Chemical Contaminants in Drinking Water: An Integrated Exposure Analysis

Rajesh Khanal

Thesis submitted to the Faculty of the

Virginia Polytechnic Institute and State University

in partial fulfillment of the requirements for the degree of

Master of Science

in

Environmental Engineering

Dr. John C. Little, Chair

Dr. Marc A. Edwards

Dr. Daniel L. Gallagher

May, 1999

Blacksburg, Virginia

Keywords: Contaminant, Uncertainty, Exposure, Monte Carlo simulation

Chemical Contaminants in Drinking Water: An Integrated Exposure Analysis

Rajesh Khanal

(ABSTRACT)

The objective of this research is to develop an integrated exposure model, which performs uncertainty analysis of exposure to the entire range of chemical contaminants in drinking water via inhalation, ingestion and dermal sorption. The study is focused on a residential environment. The various water devices considered are shower, bath, bathroom, kitchen faucet, washing machine and the dishwasher. All devices impact inhalation exposure, while showering, bathing and washing hands are considered in the analysis of dermal exposure.

A set of transient mass balance equations are solved numerically to predict the concentration profiles of a chemical contaminant for three different compartments in a house (shower, bathroom and main house). Inhalation exposure is computed by combining this concentration profile with the occupancy and activity patterns of a specific individual. Mathematical models of dermal penetration, which account for steady and non-steady state analysis, are used to estimate exposure via dermal absorption. Mass transfer coefficients are used to compute the fraction of contaminant remaining in water at the time of ingestion before estimating ingestion exposure.

Three chemical contaminant in water: chloroform, chromium and methyl parathion are considered for detailed analysis. These contaminants cover a wide range in chemical properties. The magnitude of overall exposure and comparison of the relative contribution of individual exposure pathways for each contaminant is evaluated.

The major pathway of exposure for chloroform is inhalation, which accounts for $2/3^{rd}$ of the total exposure. Dermal absorption and ingestion exposures contribute almost equally to the remaining $1/3^{rd}$ of total exposure for chloroform. Ingestion accounts for about 60% of total exposure for methyl parathion and the remaining 40% of exposure is via dermal sorption. Nearly all of the total exposure (98%) for chromium is via the ingestion pathway.

Acknowledgements

I'd like to express my sincere gratitude to my advisor, Dr. John C. Little for his constant support, encouragement and guidance during my research work at Virginia Tech. I'd also like to thank my other committee members, Dr. Daniel Gallagher and Dr. Marc Edwards for their insights and suggestions.

Gratitude is also expressed to the EPA Office of water for providing financial assistance and particularly to Dr. Nancy Chiu for her encouragement and support.

Finally, I'd like to thank my family, particularly my wife Upasana and son, Umanga without whose love, support, patience and encouragement this thesis would not have been possible.

TABLE OF CONTENTS

ABSTRACT ii

ACKNOWLEDGEMENTS iii

1. INTRODUCTION 1

2. OBJECTIVES 7

3. DESCRIPTION OF THE INTEGRATED EXPOSURE MODEL 9

3.1 PROPERTIES OF CHEMICAL CONTAMINANTS IN WATER 10
3.2 MASS TRANSFER COEFFICIENTS 11
3.3 EXPOSURE PATHWAYS 14
3.3.1 Inhalation Exposure 14
3.3.1.1 Shower/Bath 16
3.3.1.2 Bathroom 18
3.3.1.3 Main House 19
3.3.2 Ingestion 24
3.3.3 Dermal Absorption 25
3.3.4 Activity Pattern 28
3.3.4.1 Human Activity Pattern 28
3.3.4.2 Water Usage Pattern 29
3.3.5 Exposure Computations 30
3.3 UNCERTAINTY ANALYSIS 31
3.3 DEFAULT COMPUTATION 35
3.4 VISUALLY BASED COMPUTER PACKAGE 35

4. VERIFICATION OF THE MODEL 36

4.1 EXTENDED THREE COMPARTMENT MODEL 36
4.1.1 Numerical Solution 36
4.1.2 Analytical Solution 36
4.2 EXPOSURE MODEL 36
4.3 COMPARISON OF PDFS WITH EXCEL FUNCTIONS 37
4.3.1 Truncated Normal Distribution 38
4.3.2 Truncated Lognormal Distribution 39
4.3.3 Beta Distribution 41
4.3.4 Student's-t Distribution 43
4.3.5 Chi-squared Distribution 45
4.4 CONCLUSIONS 46

5. RESULTS AND DISCUSSION 47

5.1 THE MODEL OUTPUT 47
5.2 COMPARISON WITH THE PREVIOUS MODEL 54
5.3 SENSITIVITY ANALYSIS 56

6. FUTURE WORK 61

6.1 RECOMMENDATIONS ON ADDITIONAL DATA AND UNCERTAINTY ANALYSIS 61
6.2 ADDITIONAL SOURCES 62
6.3 LUNG-DEPOSITION MODEL 63
6.4 NON RESIDENTIAL ENVIRONMENTS 64
6.5 MULTI-COMPARTMENT MODEL 65

