual risk" which referred to a set of independent risks faced by one or more individuals in an exposed population, and as "population risk" which referred to the probability distribution of the actual health impacts generated by a set of individual risks.

In the last decade, increased emphasis has been placed on quantifying the variability of total human exposures to environmental pollutants, associated health risks, and uncertainty about these estimates. Air pollutant exposure models such as simulation of Hazardous Air Pollutant Exposures (SHAPE) and National Exposure Model (NEM) have been developed that have used variable concentrations and time-activity patterns to simulate differences of personal air exposures (MacIntosh, et al., 1995). The EPA has been concerned with evaluating overall exposure to common chemical contaminants in drinking water and quantifying risk associated with the different exposure pathways (EPA, 1995).

Radon and progeny exposure

Models describing the transfer of radon from water to indoor air were first developed and tested by Pritchard and Gesell (1981). The volume of the houses, the occupancy rates, air exchange rates were identified as a few important variables in the estimation of exposure. The authors experimentally measured typical radon transfer efficiencies for showers, baths, toilets, and dishwashers.

Hess et al. (1982) found that the radon levels measured in air were significantly correlated with concentrations of radon in household water supplies. They measured high concentration levels of radon (22,000 pCi/L) in the wells in the granite regions of Maine. The conditions indicated a possibility for strong emission of radon from the soil and rocks surrounding the foundations of houses, in the form of soil gas. The authors reported that high inputs of radon might occur in houses with use of water from wells with high radon content. (Hess et al., 1982).

Nazaroff et al. (1986) reported that the predominant source of ^{222}Rn in U.S. houses appeared to be the soil adjacent to the foundation. According to the authors, the other major sources were potable water and building materials which could be dominant sources in some cases and occasionally contribute significantly to indoor concentrations (Nazaroff et al., 1987). Nazaroff and Nero (1988) reported that the daughter products of radon contributed considerably to the exposure and risk attributed to radon.

Uncertainty analysis

In environmental risk assessment, there are generally three broad sources of uncertainty - scenario uncertainty, model uncertainty and variable uncertainty (EPA, 1995). Scenario uncertainty is described as "the basic appropriateness of the facts, and the inferences used to select the exposure scenarios of concern." Model uncertainty is explained as "the uncertainty and potential for error introduced by a mathematical model's simplified representation of an exposure scenario or a dose-response relationship." Variable uncertainty is characterized as "the inability to determine accurate values for the variables in an exposure or risk model, due to factors such as measurement error, systematic error or random error."

Variable uncertainty is classified into two types. The first type, natural variability is due to the heterogeneity among different members of a set population. Any variable is hence presented in the form of a range of values in the terms of statistics such as averages, medians, and percentiles (EPA, 1995). The second type of variable uncertainty results from lack of knowledge about the parameters of the variable in the model. Gathering more and better data can reduce this type of uncertainty (EPA, 1995).

Due to the inherent natural variability, the variables used in the exposure model can be defined by means of PDFs. A PDF is a mathematical formula that describes how frequently the variable will have any specific value or range of values. There are various types of PDFs such as normal, lognormal, uniform, triangular, and beta distributions. Each PDF is completely specified by one or more parameters. For example, normal and lognormal PDFs are specified by the parameters μ and σ . For a normal distribution, μ is estimated from the mean of a sample drawn from the population, while σ is estimated from the sample standard deviation. For a uniform distribution, the parameters are the minimum and the maximum values assumed by the random variate.

The parameters of a PDF are typically estimated from a limited set of observations. The data may not be representative of the entire population and sample statistics may not be accurate estimates of the true values of the population parameters. This leads to uncertainty and variability in the estimation. Hence, two types of PDFs, one that describes variability among different members of a population PDF_v and another that describes the uncertainty about a parameter PDF_u , are used to define the population.

Often in risk assessment, point estimates of risk are determined by assigning a single value to each variable. Sometimes in view of conservatism, each variable is assigned a "high end" value, the resultant value of risk being unrealistic. Hence, explicit calculation of uncertainty in exposure and risk estimates is necessary for understanding the range and likelihood of possible outcomes (Bogen and Spear, 1987). An alternative solution is the Monte Carlo simulation, which is a computerized technique of drawing repeated "samples" from a plausible set of values for each variable, and using these values to calculate risk. The Monte Carlo approach incorporates the ranges or distributions of data associated with the risk and exposure model. Because a computer can evaluate thousands of combinations of exposure variables, the probability of occurrence of any of these combinations can be easily ranked and the resultant risk can be expressed as a probability distribution, rather than a single, isolated point estimate.

The Monte Carlo simulation has a two-dimensional or nested approach. As discussed earlier, the variables in the Three-Compartment Model are characterized by PDFs. In the outer loop of the Monte Carlo simulation, the uncertain parameters (PDF_u) for the variables are evaluated and in the inner loop the actual value of the variables (PDF_v) is obtained. As different values are realized for the parameters in the outer loop, this results in a different shape and location of the distribution each time the loop is executed (EPA, 1995).

Extension to range of VOCs

Andelman (1985 a, 1985 b) recognized the growing awareness of the presence of volatile organic compounds (VOCs) in potable water and developed models to calculate exposure to trichloroethylene (TCE) through inhalation.

McKone (1987) developed a three-compartment model to simulate the 24 hour concentration profile within the shower, bathroom and remainder household volumes of a dwelling. He used this model to estimate exposures for seven VOCs – chloroform, ethylene dibromide, dibromochloropropane, methylchloroform, perchloroethylene, trichloroethylene and carbon tetrachloride and compared estimated values with measured values for chloroform.

Foster and Chrostowski (1987) evaluated inhalation exposures to VOCs by estimating the rate of VOC release from water into air, the buildup and decay of VOCs in shower room air. Andelman (1990) noted that measurements had been made indicating the presence of VOCs in

indoor air following the use of contaminated water. Studies on volatilization of VOCs from indoor water uses showed that often 50% or more of common contaminants of water supplies, such as chloroform and trichloroethylene (TCE), volatilize and constitute inhalation exposures (Andelman, 1990). Human exposures to these VOCs were thought to lead to health effects ranging from minor effects such as fatigue to more serious effects such as cancer (Wilkes et al., 1992).

Wilkes et al. (1990) developed a predictive mass balance model which considered the physical processes of chemical volatilization from water use in the home, in order to address the issue of whether residents should be advised to restrict their use of water for other non-consumptive purposes. This Model for Analysis of Volatiles and Residential Indoor-Air Quality (MAVRIQ), considered a building as a collection of well-mixed compartments interconnected by flow elements and evaluated the volatilization of VOCs from showers based on modifications of the two-film theory (Wilkes et al., 1990).

Little (1992) applied the two-resistance theory to the transfer of volatile contaminants from shower water to indoor air by means of two transient mass balance models. He used mass transfer coefficients to evaluate inhalation exposures to a range of volatiles.

3. DESCRIPTION OF EPA MODEL

This section describes the inhalation exposure model developed previously by the EPA (EPA, 1995). The objective is to replicate, as far as possible, the exact computational procedure used in the EPA model. The model, which evaluates exposure to radon gas and progeny, was based upon a similar model proposed by McKone to predict the transfer and distribution of volatile compounds inside a house (McKone, 1987). In this model, a household is assumed to consist of three compartments: shower, bathroom, and main house, as shown in Figure 1. Volatile compounds are released from water into air, depending on the water use patterns within each compartment. Air is distributed throughout the house and to the outdoors by ventilation. A transient mass balance relates the rate of change of concentration in each compartment to the different mass flow pathways, resulting in a set of simultaneous differential equations. Once solved, the profile of concentration versus time in each compartment, together with a specified human activity pattern, is used to calculate the individual exposure and associated cancer risk (EPA, 1995).

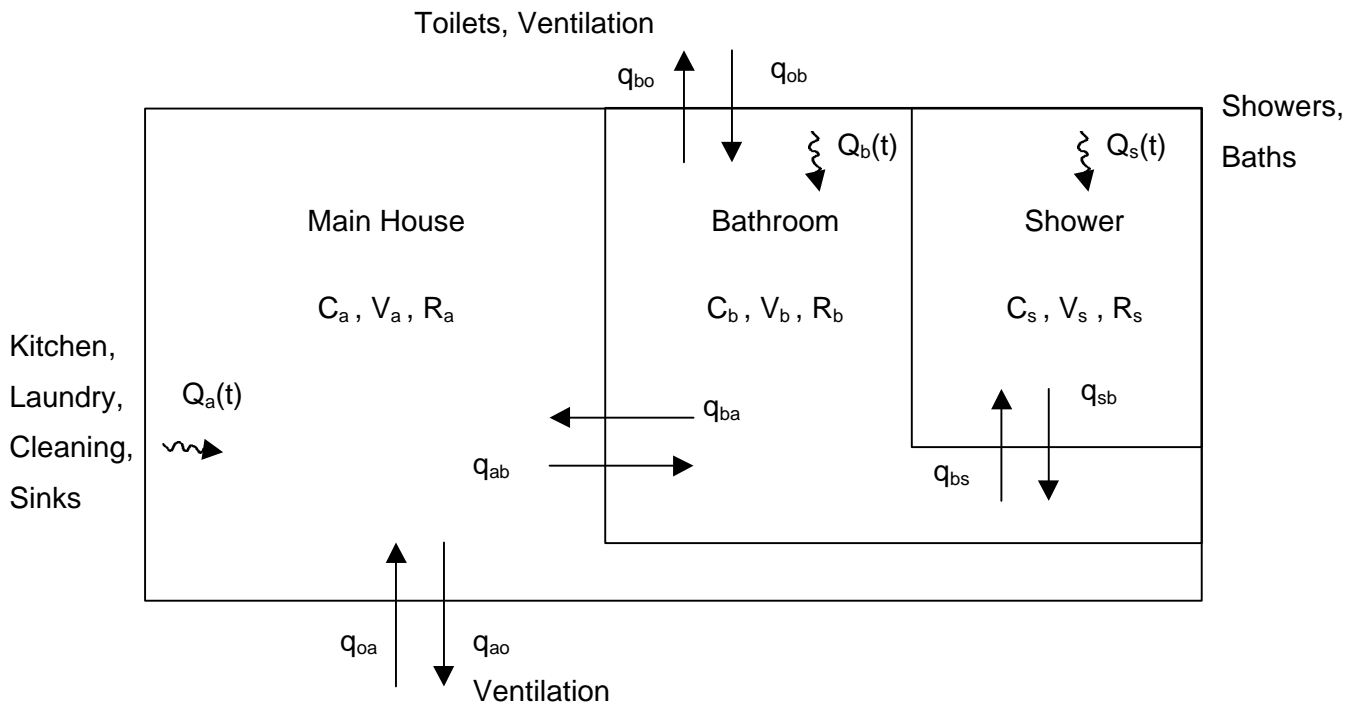


Figure 1: Three-Compartment Model (McKone, 1987)

3.1. Radon and Progeny

Radon is a highly volatile contaminant, which may be transferred from drinking water to indoor air. Once air-borne, radon decays to form radionuclides that are chemically active, although relatively short-lived. The following equation illustrates the radon decay chain and the daughter species formed. Table 1 gives the first order decay constants in terms of half-lives. It is seen that Po^{214} has a very short half-life [1.64 μ s] and its concentration does not contribute significantly to exposure or risk and hence this specific progeny was not considered in the EPA model (Nazaroff and Nero, 1988).

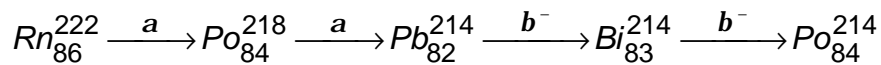


Table 1: Decay Sequence for Radon

Start Isotope	Mode of Decay	End Isotope	Half Life
Radon-222	Alpha	Polonium-218	3.823 days
Polonium-218	Alpha	Lead-214	3.05 mins
Lead-214	Beta	Bismuth-214	26.8 mins
Bismuth-214	Beta	Polonium-214 [†]	19.7 mins

Once created by decay of radon, the progeny may be removed by:

- ♦ attachment to an airborne particle,
- ♦ deposition on indoor surfaces,
- ♦ ventilation,
- ♦ further radioactive decay.

Studies reveal that the risk due to inhalation of radon progeny may be more substantial than that due to radon alone (EPA, 1995). Hence, the exposure of chief concern being to radon progeny, the basic model developed by McKone was modified by the EPA to account for the formation and loss of radon progeny by radioactive decay and for the loss of progeny due to deposition. The following sections present the mathematical details of this model, with many quoted directly from the previous published EPA Report (EPA, 1995).

3.2. Three-Compartment Model

In general the mass balance for compartment i is given (EPA, 1995) by,

$$V_i \frac{dC_i}{dt} = \sum \text{Influx}_i - \sum \text{Efflux}_i$$

where

- V_i = Volume of compartment i (L),
- C_i = Concentration in compartment i (for radon, pCi/L),
- $\sum \text{Influx}_i$ = Sum of influxes into compartment i (pCi/min),
- $\sum \text{Efflux}_i$ = Sum of effluxes out of compartment i (pCi/min).

Influx processes include:

1. Release from water used in the room into air ($Q_i(t)$) (source term for radon).
2. Transport into the compartment by ventilation from other compartments (In_v).
3. Formation of daughter species by radioactive decay of parent radionuclide (In_r).

Efflux processes include:

1. Transport out of the compartment by ventilation (Out_v).
2. Loss by radioactive decay to form daughter species (Out_r).
3. Loss by deposition (Out_p) (only for radon progeny).

3.2.1. Release from Water

Using the transfer efficiency approach, the release of radon from water is estimated (EPA, 1995) as:

$$Q_i(t) = C_w WFR_i P_i$$

where

- $Q_i(t)$ = Release of radon from water in compartment i (pCi/min),
- C_w = Concentration of radon in water (pCi/L),
- WFR_i = Water flow rate in compartment i (L/min),
- P_i = Fractional release of radon from water to air in compartment i .

3.2.2. Water Usage Patterns

In a survey of houses in the United States, it was observed that water use in the different household compartments is intermittent, especially in the showers. Based on that survey, the following assumptions were made (EPA, 1995) regarding the usage of water in the three compartments:

Shower:

- The first shower is assumed to begin at 7.00 a.m.
- There are as many showers taken as the number of occupants of the house (N).
- Water flow rate in the shower is assumed to occur for T_s minutes for each of the N showers.
- The showers are separated by T_b minutes, which is the time spent in the bathroom following each shower.

Bathroom & Main House:

- Water flow in the bathroom is assumed to be continuous, 24 hours a day.
- Water flow in the main house is assumed to begin at 7.00 a.m. and end at 11.00 p.m.

In order to account for episodic water usage, the water flow rate in each compartment is expressed as a function of time (EPA, 1995):

$$WFR_i = AWU_i H(t, t_i^0, t_i^*)$$

where

- WFR_i = Water flow rate into compartment i (L/min),
- AWU_i = Average water usage in compartment i (L/min),
- $H(t, t_i^0, t_i^*)$ = A function whose value is 1 when t is between t_i^0 and t_i^* and zero otherwise,
- t_i^0 = Time when the water usage in the compartment starts (min),
- t_i^* = Time when the water usage in the compartment ends (min).

It is assumed that the main house is occupied from 7 a.m. to 11 p.m. During that time, H for the main house assumes a value of 1. Similarly, H for the bathroom assumes a value of 1 throughout the entire day.

3.2.3. Ventilation

The basic equations describing influx and efflux due to ventilation are:

$$In_{v,i} = \sum C_j q_{j,i}$$

$$Out_{v,i} = C_i \sum q_{i,j}$$

where

- $In_{v,i}$ = Influx into compartment i by air flow from other rooms (pCi/min),
- C_j = Concentration of radionuclide in the air of compartment j (pCi/L),
- $q_{j,i}$ = Air flow from compartment j into compartment i (L/min),
- $Out_{v,i}$ = Efflux from compartment i due to ventilation to other rooms or outdoors (pCi/min),
- C_i = Gaseous concentration of radionuclide in compartment i (pCi/L),
- $q_{i,j}$ = Air flow from compartment i into compartment j (L/min).

The q 's represent the air flow rates, with the subscripts identifying the source and the end point of transfer. For example,

- q_{sb} = Air flow rate between shower, s, bathroom, b,
- q_{ba} = Air flow rate between bathroom, b, main house, a,
- q_{ao} = Air flow rate between main house, a, outside, o.

These inter-compartmental air flow rates are derived from data on the compartmental residence times (R, min) and volumes (V, L) as:

$$q = V/R$$

In the model developed by McKone, the air flux terms were considered to be constant over time. In the EPA model, these exchange rates were modified to evaluate ventilation of the bathroom under three different conditions (EPA, 1995).

It is assumed that the bathroom is unoccupied with the door open and the bathroom exhaust fan off (Case 1) during the major part of the day. When the bathroom or shower is occupied, it is assumed that the bathroom door is closed resulting in a change in the air residence time in the bathroom from R_{b1} (door open) to R_{b2} (door closed). Further, it is assumed that the occupant may either leave the bathroom exhaust fan off (Case 2) or may turn the fan on (Case 3).

In Case 3, it is assumed that the exhaust fan rate (EXFR) generates a negative pressure in the bathroom relative to the rest of the house, and that air flow from the bathroom to the house (q_{ba}) is zero. Air flow rates can then be calculated as:

Table 2: Cases for Bathroom Ventilation

Air Flux Rates	Case 1 (Bathroom door open, fan off)	Case 2 (Bathroom door closed, fan off)	Case 3 (Bathroom door closed, fan on)
q_{sb}	V_s/R_s	V_s/R_s	V_s/R_s
q_{bs}	V_s/R_s	V_s/R_s	V_s/R_s
q_{bo}	0	0	EXFR
q_{ab}	V_b/R_{b1}	V_b/R_{b2}	EXFR
q_{ba}	V_b/R_{b1}	V_b/R_{b2}	0
q_{ao}	V_a/R_a	V_a/R_a	$V_a/R_a - \text{EXFR}$

3.2.4. Radioactive Formation and Decay

The rate of loss of each radioactive species due to decay is given by:

$$\text{Out}_{r,p} = -k_p C_p V_i$$

where

- $\text{Out}_{r,p}$ = Loss of parent radionuclide due to radioactive decay (pCi/min),
- k_p = Radioactive decay constant of parent radionuclide (1/min),
- C_p = Concentration of parent radionuclide in air (pCi/L),
- V_i = Volume of compartment I (L).

The rate of formation of daughter species due to radioactive decay of parent is:

$$In_{r,d} = k_d C_d V_i$$

where

- $In_{r,d}$ = Formation of daughter radionuclide due to radioactive decay of parent (pCi/min),
- k_d = Radioactive decay constant of parent radionuclide (1/min),
- C_d = Concentration of parent radionuclide in air (pCi/L),
- V_i = Volume of compartment i (L).

Table 3 summarizes the formation and decay terms for the different radionuclide species.

Table 3: Expressions for Formation and Decay of Radon and Progeny

Radionuclide	$In_{r,p}$ (pCi/min)	$Out_{r,d}$ (pCi/min)
Radon-222	-	$k_{Rn} C_{Rn} V$
Polonium-218	$k_{Po} C_{Rn} V$	$k_{Po} C_{Po} V$
Lead-214	$k_{Pb} C_{Po} V$	$k_{Pb} C_{Pb} V$
Bismuth-214	$k_{Bi} C_{Pb} V$	$k_{Bi} C_{Bi} V$

3.2.5. Loss Due to Deposition

The rate of loss of radon progeny due to deposition is highly variable, depending on the mixing rate within a room, the surface area of walls and furniture, and the concentration of dust and other aerosol particles in air. For a well-mixed room, the following equation gives a rough estimate of the deposition rate (EPA, 1995):

$$Out_p = C_i [f_u DV_u + (1 - f_u) DV_a] A_i$$

where

- C_i = Concentration of a radon daughter in compartment i (pCi/L),
- f_u = Fraction of progeny unattached to dust or aerosol (dimensionless),
- DV_u = Deposition velocity of unattached fraction (m/min),
- DV_a = Deposition velocity of attached fraction (m/min),

A_i = Surface area of compartment i (m^2).

The surface area of a compartment, including the four walls, ceiling and floor, can be estimated from the volume of the room by assuming the room is square in shape and has a height of 2.4 m (8 ft). Then the length of the edge of the compartment is:

$$Edge_i = \sqrt{\frac{V_i}{2.4}}$$

$$A_i = 2 \cdot Edge_i^2 + 4 \cdot (2.4 \cdot Edge_i)$$

where

$Edge_i$ = Length of edge of compartment i (m),

V_i = Volume of compartment i (m^3),

A_i = Surface area of compartment i (m^2).

Summary tables listing the influx and efflux terms for radon and progeny in the different compartments are included in Appendix A.

3.2.6. Calculation of Exposure

The basic outputs from the Three-Compartment Model are the concentrations of radon and progeny in each compartment as a function of time. In order to calculate exposure to radon and progeny, it is necessary to specify the location of an individual as a function of time during the day. This is done by defining "Occupancy Factors" to characterize the time a person spends away in the home (EPA, 1995). If a person is in a room, the occupancy factor for that room in that time interval is 1. If a person is absent from the room, the occupancy factor is 0.

3.2.6.1. Radon Gas Exposure

For radon, the incremental dose (ID) over the time interval from time t to t+1 is calculated from the concentration of radon in the three compartments as:

$$ID_{t,Rn} = [\overline{C}_{s,t} OF_{s,t} + \overline{C}_{b,t} OF_{b,t} + \overline{C}_{a,t} OF_{a,t}] \Delta t$$

where

\overline{C} = Average concentration between time t and t+1,

= $0.5(C_t + C_{t+1})$

The total dose over the entire day is then the sum of the incremental doses over each of the 1440 minutes of the day. The units for the total dose are (pCi/L)(min/day).

$$Dose = \int_0^{1440} ID_t$$

Then, the exposure to radon is expressed in pCi per year. This is calculated from the average daily dose (Dose/1440) as follows:

$$\frac{\text{pCi}}{\text{year}} = \left(\frac{\text{Dose}}{1440} \right) \left(\frac{\text{pCi}}{\text{L}} \right) \cdot \left(\frac{\text{min}}{\text{day}} \right) \cdot \text{Breathing Rate} \left(\frac{\text{L}}{\text{min}} \right) \cdot \frac{365 \text{ days}}{\text{yr}}$$

3.2.6.2. Radon Progeny Exposure

In each compartment, the concentration of radon progeny (expressed in WL) is calculated from the concentration of each radon daughter (expressed in pCi/L) as:

$$WL = 0.0010 \cdot C(^{218}\text{Po}) + 0.0052 \cdot C(^{214}\text{Pb}) + 0.0038 \cdot C(^{214}\text{Bi})$$

The incremental dose for progeny is then calculated similar to radon:

$$ID_{t,Pr og} = \left[\overline{WL}_{s,t} OF_{s,t} + \overline{WL}_{b,t} OF_{b,t} + \overline{WL}_{a,t} OF_{a,t} \right] \Delta t$$

where

$$\begin{aligned} \overline{WL} &= \text{Average progeny concentration between time } t \text{ and } t+1, \\ &= 0.5(WL_t + WL_{t+1}) \end{aligned}$$

The sum of incremental doses (WL.min/day) is obtained as above and is used to calculate exposure in WLM/year as follows:

$$\frac{\text{WLM}}{\text{year}} = (WL) \cdot \left(\frac{\text{min}}{\text{day}} \right) \cdot \frac{1 \text{ hr}}{60 \text{ min}} \cdot \frac{1 \text{ Working Month}}{172 \text{ hr}} \cdot \frac{365 \text{ days}}{\text{year}}$$

The units used to express concentrations and exposure to radon and progeny used in the earlier equations are explained below.

3.2.6.3. Units for Concentration and Exposure

The units for radioactive compounds are commonly expressed in terms of activity, where activity is defined as the actual rate at which atoms decay radioactively. The SI unit for activity is the Becquerel (Bq), which is equal to a decay rate of one per second (sec^{-1}). The traditional equivalent for this unit of measure is the Curie (Ci). Either of these two units is adequate for expressing activity and concentration of radon (Nazaroff and Nero, 1988).

For radon progeny, the traditional units for concentration are working-level (WL). Units of exposure are concentration multiplied by time, hence for progeny the units are WLM, where one WLM is the exposure to one WL for a period of one working month (172 hours). (EPA, 1995). Table 4 lists conversion factors between the SI and traditional units.

Table 4: SI and Equivalent Traditional Units for Concentration and Exposure[†]

Parameter, SI unit	Conversion for traditional unit
Activity, Bq	1 Ci = 3.7×10^{10} Bq, 1 pCi = 0.037 Bq
Concentration, Bq m^{-3}	1 pCi/L = 37 Bq m^{-3}
Concentration of progeny (of Rn^{222}), Bq m^{-3}	1 WL = 3740 Bq m^{-3}
Exposure to progeny, Bq m^{-3} y	1 WLM = 73.9 Bq m^{-3}

[†] (Nazaroff and Nero, 1988).

3.2.7. Calculation of Risk

The basic equations for calculating risk based on the EPA Model are (EPA, 1995):

- Unit Risk (UR): This is the risk of death from lung cancer (Icd) per person per pCi/L of radon in water:

$$\text{UR} = \text{UD} \cdot \text{RF}$$

- Individual Risk (IR): This is the risk of lung cancer death in an individual exposed to a specific radon concentration in water:

$$\text{IR} = \text{UR} \cdot \text{C}$$

- Population Risk (PR): This is the expected number of lung cancer fatalities per year occurring in the population of U.S. residents exposed to radon in water:

$$PR = IR_{\text{mean}} \cdot N$$

3.3. Uncertainty Analysis

The uncertainty analysis used in the EPA Model is based upon a two-dimensional or nested Monte-Carlo method. This explicitly accounts for the natural variability among different members of a population (variability) as well as the lack of knowledge about the value of a specific variable (uncertainty) (EPA, 1995). Hence, two types of PDFs are used to evaluate the model variables. A PDF_v describes the natural variability among different members of a population while a PDF_u describes the uncertainty about the parameters used to define the specific distributions. This is best explained using an example.

The exposure model requires a value for the volume of the bathroom (V_b). The natural variation in bathroom size has been found to follow a lognormal distribution. This distribution is therefore referred to as a variability distribution (PDF_v). The lognormal distribution is defined by two parameters, the mean (μ) and the standard deviation (σ). The Student's-t and the Chi-square distributions are used to describe the uncertainty associated with each of these parameters. Each of these distributions is therefore referred to as an uncertainty distribution (PDF_u). Figure 2 provides a flow chart explaining this two-dimensional Monte Carlo approach, using V_b as an example.

In the outer loop, the Student's-t and the Inverse chi-square PDF_us are used to evaluate μ and σ , respectively. In each of the inner loops a value of V_b is obtained from the lognormal distribution PDF_v using the values of μ and σ found in the outer loop. Over several inner loops, the value of the parameters μ and σ are maintained constant, but a different value of V_b is obtained each time the inner loop is executed. As different values are realized for the parameters in the outer loop, this results in a different shape and location of the variability distribution each time the outer loop is executed.

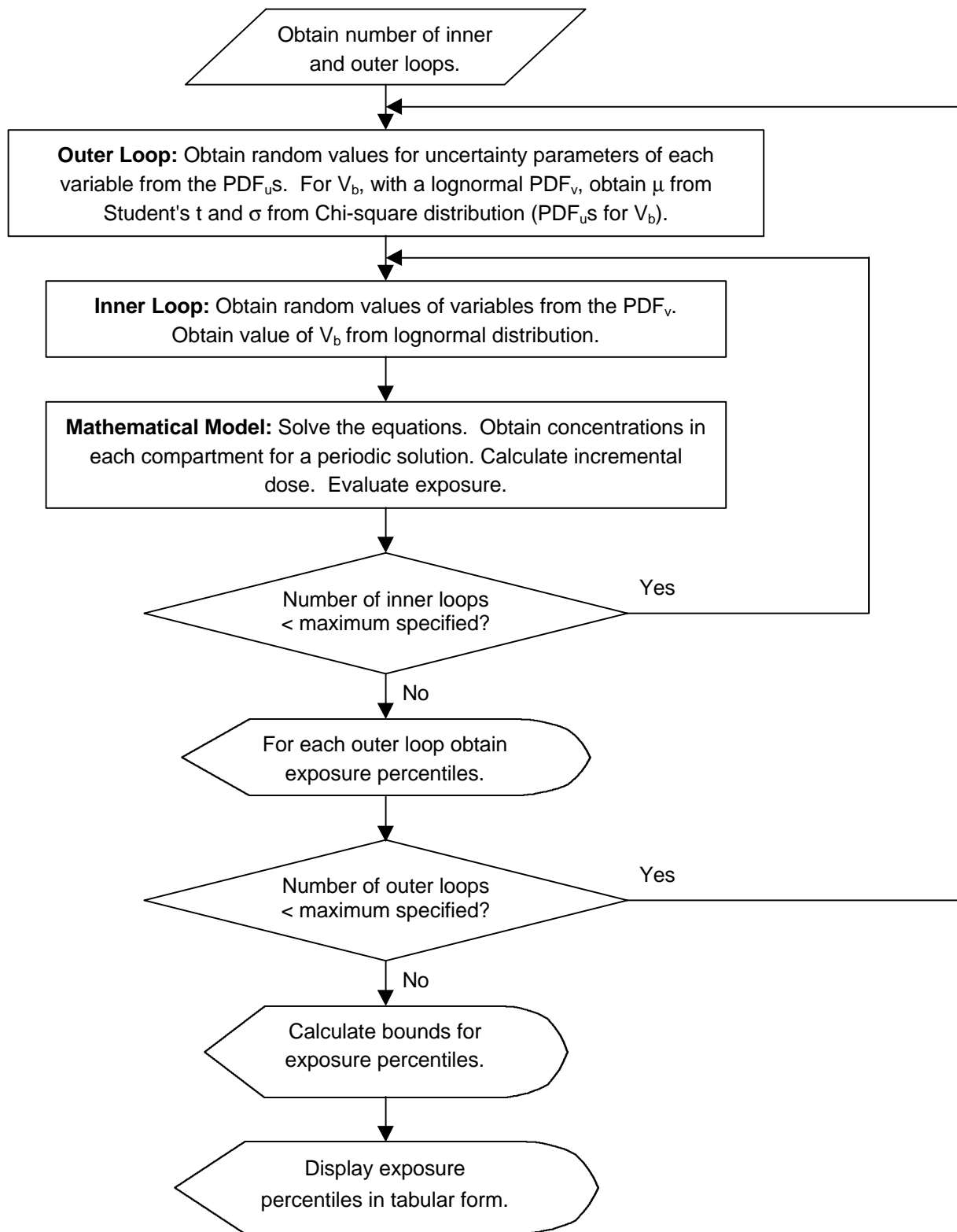


Figure 2: Flow Chart for Monte Carlo Simulation

3.4. Probability Distributions

Risk resulting from exposure to contaminants, through different pathways, is calculated by multiplying together a series of relevant terms. Each of these terms has uncertainty associated with them. The uncertainty is of two basic types: natural variability due to heterogeneity among different members of a set population and uncertainty resulting from lack of knowledge about the parameters of the variables of a model. Both types of uncertainty for a given variable can be described by probability density functions (PDFs). A PDF is a mathematical expression, denoted by $f(x)$, which gives the probability that a variable will have any specific range of values. There are many different types of PDFs like normal, lognormal, uniform, triangular, beta etc. Each PDF is specified by one or more parameters. For example, a mean and a standard deviation specify a normal PDF.

The parameters of a PDF are typically estimated from a limited set of observations. The data may not be representative of the entire population and the sample statistics may not be accurate estimates of the true values of the population parameters. This leads to uncertainty and variability in the estimation. Hence, two types of PDFs, one that describes variability among different members of the population PDF_v and another that describes the uncertainty about a parameter PDF_u are used to define a population.

In a graphical representation of a PDF (Figure 3), the y-axis indicates the probability density or relative frequency and the x-axis indicates a continuous scale for a measured variable. The total area under the PDF curve represents all the items in the original data. Hence, if an arbitrary vertical strip of a PDF curve is selected, the probability that the variable will have a value between the lower and upper bounds of the given strip is equal to the ratio of the area of the vertical strip to the total area of the curve.

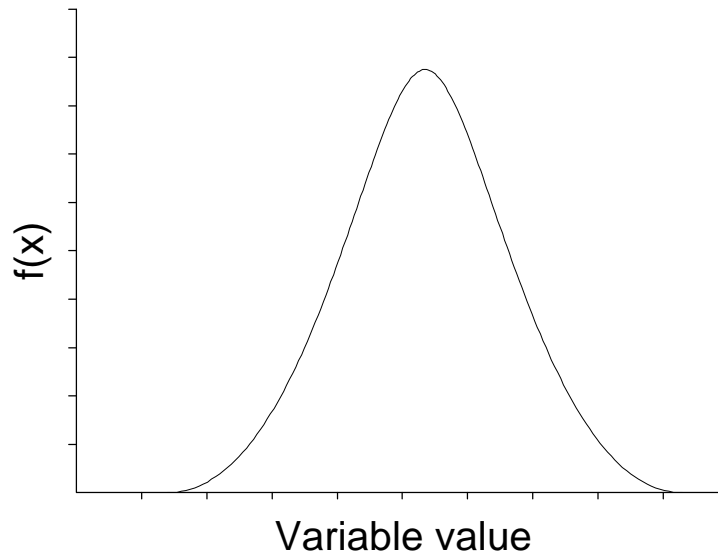


Figure 3: PDF Curve

A probability distribution can also be represented by Cumulative Distribution Function (CDF), $F(x)$. The CDF (Figure 4) is obtained by adding the individual increments of the PDF, i.e., integrating the PDF. The CDF is defined as the probability that any outcome in X is less than or equal to a stated limiting value x . Mathematically,

$$F(x) = \text{Pr ob}[X \leq x] = \int_{-\infty}^x f(x) dx$$

As x approaches infinity, the area under the curve approaches unity. Now, since the PDF is the slope of the CDF, the probability that any single item, chosen at random from a distribution, will have a given value or less can be read directly off the abscissa of the CDF plot. Conversely, once PDF and CDF of a variable is defined, a point value of the variable associated with a randomly generated probability, $F(x)$, can be obtained from the inverse of the selected CDF.

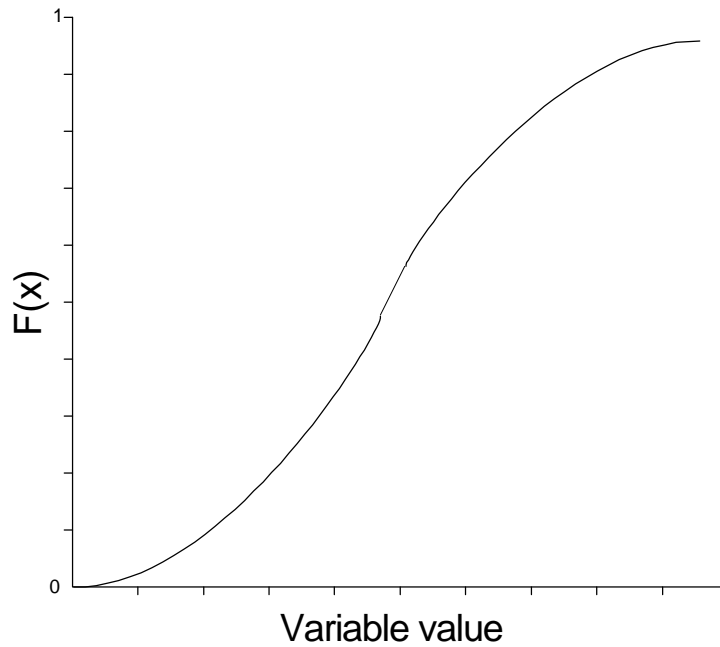


Figure 4: CDF Curve

The model employs IMSL C Numerical Libraries version 2.0 library functions to compute the inverse CDF of distributions.

The following section describes the PDFs and CDFs of different types of distributions used in the model.

3.4.1. *Uniform Distribution*

There are two parameters to the uniform distribution: minimum (min) and maximum (max). They indicate the range of values for the random variate X . If the random variate X assumes a value (x) in this range, x can be calculated knowing the PDF or the CDF. For the uniform distribution:

$$\text{PDF: } f(x) = \frac{1}{b-a} \quad a \leq x \leq b$$

$$\text{CDF: } P(a \leq X \leq x) = \int_a^x f(x) dx = \int_a^x \frac{dx}{b-a} = \frac{x-a}{b-a} \quad a \leq x \leq b$$

The uncertainty in the parameters minimum (min) and maximum (max) is again distributed uniformly. The parameter min assumes values between a and b. The parameter max assumes values between c and d. In the outer loop of the Monte Carlo simulation, the parameters (min and max) for a variable X are evaluated for a random probability generated by a random number generator.

3.4.2. *Triangular Distribution*

The PDF for the triangular distribution is:

$$\text{PDF: } f(x) = \frac{2(x-a)}{(b-a)(c-a)} \quad a \leq x \leq c$$

$$f(x) = \frac{2(b-x)}{(b-a)(b-c)} \quad c \leq x \leq b$$

There are three parameters of importance in the triangular distribution:

- the minimum: a,
- the maximum: b,
- the shape parameter or mode: c

Uncertainty about the mode (c) was usually modeled as uniform (U).

On integration of the PDF, the following equations were obtained for the CDF.

$$\text{CDF: } \text{Variable} = a + \sqrt{p \cdot (b-a) \cdot (c-a)} \quad p < \frac{c-a}{b-a}$$

$$\text{Variable} = b - \sqrt{(1-p) \cdot (b-a) \cdot (b-c)} \quad p \geq \frac{c-a}{b-a}$$

3.4.3. *Normal Distribution*

For variables such as Breathing Rate the most appropriate distribution was found to be a normal distribution (denoted by N). In some cases, however, the values were found to lie within an interval. For these cases, truncated normal distribution was used. The parameters for the normal distribution are the mean μ and the standard deviation σ . They determine the location of

the random variate and the shape of the distribution curve respectively. The PDF of the normal distribution is:

$$\text{PDF: } f(x) = \frac{1}{s\sqrt{2p}} \exp\left[-\frac{1}{2}\left(\frac{x-m}{s}\right)^2\right] \quad -\infty < x < \infty$$

The range of the variable having a normal distribution is $-\infty < x < \infty$. In order to exclude selection of random variates that are outside the range of possible values for the variable, the distribution is truncated by replacing any values selected during the simulation that are below a specified minimum or above a specified maximum with a new selection. The truncated normal distribution is referred to as TN.

The mean μ and the standard deviation σ also have uncertainty associated with them. The uncertainty about μ and σ were modeled using Student's t and Chi-square distributions respectively. The PDFs for μ and σ will be discussed in later sections.

The CDF for the normal distribution can be estimated as follows:

$$\text{CDF: } P(X \leq x) = \int_{-\infty}^x \frac{1}{s\sqrt{2p}} \exp\left[-\frac{1}{2}\left(\frac{x-m}{s}\right)^2\right] dx \quad -\infty < x < \infty$$

The truncated normal function is integrated between limits min and x.

3.4.4. Lognormal Distribution

Some of the variables were observed to have a distribution that is skewed to the right, and have values that span several order of magnitudes. Data of this type was found to be represented well by a lognormal distribution (denoted by LN). In some cases, however, the values were found to lie within an interval. For these cases, truncated lognormal distribution was used. Similar to the normal distribution, the parameters for the lognormal distribution are the mean μ and the standard deviation σ . The PDF of the lognormal distribution is:

$$\text{PDF: } f(x) = \frac{1}{xs\sqrt{2p}} \exp\left[-\frac{1}{2}\left(\frac{\ln x - m}{s}\right)^2\right] \quad 0 < x < \infty$$

An important characteristic of the lognormal distribution is that the range of the variable is $0 < x < \infty$. In order to exclude selection of random variates that are outside the range of possible values for the variable, the distribution is truncated by replacing any values selected during the simulation that are below a specified minimum or above a specified maximum with a new selection. This truncated lognormal distribution is referred to as TLN. The limits for the lognormal distribution in this case are minimum and maximum as specified in Table 24 in Appendix A.

The mean μ and the standard deviation σ are estimated from the geometric mean (gm) and the geometric standard deviation (gsd) of a sample drawn at random from the distribution.

$$gm = e^m$$

$$gsd = e^s$$

But there is uncertainty associated with this approximation. The uncertainty about μ and σ were modeled using Student's t and Chi-square distributions respectively.

The CDF for the lognormal distribution can be estimated as follows:

$$\text{CDF: } P(X \leq x) = \int_0^x \frac{1}{xs\sqrt{2p}} \exp\left[-\frac{1}{2}\left(\frac{\ln x - m}{s}\right)^2\right] dx \quad 0 < x < \infty$$

As for truncated normal, the truncated lognormal function is integrated between limits min and x.

3.4.5. *Beta Distribution*

Many variables in the mathematical model are evaluated as fractions and assume values over a narrow range (ex, between zero and one). The occupancy factor, equilibrium factor, and unattached fraction used to model inhalation exposure are included in this category. The shape of the distributions of these variables is thought to be unimodal, with a mode between the minimum and maximum values. A lot of information was not available on the mode, and hence the beta distribution was found to be suitable for incorporating data on these variables (EPA, 1995).

The beta distribution is specified by four parameters as B(a, b, min, max). The variables with beta distributions were modeled as:

$$\text{CDF: } F(x) = I_x(a, b) = \frac{1}{B(a, b)} \int_0^x t^{a-1} (1-t)^{b-1} dt \quad (a, b > 0)$$

The parameters a, and b are evaluated from the mean and the mode. a and b are related to the mean, mode, minimum and maximum by the following equations:

$$a = \frac{(\text{mean} - \text{min})(2 * \text{mode} - \text{min} - \text{max})}{(\text{mode} - \text{mean})(\text{max} - \text{min})} \quad a > 1$$

$$b = \frac{a(\text{max} - \text{mean})}{(\text{mean} - \text{min})} \quad b > 1$$

Uncertainty about the mean was usually modeled as uniform (U) and uncertainty about the mode was usually modeled as uniform (U) or triangular (TRI).

3.4.6. Student's-t Distribution

The Student's t distribution and the Chi-square distribution that follow were used as uncertainty PDFs only. The Student's-t distribution has three parameters m, s and qf. The process of choosing a random variate from the Student's-t-distribution and calculating the corresponding value of μ is designated by the function TS(m,s,qf).

The quality factor denoted by 'qf' is used to replace 'n', the number of samples considered in the study, and reflects on how well the sample is judged to represent the population of interest. Based on the number of observations drawn from a population a quality factor of 10, 25 or 100 was chosen.

$$\frac{m - \mathbf{m}}{s/\sqrt{n}} = T_{n-1}$$

$$\frac{(n-1) s^2}{s^2} = CHISQ_{n-1}$$

The t-variate having (qf-1) degrees of freedom is expressed as,

$$T_{qf-1} = \frac{m - \bar{m}}{s / \sqrt{qf}}$$

where

- m = ln(gm) of a sample drawn from the normal population $N(\mu, \sigma^2)$,
- s = ln(gsd) of a sample drawn from the normal population $N(\mu, \sigma^2)$.

Hence, corresponding to a probability (generated randomly) and the number of degrees of freedom ($qf-1$) the value of T is calculated. Since m, s, qf are known, μ can be calculated.

3.4.7. Chi-square Distribution

The important parameters of a Chi-squared distribution are m and qf. The process of choosing a random variate from the chi-squared distribution and calculating the corresponding value of σ is designated by the function INVCH(s,qf).

The χ^2 variate with $qf-1$ degrees of freedom is expressed as,

$$\chi^2_{qf-1} = \frac{(qf - 1)s^2}{s^2}$$

where

- m = ln(gm) of a sample drawn from the normal population $N(\mu, \sigma^2)$,
- s = ln(gsd) of a sample drawn from the normal population $N(\mu, \sigma^2)$.

Again, corresponding to a probability and the number of degrees of freedom ($qf-1$) the value of χ^2 is calculated. Since m, s, qf are known, σ can be calculated.

3.5. Exposure Model Variables

This section presents the derivation of Probability Distribution Functions (PDFs) to describe both the variability (PDF_v) and uncertainty (PDF_u) in each of the Three-Compartment Model parameters. All the data in this section is taken from the EPA Report (EPA, 1995).

3.5.1. Number of People per House (PNUM)

The EPA Model used information that was based on a survey of 6051 randomly selected U.S. residences conducted by the U.S. DOE (1982). Based on this survey the relative frequency of homes as a function of number of residents (PNUM) is given as:

Table 5: Parameters of Empirical Distribution for PNUM

Number of People in House (PNUM)	Relative Frequency
1	0.192
2	0.328
3	0.183
4	0.164
5	0.083
6	0.049

Since PNUM can assume only integral values, the variable is expressed in terms of an empirical PDF_v, assuming values from 1 to 6 in proportion to the frequency given in Table 5. Since this distribution is based on over 6000 observations, PNUM is not treated as an uncertain variable.

3.5.2. Compartment Volumes

3.5.2.1. Volume of Shower (V_s)

Since limited information was available on shower volume, the EPA modeled V_s as a uniform distribution with uncertain minimum and maximum values.

PDF_v (V_s) ~ U(min, max)

PDF_u (min) ~ U(1000, 1500)

PDF_u (max) ~ U(2500, 3000)

3.5.2.2. *Volume of Bathroom (V_b)*

The EPA found that the data collected by the NKBA (National Kitchen and Bath Association) on the size of the bathrooms in households are well fit by a lognormal distribution with uncertain gm and gsd and fixed lower and upper bounds. The data set used to derive this PDF_v was assumed to be large and reasonably representative, but since no details were provided on the sample set, an intermediate qf of 25 was assigned.

$$PDF_v(V_b) \sim TLN(gm, gsd, min, max)$$

$$PDF_u(\ln(gm)) \sim TS(m, s, qf)$$

$$PDF_v(\ln^2(gsd)) \sim INVCH(s, qf)$$

$$m = \ln(14000)$$

$$s = \ln(1.66)$$

$$qf = 25$$

$$min = 4000$$

$$max = 60000$$

3.5.2.3. *Volume of the Main House (V_a)*

The U.S. DOE (1982) collected data on house volume through a survey of 6051 randomly selected homes in the U.S. Each house was assigned to one of seven different size categories, based on the total heated floor space.

Nazaroff et al. (1987) estimated the house volume from the floor area by assuming a wall height of 2.4 m (8 ft). They obtained the per capita volume (V_t) by dividing the house volume by the number of people. The authors found that the resulting distributions were well fit by lognormal PDFs and hence they modeled the value of V_t as a set of truncated lognormal distributions, based on the number of people in the house.

Table 6: Parameters of Lognormal Distribution for V_t

PNUM	gm (L/person)	gsd	min	max
1	205000	1.78	35000	1100000
2	144000	1.74	30000	700000
3	99000	1.68	25000	450000
4	89000	1.67	20000	400000
5	75000	1.70	15000	350000
6	54000	1.78	10000	300000

The maximum and minimum values shown in Table 6 are approximately equal to the 99th and the 1st percentile values, estimated from graphs of data presented by the authors. Since the study involved a large number of homes from different cities across the U.S. a qf of 100 was assigned.

Using the distributions formulated by Nazaroff et al., EPA estimated the value of the main house volume as follows: A value is selected for the number of the people in the house (PNUM). The value of V_a (volume of the main house) is then calculated by choosing a value from the corresponding total volume per capita (V_t) PDF. Then:

$$V_a = \text{PNUM} \cdot V_t - V_b - V_s$$

This method for calculating V_a allows for choosing large values for the volume of the shower and/or the bathroom while choosing a small volume for total house volume, and occasionally this approach leads to unrealistic values for V_a . This problem could be solved by specifying a correlation coefficient that describes the degree of correlation between the size of each of the three house compartments.