6.6 COUPLING WITH PBPK MODEL 66

REFERENCES 67

APPENDIX A 71

APPENDIX B 74

APPENDIX C 82

VITA 96

LIST OF TABLES

1. PROPERTIES OF REPRESENTATIVE CONTAMINANTS 11
2. CASES FOR BATHROOM VENTILATION 19
3. INPUT VARIABLES FOR WASHING MACHINE 20
4. INPUT VARIABLES FOR DISHWASHER 22
5. COMPARISON OF EXCEL RESULTS FROM PROGRAM AND EXCEL 37
6. COMPARISON OF TRUNCATED NORMAL VARIABLE VALUES 38
7. COMPARISON OF TRUNCATED LOG NORMAL VARIABLE VALUES 40
8. COMPARISON OF BETA VARIABLE VALUES 42
9. COMPARISON OF STUDENT'S t VARIABLE VALUES 44
10. COMPARISON OF CHI SQUARED VARIABLE VALUES 45
11. PARAMETERS OF PDFs FOR TOTAL EXPOSURE 54
12. DEFAULT VALUES OF INPUT VARIABLES IN THE MODEL 57
13. RATE OF CHANGE OF EXPOSURE 59
14. VARIABLES REQUIRING ADDITIONAL DATA 62
15. SOURCE/SINK TERMS IN THE MATHEMATICAL MODEL 72
16. PARAMETERS FOR EMPIRICAL DISTRIBUTION FOR PNUM 83
17. PARAMETERS OF LOG NORMAL DISTRIBUTION FOR V_t 85
18. PDFs FOR R_b BASED ON CASES OF BATHROOM VENTILATION 88
19. SUMMARY OF MODEL VARIABLES WITH KNOWN PDFs 92
20. EXPERIMENTAL DATA USED BY THE MODEL 95

LIST OF FIGURES

1. Modified Three-Compartment Model 10
2. Change in Concentration of Chloroform in Bath Water 18
3. Schematic of Dermal Sorption Process 25
4. Flow Chart for the Computer Program 34
5. Comparison of Normal Variable Values from Program and Excel 39
6. Comparison of Log Normal Variable Values from Program and Excel 41
7. Comparison of Beta Variable Values from Program and Excel 43
8. Comparison of Student's t Variable Values from Program and Excel 44
9. Comparison of Chi Squared Variable Values from Program and Excel 46
10a. Concentration Profile of Chloroform – Washing Machine - Off 48
10b. Concentration Profile of Chloroform – Washing Machine - On 48
11a. Concentration Profile of Methyl parathion – Washing Machine - Off 49
11b. Concentration Profile of Methyl parathion – Washing Machine - On 49
12. Impact of Each Exposure Pathway for Chloroform 50
13. Impact of Each Exposure Pathway for Methyl parathion 50
14. Impact of Each Exposure Pathway for Chromium 51
15. Median Values of Exposures for the Three Contaminants 51
16. Bounds of Total Exposure for Chloroform 52
17. Bounds of Total Exposure for Methyl parathion 53
18. Bounds of Total Exposure for Chromium 53
19. Bounds of Inhalation Exposure to Radon 55
20. Schematic Representation of Lung Model 64
21. User-Defined Multi-Compartment Model 65
22. PDF Curve 75
23. CDF Curve 76

1. INTRODUCTION

Potable water can be 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" (AWWA, 1990). Although, biological contaminants have traditionally received more attention from a public health standpoint, in recent years, there has been growing concern for chemical contaminants present in drinking water that might be hazardous to human health.

Exposure to many contaminants in water is thought to lead to human health problems ranging from minor effects such as fatigue to more serious effects such as cancer (Wilkes et al., 1992). A large number of public and private water supplies serving community households are contaminated with potentially hazardous chemicals. Most public water supplies depend on a chlorine disinfection process, which may produce water containing chloroform and other trihalomethanes (Lindstrom and Pleil, 1996). In addition, a wide variety of volatile and synthetic organic chemicals, pesticides, inorganic chemicals and radionuclides have been detected in water supplies (AWWA, 1990). Drinking tap water and using different water devices in indoor environments can, therefore, be potential sources of exposure to chemical contaminants.

The establishment of safety standards (maximum contaminant levels) for chemicals in drinking water has generally, been based on the assumption that ingestion is the primary route for human exposure. However, recent research has shown that inhalation exposure, during water use activities like showering and bathing, can have an equally significant, if not higher, impact on human exposure (Andelman, 1990). Also, exposure due to dermal absorption of chemicals during bathing has been shown to be comparable to direct ingestion of water (Brown et al., 1984).

Radon was one of the first contaminants studied extensively while considering the inhalation exposure route for the indoor environment. A study by Pritchard and Gessel (1981) concluded that the negative health impact of radon in drinking water is nearly comparable to the effect of radon released during mining and milling of uranium in the U.S. The EPA, during the discussion of the possible revision of its drinking water regulations (EPA, 1983) noted that "Airborne exposure from radon released into the home from water might be more significant than

direct ingestion from drinking water" and that "It appears that radon may contribute one of the most significant cancer risks of any substance in drinking water." Nazaroff et al (1987) concluded that potable water might occasionally be a dominant source of radon concentrations in indoor air. Additional studies on ingestion and inhalation exposure to radon and its progenies (EPA, 1995, Giardino and Hageman, 1996, Little et al., 1998) have reinforced the significance of the inhalation exposure route.

Much research on inhalation exposure to an individual or a specific group of contaminants has been completed. Andelman (1985a and 1985b) looked at the volatilization of trichloroethylene (TCE) during a shower. The differences in chloroform concentration between occupied and unoccupied apartments were compared by Stern and Andrews (1988) with the assumption that the sources of chloroform were the water use activities in the apartment. Jo et al. (1990) considered chloroform exposure from showering on the basis of exhaled breath analysis. Tancrede et al. (1991) performed experiments to analyze simultaneous release of five volatile contaminants (chloroform, carbon tetrachloride, TCE, 1, 2, 3-trichloropropane, tetrachloroethlyene (PCE)) from full size experimental showers. Emissions of TCE and 1, 2,-dibromo-3-chloropropane in an experimental shower were characterized by Giardino and Andelman (1995).