Since no information is available on the nature or magnitude of this correlation, the problem of unrealistic combinations of selected compartment volumes was addressed by imposing a "reality check" on the calculated value of V_a . If the value of V_a was smaller than 50% of the value of total house volume ($\text{PNUM} \cdot V_t$), then new values were selected for each of the variables V_s , V_b , and V_t , and the reality check was performed again.

3.5.3. Water Usage

3.5.3.1. Shower Flow Rate (SFR)

The EPA (1995) stated that typical shower flow rates range from 5 to 15 gal/min, which appears to be significant over-estimate, since most literature values fall between 5 and 20 L/min. James and Knuiman conducted extensive research on shower flow rates and reported arithmetic mean and standard deviation values of 7.1 and 1.54 respectively. Since the study by James and Knuiman involved a large number of people, a qf of 100 was assigned for this study. The EPA Model utilized these values to fit a truncated lognormal PDF for the shower flow rate. The SFR was hence modeled as:

$$PDF_v(SFR) \sim TLN(gm, gsd, min, max)$$

$$PDF_u(\ln(gm)) \sim TS(m, s, qf)$$

$$PDF_u(\ln^2(gsd)) \sim INVCH(s, qf)$$

$$m = \ln(7.1)$$

$$s = \ln(1.54)$$

$$qf = 100$$

$$min = 3$$

$$max = 24$$

3.5.3.2. Total per capita water use in shower

Information collected by the EPA shows that all reported values on per capita water use during showering fall between 30 and 60 L/person/shower. A value of 50 L/person/day was obtained, by multiplying the 50th percentile of the distribution generated PDF for SFR by the PDF for T_s . This suggests that the PDFs selected for these variables are reasonable.

3.5.3.3. Water Use in Bathroom (I_b)

Although there are a number of studies on this variable, no information was available on the shape and range of the distribution for I_b . Therefore, the EPA modeled the value of I_b as a function of the total per capita water use in the bathroom (WU_b) with WU_b evaluated by an uncertain uniform distribution.

$$I_b = \text{PNUM} \cdot \text{WU}_b$$

$$\text{PDF}_v(\text{WU}_b) \sim \text{U}(\text{min}, \text{max})$$

$$\text{PDF}_u(\text{min}) \sim \text{U}(15, 20)$$

$$\text{PDF}_u(\text{max}) \sim \text{U}(75, 85)$$

3.5.3.4. Water Use in Main House (I_a)

Nazaroff et al. (1987) combined the data from several studies and found that the CDF representing the water use in the main house was well fit by a lognormal distribution. However, according to Brown and Caldwell the water use per capita depends to a certain extent on the number of people in the house. They stratified the data on water use by number of people and reported the means and standard deviations along with graphs. These graphs were used to identify the minimum and maximum values for each distribution, and because of the modest number of homes surveyed in each stratum, qfs of 25 and 10 were chosen for the strata. The resulting values of gm, gsd, min, max and qf needed to characterize the truncated lognormal distributions are listed below:

Table 7: Parameters of Lognormal Distribution for WUt based on PNUM

N	Per Capita Total Water Use (WUt) (L/person/day)	
	Mean	Std
1	316	90
2	266	76
3	264	59
4	238	55
5	216	32
6	184	--

Based on this information, the value of I_a was calculated by the EPA as follows:

$$I_a = \text{PNUM} \cdot \text{WUt}_i - \text{PNUM} \cdot \text{SFR} \cdot T_s - I_b$$

$$\text{PDF}_v(\text{WUt}_i) \sim \text{TLN}(\text{gm}, \text{gsd}, \text{min}, \text{max})$$

$$\text{PDF}_u(\ln(\text{gm})) \sim \text{TS}(\text{m}, \text{s}, \text{qf})$$

$$\text{PDF}_u(\ln^2(\text{gsd})) \sim \text{INVCH}(s, \text{qf})$$

In practice this method for calculating I_a allows for choosing large values for SFR and/or I_b , while choosing a small value for total house water use. Occasionally this approach leads to unrealistic values for I_a (including values that are negative). There is no information available on the any possible correlation between the water use in each of the three compartments.

Hence, the problem of unrealistic combinations of selected compartment volumes was addressed by imposing a "reality check" on the calculated value of I_a . If the value of I_a was smaller than 50% of the value of total water use ($\text{PNUM} \cdot \text{WU}_t$), then new values were selected for each of the variables T_s , SFR, WU_b , and WU_t and the reality check was performed again.

3.5.4. *Compartment Ventilation Rates*

Ventilation rate (VR) is described either in terms of air exchanges per hour (ACH), or in terms of air residence time (R) (1/min). The ventilation rate (VR) and the residence time are related as:

$$R = \frac{60}{\text{VR}}$$

3.5.4.1. *Main House Residence Time (R_a)*

Taking into consideration various values for ventilation rates and residence times in the main house that were reported from studies VR_a was modeled as:

$$\text{PDF}_v(\text{VR}_a) \sim \text{TLN}(\text{gm}, \text{gsd}, \text{min}, \text{max})$$

$$\text{PDF}_u(\ln(\text{gm})) \sim \text{TS}(m, s, \text{qf})$$

$$\text{PDF}_u(\ln^2(\text{gsd})) \sim \text{INVCH}(s, \text{qf})$$

$$m = \ln(0.68)$$

$$s = \ln(2.01)$$

$$\text{qf} = 25$$

$$\text{min} = 0.1/\text{hr}$$

$$\text{max} = 3.5/\text{hr}$$

The residence time in the main house is then calculated from the ventilation rate as:

$$R_a = 60 / VR_a$$

As the analysis of house size and ventilation rate did not reveal any significant correlation between these variables, the ventilation rate was modeled as independent of house size by the EPA.

3.5.4.2. Bathroom Residence Time (R_b)

Ventilation of bathroom is found to occur by two main pathways:

1. Simple exchange with air from the main house, driven by forced air movement from furnaces or air conditioners, and
2. Forced air exhaust via a bathroom fan vented to outdoors.

Normal exhaust rates for different fans supplied by different manufacturers range from about 40 to 160 ft³/min with most mid-range fans discharging about 70 to 90 ft³/min. Based on these data, the EPA modeled the air flow rates into and out of the bathroom separately for three different conditions. These cases have been described in Section 3.2.3.

Table 8: PDFs for R_b Based on Cases of Bathroom Ventilation

Case	Description	PDFs	Values
1	Door open, fan off	$R_{b1} \sim U(\min, \max)$	min ~ U(20, 30) max ~ U(40, 50)
2	Door closed, fan off	$R_{b2} \sim U(\min, \max)$	min ~ U(20, 30) max ~ U(150, 250)
3	Door closed, fan on	$R_{b3} = V_b / \text{EXFR}$ $\text{EXFR} \sim \text{TRI}(\min, \max, \text{mode})$	mode ~ U(2000, 2500) min = 1000 max = 5000

In case 3 it is assumed that the exhaust rate (EXFR) is the only source of ventilation in the bathroom. No information was available on the fraction of people who turn the bathroom fan on when in the shower or bathroom. In the absence of data, the probability of having the fan on

was assumed to be 0.5. Therefore, each individual in the house was assigned at random to either case 2 (fan off) or to case 3 (fan on), with a 50% likelihood of being assigned to either case.

3.5.4.3. Shower Residence Time (R_s)

The only pathway for ventilation of the shower is air exchange into the bathroom. The rate of air mixing depends on the physical structure of the shower (closed stall, tub with curtain, etc.) and is driven mainly by thermal gradients generated during showering. Based on this, Wilkes et al. suggested that the residence time in the shower is relatively brief. Hence, the value of R_s was modeled by the EPA as:

$$PDF_v(R_s) \sim U(\min, \max)$$

$$PDF_u(\min) \sim U(2, 3)$$

$$PDF_u(\max) \sim U(4, 6)$$

3.5.5. Human Activity Patterns

Some of the important terms in tracking human activity through the house are:

- SS: Time start shower,
- ES: Time end shower ($ES = SS + T_s$),
- LB: Time leave bathroom after shower ($LB = ES + TB$),
- LH: Time leave house after leaving bathroom,
- RH: Time return home,
- OF: Occupancy Factor (time away from home),
- BR: Breathing Rate.

According to the assumptions made about human activity patterns in the household (Section 3.2.2):

- ♦ There are N showers in the house.
- ♦ First shower starts at 7.00 a.m., i.e., SS_1 is 7.00 a.m. or 420 minutes.
- ♦ $ES_1 = 420 + T_{s1}$

- The second shower starts after the first person finishes his shower and leaves the bathroom. The time spent in the bathroom is assumed to be the same for all occupants of the house (T_b).
- $SS_2 = ES_1 + T_b$
- The times of start and end of other showers are calculated similarly.

3.5.5.1. *Time in Shower (T_s)*

In 1984, data was collected on the showering habits of 345 people and it was reported that these people took an average of 5.2 showers/week, with average shower duration of 10.4 minutes. A survey conducted in 1987 gathered information on the showering habits of people in 2500 households. The EPA used a lognormal distribution, with a geometric mean 6.8 minutes and geometric standard deviation of 1.60, to fit the data on shower duration. A qf of 100 was assigned for this study, because a large number of people were involved. Hence, T_s was modeled as:

$$PDF_v(T_s) \sim TLN(gm, gsd, min, max)$$

$$PDF_u(\ln(gm)) \sim TS(m, s, qf)$$

$$PDF_u(\ln^2(gsd)) \sim INVCH(s, qf)$$

$$m = \ln(6.8)$$

$$s = \ln(1.6)$$

$$qf = 100$$

$$min = 1$$

$$max = 30$$

3.5.5.2. *Time in Bathroom After Shower (T_b)*

EPA's exposure assessment predicts the time a person spends in the bathroom to be about 4 - 5 hours/week. This includes the time spent bathing (average = 7 - 8 min/day), as well as periodic uses of the bathroom throughout the day. The average time spent in the bathroom after bathing is found to be 10 - 20 minutes, with a range of 1 to 30 minutes. T_b was hence modeled as:

$$\text{PDF}_v(T_b) \sim U(\text{min}, \text{max})$$

$$\text{PDF}_u(\text{min}) \sim U(1, 10)$$

$$\text{PDF}_u(\text{max}) \sim U(20, 30)$$

3.5.5.3. *Time Leave Home (LH)*

LH denotes the time a person leaves home. LH_{min} and LH_{max} respectively, are the earliest and latest time when a person can leave home. LH is chosen at random, subject to the constraints that the selected time must be no earlier than LH_{min} and no later than LH_{max} . LH_{max} is calculated as the difference between 12.00 midnight and the time away from home. That is:

$$LH_{\text{max}} = \text{OF} \cdot 1440$$

Then LH is modeled as: $LH \sim U(LH_{\text{min}}, LH_{\text{max}})$

3.5.5.4. *Time Return Home (RH)*

The time a person returns home is calculated from the value of LH and OF as:

$$RH = LH + 1440 \cdot (1.0 - \text{OF})$$

3.5.5.5. *Occupancy Factor (OF)*

The EPA (1995) defined an Occupancy Factor to characterize the time a person spends away from home. The occupancy factor varies with age and occupational status. Based on the presence or absence of a person in a room, a value of one or zero is assigned to the occupancy factor. Studies reviewed by ORIA found a value of 0.75 as the most appropriate point estimate of the mean, with a credibility interval around the mean of 0.65 - 0.80. The minimum plausible value is estimated to be 0.33, based on the expectation that nearly all people will spend an average of about 8 hours/day at home. The maximum plausible value was set at 1.0 (24 hours/day). Based on these values, the occupancy factor was modeled as:

$$\text{PDF}_v(\text{OF}) \sim \text{BETA}(\text{mean}, \text{mode}, \text{min}, \text{max})$$

$$\text{PDF}_u(\text{mean}) \sim U(0.65, 0.80)$$

$$\text{PDF}_u(\text{mode}) \sim U(\text{min}, \text{mean}) \quad \text{if } (\text{mean} < 0.5 \cdot (\text{min} + \text{max}))$$

$$\sim U(\text{mean}, \text{max}) \quad \text{if } (\text{mean} > 0.5 \cdot (\text{min} + \text{max}))$$

min = 0.33

max = 1.0

Sometimes during the Monte Carlo simulation, an occupancy factor is selected that calls for the person to be away from the house longer than the time interval between the earliest possible time to leave the house (LH_{min}) and 12.00 midnight. To avoid this error, the smallest possible value of occupancy factor (OF_{min}) is calculated and if the value of OF selected is smaller than OF_{min} , then the value of OF_{min} is substituted for OF.

Leave Bathroom (LB) = End of Shower (ES) + Time in Bathroom (T_b)

Earliest time to leave house (LH_{min}) = LB + 10

(LH_{min} is assumed to be 10 minutes after leaving the bathroom after shower)

$OF_{min} = LH_{min}/1440$

3.5.5.6. *Breathing Rate (BR)*

The EPA (1989) collected and tabulated data on breathing rate of humans as a function of age and activity level. Based on available data, the breathing rate was modeled as a Truncated Normal distribution. Because of uncertainty in the accuracy of the factors selected for determining the distributions, a low value of qf (10) was selected.

$PDF_v(BR) \sim TN(\text{mean}, \text{std}, \text{min}, \text{max})$

$PDF_u(\text{mean}) \sim TS(m, s, \text{qf})$

$PDF_u(\text{std}^2) \sim INVCH(s, \text{qf})$

m = 9.1

s = 2.0

qf = 10

min = 2.6

max = 46.6

3.5.6. *Unattached Fraction (Ufract)*

The Unattached Fraction (also denoted by f_u) depends mainly on the concentration of aerosol in air and the attachment rates, both of which are highly variable. Based on data collected from several studies:

$$\text{PDF}_v(\text{Ufract}) \sim U(\text{min}_i, \text{max}_i)$$

$$\text{PDF}_u(\text{mean}) \sim U(0.05, 0.15)$$

$$\text{PDF}_u(\text{mode}) \sim \text{TRI}(\text{min}, \text{mean}, 0.5 \cdot (\text{min} + \text{mean}))$$

$$\text{min} = 0$$

$$\text{max} = 1$$

3.5.7. *Radon Progeny Deposition Velocity*

3.5.7.1. *Deposition Velocity of Unattached Fraction*

The deposition velocity of unattached radon progeny is determined by the degree of air mixing within a room. Knuston (1988) reviewed a number of studies on deposition rate and concluded that the average value fell within the range of 5 - 10 m/hr, and recommended a value of 8 m/hr as the best estimate. The theoretical lower bound is 0.5 m/hr, and data from several studies suggest that values of 1 - 4 m/hr may occur in calm (non-turbulent) rooms. Studies performed in rooms or chamber with good air mixing yielded values from 16 to 22 m/hr.

Based on this information, the value for DV_u (expressed in units of m/min) was modeled by the EPA as:

$$\text{PDF}_v(DV_u) \sim (1/60) \cdot U(\text{min}, \text{max})$$

$$\text{PDF}_u(\text{min}) \sim U(1, 4)$$

$$\text{PDF}_u(\text{max}) \sim U(16, 22)$$

3.5.7.2. *Deposition Velocity of Attached Fraction*

The deposition velocity of radon progeny which have become attached to aerosol particles is dictated both by the size distribution of the particles and by the air mixing rate in the

room. From Knuston's review (1988) of several studies on the deposition rate of various aerosol types, a range of 0.03 - 0.2 m/hr with a midpoint of 0.08 m/hr was found to be typical. But there is some uncertainty due to lack of extensive data and the variability in particle size and concentration, season, and air mixing rates. Hence the EPA modeled the value of DV_a as:

$$PDF_v(DV_a) \sim (1/60) * U(\min, \max)$$

$$PDF_u(\min) \sim U(0.01, 0.05)$$

$$PDF_u(\max) \sim U(0.1, 0.3)$$

Table 25 in Appendix A gives a summary of the model variables and the PDFs used to characterize them.

4. VERIFICATION OF RE-IMPLEMENTED EPA MODEL

4.1. *Three-Compartment Model*

The concentrations of radon and progeny used to calculate exposure were obtained by solving the differential equations representing the mass balance for radon and progeny in the three compartments. The function used in the program to solve these equations was verified by comparing the numerical program solution with an analytical solution.

4.1.1. *Numerical Solution*

The differential equations in the mass balance for radon and progeny were solved simultaneously using the fourth order Runge-Kutta Method. There are four sets of simultaneous differential equations in the case of radon and progeny, whereas in the case of a VOC, there is only one set of simultaneous differential equations. The implementation of the Runge-Kutta Method for a single set of differential equations is shown in Appendix A. Figures 5 & 6 show the concentrations of radon and progeny, in the three compartments, obtained using the numerical solution. In figures 5 through 8, C_s , C_b , and C_a respectively denote the concentrations in the shower, the bathroom and the main house.

4.1.2. *Analytical Solution*

In order to verify the concentration profiles given by the program, the mathematical model was solved using Mathematica. The model was simplified using the coefficients of the concentration terms and the source terms. The details of the analytical solution are given in Appendix B. Figures 7 & 8 show the concentrations of radon and progeny, in the three compartments, obtained using the analytical solution.

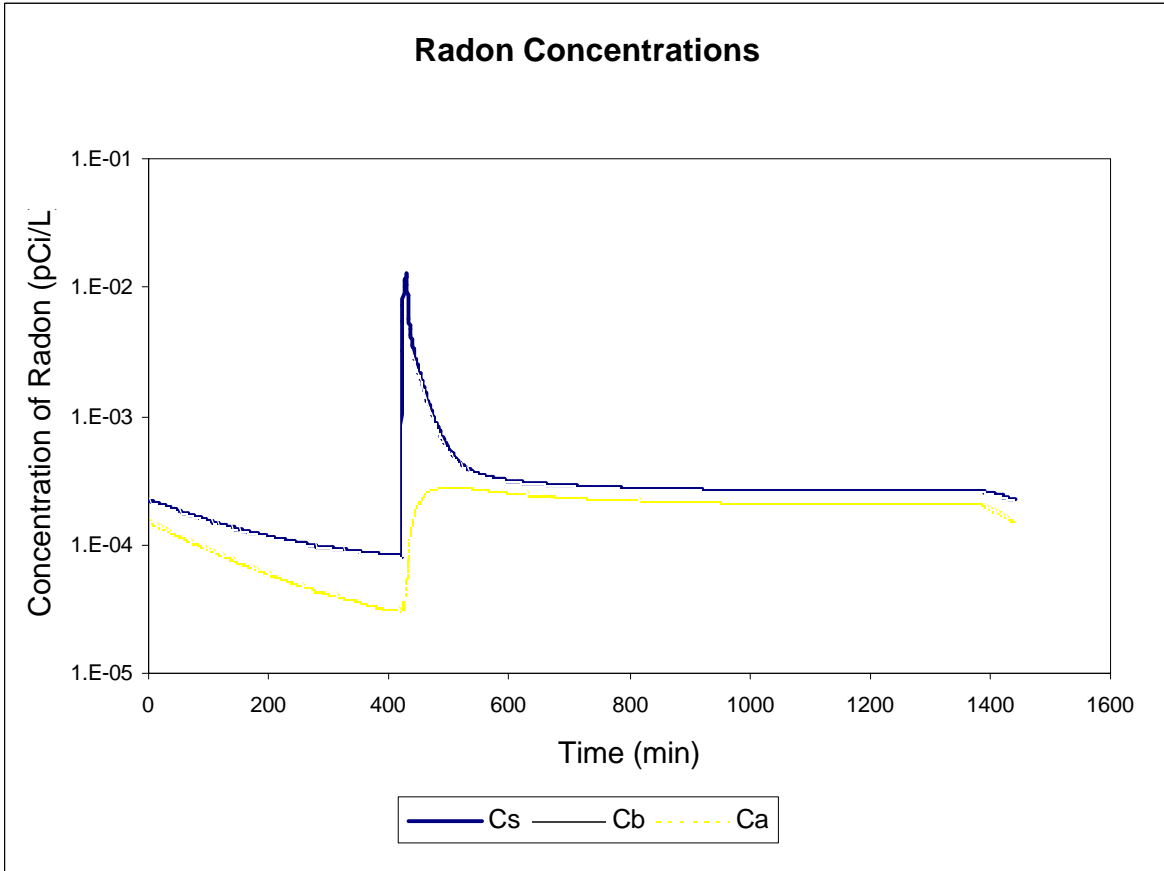


Figure 5: Radon concentration given as a function of time by the numerical solution

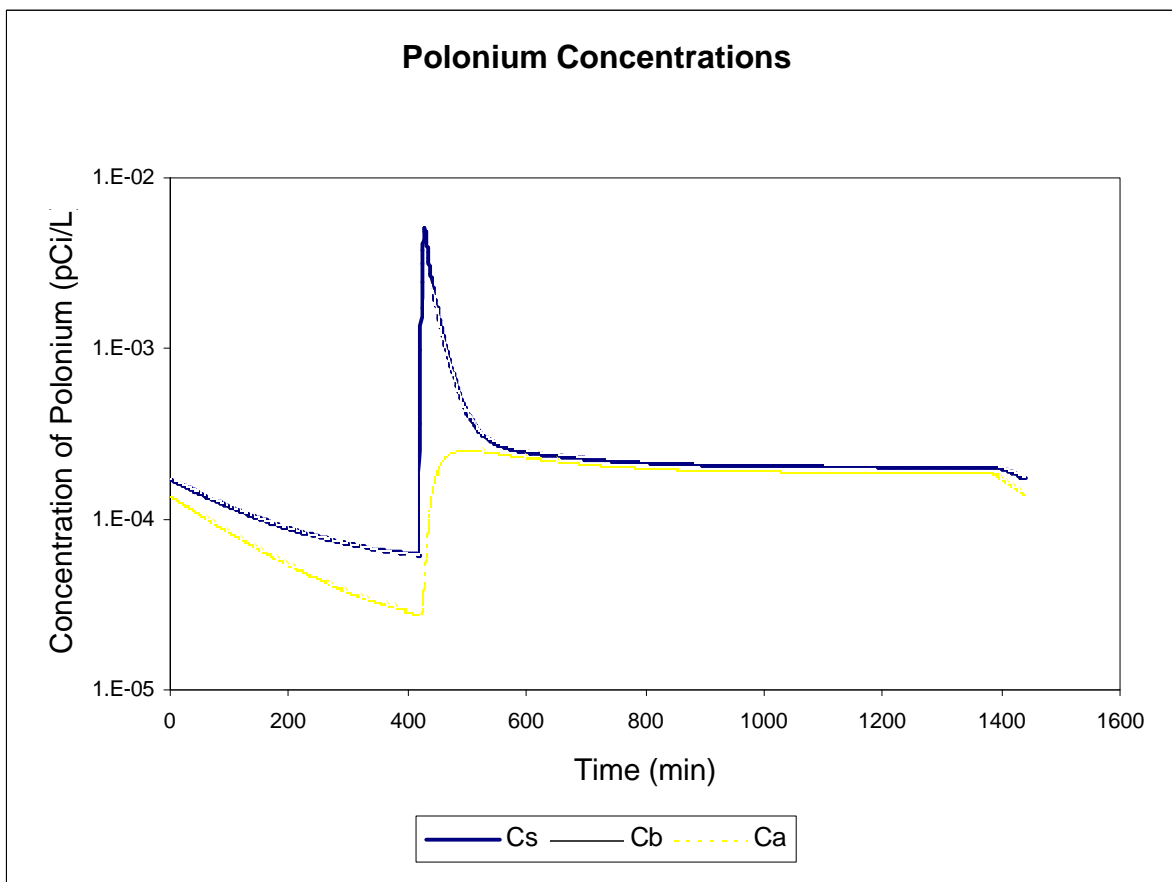


Figure 6: Polonium concentration given as a function of time by the numerical solution

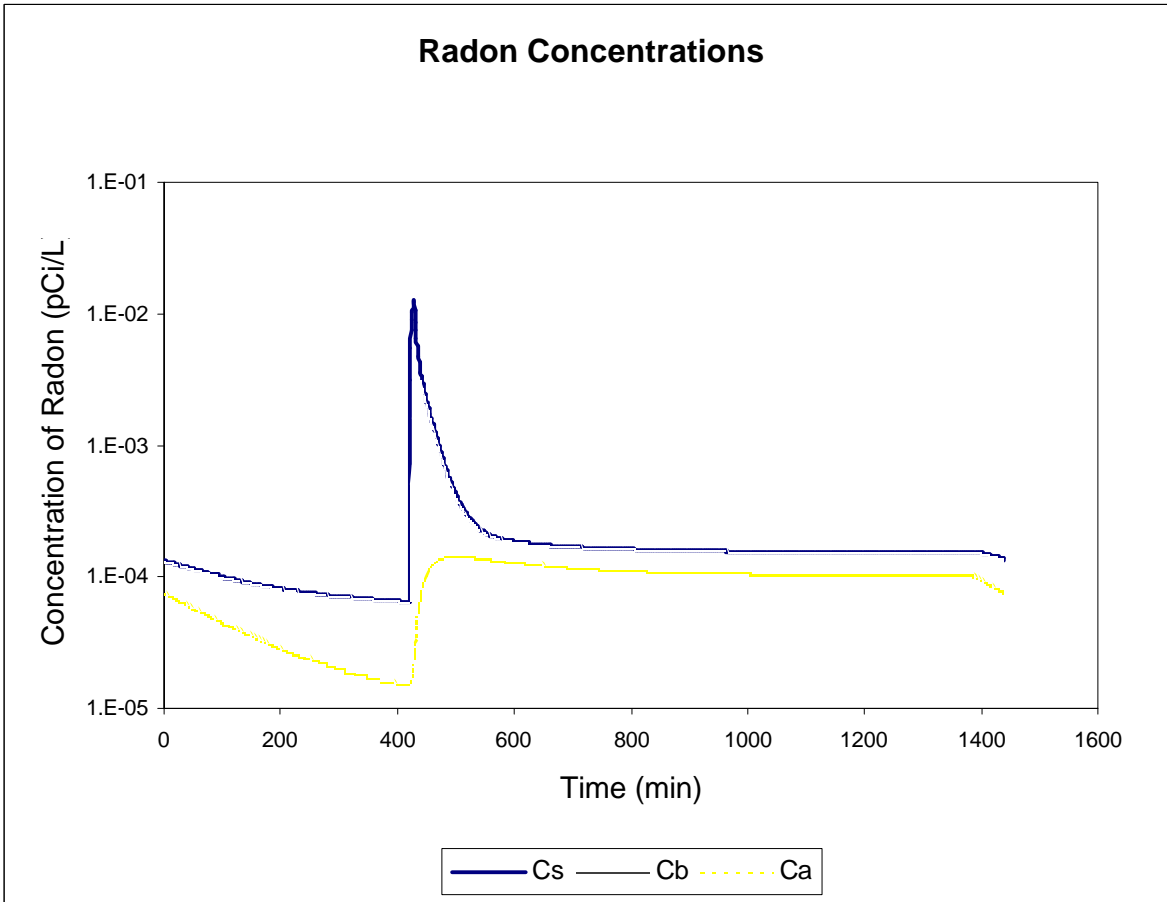


Figure 7: Radon concentration given as a function of time by the analytical solution

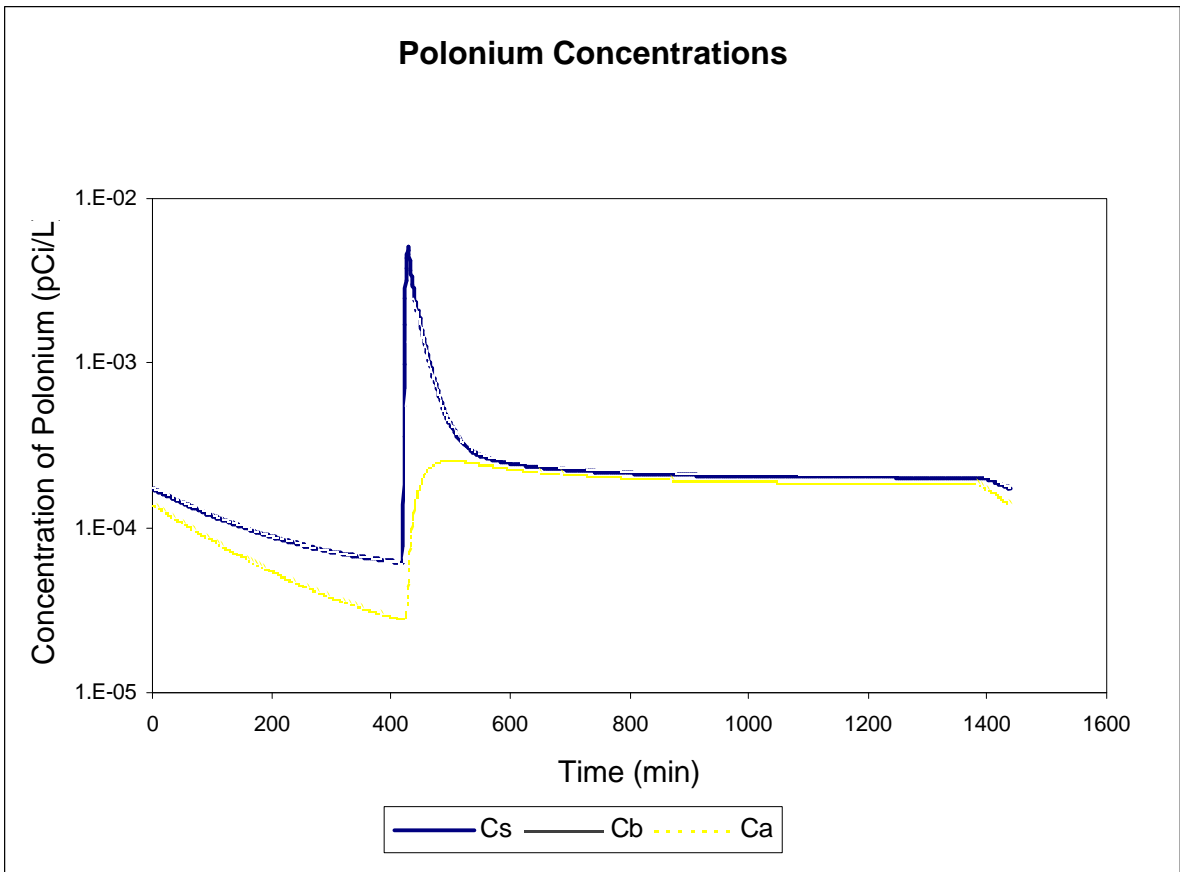


Figure 8: Polonium concentration given as a function of time by the analytical solution

4.2. Exposure Model

The exposure model given in the EPA Report (EPA, 1995) was verified through calculations in an Excel spreadsheet similar to the ones used in the program. A comparison of the exposure results given by the program and by the Excel spreadsheet is shown in Table 9.

Table 9: Comparison of Exposure Results from Program and Excel

Results	Radon Exposure	Progeny Exposure
Program	480.	1.664E-05
Excel	479.9	1.665E-05

4.3. Comparison of PDFs with Excel Functions

In the following sub-sections, the values of variables with normal (truncated), lognormal (truncated), beta, student's t and chi-square distribution obtained from the program are compared with the values obtained from the corresponding statistical functions in Excel. Samples from this comparison are shown in the tables.

4.3.1. Normal Distribution

In Excel the variable with normal distribution is calculated as follows:

$$\text{Var} = \text{NORMSINV}(p, \text{gm}, \text{gsd})$$

where

- p = Probability
- gm = Geometric mean
- gsd = Geometric standard deviation

Table 10: Comparison of Normal Variable Values

P	gm	gsd	Variable from Program	Variable from Excel	% Difference in Variable values
0.147	10.031	2.392	7.520	7.520	0.000
0.278	8.549	2.549	7.047	7.047	0.000
0.951	10.718	2.153	14.280	14.280	0.000
0.237	9.316	2.604	7.453	7.453	0.000
0.229	8.138	2.432	6.331	6.331	0.000
0.454	8.122	3.251	7.747	7.747	0.000
0.225	9.125	2.237	7.435	7.435	0.000
0.184	8.515	1.629	7.046	7.046	0.001
0.382	9.579	3.390	8.564	8.564	0.001
0.030	9.519	1.949	5.843	5.843	0.001

Figure 9 shows a plot of the comparison between Normal variable values from the program and those from Excel.

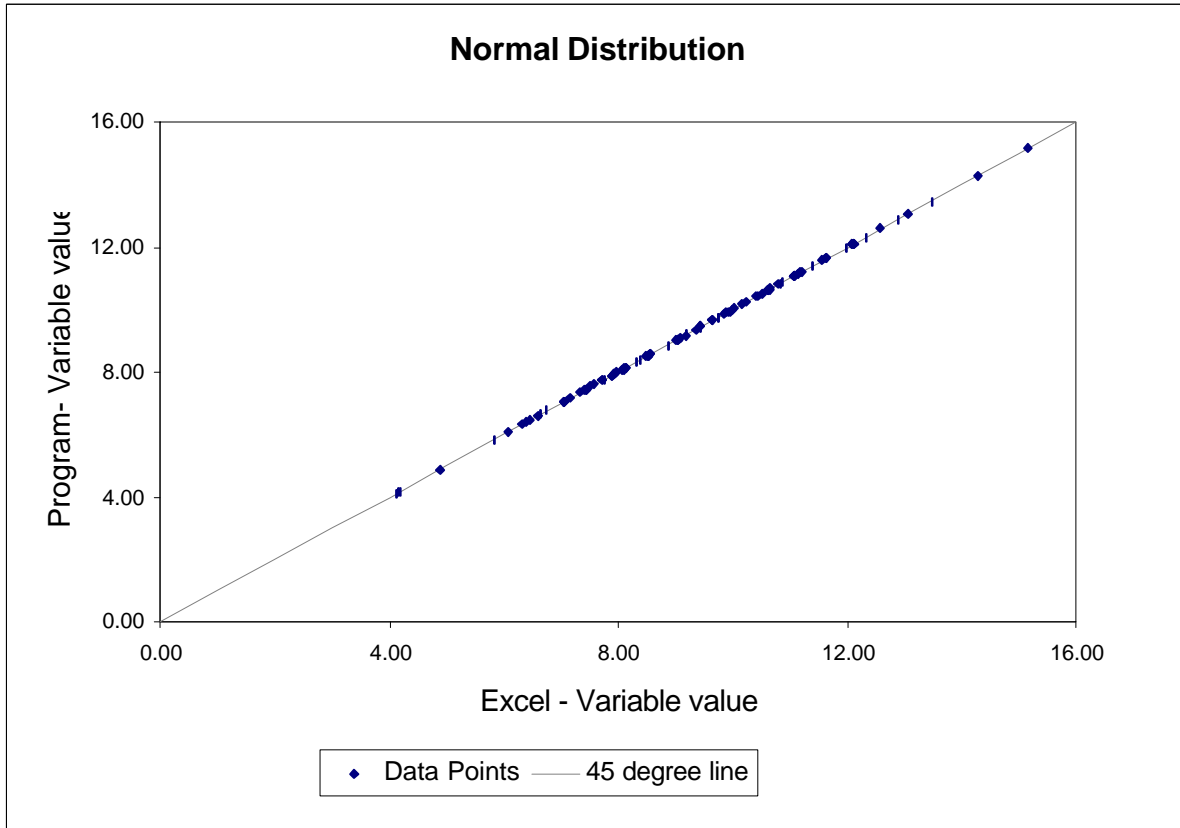


Figure 9: Comparison of Normal variable values from the program and Excel

4.3.2. Lognormal Distribution

In Excel the variable with lognormal distribution is calculated as follows:

$$\text{Var} = \text{LOGINV}(p, gm, gsd)$$

where

- P = Probability
- Gm = Geometric mean
- Gsd = Geometric standard deviation

Table 11: Comparison of Lognormal Variable Values

P	gm	gsd	Variable from Program	Variable from Excel	% Difference in Variable values
0.891	9.506	0.469	23957.991	23958.108	0.000
0.704	9.565	0.586	19508.136	19508.235	0.001
0.540	9.450	0.420	13254.001	13253.933	0.001
0.871	9.729	0.455	28109.463	28109.610	0.001
0.594	9.460	0.680	15081.095	15081.179	0.001
0.383	9.712	0.467	14368.961	14369.042	0.001
0.784	9.522	0.457	19564.144	19564.256	0.001
0.704	9.652	0.422	19499.557	19499.672	0.001
0.131	9.361	0.441	7094.310	7094.268	0.001
0.807	9.627	0.603	25593.618	25593.464	0.001

Figure 10 shows a plot of the comparison between Lognormal variable values from the program and those from Excel.

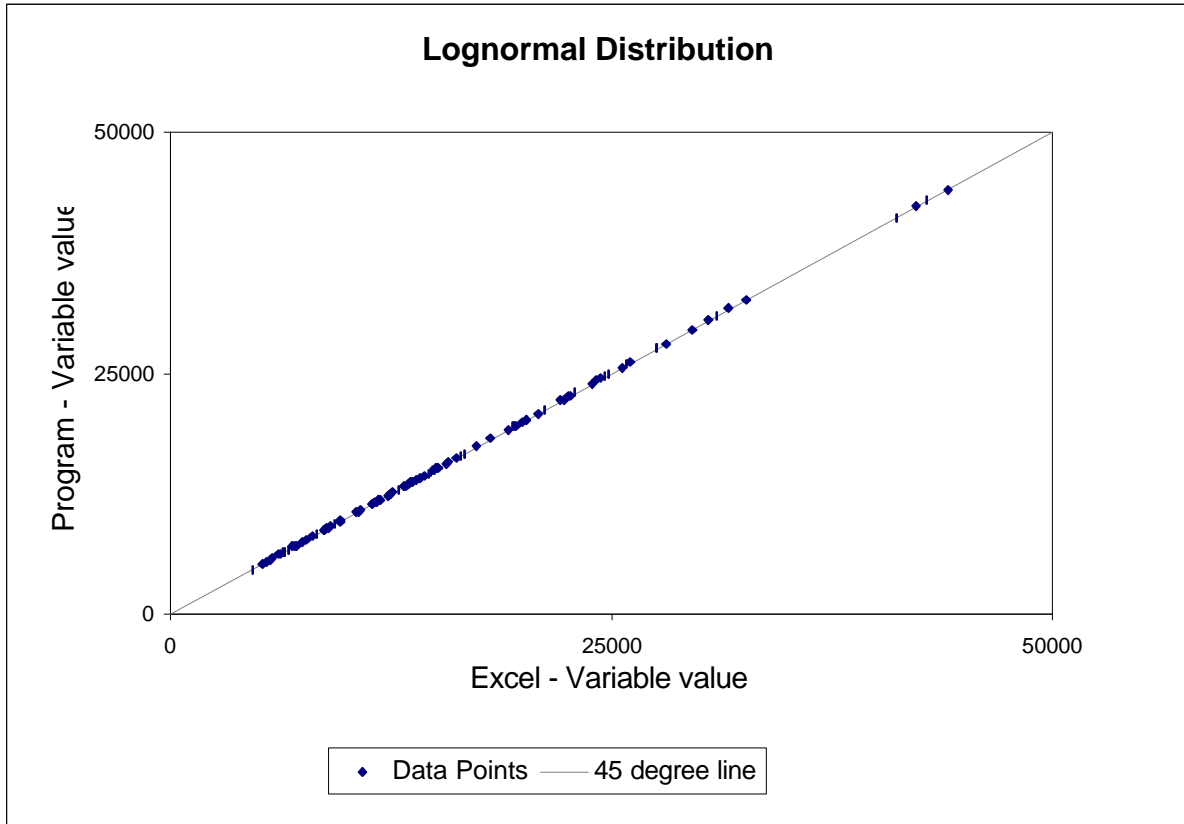


Figure 10: Comparison of Lognormal variable values from the program and Excel

4.3.3. Beta Distribution

In Excel the variable with Beta distribution is calculated as follows:

$$\text{Var} = \text{BETAINV}(p, \text{alpha}, \text{beta}, \text{min}, \text{max})$$

where

- P = Probability
- A = Parameter 1 for Beta Distribution
- B = Parameter 2 for Beta Distribution

Table 12: Comparison of Beta Variable Values

P	a	b	Variable from Program	Variable from Excel	% Difference in Variable values
0.5712	1.1780	1.0790	0.7287	0.7287	0.0000
0.4530	1.2786	1.0263	0.6850	0.6850	0.0000
0.8566	1.3429	1.0767	0.9154	0.9154	0.0000
0.6109	2.0208	1.0981	0.8379	0.8379	0.0001
0.4150	2.8056	1.3979	0.7613	0.7613	0.0001
0.4190	2.6198	1.6783	0.7163	0.7163	0.0001
0.2982	1.4316	1.0708	0.6049	0.6049	0.0009
0.3141	1.2641	1.0737	0.5848	0.5848	0.0009
0.2114	1.1909	1.0378	0.5064	0.5064	0.0010
0.1819	1.6842	1.4817	0.5156	0.5156	0.0010

Figure 11 shows a plot of the comparison between Beta variable values from the program and those from Excel.

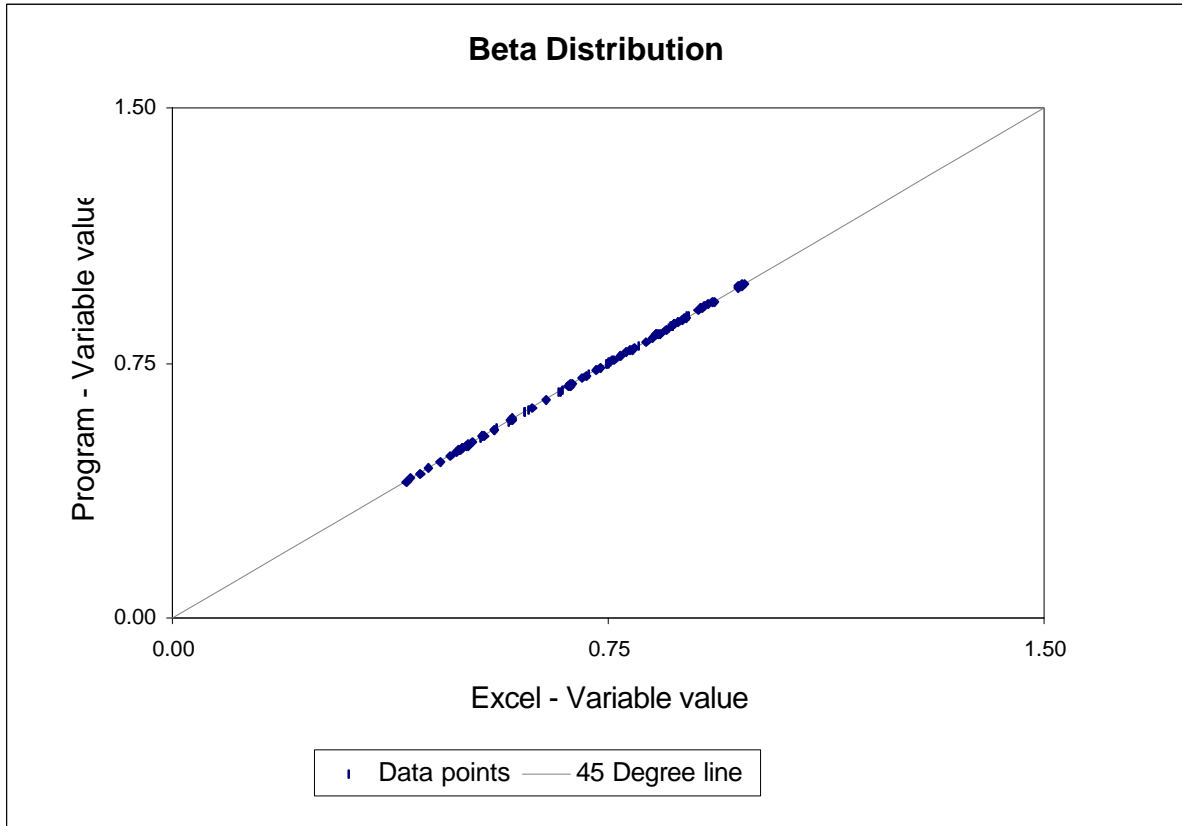


Figure 11: Comparison of Beta variable values from the program and Excel

4.3.4. Student's *t* Distribution

In Excel the variable with Student's *t* distribution is calculated as follows:

$$\text{Var} = \text{TINV}(p, \text{df})$$

where

- P = Probability
- Df = Degrees of freedom

Table 13: Comparison of Student's t Variable Values

p	qf	Variable from Program	Variable from Excel	% Difference in Variable values
0.2995	24.0000	-0.5330	-0.5330	0.0023
0.3141	24.0000	-0.4905	-0.4905	0.0013
0.3157	24.0000	-0.4860	-0.4860	0.0010
0.3334	24.0000	-0.4360	-0.4360	0.0030
0.4935	24.0000	-0.0166	-0.0166	0.0691
0.4980	24.0000	-0.0051	-0.0051	0.0812
0.5117	24.0000	0.0297	0.0297	0.0333
0.9569	24.0000	1.7895	1.7895	0.0003
0.9652	24.0000	1.8989	1.8989	0.0005
0.9730	24.0000	2.0252	2.0253	0.0036

Figure 12 shows a plot of the comparison between Student's t variable values from the program and those from Excel.

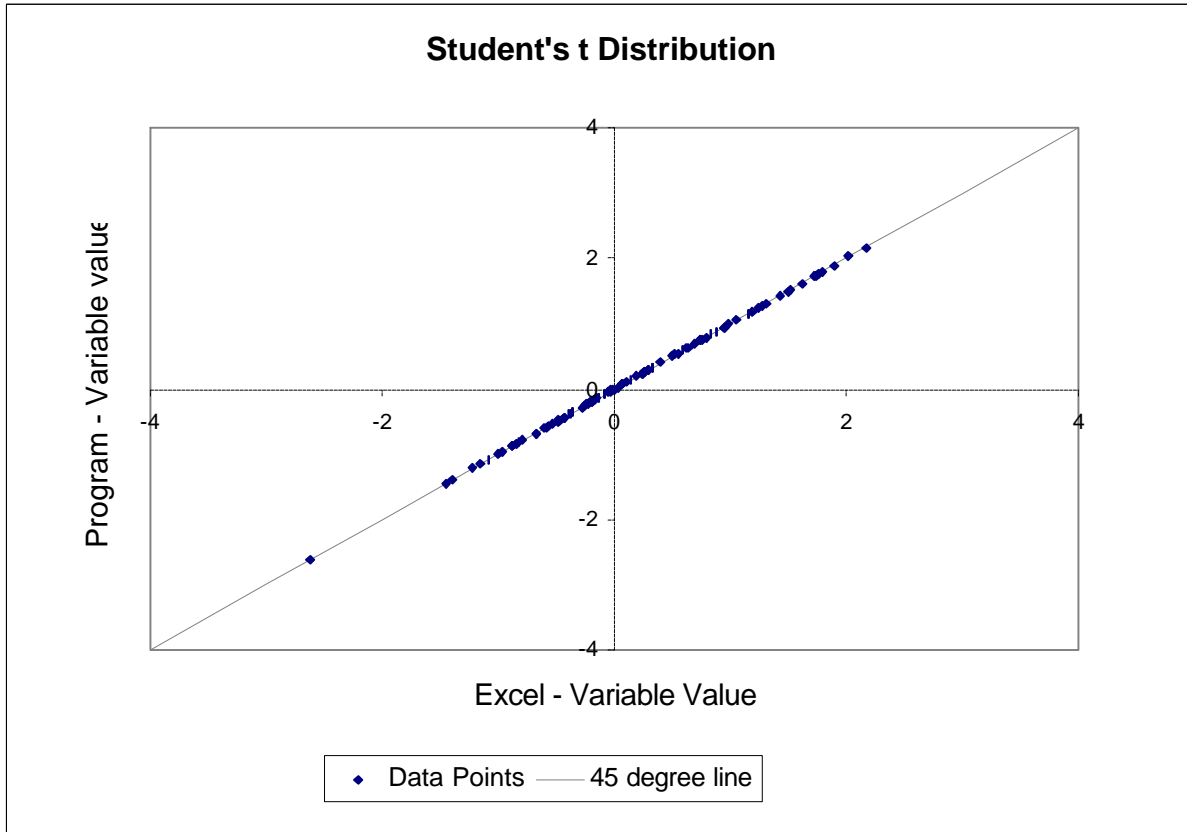


Figure 12: Comparison of Student's t variable values from the program and Excel

4.3.5. Chi-square Distribution

In Excel the variable with Student's t distribution is calculated as follows:

$$\text{Var} = \text{CHIINV}(1 - p, \text{df})$$

where

- p = Probability
- df = Degrees of freedom

Table 14: Comparison of Chi-square Variable Values

P	qf	Variable from Program	Variable from Excel	% Difference in Variable values
0.1694	24.0000	17.4120	17.4119	0.0004
0.1932	24.0000	17.9205	17.9204	0.0001
0.2010	24.0000	18.0822	18.0823	0.0005
0.2027	24.0000	18.1164	18.1163	0.0003
0.3984	24.0000	21.6249	21.6250	0.0001
0.4123	24.0000	21.8587	21.8587	0.0002
0.4190	24.0000	21.9702	21.9701	0.0002
0.6937	24.0000	26.9595	26.9596	0.0003
0.7044	24.0000	27.1921	27.1921	0.0001
0.7093	24.0000	27.2987	27.2988	0.0003

Figure 13 shows a plot of the comparison between Chi-square variable values from the program and those from Excel.