Of the different water using devices within an indoor environment, the shower is one of the most important mediums for volatilization of chemical contaminants from water into the surrounding air. Consequently, it has been the most widely studied water device. Extensive theoretical assessment and development of mathematical model for showers have been made. McKone and Knezovich (1991) measured the influent and effluent concentrations of TCE in the shower compartment to measure its transfer efficiency from water to air. Little (1992) applied two-resistance theory to the volatilization of contaminants in showers. Assessment of the factors affecting the volatilization of TCE from a shower spray as a function of the drop size distribution was performed by Giardino et al. (1992).

Very few studies are available characterizing volatilization of chemicals from other water devices like bath, toilet, faucets, washing machines, dishwashers and humidifiers. The Three Compartment model (McKone, 1987) utilizes the measured transfer efficiency data of radon in the different compartments (shower, bathroom and the main house) of the model. The Three Compartment model does not consider each of the water devices, except the shower, separately.

The EPA model (EPA, 1995) for inhalation exposure analysis of radon and progeny is based on McKone's Three Compartment model. The Model for Analysis of Volatiles and Residential Indoor-air Quality, MAVRIQ (Wilkes et al., 1992) utilizes the estimates of a dimensionless mass transfer coefficients for different water devices in its computation of volatilization of the contaminant during water use events. The mass transfer coefficients used in MAVRIQ are based on estimates of residence time (duration of contact between water and air) for the different devices and the values reported for radon volatilization (Pritchard and Gessel, 1981). More recently, mass transfer coefficients for kitchen faucet (Howard and Corsi, 1996), shower, bath, washing machine, and dishwasher (Corsi and Howard, 1998) have been experimentally measured for different operating conditions.

For inhalation exposure computations, the concentration of the contaminant in the compartment air should be known for any instant throughout the day. Hence, the air exchange between the different compartments and/or with the outside air needs to be accounted for. The Three Compartment model (McKone, 1987) bases its air exchange rates on the volume and residence times in each compartments. The EPA model (EPA, 1985) extends the idea by incorporating three additional scenarios for the bathroom. The MAVRIQ model (Wilkes et al., 1992) uses measured values of the air exchange rate (Air Changes per Hour or ACH) for its ventilation rates.

An additional component that is important in inhalation exposure analysis is the human activity pattern, both in terms of occupancy of the different compartments and the usage of different water devices. The Three Compartment and the MAVRIQ models use a series of assumptions and survey data to account for activity patterns.

Another important exposure pathway associated with drinking water is the absorption of contaminants through the skin during water use activities. Primary activities resulting in skin contact with contaminated water are bathing and showering (Olin et al., 1998). Brown et al. (1984) conducted a human volunteer study and discussed the applicability of a Fickian diffusion model to describe dermal absorption of solutes from dilute aqueous solutions. Jo et al. (1990) estimated that dermal uptake from showering for ^{14}C labeled chloroform constituted 90% of that due to inhalation alone. Percutaneous absorption of dilute aqueous chloroform, TCE and PCE in hairless guinea pigs was measured by Bogen et al. (1992) and the values of the permeability constants obtained were recommended to be useful for human skin absorption computations.

Cleek and Bunge (1993) simplified Crank's equation (Crank, 1975) for chemical uptake through a pseudo homogeneous membrane, to compute dermal uptake through the skin. Bunge and McDougal (1996) developed correlation equations to compute the permeability coefficient across the stratum corneum (the outermost layer of the skin) (P_{sc}) and the equilibrium partition coefficient between the stratum corneum and water ($K_{sc/w}$) for a given contaminant on the basis of the more readily available properties, octanol-water partition coefficient and molecular weight.

Risk is defined as the probability of incurring a particular class of disease(s) caused by the environmental agent(s) under consideration. If there is background incidence for this disease class, then "risk" represents the incremental risk imposed by a given exposure scenario (Bogen and Spear, 1987).

In environmental exposure and risk assessment, there are generally three broad sources of uncertainty - scenario uncertainty, model uncertainty and variable uncertainty (EPA, 1995). Scenario uncertainty involves "the basic appropriateness of the facts, and the inferences used to select the exposure scenarios of concern." Model uncertainty refers to "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 refers to "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 of two types: The first type of uncertainty (natural variability) is due to the heterogeneity among different members of a given population. For example, there are differences in the amount of water consumed, the body surface area of an individual, the time spent in a particular compartment and the sizes and volumes of the compartments. There is hence no unique answer to a question such as "What is the exposure from a contaminant in water?" The answer is presented in the form of a range of values or in 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. For example, there is uncertainty in the data on the mean and standard deviation of variables such as volume and water usage in each of the compartment (EPA, 1995).

Due to the inherent natural variability, the variables of a model can be defined in terms of a Probability Density Function (PDF). A PDF is a mathematical formula that describes how frequently a variable will have any specific value or range of values. There are various types of PDF 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 mean (μ) and standard deviation (σ) of a sample drawn from the population. 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 procedure. 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.

One effective method that incorporates the uncertainty and the variability of a population in the estimation procedure is the Monte Carlo simulation. The process involves 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 method 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.

In the nested Monte Carlo approach (EPA, 1995, Macintosh et al., 1995), the uncertain parameters (PDF_u) for the variables are evaluated in an outer loop and actual value of the variables (PDF_v) are obtained in the inner loop. Hence, after each outerloop, predicted exposure will assume a range of values and can typically be described by a new PDF. Over a number of outerloops, the two PDF curves representing the lowest and the highest range can be expressed as the bounds of the exposure. The lowest and the highest PDF curves are then identified from the median values of exposure for each outerloop (Macintosh et al., 1995).

The objective of an integrated exposure model is to simulate all aspects of a subject's environment that can affect his/her exposure, and to estimate that exposure. In addition, a versatile model must be able to analyze an entire range of chemical contaminant in drinking water. The characteristics of the physical environment that must be considered are the contaminant formation and chemistry (i.e. the concentration of the contaminant in the water, types and characteristics of water sources in the home, volatilization rates, Henry's Law constant, etc.) and the transport mechanisms (i.e. infiltration rates, physical boundaries, etc.). The model must also include characteristics of the persons being modeled. These include the water-use activities that lead to exposure (showering, bathing, drinking water etc.), the location of the occupants and their exposure characteristics (i.e. breathing rates). By correlating these physical and personal aspects, the model can predict pollutant transport via the different pathways and subsequently estimate the subject's total exposure to a contaminant.

2. OBJECTIVES

Water using devices within an indoor environment represent potential sources of human exposure to chemical contaminants in drinking water. The primary pathways for exposure to chemical substances are ingestion, inhalation and dermal sorption. The presence of a wide range of contaminants in drinking water makes it essential to limit their concentration levels in order to safeguard human health. The relative impact of each of the exposure pathways depends upon the physical and the chemical nature of the contaminant, the types and usage of the various water devices, and the human activity pattern. Typically, previous research has focused on a single exposure pathway, chemical contaminant, or water-using device. Development of an integrated model analyzing exposure due to ingestion, inhalation and dermal sorption for a wide range of chemical contaminants via different water devices will provide valuable information for risk assessment and the subsequent establishment of Maximum Contamination Levels (MCLs) in drinking water.

The present model is an extension of the EPA model (EPA, 1995) that estimates inhalation and ingestion exposure to radon and its progeny. The current model performs uncertainty analysis of integrated exposure, incorporating the pathways of ingestion, inhalation and dermal sorption, to a wide range of chemical contaminants in drinking water. The model considers the use of shower, bath, toilet, faucet, washing machines and dishwashers as potential sources of chemical contaminants. The EPA model was based on an estimated transfer efficiency (essentially the fraction released while the water is being used) and considered radon as the only volatile compound. 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 (m)), 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). Hence, the current model utilizes experimentally determined mass transfer coefficients, for various water devices (Corsi and Howard, 1998), to replace transfer efficiency factors used in the previous models.

The EPA model considered only one water-using source in each of its three compartments. To make the model more realistic, additional water using devices (bathtubs, faucets, washing machines and dishwashers) will be added to appropriate compartments of the model. In addition, each device will be correctly represented using an idealized flow model.

To be of any practical significance, a model must consider all major exposure pathways. The focus of the EPA model was the analysis of inhalation and ingestion pathways of exposure to radon and progeny. An integrated exposure model will require not only the ability to perform exposure analysis of other contaminants in drinking water but also the incorporation of the dermal absorption pathway.

To facilitate easy analysis and further development of the model, a visually based computer software program is essential. Such a package will simplify management of the model including the addition of new components.

Specifically, the objectives of this study are to:

- Reformulate the EPA model to use mass transfer coefficient to facilitate exposure analysis of other chemical contaminants in drinking water.
- Incorporate additional water using devices: bathtub, faucet, washing machine and dishwasher, to the model.
- Develop an integrated exposure model, incorporating inhalation, ingestion and dermal uptake, to different chemical contaminants in drinking water in a residential environment and
- Develop a visually based computer software package for the model.

The current model makes possible the estimation of exposure (and hence risks) associated with chemical contaminants in drinking water. The model should prove valuable in establishing MCLs for the entire range of chemicals 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 reducing risk.

In the longer term, the model will be made more flexible and user defined to facilitate exposure analysis in non-residential environments. Extensive studies on human activity patterns and specific water devices in these environments are necessary to extend the model to incorporate other exposure environments. This completed multi-compartment model will then be suitably integrated with a physiologically-based pharmacokinetic (PBPK) model.

3. DESCRIPTION OF THE INTEGRATED EXPOSURE MODEL

This section describes the components of the exposure model developed in this study. The model is an extension of the exposure model developed previously by the EPA (EPA, 1995), which evaluated exposure to radon gas and its progenies. The EPA model was based upon a similar model proposed by McKone to predict the transfer and distribution of volatile compounds inside a house (McKone, 1987).

The model developed in this work performs an uncertainty analysis of integrated exposure, incorporating ingestion, inhalation and dermal exposure pathways, to the entire range of chemical contaminants in drinking water. In the model, a household is assumed to consist of three compartments: shower, bathroom, and main house. The locations of the water using devices in the different compartments are shown in Figure 1. The shower compartment consists of the shower and the bathtub. The devices in the bathroom compartment are lumped together and represented as a continuous, but low flow, water using device. The main house compartment has the kitchen faucet, washing machine and dishwasher. Air exchange between the different compartments and/or with the outside air is indicated using arrows in Figure 1.

For inhalation exposure computations, volatilization of the contaminants as they are released from different water using devices into the air and their redistribution throughout the house and the outdoors, needs to be predicted. Volatilization of a contaminant from a device can be characterized by the overall mass transfer coefficient which is a function of both the nature of the device and the chemical properties of the contaminant, specifically, the diffusion coefficients and the Henry's law constant. The Henry's constant is a measure of the volatility of a compound. The ventilation rates, between the compartments and the outside, can be calculated from the residence times and the volumes of the different compartments. From these quantities, a set of transient mass balance differential equations can be set up and solved to obtain the concentration in the different compartments of the model as a function of time. The profile of concentration versus time in the individual compartments coupled with the specified human activity, is then used to calculate the individual exposure via inhalation (Little et al., 1998).