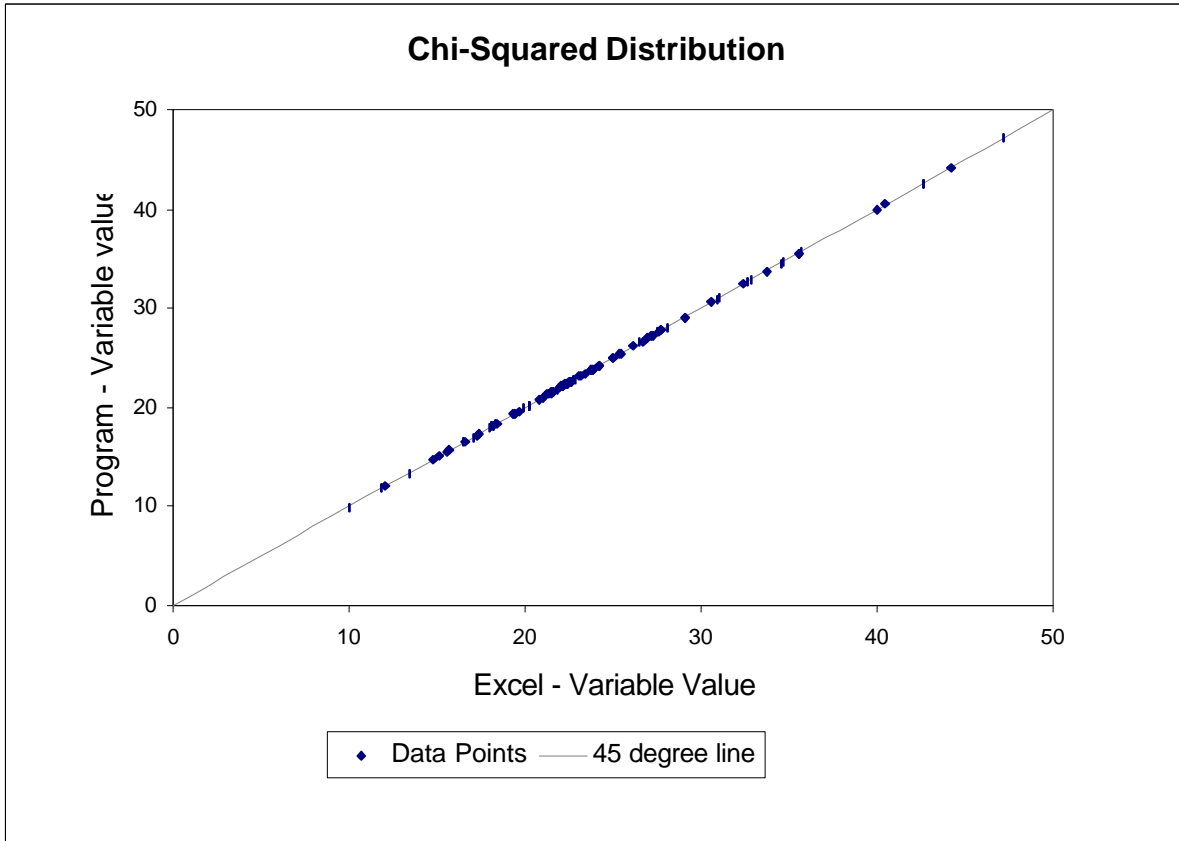


Figure 13: Comparison of Student's *t* variable values from the program and Excel

5. RESULTS

5.1. Percentiles

The output variables from the Three-Compartment Model are exposure and risk evaluated from the concentrations of chemical contaminants. Multiple estimates of the output variable are made through the Monte Carlo Simulation. The distribution of these results is used to calculate statistics of interest (mean, median, percentiles). In the outer Monte Carlo loop, the uncertain parameters are selected and with these values held constant, a number of iterations are performed in the inner Monte Carlo loop to characterize the variability of the output PDF.

From the results of the inner loop, a range of statistics such as the 5th, 25th, 50th, 75th, 95th percentiles and the mean of the output variables are calculated. This characterizes the uncertainty in the output. The variability in the output is determined by calculating the minimum, median, and maximum for these percentiles over several outer loops. Comparison of the exposure results for radon and progeny from Monte Carlo simulation (for a 250 by 2000 simulation) with results obtained by the EPA in 1995 is shown in Tables 15 & 16.

Table 15: Variability and Uncertainty in Exposure to Radon Gas

Results	Variability Statistic	Uncertainty (pCi/yr per pCi/L)		
		Lower Bound	Median	Upper Bound
Program	5 th percentile	86	137	228
	Mean	355	548	897
	95 th percentile	831	1332	2155
EPA	5 th percentile	86	120	150
	Mean	430	550	700
	95 th percentile	1100	1400	1900

Table 16: Variability and Uncertainty in Exposure to Radon Progeny

Results	Variability Statistic	Uncertainty (WLM/yr per pCi/L)		
		Lower Bound	Median	Upper Bound
Program	5 th percentile	1.5E-06	2.5E-06	3.9E-06
	Mean	8.5E-06	1.6E-05	2.6E-05
	95 th percentile	2.4E-05	4.9E-05	9.0E-05
EPA	5 th percentile	1.4E-06	2.1E-06	2.8E-06
	Mean	1.2E-06	1.6E-06	2.4E-06
	95 th percentile	3.9E-05	5.2E-05	7.9E-05

5.2. Sensitivity Analysis

The two-dimensional Monte Carlo analysis gives an output in the form of exposure and risk values for radon, progeny and VOCs. This does not provide any information on the relative importance of each variable in the calculations, and which variables contribute primarily to the variability and uncertainty in the output parameters. In order to explore these issues, a local rate of change analysis was performed.

The sensitivity of the model is assessed by calculating the percent change in the output variable per small unit increase (1% for the EPA model) in an input variable. Usually, the rate of change of the output variable depends on the values selected for each of the model inputs. Sensitivity analysis was performed on the EPA model, by incrementing default variable inputs to the model by 1%. Output changes on the scale of +1% or -1% were observed for variables that were important in determining dose and risk. Variables that had little impact on the output had a rate of change close to zero. The default values of the input variables are presented in Table 18.

Table 17: Default Values of the Input Variables in the EPA Model

Variable	Units	Values
No. of people in the house (PNUM)	-	1
Occupancy factor (OF)	-	0.783
Volume of main house (Va)	L	400000
Volume of bathroom (Vb)	L	10000
Volume of shower (Vs)	L	2000
Total water use in main house (Ia)	L/day	350
Total water use in bathroom (Ib)	L/day	125
Total water use in the shower (Is)	L/day	60
Time in shower (Ts)	min	8.0
Transfer efficiency in main house (Pa)	-	0.670
Transfer efficiency in bathroom (Pb)	-	0.30
Transfer efficiency in shower (Ps)	-	0.70
Shower flow rate (SFR)	L/min	10
Time in bathroom (Tb)	min	10
Time leave home (LH)	minutes	450
Time return home (RH)	Minutes	762
Breathing rate (BR)R	L/min	7

The following tables show comparison of results from the sensitivity analysis conducted using the computer program for radon and radon progeny with results tabulated in the EPA Report (1995).

Table 18: Rate of Change in Radon Gas Exposure

Variable	Variable	Average % Change in Exposure per	
		1% Increase in Variable Value	
		Program	EPA
Breathing Rate	BR	1.00	1.00
Time in shower	ts[1]	0.00	0.00
Occupancy factor	OF	0.67	0.71
Transfer efficiency in shower	Ps	0.55	0.55
Shower flow rate	SFR	0.55	0.55
Volume of main house	Va	-0.46	-0.44
Residence time in main house	Ra	0.52	0.42
Transfer efficiency in main house	Pa	0.38	0.33
Total water use in main house	Ia	0.38	0.33
Volume of shower	Vs	-0.34	-0.27
Volume of bathroom	Vb	-0.19	-0.17
Residence time in shower	Rs	0.12	0.12
Time in bathroom after shower	Tb	0.00	0.11
Transfer efficiency in bathroom	Pb	0.07	0.07
Total water use in bathroom	Ib	0.07	0.07
Bathroom exhaust fan rate	EXFR	-	-0.06
Residence time in bath (door open)	Rb1	-	0.02
Residence time in bath (door closed)	Rb2	-	-0.01
Residence time in bath (average)	Rb	0.07	-

Table 19: Rate of Change in Radon Progeny Exposure

Variable	Variable	Average % Change in Exposure per	
		1% Increase in Variable Value	
		Program	EPA Report
Occupancy factor	OF	1.21	1.12
Risk Factor	RF	0.00	1.00
Concentration of radon in water	CW	0.00	1.00
Residence time in main house	Ra	1.07	0.79
Volume of main house	Va	-0.79	-0.64
Transfer efficiency in main house	Pa	0.70	0.51
Total water use in main house	Ia	0.70	0.51
Deposition velocity (unattached fraction)	DVu	-0.36	-0.41
Unattached fraction	Ufrac	-0.35	-0.40
Time in shower	Ts	0.00	0.37
Shower flow rate	SFR	0.19	0.29
Transfer efficiency in shower	Ps	0.19	0.29
Time in bathroom	Tb	0.00	0.11
Transfer efficiency in bathroom	Pb	0.12	0.10
Total water use in bathroom	Ib	0.12	0.10
Volume of bathroom	Vb	-0.09	-0.09
Volume of shower	Vs	-0.05	-0.04
Bathroom exhaust fan rate	EXFR	-	-0.04
Deposition velocity (attached fraction)	DVa	-0.03	-0.04
Residence time in shower	Rs	0.02	0.03
Residence time in bath (door open)	Rb1	-	-0.01
Residence time in bath (door closed)	Rb2	-	0.01
Residence time in bath (average)	Rb	0.05	-

5.3. Discussion of Comparison

Tables 15 and 16 present a comparison of the percentiles generated by the program with those given by the EPA (EPA, 1995). It is seen that the ranges of percentiles match quite well. There is however a difference in the exact values (say, for the 5th percentile) because the Monte Carlo Simulation chooses random values for the variables during each run and it is not possible to exactly replicate the simulation as conducted by the EPA. Hence it is impossible to obtain identical results.

The variability in unit dose between different people in different houses from the program is indicated by the ratio of the 95th percentile to the 5th percentile (EPA, 1995). Uncertainty in a particular exposure statistic is characterized as the ratio of the upper bound divided by the lower bound (EPA, 1995). Variability and uncertainty ratios were calculated for radon and progeny from the program percentiles and compared with those obtained from the EPA results. It is seen the program as compared to the EPA results exhibits a greater degree of uncertainty and a lesser degree of variability.

Table 20: Comparison of Variability and Uncertainty Ratios

Compound	Values	Variability (ratio)	Uncertainty (ratio)
Radon	Program	9 - 10	2.5 - 2.7
	EPA	11 - 12	1.6 - 1.7
Progeny	Program	15 - 25	2.6 - 3.8
	EPA	25 - 30	2.0

The results from a sensitivity analysis conducted on the program are slightly different from the results tabulated by the EPA (EPA, 1995). The program results for radon are seen to be in better agreement with the EPA results than those for the progeny. However, the significance of the variables (indicated by the magnitude and sign of the rate of change) is seen to remain almost the same. That is, the order of importance of the variables remains the same. It appears that the discrepancy is either due a different set of default values used by the EPA (no indication was given in the EPA Report) or to small differences in the mathematical model.

For some variables such as the Risk Factor (RF) and Concentration of Radon in Water (CW), the data given by the EPA (EPA, 1995) was not found to be sufficient to model those variables correctly. For such variables the rate of change was not evaluated. Since certain variables such as bathroom exhaust fan rate (EXFR), residence time in bath (door open) (Rb1) and residence time in bath (door closed) (Rb2) were not used in the default calculations, the rate of change for these variables was not evaluated. Instead the rate of change for the average residence time in the bath was calculated.

To obtain a clearer understanding of the distinction between the percentile values generated by the program and those found by the EPA, the entire Monte Carlo Simulation was performed several times (250 outer loops times 2000 inner loops). The average and standard deviation for each of the percentiles of the lower, median and upper bounds of exposure to radon and progeny were determined. The values were plotted in Figures 14-19. The comparative point values of the EPA result are also indicated.

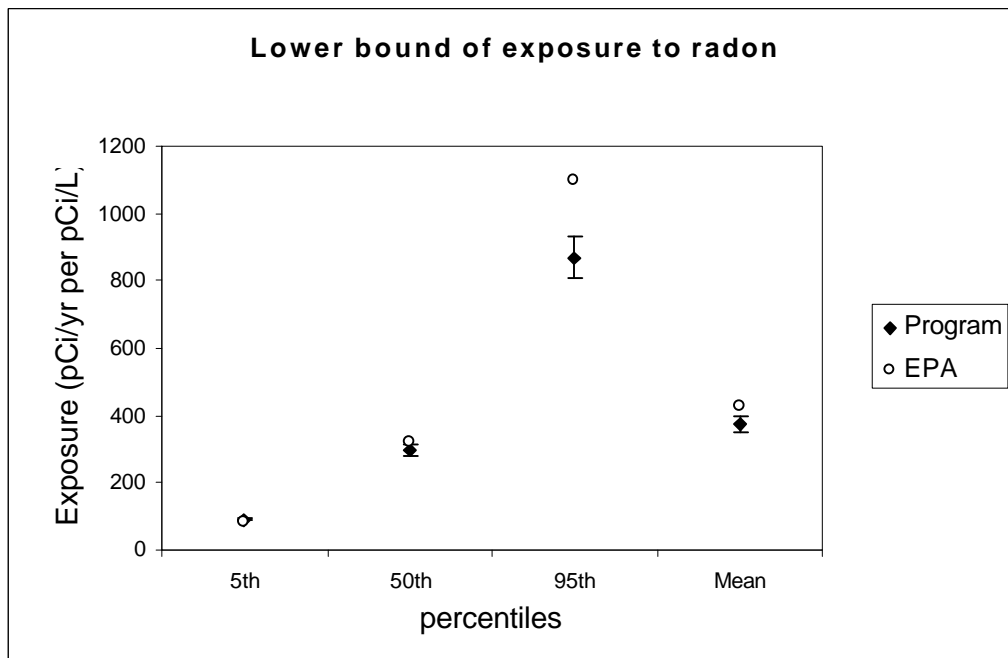


Figure 14: Lower Bound of Exposure to Radon

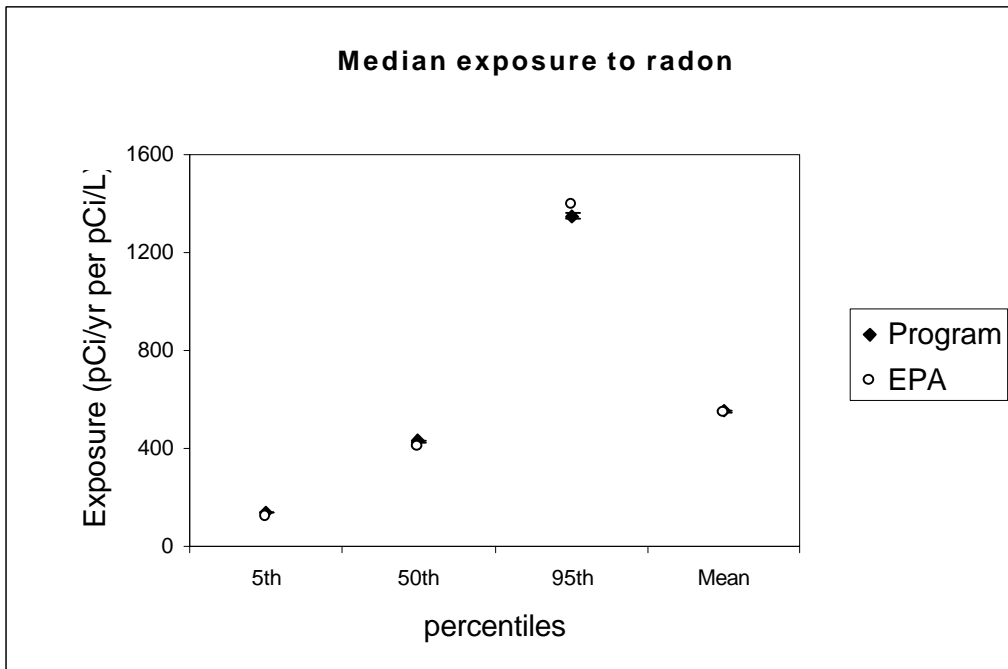


Figure 15: Median Exposure to Radon

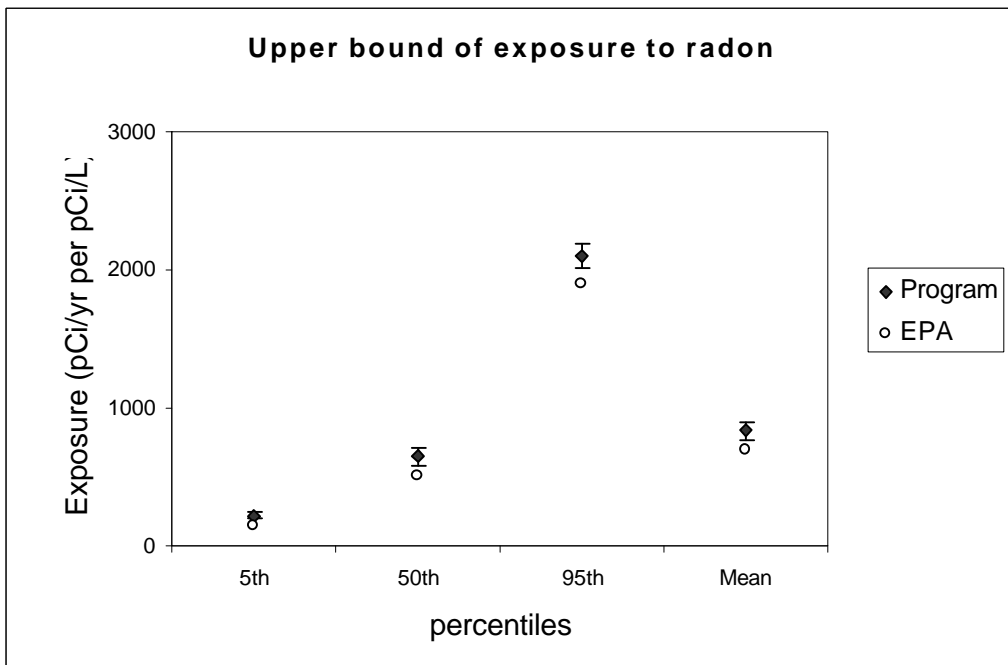


Figure 16: Upper Bound of Exposure to Radon

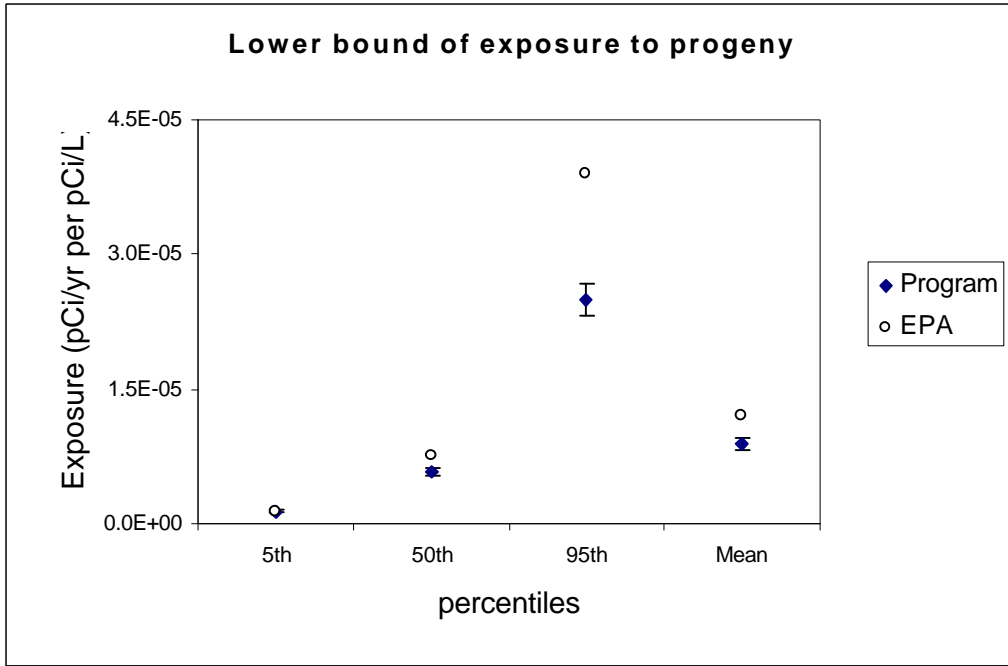


Figure 17: Lower Bound of Exposure to Progeny

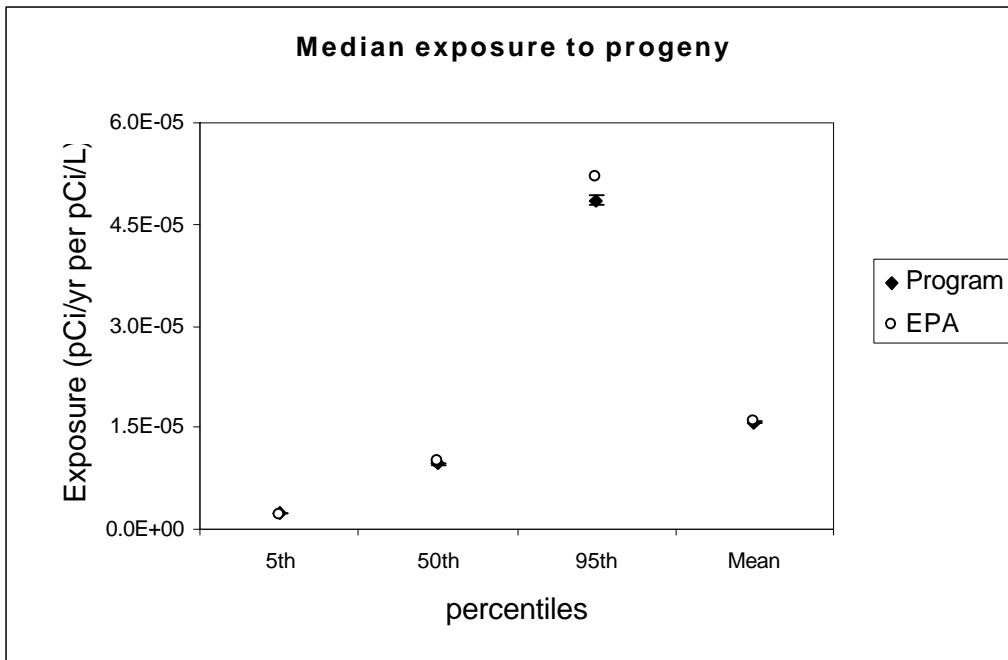


Figure 18: Median Exposure to Progeny

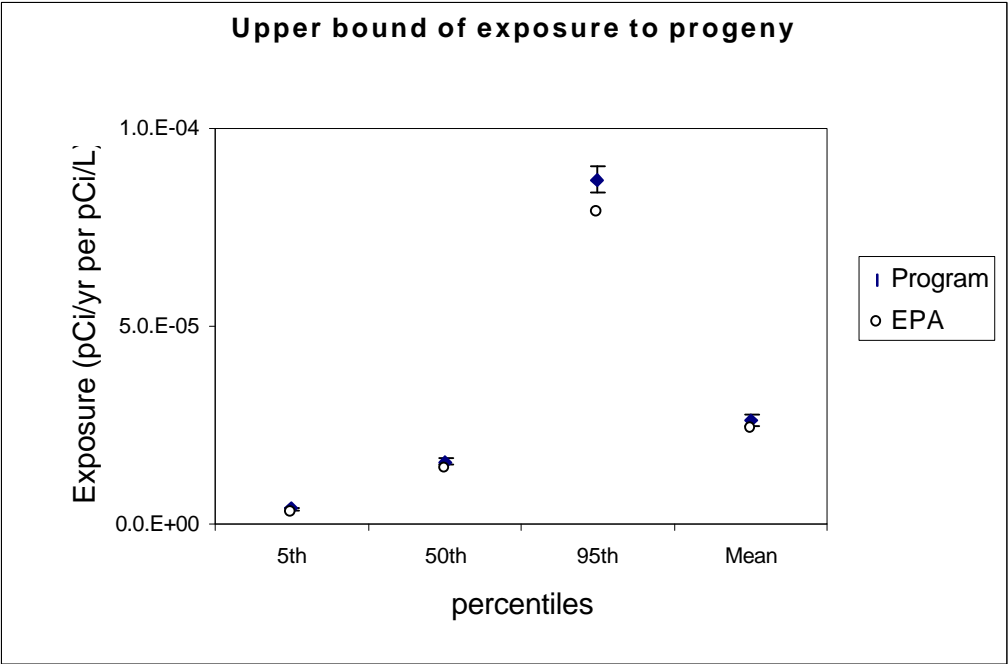


Figure 19: Upper Bound of Exposure to Progeny

The median values from the program and the EPA results appear close enough, as do the results in all percentiles of upper and lower bounds. However, for the 95th percentile there is a greater discrepancy. Small discrepancies can be attributed to the inherent random element in the computational procedure. Other differences, however, are not large enough to be of serious concern.