Ingestion exposure computation requires the daily volume of water ingested and the concentration of the contaminant in water. Human activity pattern in terms of movement within and outside the house has no relevance in the ingestion analysis. The current model assumes that

the ingested water is drawn from the kitchen faucet and utilizes its overall mass transfer coefficient to compute the contaminant concentration remaining in the water.

The activities of showering, bathing and washing hands are considered in the dermal exposure analysis. The Permeability Coefficient (P_{sc}) for the outermost layer of the skin, the stratum corneum (sc), is a measure of a contaminant's capacity to permeate through it. Equilibrium partitioning coefficient ($K_{sc/w}$) represents the partitioning of the contaminant between the sc and the film of water on the surface of the skin. Both P_{sc} and $K_{sc/w}$ for a contaminant are required to estimate exposure via the dermal pathway. Commonly available properties of molecular weight (MW) and octanol-water partitioning coefficient (K_{ow}) of a contaminant are utilized to estimate P_{sc} and $K_{sc/w}$.

Finally, a nested Monte Carlo approach is employed to perform uncertainty analysis of exposure to both the individual and the combination of the three exposure pathways considered. Out of a number of people in the house, the model is designed to track a particular individual, randomly selected, for exposure analysis.

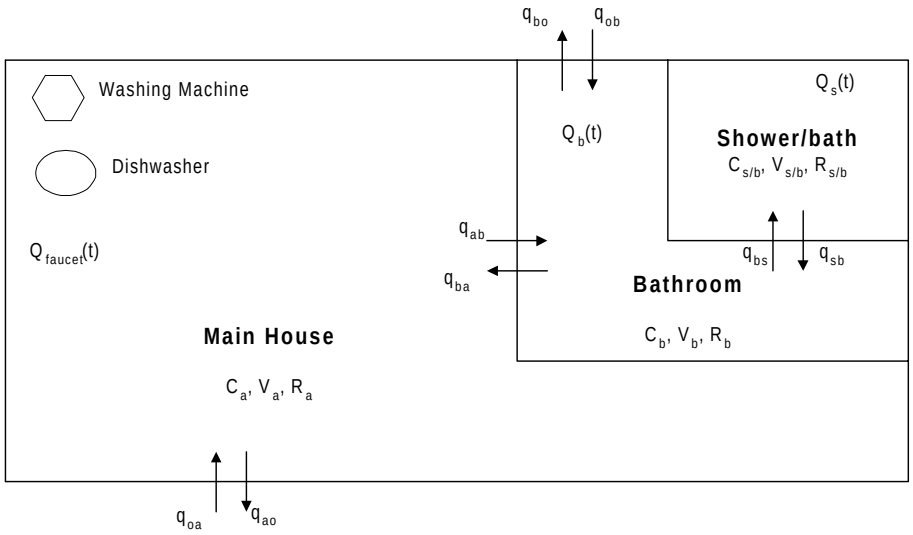

Figure 1: Modified Three Compartment Model

3.1 Properties of Chemical Contaminants in Water

The physical and chemical properties of the contaminant (in conjunction with their mass transfer coefficient for different water using devices), constitute major factors that determine the level of significance of each exposure pathway. The overall mass transfer coefficient is a function of the diffusion coefficients in air and water and Henry's law constant of the

contaminant. Contaminants with high values of Henry's constant and overall mass transfer coefficient would impact most through the inhalation pathway. Henry's law constant increases with temperature and volatilization would be even greater from devices using water at higher temperatures. For compounds with low volatility, ingestion is generally the major exposure pathway. Dermal exposure would be high for contaminants with low molecular weight and high permeability coefficient.

Three compounds, namely, chloroform, methyl parathion, and chromium were chosen for this study specifically because of the substantial variations in the values of their chemical properties. Table 1 lists the salient properties of these contaminants.

Table 1: Properties of the Representative Contaminants

Contaminant	Molecular Weight	Henry's m (-)	Log K_{ow} (-)	P_{sc} (cm/hr)	$R_{sc/w}$ (-)
Chloroform	120	0.12	1.93	0.0084	23.5
Methyl parathion	263	8.0×10^{-6}	2.86	0.005	107
Chromium	52.0	0.00	NA	0.0021	0.10

3.2 Mass Transfer Coefficients

This section explains the procedure used to determine the overall mass transfer coefficient ($K_{OL}A$) of a contaminant, using a known value for a reference contaminant, chloroform, for the different water using devices. The procedure to account for the variations in the Henry's law constant with water temperature is also explained.

Chloroform is the reference contaminant for this study. The values of the overall mass transfer coefficient for chloroform ($K_{OL}A_b$) for different water devices like shower, bath, washing machine, dishwasher and kitchen faucet for different sets of experimental conditions were computed from experimental data available for Toluene (Corsi and Howard, 1998). The computed values for chloroform are presented in Table 20 in Appendix C. These values, in combination with the diffusion coefficients and Henry's constant of a contaminant and the water temperature of the particular device, are employed to determine the overall mass transfer coefficient of the contaminant of interest ($K_{OL}A_i$) for the given device. The model uses the following sequence of equations (Corsi and Howard, 1998):

$$\varphi_l = \left(\frac{D_{L,i}}{D_{L,b}} \right)^{2/3}$$

$$\varphi_g = \left(\frac{D_{G,i}}{D_{G,b}} \right)^{2/3}$$

$$\varphi_m = \frac{K_{OL}A_i}{K_{OL}A_b} = \varphi_l \varphi_g \left(\frac{m_i}{m_b} \right) \left(\frac{1 + \left(\frac{K_{G,b}}{K_{L,b}} \right) m_b}{\varphi_l + \varphi_g m_i \left(\frac{K_{G,i}}{K_{L,i}} \right)} \right)$$

$$K_{OL}A_i = \varphi_m \cdot K_{OL}A_b$$

where,

φ_m = overall mass transfer relational parameter (-)

φ_l = liquid phase mass transfer relational parameter (-)

φ_g = gas phase mass transfer relational parameter (-)

$K_{OL}A_i$ = overall mass transfer coefficient for contaminant i (L/min)

$K_{OL}A_b$ = overall mass transfer coefficient for the reference contaminant (L/min)

$K_{L,i}$ = liquid phase mass transfer coefficient for contaminant i (L/min)

$K_{L,b}$ = liquid phase mass transfer coefficient for the reference contaminant (L/min)

$K_{G,i}$ = gas phase mass transfer coefficient for contaminant i (L/min)

$K_{G,b}$ = gas phase mass transfer coefficient for the reference contaminant (L/min)

$D_{L,i}$ = liquid phase diffusion coefficient for contaminant i (cm^2/min)

$D_{L,b}$ = liquid phase diffusion coefficient for the reference contaminant (cm^2/min)

$D_{G,i}$ = gas phase diffusion coefficient for contaminant i (cm^2/min)

$D_{G,b}$ = gas phase diffusion coefficient for the reference contaminant (cm^2/min)

m_i = Henry's law constant for the contaminant i (-)

m_b = Henry's law constant for the reference contaminant b(-)

For temperatures other than 20 °C, the Henry's law constant is adjusted according to (Selleck et al., 1988)

$$m_{T_2,i} = \frac{m_{T_1,i} \cdot T_1 \cdot 10^{(B_i/T_1)}}{T_2 \cdot 10^{(B_i/T_2)}}$$

where,

T_1 = Standard temperature in degree Kelvin (293 °K or 20 °C)

T_2 = Operating water temperature (°K)

B_i = Henry's constant temperature correction coefficient for contaminant i (-)

$m_{T_1,i}$ = Henry's law constant for contaminant i at temperature T_1 (-)

$m_{T_2,i}$ = Henry's law constant for contaminant i at temperature T_2 (-)

The computation procedure of the mass transfer coefficient for the bathroom follows a different procedure due to the lack of specific mass transfer data for the toilet. In the absence of this data, the transfer efficiency for radon (Little et al., 1998) together with the ratio K_G/K_L is used to calculate the K_G and K_L values for the bathroom as follows:

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

$$K_{OL}A_i = \frac{1}{\left(\frac{1}{K_L A} + \frac{1}{m_i \cdot K_G A}\right)}$$

$$K_L A = K_{OL}A_b \frac{\left(\frac{K_G}{K_L} \cdot m_b + 1\right)}{\left(\frac{K_G}{(K_L \cdot m_b + 1)}\right)}$$

where,

$K_{OL}A_i$ = overall mass transfer coefficient for contaminant i (L/min)

$K_{OL}A_b$ = overall mass transfer coefficient for the reference contaminant (radon) (L/min)

$K_L A$ = liquid phase mass transfer coefficient (L/min)

$K_G A$ = gas phase mass transfer coefficient (L/min)

m_i = Henry's law constant for the contaminant i (-)

m_b = Henry's law constant for the reference contaminant (-)

TE = Transfer efficiency of the reference contaminant (radon) in the bathroom.

Q_L = Liquid flow rate in the bathroom (L/min)

3.3 Exposure Pathways

A person's exposure to a contaminant present in drinking water in indoor environments arises primarily from three distinct pathways:

- The contaminant may volatilize from water in showers, faucets, dishwashers and washing machines and be inhaled as the individual breathes,
- water ingested directly with some fraction of the contaminant still in water,
- the contaminant absorbed through the skin during activities like showering, bathing, and washing hands.

The relative contribution of each exposure pathway to the total exposure is a combination of many factors. The physical and chemical properties of the contaminant, its chemical concentration in water, the type of water using device and a person's activity pattern, both in terms of water use and occupancy, determine the significance of each pathway. Hence, a complete integrated exposure analysis for a broad range of chemical contaminants in water must incorporate contributions from the three major exposure pathways.

The following sections consider the individual exposure pathways and their incorporation in the model in greater detail.

2.3.1 Inhalation Exposure

There are three important components to the inhalation exposure analysis of contaminants in drinking water:

- Volatilization of the contaminant from different water using devices and its resulting concentration in the compartment at any given time,
- the movement of the contaminated air between compartments,
- the presence of a person in the compartment.

Volatilization of a contaminant from water may occur while showering, bathing, or using faucets, washing machines, and dishwashers. Major factors that contribute to the volatilization of

a contaminant are the water flow rate used, the temperature of the water and the contaminant's volatility, expressed by its Henry's constant (Olin et al., 1998).

In general, the mass balance equation for a compartment consists of the summation of the source and sink terms.

Source terms include:

- Release from the water device(s) used in the compartment into air.
- Transport into the compartment by ventilation from other compartments.

Sink terms include:

- Transport out of the compartment by ventilation.

Room furniture, floorings and carpets are other possible sinks. The mass of contaminant retained by the lung while an occupant breathes the compartment air will also have a sink effect. These additional sinks were not considered for this study.