6. EXTENDED MODEL FOR VOCS

6.1. Henry's Law and Two-Resistance Theory

Henry's Law gives the phase equilibrium between air and a dilute aqueous solution of dissolved gas.

$$y = m C$$

where

- y = Gas phase concentration,
- C = Aqueous phase contaminant concentration at equilibrium,
- m = Henry's constant for VOC (dimensionless).

The Henry's constant varies with temperature (Selleck et al., 1988) as:

$$m \propto \left(\frac{1}{T}\right) 10^{-\left(\frac{B}{T}\right)}$$

where

- B = Temperature correction coefficient,
- T = Absolute temperature (K).

There exists a concentration driving force between the gaseous and the aqueous phases, when they are brought into contact. This results in a mass transfer flux, J, which is proportional to the driving force as:

$$J = K_{OL} \left(C - \frac{y}{m} \right)$$

where

- K_{OL} = Overall mass transfer coefficient based on liquid phase concentrations
- C = Bulk aqueous phase concentration,
- y = Bulk gas phase concentration,

The Two-Resistance Theory (Lewis and Whitman, 1924) relates the overall mass-transfer coefficient to the individual liquid phase and gas phase mass transfer coefficients, K_L and K_G , respectively:

$$\frac{1}{K_{OL}} = \frac{1}{K_L} + \frac{1}{m K_G}$$

The mass transfer flux passes through the interfacial area A that exists between the gaseous and aqueous phases. As this active interfacial area is usually difficult to measure directly, it is usually lumped together with the mass-transfer coefficient, and the combined parameter is measured experimentally. Hence, the Two-Resistance Theory is modified as:

$$\frac{1}{(K_{OL}A)} = \frac{1}{(K_L A)} + \frac{1}{m(K_G A)}$$

The values of K_L and K_G depend on the degree of turbulence, the fluid temperature, and the diffusion coefficient of the compound being transferred in both the phases. Theoretical and experimental studies indicate that turbulent mass transfer coefficients generally depend on the diffusion coefficient raised to some power, the magnitude of which lies between 1/2 and 2/3 (Little, 1992). If no better information is available, the following relationships are often assumed (Little, 1992):

$$K_L \propto D_L^{1/2}$$

and

$$K_G \propto D_G^{2/3}$$

where D_L and D_G are the diffusion coefficients of the compounds in water and air, respectively.

Using these relationships, a mass transfer coefficient measured for one compound to the can be adjusted to an equivalent mass transfer coefficient for another compound, when the diffusion coefficients for the two compounds are known. Table 20 provides information on the Henry's constant and the diffusion coefficients for some volatile contaminants.

Table 21: Volatile Compound data (Selleck et al. 1988).

Compound	$m^{\dagger}(20^{\circ}\text{C})$	B (K)
1,1,2-Trichlorotrifluoroethane	9.9	1600
Radon	3.9	1340
Fluorotrichloromethane	3.0	1030
Carbon tetrachloride	0.88	1820
1,1,1-Trichloroethane (TCA)	0.57	1770
Tetrachloroethylene (PCE)	0.54	1930
Trichloroethylene (TCE)	0.32	1960
Ethylbenzene	0.28	1700
Trans-1,2-Dichloroethylene	0.30	1820
m- & p-Xylenes	0.22	1900
Toluene	0.22	1630
1,1-Dichloroethane	0.18	1800
o-Xylene	0.16	1900
cis-1,2-Dichloroethylene	0.12	1820
m-Dichlorobenzene	0.12	1600
Chloroform	0.12	1930
Monochlorobenzene	0.11	1500
1,2-Dichloropropane	0.092	1620
Methylene chloride	0.090	1620
Dichlorobromomethane	0.067	2050
o-Dichlorobenzene	0.047	1600
1,2-Dichloroethane	0.040	1540
Ethylene dibromide	0.040	2000
Chlorodibromomethane	0.036	2050
1,1,2-Trichloroethane	0.028	1600
Bromoform	0.017	2170
1,1,2,2-Tetrachloroethane	0.012	1600
1,2-Dibromo-3-chloropropane (DBCP)	0.0056	2350

$${}^{\dagger} m_{\infty} \left(\frac{1}{T} \right) 10^{-\left(\frac{B}{T} \right)}$$

6.1.1. Values of Mass Transfer Coefficients

The two-resistance theory illustrates the relationship between the individual liquid- and gas-phase mass transfer coefficients. For example, the overall resistance to mass transfer ($1/K_{OL}$) equals the sum of two resistances in series; one for the liquid phase ($1/K_L$) and one for the gas phase ($1/mK_G$). For highly volatile compounds (large m) the gas-phase resistance is negligible and the rate of mass transfer is controlled by the liquid-phase resistance. In contrast, for compounds of low volatility (small m), the gas-phase resistance controls. To predict the rate of mass transfer for a series of compounds spanning a wide range of volatility, reliable estimates are required of both the liquid-phase and gas-phase mass transfer coefficients.

Earlier workers have found that the K_G/K_L ratio appears to be reasonably constant under similar conditions for a given mass-transfer system. If the ratio is known, it can be used to obtain an estimate of either K_{LA} or K_{GA} when only the other is known. Having an estimate of the K_G/K_L ratio is especially valuable as, in many cases, K_{OLA} is measured using only highly volatile compounds. Since liquid-phase resistance usually dominates under these conditions, the value of K_{OLA} inferred from the experimental data is essentially equal to the value of K_{LA} . To predict the extent of volatilization of low volatility compounds present, an estimate of K_{GA} is required. The only way to obtain this is either through additional experimental measurements, or by calculation using an estimate of the K_G/K_L ratio. The latter approach is clearly less accurate, but may suffice for a first approximation (Little, 1992). The liquid-side mass transfer coefficients for the different compartments of the house and the ratio of the liquid and gas-side mass transfer coefficients are (Little, 1992):

Shower: $K_{Ls} = 15$ L/min
 $(K_G/K_L)_s = 17$

Bathroom: $K_{Lb} = 0.032$ L/min
 $(K_G/K_L)_b = 40$

Main House: $K_{La} = 0.041$ L/min
 $(K_G/K_L)_a = 40$

The value of the gas-side mass transfer coefficient (K_G) is calculated as:

$$K_G = (K_G/K_L) * K_L$$

6.2. Conversion of TE values to Mass Transfer Coefficients

The Three-Compartment Model for radon is based on transfer efficiency data and applies only to the specific volatile contaminant (in this case radon and progeny). In order to extend the Three-Compartment Model to include VOCs in drinking water, a more general approach using mass transfer coefficients was developed. Transfer Efficiency (TE) values can be converted to corresponding values of mass transfer coefficients to implement this approach. This approach of TE conversion can be used until the mass transfer coefficients for various water-using devices are measured over a range of operating conditions.

Transfer Efficiency is defined as the fractional volatilization when the gas phase concentration is zero and the system is at steady state.

$$\frac{C_{out}}{C_{in}} = (1 - TE)$$

For the shower a steady state plug flow model with gas phase concentration equal to zero is assumed. Then the concentrations can be expressed (Little and Chiu, 1998) as:

$$\frac{C_{out}}{C_{in}} = \exp\left(-\frac{K_{OL}A}{Q_L}\right)$$

On substituting in the earlier equation:

$$K_{OL}A = -Q_L \ln(1 - TE)$$

Hence if the values of Q_L and TE are known, $K_{OL}A$ can be evaluated for the corresponding volatile contaminant under the given operating conditions. With the absence of data on operating conditions in the bathroom and in the main house, a similar approach is used in these compartments.

6.3. Modified Three-Compartment Model for VOCs

When applied to VOCs, the terms related to formation, decay and deposition out of radon progeny were dropped from the Three-Compartment Model. The model then consists of three simultaneous equations

$$V_s \frac{dC_s(t)}{dt} = -q_{sb}C_s(t) + q_{bs}C_b(t) + Q_s(t)$$

$$V_b \frac{dC_b(t)}{dt} = q_{sb}C_s(t) - (q_{bs} + q_{b0} + q_{ba})C_b(t) + q_{ab}C_a(t) + Q_b(t)$$

$$V_a \frac{dC_a(t)}{dt} = q_{ba}C_b(t) - (q_{ab} + q_{a0})C_a(t) + Q_a(t)$$

The $Q_i(t)$'s represent the source terms for the VOC in compartment i , which are computed using the mass transfer approach. Using Henry's Law for the concentration of VOC in air, the release of VOC from water is

$$\begin{aligned} In_{w,i} &= K_{v,i} \left(C_w - C_i/m \right) \\ K_{v,i} &= WFR_i [1 - \exp(Z_i)] \\ Z_i &= -(K_{OL}A)_i / AWU_i \end{aligned}$$

where

- $In_{w,i}$ = Release of VOC from water in compartment i (pCi/min),
- $K_{v,i}$ = Volatilization fraction into compartment i (L/min),
- C_w = Concentration of VOC in water (pCi/L),
- C_i = Concentration of VOC in air in compartment i (pCi/L),
- m = Henry's constant for VOC (dimensionless)
- WFR_i = Water flow rate into compartment i (L/min),
- AWU_i = Average water usage in compartment i (L/min).

The average water usage for the different compartments is computed as a ratio of the total water used in the compartment and the total time the compartment is occupied during the day.

Shower: $AWU_s = I_s / (NT_{s,avg})$

$$\text{Bathroom: } AWU_b = \frac{I_b}{(EWUB - SWUB)}$$

$$\text{Main House: } AWU_a = \frac{I_a}{(EWUA - SWUA)}$$

where

- I_s = Water use in the shower (L/day),
- $T_{s,avg}$ = Average time spent by a person in the shower (computed from the total time spent in the shower) (min),
- I_b = Water use in the bathroom (L/day),
- $SWUB$ = Time water use in the bathroom begins (12.00 a.m.) (min),
- $EWUB$ = Time water use in the bathroom ends (12.00 a.m.) (min),
- I_a = Water use in the main house (L/day),
- $SWUA$ = Time water use in the main house begins (7.00 a.m.) (min),
- $EWUA$ = Time water use in the main house ends (11.00 p.m.) (min).

Incorporating the above terms in the Three-Compartment Model, the complete mathematical model representing the mass balance for the concentration of VOC in the three compartments is:

$$V_s \frac{dC_s(t)}{dt} = - \left(q_{sb} + \frac{K_{v,s}}{m} \right) C_s(t) + q_{bs} C_b(t) + K_{v,s} C_w$$

$$V_b \frac{dC_b(t)}{dt} = q_{sb} C_s(t) - \left(q_{bs} + q_{b0} + q_{ba} + \frac{K_{v,b}}{m} \right) C_b(t) + q_{ab} C_a(t) + K_{v,b} C_w$$

$$V_a \frac{dC_a(t)}{dt} = q_{ba} C_b(t) - \left(q_{ab} + q_{a0} + \frac{K_{v,a}}{m} \right) C_a(t) + K_{v,a} C_w$$

6.4. Effect of Variation in Volatility

The volatility of the contaminant is directly proportional to the value of Henry's constant (m). Under similar conditions a contaminant with a higher m (more volatile) would have a higher inhalation exposure compared to a contaminant with a lower value m (less volatile). Figure 20 illustrates the variation in radon exposure with volatility.

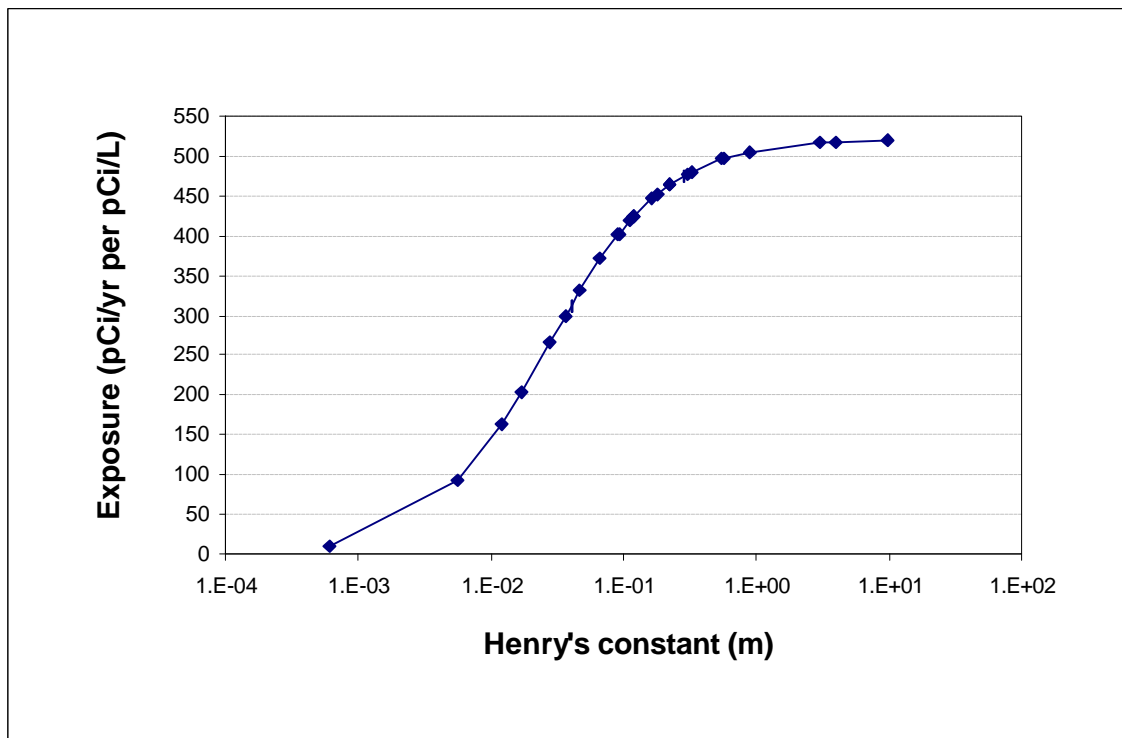


Figure 20: Effect of Volatility on Radon Inhalation Exposure

Figure 20 illustrates that the contaminants with the highest volatility have an almost constant value of exposure. This is due to the fact that, as volatility increases, the gas side resistance becomes insignificant and the liquid side resistance controls the mass transfer between the two phases. The value of $K_{OL}A$ is then independent of m , that is $K_{OL}A \cong K_LA$. And the exposure is independent of the Henry's constant and is evaluated from the concentration of the volatile contaminants in the gaseous phase, which remains the same.

The exposure was divided into its components from the three compartments. The results indicate that the main house contributes about 79% of the total exposure. This could be explained by the fact that the occupants of the house spend the maximum amount of time in this compartment. The percentage of total exposure contributed by the three compartments has been plotted on a pi chart shown in Figure 21.

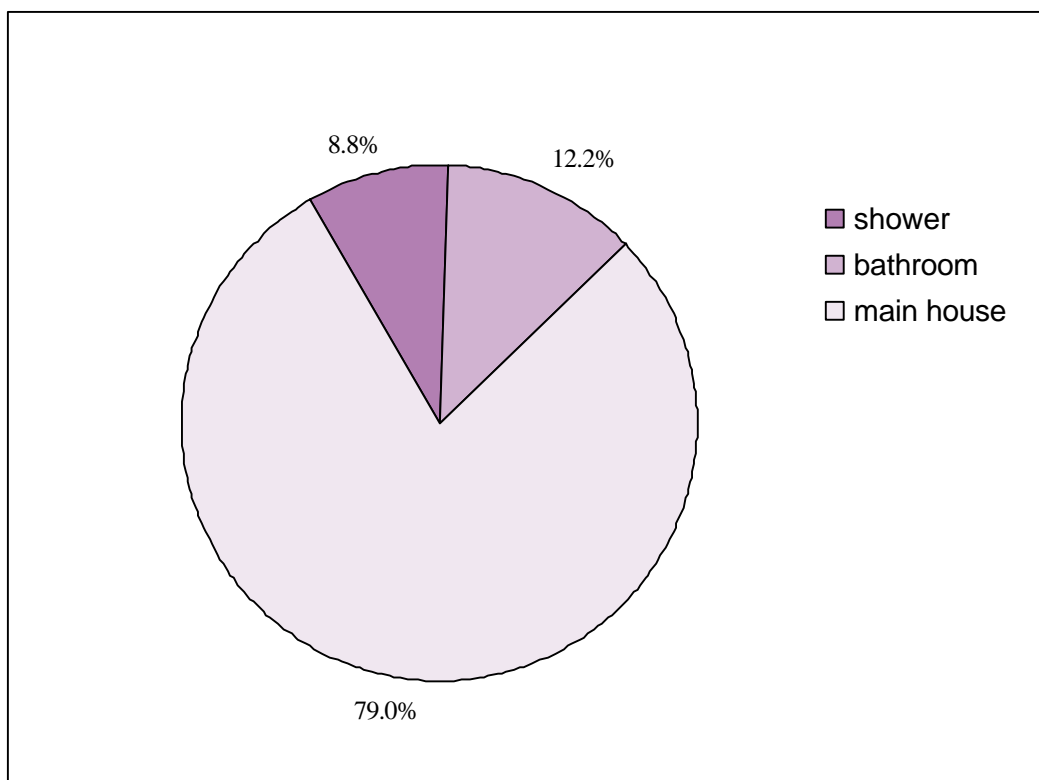


Figure 21: Percentage of exposure to radon from the different compartments.

Three different VOCs with Henry's constant ranging from 0.005 to 3.0 were chosen. The concentrations of these VOCs in the three compartments were obtained from the program. It is seen that the more volatile VOCs have a higher concentration in the each of the three compartments. The VOCs selected and their Henry's constants are given in Table 21. A comparison of the concentrations of VOCs in the shower is shown in Figure 22.

Table 22: Henry's constant for selected VOCs

Compound	m
Fluorotrichloromethane (CCl ₃ F)	3.0
Chloroform (CHCl ₃)	0.12
1,2-dibromo-3-chloropropane (DBCP)	0.005

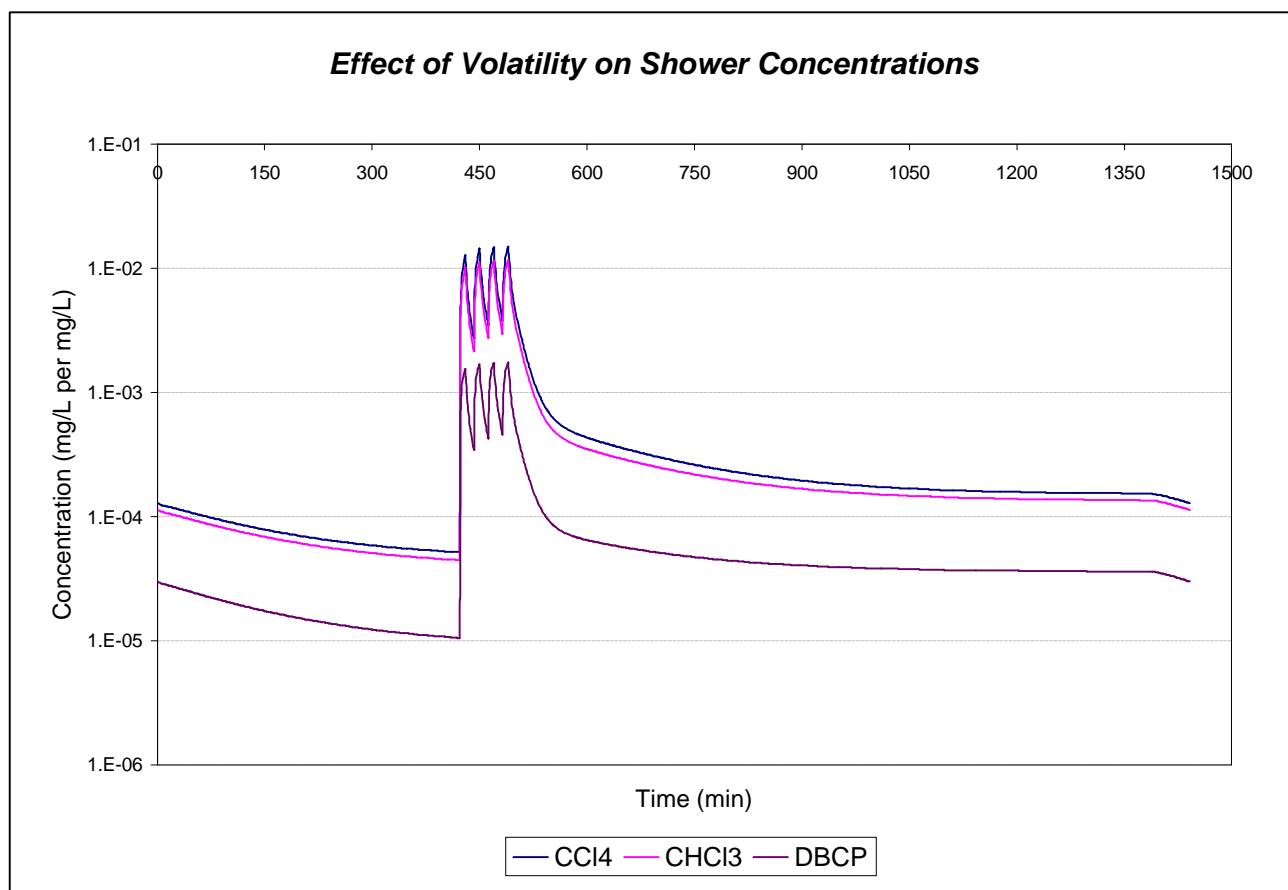


Figure 22: Effect of Volatility on Shower Concentrations

The effect of the release of VOC from water in the shower, bathroom and main house on exposure to Fluorotrichloromethane (CFCl_3), Chloroform (CHCl_3) and 1,2-dibromo-3-chloropropane (DBCP) was analyzed by turning the water release terms on and off in the three compartments. Sh, Ba and Mh respectively denote the Shower, Bathroom and Main House. Therefore, “Sh On”, “Ba On” and “Mh On” represent the cases where the VOCs are released only in the shower, bathroom and main house respectively. “All On” represents the case where the VOCs are released in all the three compartments. In the following analyses, the cases “All On”, “Sh On”, “Ba On”, and “Mh On” are respectively referred to as cases 1, 2, 3, and 4.