The rate of change of concentration with time of contaminant i in compartment a, is expressed by the following transient mass balance equation:

$$V_a \frac{dy_{i,a}(t)}{dt} = -(q_{ab} + q_{ao}) \cdot y_{i,a}(t) + (q_{ba} + q_{oa}) \cdot y_{i,b}(t) + Q_{i,x/a}(t)$$

where

$y_{i,a}(t)$ = gas phase concentration of contaminant i in compartment a (mg/L)

V_a = the volume of compartment a (L)

$Q_{i,x/a}(t)$ = the source term for contaminant i from device x in compartment a (mg/min)

q_{ab} = the air flow rate from compartment a to compartment b (L/min)

q_{ao} = the air flow rate between compartment a and the outside (L/min)

The generalized source term, $Q_{i,x/a}(t)$, used to account for the input of a volatile contaminant from a water device into the compartment air is expressed as:

$$Q_{i,x/a}(t) = H(t, \tau_1^o, \tau_1^*) \cdot K_{v,i/x} \cdot \left(C_w - \frac{y_{i,a}(t)}{m_i} \right)$$

where

$K_{v,i/x}$ = volatilization fraction of the contaminant i from device x.

$H(t, \tau_1^o, \tau_1^*)$ = function equal to 1 when t is between τ_i^o and τ_i^* or zero otherwise,

τ_i^o = time at which activity in the compartment i starts,

τ_i^* = time at which activity in the compartment i ends,

C_w = contaminant concentration in the water supply, mg/L.

m_i = Henry law constant of contaminant i.

The change in the concentration of the contaminant in the compartment air due to ventilation is accounted for by the appropriate air exchange rates. The inter-compartmental air flow rates are derived from data on the compartmental residence times (R, min) and volumes (V, L) as:

$$q = V/R$$

The following section considers the sources and sinks in the three different compartments.

3.3.1.1 Shower/Bath

The mass balance in the shower compartment is:

$$V_s \cdot \frac{dy_{i,s}(t)}{dt} = Q_s(t) + [q_{bs} \cdot y_{i,b}(t)] - [q_{sb} \cdot y_{i,s}(t)]$$

where

$y_{i,s}(t)$ = gas phase concentration of contaminant i in the shower/bath (mg/L)

V_s = the volume of the shower compartment (L)

$Q_s(t)$ = the source term for contaminant i from shower in the compartment (mg/min).

$q_{s,b}$ = the air exchange rates from shower to the bathroom (L/min)

$q_{b,s}$ = the air exchange rates from bathroom to the shower (L/min)

The source term $Q_s(t)$ is

$$Q_s(t) = H(t, \tau_1^o, \tau_1^*) \cdot K_{v,i/x} \cdot \left(C_w - \frac{y_{i,s}(t)}{m_i} \right)$$

Calculation of the volatilization fraction ($K_{v,i/x}$) follows a different procedure depending upon whether a showering or a bathing event is under consideration. The shower device is considered to follow a plug flow model (PFM) (Little, 1992). The volatilization fraction for the shower device is given by:

$$K_{v,i/s} = 1 - \exp\left(-K_{OL}A_{i,s}\right)$$

where

$K_{v,i/s}$ = Volatilization fraction of contaminant i from shower (L/min),

$K_{OL}A_{i,s}$ = overall mass transfer coefficient for contaminant i in the shower (L/min)

For the bathing event, the shower compartment is divided into two volumes, the liquid volume in the bathtub and the air volume in the rest of the compartment. The liquid volume is considered to be a batch reactor while the gas volume is a Completely Mixed Flow Model (CMFM) (Corsi and Howard, 1998). During bathing, surface volatilization is the most significant contributor to total exposure via inhalation (Corsi and Howard, 1998). Hence, only surface volatilization was considered for this study. The volatilization fraction for surface volatilization is the same as the overall mass transfer coefficient $K_{OL}A$, or

$$K_{v,i/bath} = \left(K_{OL}A\right)_{i/bath}$$

The model also accounts for the change in concentration of the contaminant in the pool of bath water (C_{bath}) due to surface volatilization during bathing. The appropriate differential equation is:

$$V_{bath} \cdot \frac{dC_{bath}(t)}{dt} = -K_{OL}A \cdot \left[C_{bath}(t) - \frac{y_s(t)}{m} \right]$$

Figure 2 shows the change in concentration of chloroform in the bath water during a bathing event of 20-minute duration.

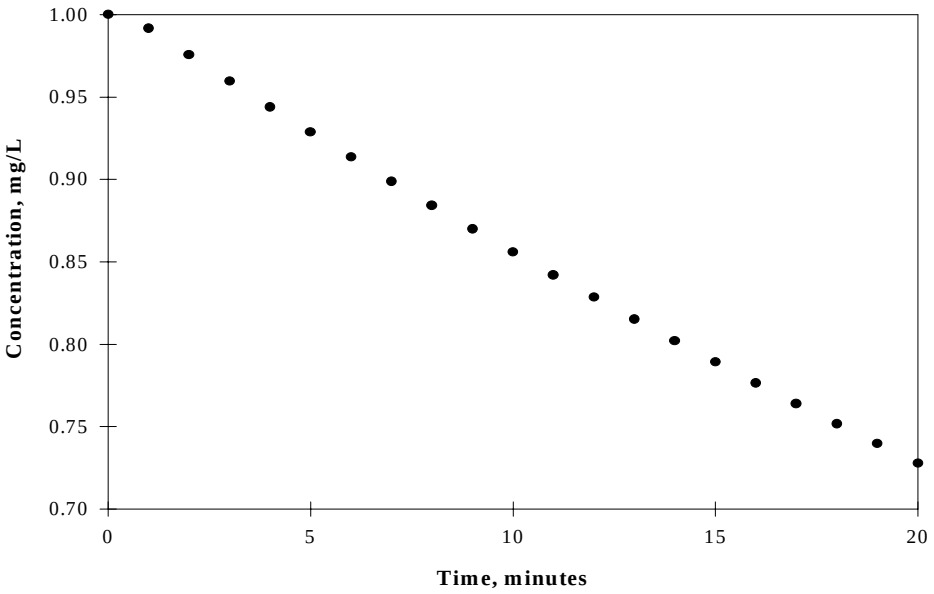

Figure 2: Change in Concentration of Chloroform in Bath Water

3.3.1.2 Bathroom

As explained previously, the mass transfer coefficient for water use in the bathroom is calculated on the basis of transfer efficiency. However, the release of contaminant from the bathroom into the compartment air is calculated in a manner similar to the shower. The mass balance equation for the bathroom is:

$$V_b \cdot \frac{dy_{i,b}(t)}{dt} = Q_b(t) + \left[q_{sb} \cdot y_{i,s}(t) + q_{ab} \cdot y_{i,a}(t)\right] - \left[(q_{bs} + q_{bo} + q_{ba}) \cdot y_{i,b}(t)\right]$$