Exposures in the different compartments obtained from Case 1 are the sum of the exposures in from Cases 2, 3 and 4. This is illustrated by the calculations for CFCl_3 in the following table.

Table 23: Release Term Cases for CFCI₃

Case No.	Exposure to CFCI ₃		
	Shower	Bath	Main House
1	181.99	103.13	226.01
2	180.64	101.07	11.17
3	1.22	1.83	29.05
4	0.12	0.24	185.79
Σ(Sh + Ba + Mh)	181.99	103.13	226.01

By comparing the exposures in the compartments from Cases 2, 3 and 4 with the exposure from Case 1, the major factors contributing to the exposure in each of the compartments can be deduced. Also to examine the importance of volatility on the exposure, the K_{OL}A values in the three compartments for CFCI₃, CHCl₃ and DBCP were computed and are presented in Table 23.

Table 24: K_{OL}A values for VOCs

Compartment	K _{OL} A values (L/min)		
	CFCI ₃ (m = 3)	CHCl ₃ (m = 0.12)	DBCP (m = 0.005)
Shower	14.71	10.07	1.18
Bathroom	0.0317	0.0265	0.0053
Main House	0.0407	0.0339	0.0068

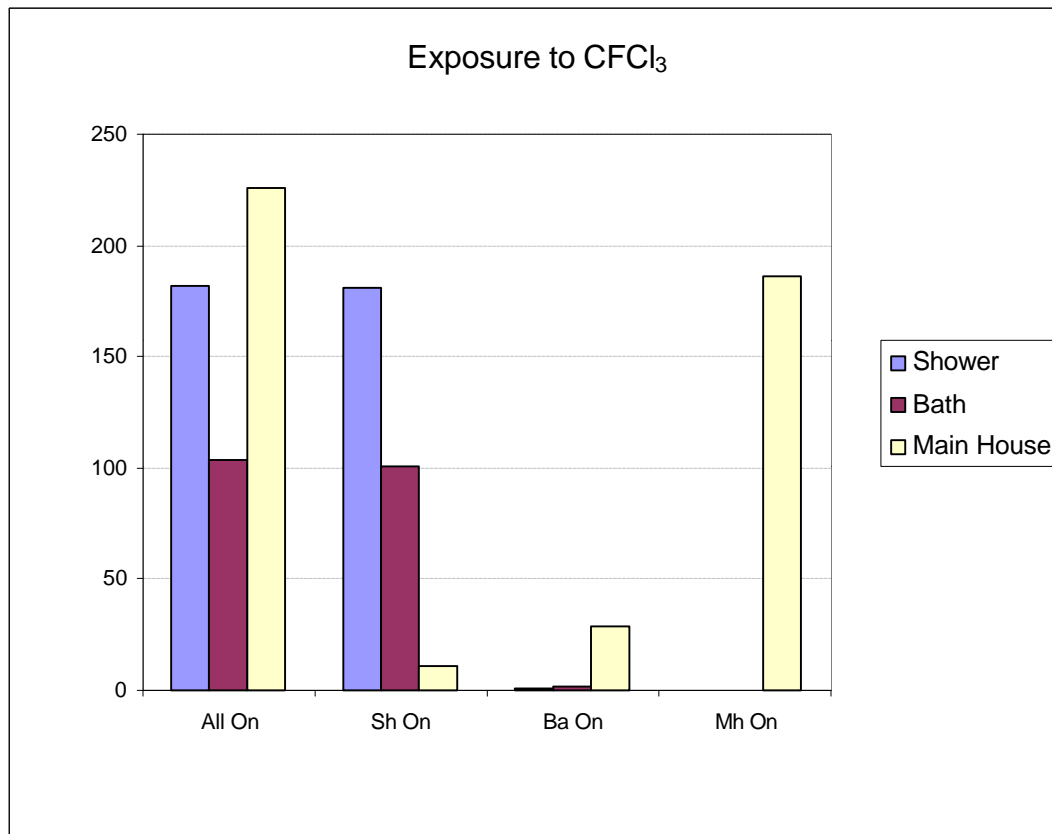


Figure 23: Effect of individual release terms on exposure to CFC₁₃

The effects of the different cases on exposure are seen in Figure 23.

- Case 2 reveals that the shower release term contributes primarily to the exposure in the shower and the bathroom. The $K_{OL}A$ for the shower is very high compared to the $K_{OL}A$ for the bathroom and the main house (Table 22). Hence, the magnitude of the release term for VOC, from the aqueous to the gaseous phase in the shower is quite substantial. Also the air in the shower is vented out only to the bathroom. Therefore, the shower release term also contributes to the exposure in the bathroom.
- Case 3 shows that the bathroom release term contributes minimally to the exposure in the main house and just barely to the exposure in the bathroom and the shower. The fact that the $K_{OL}A$ for the bathroom is quite low compared to the $K_{OL}A$ for the other compartments explains the low exposures in the compartments. The air in the bathroom is vented to the

main house and to the outside. Hence, the release of VOC in the bathroom does not contribute majorly to the exposure in the bathroom.

- Case 4 indicates that the major contribution to the exposure in the main house comes from the main house release term. The $K_{OL}A$ in the main house is quite high, which means that the magnitude of release of VOC from the water in the main house is quite substantial. Also the volume of the main house is quite large (~400,000 L), and hence the ventilation from the main house should not majorly decrease the exposure in the main house.

The effects of the release terms on exposures to $CHCl_3$ and DBCP are shown in Figures 18 and 19. These figures are very similar to Figure 17, the only difference being the magnitude of the exposure. The magnitude of the exposure in the three compartments is found to decrease with the decrease in the volatility of the VOC from $CFCl_3$ to DBCP.

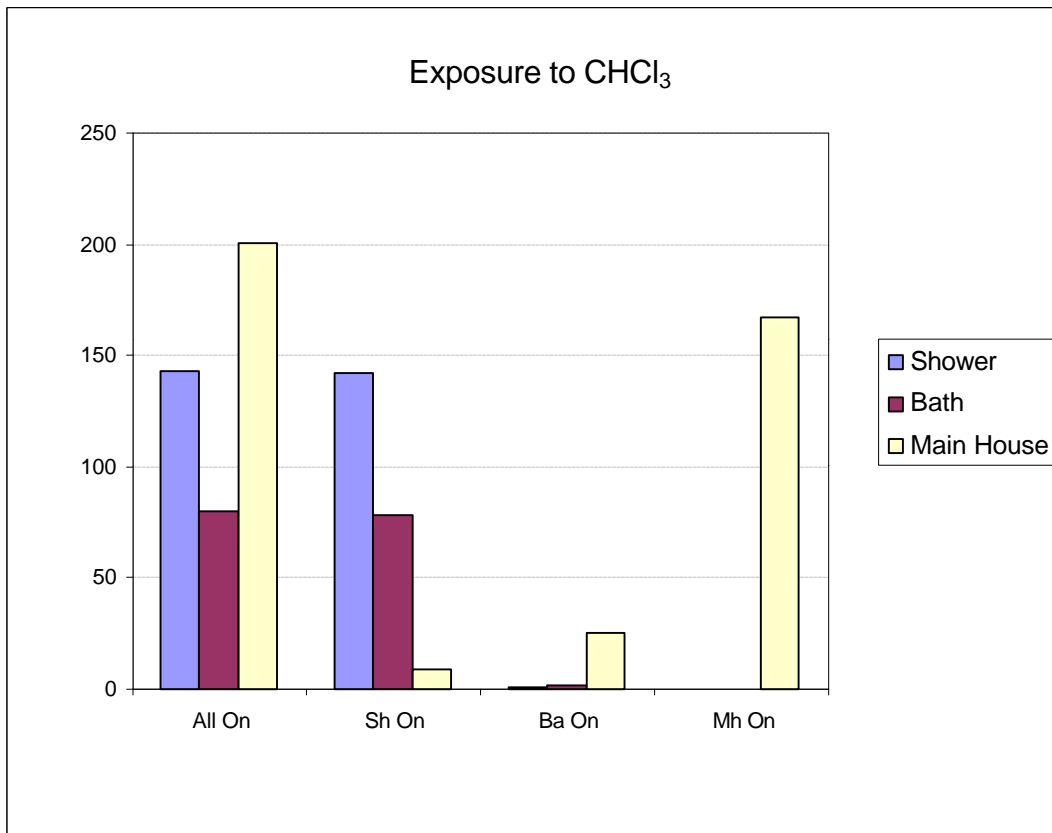


Figure 24: Effect of individual release terms on exposure to $CHCl_3$

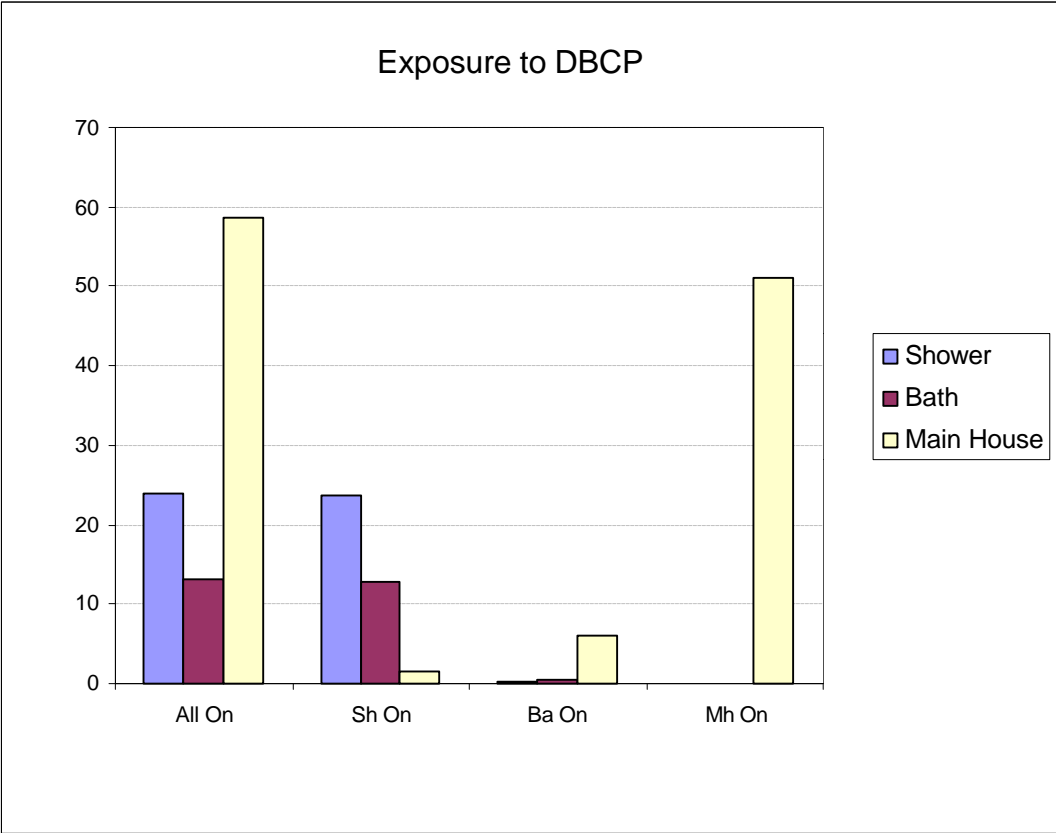


Figure 25: Effect of individual release terms on exposure to DBCP

SUMMARY, CONCLUSIONS AND FUTURE WORK

SUMMARY AND CONCLUSIONS

A previously developed EPA exposure model was re-implemented and used to calculate inhalation exposure to radon and daughter products originating in drinking water. The calculations were performed using a computer program developed in the C programming language. The program comprised three main features: a three compartment model that estimated the gas-phase concentrations in each of three different zones within a house, an exposure model that predicted exposure based on the concentration profiles as a function of time in each of the three compartments, and an uncertainty analysis carried out using a two-dimensional Monte-Carlo approach. Each of these three features of the program was independently verified and found to be reliable. The exposure estimates and associated uncertainty obtained from the program were compared with results obtained previously by the EPA for both radon and progeny, and found to be very similar. A sensitivity analysis was conducted to identify the most important variables that affect the exposure calculations, as well as to provide a further point of comparison between the previously developed computer code and that implemented in this project. Finally, the theoretical basis of the exposure model was extended to include the full range of VOCs and the effect of variation of volatility on inhalation exposure was evaluated. Inhalation exposure was found to decrease substantially for compounds of low volatility.

FUTURE WORK

The proposed future work includes:

- addition of other water using devices such as dishwashers, washing machines and kitchen sinks to the Three-Compartment Model using data collected by Richard Corsi (1995),
- formulation of exposure models for ingestion and dermal sorption,
- evaluation of exposure in non-residential environments such as schools and hospitals; improvement of the current model to facilitate incorporation of additional user-specified components,
- investigation of the impact of aerosols on exposure.

REFERENCES

1. Abramowitz, M. and Stegun, I. A., Handbook of mathematical functions with formulas, graphs and mathematical tables, U. S. Govt. Print. Off, Washington, DC, 1972.
2. Aggazzotti, G., Fantuzi, G., Tartoni, P.L., and Predieri, G., Plasma chloroform concentrations in swimmers using indoor swimming pools, *Arch. Envir. Health* 45, 175-179, 1990.
3. Andelman, J. B., Inhalation exposure in the home to volatile organic contaminants of drinking water, *The Science of The Total Environment* 47, 443-460, 1985 a.
4. Andelman, J. B., Human Exposures to Volatile Halogenated Organic Chemicals in Indoor and Outdoor Air, *Environmental Health Perspectives* 62, 313-318, 1985 b.
5. Andelman, J. B., Total exposure to volatile organic compounds in potable water, in *Significance and treatment of volatile organic compounds in water supplies*, Ram, N., Christman, R. and Cantor, K., Eds., Lewis Publishers, Ann Arbor, 485-504, 1990.
6. Bogen, K. T. and Spear, R. C., Integrating uncertainty and interindividual variability in environmental risk assessment, *Risk Analysis* 7, 427-436, 1987.
7. Bogen, K. T., Colston, B. W. and Machiao, L. K., Dermal absorption of dilute aqueous chloroform, trichloroethylene, and tetrachloroethylene in hairless guinea pigs, *Fundamental and Applied Toxicology*. 18, 30-39, 1992.
8. Coombes, et al., *Differential Equations with Mathematica*, John Wiley & sons, 1995.
9. Foster, S. A., and Chrostowski, P. C., Inhalation exposures to volatile organic contaminants in the shower, APCA – For presentation at the 80th Annual Meeting of the APCA, New York, New York, June 21-26, 1987.
10. Foster, S. A., and Chrostowski, P. C., Total exposure from contaminated tap water, APCA – For presentation at the 80th Annual Meeting of the APCA, New York, New York, June 21-26, 1987.
11. Georgopoulos, et al., Integrated Exposure and Dose Modeling and Analysis System. Formulation and Testing of Microenvironmental and Pharmacokinetic Components, *Environmental Science & Technology* 31,17-27, 1997.
12. Giardino, N. J., Esmen, N. A. and Andelman, J. B., Modeling volatilization of trichloroethylene from a domestic shower spray: the role of drop size distribution, *Environmental Science & Technology*, 26, 1602-1606, 1992.
13. Giardino, N. J. and Hageman, J. P., Pilot study of radon volatilization from showers with implications for dose, *Environmental Science & Technology*, 30, 1242-1244, 1996.

14. Hess, C. T., Weiffenbach, C. V. and Norton, S. A., Variations of airborne and waterborne Rn-222 in houses in Maine, *Environment International*, 8, 59-66, 1982.
15. Hopke, P. K., Radon and its decay products: occurrence, properties and health effects, American Chemical Society, Washington, DC, 1987.
16. Jo, W. K., Weisel, C. P. and Liroy, P. J., Routes of chloroform exposure and body burden from showering with chlorinated tap water, *Risk Analysis*, 10, 575-580, 1990 a.
17. Jo, W. K., Weisel, C. P. and Liroy, P. J., Chloroform exposure and the health risk associated with multiple uses of chlorinated tap water, *Risk Analysis*, 10, 581-585, 1990 b.
18. Lindstrom, A. B. and Pleil, J.D., A methodological approach for exposure assessment studies in residences using volatile organic compound – contaminated water, *Journal of the Air & Waste Management Association*, 46, 1058-1066, 1996.
19. Little, J. C., Applying the two-resistance theory to contaminant volatilization in showers, *Environmental Science & Technology*, 26, 1341-1349, 1992.
20. Macintosh, D. L., Xue, J., Ozkaynak, H., Spengler, J. D. and Ryan, P. B., A population based exposure model for Benzene, *Journal of Exposure Analysis and Environmental Epidemiology*, 5, 375-403, 1995.
21. McKone, T. E., Human exposure to volatile organic compounds in household tap water: The indoor inhalation pathway. *Environmental Science & Technology*, 21, 1194-1201, 1987.
22. McKone, T. E. and Howd, R. A., Estimating dermal uptake of nonionic organic chemicals from water and soil: I. Fugacity – based models for risk assessments. *Risk Analysis*, 12, 543-557, 1992.
23. McKone, T. E. and Knezovich, J. P., The transfer of trichloroethylene (TCE) from a shower to indoor air: experimental measurements and their implications, *Journal of the Air & Waste Management Association*, 41, 832-837, 1991.
24. Nazaroff, W. W, Doyle, S. M., Nero, A. V. and Sextro, R. G., Potable Water as a source of airborne ²²²Rn in U.S. Dwellings: A review and assessment, *Health Physics*, 52, 281-295, 1987.
25. Nazaroff, W. W and Nero, A. V., Radon and its decay products in indoor air, John Wiley & Sons, 1988.
26. Patel, J. K., Kapadia, C. H. and Owen, D. B., Handbook of statistical distributions. Marcel Dekker, New York, 1976.
27. Prichard, H. M. and Gesell, T. F., An estimate of population exposures due to radon in public water supplies in the area of Houston Texas, *Health Physics*, 41, 599-606, 1981.

28. Stern, A. H. and Andrews, L. R., The contribution of domestic water use to indoor air concentrations of chloroform in New York City apartments - a pilot study, *Toxicological and Environmental Chemistry*, 24, 71-81, 1989.
29. Tancrede, M., Yanagisawa, Y. and Wilson, R., Volatilization of volatile organic compounds from shower – I. Analytical method and quantitative assessment, *Atmospheric Environment*, 26A, 1103-1111, 1992.
30. Wallace, L. A., and Clayton, C. A., Volatile organic compounds in 600 US homes: Major sources of personal exposure. In *Indoor Air '87* Vol. 1, 183-187. Institute for Water, Soil and Air Hygiene, Berlin, 1987.
31. Wilkes, C. R., Small, M. J., Andelman, J. B., Giardino, N. J. and Marshall, J., Air quality model for volatile constituents from indoor uses of water, *Indoor Air '90 – Proceedings of the 5th International Conference on Indoor Air Quality and Climate*, 29th July – 3rd August 1990, Toronto.
32. Wilkes, C. R., Small, M. J., Andelman, J. B., Giardino, N. J. and Marshall, J., Inhalation exposure model for volatile chemicals from indoor uses of water, *Atmospheric Environment*, 26A, 2227-2236, 1992.

APPENDIX A

Influx and Efflux Terms for Radon and Progeny in the Three Compartments

Table 25: Influx Terms in the Mathematical Model

Contaminant	Compartment	Q_i	In_v	In_r
Radon	Shower	$C_w WFR_s P_s$	$q_{bs} C_{b,Rn}$	-
	Bathroom	$C_w WFR_b P_b$	$q_{sb} C_{s,Rn} + q_{ab} C_{a,Rn}$	-
	Main House	$C_w WFR_a P_a$	$q_{bs} C_{b,Rn}$	-
Polonium	Shower	-	$q_{bs} C_{b,Po}$	$k_{Po} C_{s,Rn} V_s$
	Bathroom	-	$q_{sb} C_{s,Po} + q_{ab} C_{a,Po}$	$k_{Po} C_{b,Rn} V_b$
	Main House	-	$q_{bs} C_{b,Po}$	$k_{Po} C_{a,Rn} V_a$
Lead	Shower	-	$q_{bs} C_{b,Pb}$	$k_{Pb} C_{s,Po} V_s$
	Bathroom	-	$q_{sb} C_{s,Pb} + q_{ab} C_{a,Pb}$	$k_{Pb} C_{b,Po} V_b$
	Main House	-	$q_{bs} C_{b,Pb}$	$k_{Pb} C_{a,Po} V_a$
Bismuth	Shower	-	$q_{bs} C_{b,Bi}$	$k_{Bi} C_{s,Pb} V_s$
	Bathroom	-	$q_{sb} C_{s,Bi} + q_{ab} C_{a,Bi}$	$k_{Bi} C_{b,Pb} V_b$
	Main House	-	$q_{bs} C_{b,Bi}$	$k_{Bi} C_{a,Pb} V_a$

Table 26: Efflux Terms in the Mathematical Model

Contaminant	Compartment	Out _v	Out _r	Out _p
Radon	Shower	$q_{sb} C_{s,Rn}$	$k_{Rn} C_{s,Rn} V_s$	-
	Bathroom	$(q_{bs} + q_{bo} + q_{ba}) C_{b,Rn}$	$k_{Rn} C_{b,Rn} V_b$	-
	Main House	$(q_{ab} + q_{ao}) C_{a,Rn}$	$k_{Rn} C_{a,Rn} V_a$	-
Polonium	Shower	$q_{sb} C_{s,Po}$	$k_{Po} C_{s,Po} V_s$	$[f_u DV_u + (1-f_u) DV_a] A_s C_{s,Po}$
	Bathroom	$(q_{bs} + q_{bo} + q_{ba}) C_{b,Po}$	$k_{Po} C_{b,Po} V_b$	$[f_u DV_u + (1-f_u) DV_a] A_s C_{b,Po}$
	Main House	$(q_{ab} + q_{ao}) C_{a,Po}$	$k_{Po} C_{a,Po} V_a$	$[f_u DV_u + (1-f_u) DV_a] A_s C_{a,Po}$
Lead	Shower	$q_{sb} C_{s,Pb}$	$k_{Pb} C_{s,Pb} V_s$	$[f_u DV_u + (1-f_u) DV_a] A_s C_{s,Pb}$
	Bathroom	$(q_{bs} + q_{bo} + q_{ba}) C_{b,Pb}$	$k_{Pb} C_{b,Pb} V_b$	$[f_u DV_u + (1-f_u) DV_a] A_s C_{b,Pb}$
	Main House	$(q_{ab} + q_{ao}) C_{a,Pb}$	$k_{Pb} C_{a,Pb} V_a$	$[f_u DV_u + (1-f_u) DV_a] A_s C_{a,Pb}$
Bismuth	Shower	$q_{sb} C_{s,Bi}$	$k_{Bi} C_{s,Bi} V_s$	$[f_u DV_u + (1-f_u) DV_a] A_s C_{s,Bi}$
	Bathroom	$(q_{bs} + q_{bo} + q_{ba}) C_{b,Bi}$	$k_{Bi} C_{b,Bi} V_b$	$[f_u DV_u + (1-f_u) DV_a] A_s C_{b,Bi}$
	Main House	$(q_{ab} + q_{ao}) C_{a,Bi}$	$k_{Bi} C_{a,Bi} V_a$	$[f_u DV_u + (1-f_u) DV_a] A_s C_{a,Bi}$

The mass balance for radon and progeny in the Three-Compartment Model can be expressed as:

Radon:

$$V_s \frac{dC_{s,Rn}(t)}{dt} = -(q_{sb} + V_s k_{Rn} + C_w WFR_s P_s) C_{s,Rn}(t) + q_{bs} C_{b,Rn}(t)$$

$$V_b \frac{dC_{b,Rn}(t)}{dt} = q_{sb} C_{s,Rn}(t) - (q_{bs} + q_{b0} + q_{ba} + V_b k_{Rn} + C_w WFR_b P_b) C_{b,Rn}(t) + q_{ab} C_{a,Rn}(t)$$

$$V_a \frac{dC_{a,Rn}(t)}{dt} = q_{ba} C_{b,Rn}(t) - (q_{ab} + q_{a0} + V_a k_{Rn} + C_w WFR_a P_a) C_{a,Rn}(t)$$

Polonium:

$$V_s \frac{dC_{s,Po}(t)}{dt} = -(q_{sb} + V_s k_{Po} + [f_u DV_u + (1 - f_u) DV_a] A) C_{s,Po}(t) + q_{bs} C_{b,Po}(t) + V_s k_{Po} C_{s,Rn}(t)$$

$$V_b \frac{dC_{b,Po}(t)}{dt} = q_{sb} C_{s,Po}(t) - (q_{bs} + q_{b0} + q_{ba} + V_b k_{Po} + [f_u DV_u + (1 - f_u) DV_a] A) C_{b,Po}(t) + q_{ab} C_{a,Po}(t) + V_b k_{Po} C_{b,Rn}(t)$$

$$V_a \frac{dC_{a,Po}(t)}{dt} = q_{ba} C_{b,Po}(t) - (q_{ab} + q_{a0} + V_a k_{Po} + [f_u DV_u + (1 - f_u) DV_a] A) C_{a,Po}(t) + V_a k_{Po} C_{a,Rn}(t)$$

Lead:

$$V_s \frac{dC_{s,Pb}(t)}{dt} = -(q_{sb} + V_s k_{Pb} + [f_u DV_u + (1 - f_u) DV_a] A) C_{s,Pb}(t) + q_{bs} C_{b,Pb}(t) + V_s k_{Pb} C_{s,Po}(t)$$

$$V_b \frac{dC_{b,Pb}(t)}{dt} = q_{sb} C_{s,Pb}(t) - (q_{bs} + q_{b0} + q_{ba} + V_b k_{Pb} + [f_u DV_u + (1 - f_u) DV_a] A) C_{b,Pb}(t) + q_{ab} C_{a,Pb}(t) + V_b k_{Pb} C_{b,Po}(t)$$

$$V_a \frac{dC_{a,Pb}(t)}{dt} = q_{ba} C_{b,Pb}(t) - (q_{ab} + q_{a0} + V_a k_{Pb} + [f_u DV_u + (1 - f_u) DV_a] A) C_{a,Pb}(t) + V_a k_{Pb} C_{a,Po}(t)$$

Bismuth:

$$V_s \frac{dC_{s,Bi}(t)}{dt} = -(q_{sb} + V_s k_{Bi} + [f_u DV_u + (1 - f_u) DV_a] A) C_{s,Bi}(t) + q_{bs} C_{b,Bi}(t) + V_s k_{Bi} C_{s,Pb}(t)$$

$$V_b \frac{dC_{b,Bi}(t)}{dt} = q_{sb} C_{s,Bi}(t) - (q_{bs} + q_{b0} + q_{ba} + V_b k_{Bi} + [f_u DV_u + (1 - f_u) DV_a] A) C_{b,Bi}(t) + q_{ab} C_{a,Bi}(t) + V_b k_{Bi} C_{b,Pb}(t)$$

$$V_a \frac{dC_{a,Bi}(t)}{dt} = q_{ba} C_{b,Bi}(t) - (q_{ab} + q_{a0} + V_a k_{Bi} + [f_u DV_u + (1 - f_u) DV_a] A) C_{a,Bi}(t) + V_a k_{Bi} C_{a,Pb}(t)$$

Table 27: Summary of PDFs Used in Three-Compartment Model

Variable	PDF _v	PDF _u	Values	
Number of people	PNUM ~ empirical	NA	1 = 0.192	4 = 0.164
			2 = 0.328	5 = 0.083
			3 = 0.183	6 = 0.049
Volume of shower	V _s ~ U(min, max)	min ~ U(a, b)	a = 1000	b = 1500
		max ~ U(c, d)	c = 2500	d = 3000
Volume of bathroom	V _b ~ TLN(gm, gsd, min, max)	ln ₂ (gm) ~ TS(m, s, qf)	m = ln(14)	min = 4
		ln(gsd) ~ INVCH(m, qf)	s = ln(1.66) qf = 25	max = 60
Total per capita volume of house	Vt1 ~ TLN(gm, gsd, min, max)	ln ₂ (gm) ~ TS(m, s, qf)	m = ln(205,000)	min = 35,000
		ln(gsd) ~ INVCH(m, qf)	s = ln(1.78) qf = 100	max = 1,100,000
	Vt2 ~ TLN(gm, gsd, min, max)	ln ₂ (gm) ~ TS(m, s, qf)	m = ln(144,000)	min = 30,000
		ln(gsd) ~ INVCH(m, qf)	s = ln(1.74) qf = 100	max = 700,000
Vt3 ~ TLN(gm, gsd, min, max)	ln ₂ (gm) ~ TS(m, s, qf)	m = ln(99,000)	min = 25,000	
	ln(gsd) ~ INVCH(m, qf)	s = ln(1.68) qf = 100	max = 450,000	
Vt4 ~ TLN(gm, gsd, min, max)	ln ₂ (gm) ~ TS(m, s, qf)	m = ln(89,000)	min = 20,000	
	ln(gsd) ~ INVCH(m, qf)	s = ln(1.67) qf = 100	max = 400,000	

	Vt5 ~ TLN(gm, gsd, min, max)	$\ln_2(\text{gm}) \sim \text{TS}(m, s, \text{qf})$ $\ln(\text{gsd}) \sim \text{INVCH}(m, \text{qf})$	$m = \ln(75,000)$ $s = \ln(1.70)$ $\text{qf} = 100$	min = 15,000 max = 350,000
	Vt6 ~ TLN(gm, gsd, min, max)	$\ln_2(\text{gm}) \sim \text{TS}(m, s, \text{qf})$ $\ln(\text{gsd}) \sim \text{INVCH}(m, \text{qf})$	$m = \ln(54,000)$ $s = \ln(1.78)$ $\text{qf} = 100$	min = 10,000 max = 300,000
Shower flow rate	SFR ~ TLN(gm, gsd, min, max)	$\ln_2(\text{gm}) \sim \text{TS}(m, s, \text{qf})$ $\ln(\text{gsd}) \sim \text{INVCH}(m, \text{qf})$	$m = \ln(7.1)$ $s = \ln(1.54)$ $\text{qf} = 100$	min = 3 max = 24
Per capita water use in bathroom	WUb ~ U(min, max)	min ~ U (a, b) max ~ U (c, d)	a = 15 c = 75	b = 20 d = 80
Total per capita water use	Wut1 ~ TLN(gm, gsd, min, max)	$\ln_2(\text{gm}) \sim \text{TS}(m, s, \text{qf})$ $\ln(\text{gsd}) \sim \text{INVCH}(m, \text{qf})$	$m = \ln(304)$ $s = \ln(1.32)$ $\text{qf} = 25$	min = 150 max = 560
	Wut2 ~ TLN(gm, gsd, min, max)	$\ln_2(\text{gm}) \sim \text{TS}(m, s, \text{qf})$ $\ln(\text{gsd}) \sim \text{INVCH}(m, \text{qf})$	$m = \ln(256)$ $s = \ln(1.32)$ $\text{qf} = 25$	min = 130 max = 520
	Wut3 ~ TLN(gm, gsd, min, max)	$\ln_2(\text{gm}) \sim \text{TS}(m, s, \text{qf})$ $\ln(\text{gsd}) \sim \text{INVCH}(m, \text{qf})$	$m = \ln(258)$ $s = \ln(1.23)$ $\text{qf} = 25$	min = 110 max = 480
	Wut4 ~ TLN(gm, gsd, min, max)	$\ln_2(\text{gm}) \sim \text{TS}(m, s, \text{qf})$ $\ln(\text{gsd}) \sim \text{INVCH}(m, \text{qf})$	$m = \ln(232)$ $s = \ln(1.26)$ $\text{qf} = 25$	min = 90 max = 440

	Wut5 ~ TLN(gm, gsd, min, max)	$\ln_2(\text{gm}) \sim \text{TS}(m, s, \text{qf})$ $\ln(\text{gsd}) \sim \text{INVCH}(m, \text{qf})$	$m = \ln(214)$ $s = \ln(1.16)$ $\text{min} = 70$	$\text{max} = 400$ $\text{qf} = 10$
	Wut6 ~ TLN(gm, gsd, min, max)	$\ln_2(\text{gm}) \sim \text{TS}(m, s, \text{qf})$ $\ln(\text{gsd}) \sim \text{INVCH}(m, \text{qf})$	$m = \ln(214)$ $s = \ln(1.16)$ $\text{min} = 70$	$\text{max} = 400$ $\text{qf} = 10$
Shower air residence time	$R_a \sim U(\text{min}, \text{max})$	$\text{min} \sim U(a, b)$ $\text{max} \sim U(c, d)$	$a = 2$ $c = 4$	$b = 3$ $d = 6$
Bathroom air residence time (door open)	$R_{b1} \sim U(\text{min}, \text{max})$	$\text{min} \sim U(a, b)$ $\text{max} \sim U(c, d)$	$a = 20$ $c = 40$	$b = 30$ $d = 50$
Bathroom air residence time (door closed)	$R_{b2} \sim U(\text{min}, \text{max})$	$\text{min} \sim U(a, b)$ $\text{max} \sim U(c, d)$	$a = 20$ $c = 150$	$b = 30$ $d = 250$
Bathroom fan exhaust rate	$\text{EXFR} \sim \text{TRI}(\text{min}, \text{max}, \text{mode})$	$\text{mode} \sim U(a, b)$	$\text{min} = 1000$ $\text{max} = 5000$	$a = 2000$ $b = 2500$
Main house ventilation rate	$\text{VR}_a \sim \text{TLN}(\text{gm}, \text{gsd}, \text{min}, \text{max})$	$\ln_2(\text{gm}) \sim \text{TS}(m, s, \text{qf})$ $\ln(\text{gsd}) \sim \text{INVCH}(m, \text{qf})$	$m = \ln(0.68)$ $s = \ln(2.01)$ $\text{qf} = 25$	$\text{min} = 0.1$ $\text{max} = 2$
Radon transfer efficiency in Shower	$P_s \sim U(\text{min}, \text{max})$	$\text{min} \sim U(a, b)$ $\text{max} \sim U(c, d)$	$a = 0.5$ $c = 0.7$	$b = 0.6$ $d = 0.8$
Radon transfer efficiency in Bathroom	$P_b \sim U(\text{min}, \text{max})$	$\text{min} \sim U(a, b)$ $\text{max} \sim U(c, d)$	$a = 0.15$ $c = 0.35$	$b = 0.25$ $d = 0.45$
Radon transfer efficiency in Main House	$P_a \sim U(\text{min}, \text{max})$	$\text{min} \sim U(a, b)$ $\text{max} \sim U(c, d)$	$a = 0.4$ $c = 0.7$	$b = 0.5$ $d = 0.8$

Unattached fraction	UFRACT ~ B(mean, mode, min, max)	mean ~ U(a, b)	a = 0.05	min = 0
		mode ~ TRI(min, mean, 0.5*(min mean))	b = 0.15	max = 1
Deposition velocity of unattached fraction	DVu ~ U(min, max)	min ~ U(a, b)	a = 1	c = 16
		max ~ U(c, d)	b = 4	d = 22
Deposition velocity of attached fraction	DVu ~ U(min, max)	min ~ U(a, b)	a = 0.01	c = 0.1
		max ~ U(c, d)	b = 0.05	d = 0.3
Time in shower	Ts ~ TLN(gm, gsd, min, max)	ln ₂ (gm) ~ TS(m, s, qf)	m = ln(6.8)	min = 1
		ln(gsd) ~ INVCH(m, qf)	s = ln(1.6)	max = 30
			qf = 100	
Time in bathroom	Tb ~ U(min, max)	min ~ U(a, b)	a = 1	c = 20
		max ~ U(c, d)	b = 10	d = 30
Breathing rate	BR ~ TN(mean, std, min, max)	mean ~ TS(m, s, qf)	m = 9.1	min = 2.6
		std ² ~ INVCH(m, qf)	s = 2.0	max = 46.6
			qf = 10	
Occupancy factor	OF ~ B(mean, mode, min, max)	mean ~ U(a, b)	a = 0.65	min = 0.33
		mode ~ U(mean, max) or U(min, mean)	b = 0.80	max = 1.0

APPENDIX B

Details of Numerical Solution to the Mathematical Model

The mass balance for radon/VOC can be rewritten as:

$$\frac{dC_s}{dt} = \dot{C}_s = e(t, C_s, C_b, C_a)$$

$$\frac{dC_b}{dt} = \dot{C}_b = f(t, C_s, C_b, C_a)$$

$$\frac{dC_a}{dt} = \dot{C}_a = g(t, C_s, C_b, C_a)$$

where

$$e = a_{11}C_s + a_{12}C_b + a_{13}C_a + Q_s$$

$$f = a_{21}C_s + a_{22}C_b + a_{23}C_a + Q_b$$

$$g = a_{31}C_s + a_{32}C_b + a_{33}C_a + Q_a$$

The fourth order Runge Kutta method for solving the above system of equations is:

- For shower air concentration, C_s

$$k_1 = he(t_0, C_{s0}, C_{b0}, C_{a0})$$

$$k_2 = he\left(t_0 + \frac{1}{2}h, C_{s0} + \frac{1}{2}k_1, C_{b0} + \frac{1}{2}m_1, C_{a0} + \frac{1}{2}n_1\right)$$

$$k_3 = he\left(t_0 + \frac{1}{2}h, C_{s0} + \frac{1}{2}k_2, C_{b0} + \frac{1}{2}m_2, C_{a0} + \frac{1}{2}n_2\right)$$

$$k_4 = he(t_0 + h, C_{s0} + k_3, C_{b0} + m_3, C_{a0} + n_3)$$

$$C_{s1} = C_{s0} + \frac{(k_1 + 2k_2 + 2k_3 + k_4)}{6}$$

- For bathroom air concentration, C_b

$$m_1 = hf(t_0, C_{s0}, C_{b0}, C_{a0})$$

$$m_2 = hf\left(t_0 + \frac{1}{2}h, C_{s0} + \frac{1}{2}k_1, C_{b0} + \frac{1}{2}m_1, C_{a0} + \frac{1}{2}n_1\right)$$

$$m_3 = hf\left(t_0 + \frac{1}{2}h, C_{s0} + \frac{1}{2}k_2, C_{b0} + \frac{1}{2}m_2, C_{a0} + \frac{1}{2}n_2\right)$$

$$m_4 = hf(t_0 + h, C_{s0} + k_3, C_{b0} + m_3, C_{a0} + n_3)$$

$$C_{b1} = C_{b0} + \frac{(m_1 + 2m_2 + 2m_3 + m_4)}{6}$$

- For main house air concentration, C_a

$$n_1 = hg(t_0, C_{s0}, C_{b0}, C_{a0})$$

$$n_2 = hg\left(t_0 + \frac{1}{2}h, C_{s0} + \frac{1}{2}k_1, C_{b0} + \frac{1}{2}m_1, C_{a0} + \frac{1}{2}n_1\right)$$

$$n_3 = hg\left(t_0 + \frac{1}{2}h, C_{s0} + \frac{1}{2}k_2, C_{b0} + \frac{1}{2}m_2, C_{a0} + \frac{1}{2}n_2\right)$$

$$n_4 = hg(t_0 + h, C_{s0} + k_3, C_{b0} + m_3, C_{a0} + n_3)$$

$$C_{a1} = C_{a0} + \frac{(n_1 + 2n_2 + 2n_3 + n_4)}{6}$$

In the above equations the first subscript denotes the concentration C_s , C_b , C_a and the second subscript denotes the value of C_i 's being calculated corresponding to the t value being used, i.e., C_{s0} is the value of C_s corresponding to t_0 . Also the calculation is shown for $t = t_0$, after one such calculation the time t is increased to $t_1 = t_0 + h$ where 'h' is the time step used. Time step used is $h = 1$ min.

The Q_i 's are evaluated based on the compartment usage patterns. The numerical integration using the Runge Kutta procedure is carried out a few times until a periodic solution reaching steady state is obtained. Hence any reasonable value might be used as a first guess for the initial conditions, C_{s0} , C_{b0} , C_{a0} .

APPENDIX C

Details of Analytical Solution to the Mathematical Model

The set of simultaneous differential equations describing change of concentrations in the Three-Compartment Model is:

$$\begin{aligned}\frac{dC_s}{dt} &= a_{11}C_s + a_{12}C_b + a_{13}C_a + b^1(t) \\ \frac{dC_b}{dt} &= a_{21}C_s + a_{22}C_b + a_{23}C_a + b^2(t) \\ \frac{dC_a}{dt} &= a_{31}C_s + a_{32}C_b + a_{33}C_a + b^3(t)\end{aligned}$$

For a homogeneous linear system of form,

$$\frac{dX}{dt} = A X$$

a straight-line solution may be found as,

$$X(t) = \exp(I t) X_0$$

where X_0 is a non-zero constant vector which satisfies

$$A X_0 = I X_0$$

The constant λ is called an eigenvalue of the matrix A, and X_0 is called an eigenvector associated to the eigenvalue λ of the matrix A.

Therefore, the above set of simultaneous differential equations can be represented in the matrix form and solved to obtain eigenvalues:

$$|A - I\lambda| = 0$$

where

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

λ_i = Eigenvalues of the equation.

I = Identity matrix of order 3.

The Identity Matrix for this equation would be of order 3 x 3:

$$I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The eigenvectors are obtained from the following equation:

$$(A - I_i I) X^{(i)} = 0$$

where

$$X^{(i)} = \text{Column eigenvector for a particular eigenvalue } \lambda_i.$$

Based on the eigenvectors calculated for the different time intervals, general and particular solutions are obtained as:

Particular solution:

$$d_i = \begin{bmatrix} d_1^i \\ d_2^i \\ d_3^i \end{bmatrix} \quad \text{from} \quad A d_i = -b_i$$

General Solution (if λ_i are distinct):

$$C^i(t) = d_i + \sum_{j=1}^3 k_j^i X^{(j)} e^{\lambda_j t}$$

Constant k_j is determined from initial conditions at $t = 0$

$$C^i(0) = d_i + \sum_{j=1}^3 k_j^i X^{(j)}$$

that is,

$$E(t) = \begin{bmatrix} e^{\lambda_1 t} & 0 & 0 \\ 0 & e^{\lambda_2 t} & 0 \\ 0 & 0 & e^{\lambda_3 t} \end{bmatrix}$$

$$F = \begin{bmatrix} X^{(1)} & X^{(2)} & X^{(3)} \end{bmatrix}$$

For the different time intervals,

$$0 \leq t \leq T_1$$

$$E(T_1) = \begin{bmatrix} e^{I_1 T_1} & 0 & 0 \\ 0 & e^{I_2 T_1} & 0 \\ 0 & 0 & e^{I_3 T_1} \end{bmatrix}$$

$$T_1 \leq t \leq T_2$$

$$E(T_2) = \begin{bmatrix} e^{I_1 T_2} & 0 & 0 \\ 0 & e^{I_2 T_2} & 0 \\ 0 & 0 & e^{I_3 T_2} \end{bmatrix}$$

and so on...

The particular solutions are obtained by solving the equation $Ad_j = -b_j$ for each time interval.

For the first time interval: $0 \leq t \leq T_1$

$$Ad_1 = -b_1$$

For this time interval the concentrations are given by:

$$C^1(t) = d_1 + \sum_{j=1}^3 k_j^1 X^{(j)} e^{I_j t} = d_1 + FE(t)k^1$$

Using the initial condition:

$$C^1(0) = d_1 + Fk^1$$

For the second time interval: $T_1 \leq t \leq T_2$

$$Ad_2 = -b_2$$

For this time interval the concentrations are given by:

$$C^2(t) = d_2 + \sum_{j=1}^3 k_j^2 X^{(j)} e^{I_j t} = d_2 + FE(t)k^2$$

Using the initial condition:

$$\begin{aligned} C^1(T_1) &= C^2(T_1) \\ \Rightarrow d_1 + FE(T_1)k^1 &= d_2 + FE(T_2)k^2 \end{aligned}$$

For the third time interval: $T_2 \leq t \leq T_3$

$$Ad_3 = -b_3$$

For this time interval the concentrations are given by:

$$C^3(t) = d_3 + \sum_{j=1}^3 k_j^3 X^{(j)} e^{I_j t} = d_3 + FE(t)k^3$$

Using the initial condition:

$$\begin{aligned} C^2(T_2) &= C^3(T_2) \\ \Rightarrow d_2 + FE(T_2)k^2 &= d_3 + FE(T_3)k^3 \end{aligned}$$

For the fourth time interval: $T_3 \leq t \leq T_4$

$$Ad_4 = -b_4$$

For this time interval the concentrations are given by:

$$C^4(t) = d_4 + \sum_{j=1}^3 k_j^4 X^{(j)} e^{I_j t} = d_4 + FE(t)k^4$$

Using the initial condition:

$$\begin{aligned} C^3(T_3) &= C^4(T_3) \\ \Rightarrow d_3 + FE(T_3)k^3 &= d_4 + FE(T_4)k^4 \end{aligned}$$

$$k^1 = F^{-1}[C^1(0) - d_1]$$

$$k^2 = k^1 + E^{-1}(T_1)F^{-1}[d_1 - d_2]$$

$$k^3 = k^2 + E^{-1}(T_2)F^{-1}[d_2 - d_3]$$

$$k^4 = k^3 + E^{-1}(T_3)F^{-1}[d_3 - d_4]$$

Simplifying,

$$k^2 = F^{-1}[C^1(0) - d_1] + E^{-1}(T_1)F^{-1}[d_1 - d_2]$$

$$k^3 = F^{-1}[C^1(0) - d_1] + E^{-1}(T_1)F^{-1}[d_1 - d_2] + E^{-1}(T_2)F^{-1}[d_2 - d_3]$$

$$k^4 = F^{-1}[C^1(0) - d_1] + E^{-1}(T_1)F^{-1}[d_1 - d_2] + E^{-1}(T_2)F^{-1}[d_2 - d_3] + E^{-1}(T_3)F^{-1}[d_3 - d_4]$$

Using the values of the k vectors, the concentrations in the different compartments can be evaluated as:

$$0 \leq t \leq T_1$$

$$C^1(t) = d_1 + F E(t)F^{-1}[C^1(0) - d_1]$$

$$T_1 \leq t \leq T_2$$

$$C^2(t) = d_2 + F E(t)\{F^{-1}[C^1(0) - d_1] + E^{-1}(T_1)F^{-1}[d_1 - d_2]\}$$

$$T_2 \leq t \leq T_3$$

$$C^3(t) = d_3 + F E(t)\{F^{-1}[C^1(0) - d_1] + E^{-1}(T_1)F^{-1}[d_1 - d_2] + E^{-1}(T_2)F^{-1}[d_2 - d_3]\}$$

$$T_3 \leq t \leq T_4$$

$$C^4(t) = d_4 + F E(t)\left\{F^{-1}[C^1(0) - d_1] + E^{-1}(T_1)F^{-1}[d_1 - d_2] + E^{-1}(T_2)F^{-1}[d_2 - d_3] + E^{-1}(T_3)F^{-1}[d_3 - d_4]\right\}$$

By substituting we obtain the initial concentration

$$C^1(0) = \left[I - F E(T_4) F^{-1} \right]^{-1} \{ d_4 + F E(T_3) L \}$$

where

$$L = -F^{-1} d_1 + E^{-1}(T_1) F^{-1} [d_1 - d_2] + E^{-1}(T_2) F^{-1} [d_2 - d_3] + E^{-1}(T_3) F^{-1} [d_3 - d_4]$$

VITA

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