In addition to ventilating to the shower and the main house, the bathroom also ventilates to the outside air which is represented by the air exchange rate, q_{bo}. To reflect a more realistic situation for ventilation in the bathroom, three different cases are considered (EPA, 1995). First 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. Then, 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 shown in Table 2.

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

3.3.1.3 Main House

Unlike the shower and the bathroom where there is one source per compartment, the main house has three different sources. The mass balance equation for the main house is:

$$V_a \cdot \frac{dy_a(t)}{dt} = Q_{kf}(t) + E_{wm}(t) + E_{dw}(t) + [q_{ba} \cdot y_b(t)] - [(q_{ab} + q_{a0}) \cdot y_a(t)]$$

where Q_{kf} is the source term for the kitchen faucet and E_{wm} and E_{dw} are the emission terms for the washing machine and the dishwasher, respectively. The computational procedure to obtain each of these terms is explained in the following sections.

Kitchen faucet:

The kitchen faucet is modeled as a PFM similar to the shower (Little, 1992). The release of contaminant from the kitchen faucet is immediately distributed uniformly throughout the volume of the main house. In essence, the faucet is interacting with the entire air volume of the compartment.

Washing Machine:

Unlike the kitchen faucet, the washing machine is considered to be an independent source since the device does not interact with the entire volume of the main house. The washing machine contributes to the contaminant concentration in the compartment with a continuous

emission during its time of operation. The device volume itself is divided into two sub compartments: the liquid phase and gas phase. Both volumes are considered to be CMFMs (Corsi and Howard, 1998). The following sequence of cycles is considered for the washing machine (Corsi and Howard, 1998):

> Fill cycle (4 min) – Wash cycle (10 min) – Drain & Spin (4 min) – Fill cycle (4 min) – Rinse cycle (4 min) -- Drain & Spin (6 min)

The data used to compute the source emission rate for the washing machine are presented in Table 3.

Table 3: Input Variables for the Washing Machine

Variable	Value
Henry's law constant for the base compound (chloroform), m_b (-)	0.126
Water flow rate into the washing machine, Q_l (L/min)	13.8
Air flow rate in the washing machine (average for all cycles), Q_g (L/min)	54.0
Volume of water in the washing machine, V_l (L)	45.8
Initial concentration of the contaminant in washing machine water, C_0(mg/L)	1.00
Initial concentration of the contaminant in washing machine air, y_o (mg/L)	0.00
$K_{OL}A$ for the base compound (chloroform) – Fill cycle, (L/min)	2.14
$K_{OL}A$ for the base compound (chloroform) – Wash cycle, (L/min)	0.39
$K_{OL}A$ for the base compound (chloroform) – Rinse cycle, (L/min)	0.71
K_G/K_L for the base compound (chloroform) - Fill cycle, (L/min)	4.50
K_G/K_L for the base compound (chloroform) - Wash cycle, (L/min)	1.60
K_G/K_L for the base compound (chloroform) - Rinse cycle, (L/min)	8.60
Temperature of the water, t (°C)	21.0

The steps to compute the source emission rate from the washing machine are (Corsi and Howard, 1998):

1. With chloroform as the base compound (contaminant b), determine the appropriate values of $K_{OL}A$ and K_G/K_L for the device under consideration. For example, for the fill cycle of

the washing machine, the values for $K_{OL}A$ ands K_G/K_L are 2.14 L/min and 4.50, respectively.

2. Estimate values of φ_l and φ_g for the base compound and the contaminant of interest (contaminant i) using the following equations:

$$\varphi_l = \left(\frac{D_{L,i}}{D_{L,b}} \right)^{2/3}$$

$$\varphi_g = \left(\frac{D_{G,i}}{D_{G,b}} \right)^{2/3}$$

3. Estimate φ_m for the base compound and the contaminant of interest.

$$\varphi_m = \frac{K_{OL}A_i}{K_{OL}A_b} = \varphi_l \varphi_g \left(\frac{m_i}{m_b} \right) \left(\frac{1 + \left(\frac{K_{G,b}}{K_{L,b}} \right) m_b}{\varphi_l + \varphi_g m_i \left(\frac{K_{G,i}}{K_{L,i}} \right)} \right)$$

4. Calculate $K_{OL}A$ for the contaminant of interest.

$$K_{OL}A_i = \varphi_m \cdot K_{OL}A_b$$

5. The mass balance equations for the liquid and gas phases in the washing machine are solved simultaneously, using a second order Runge-Kutta solution technique (Corsi and Howard, 1998). The process of computing the liquid and gas phase concentration of the contaminant is repeated for all the cycles of the washing machine in proper sequence.

6. The ventilation decay rate between cycles and during the drain period is:

$$y(t) = y_0 \exp\left(-\frac{Q_g}{V_g} \cdot t \right)$$

7. Finally, the source emission rate at any time t :

$$E_{wm} = Q_g \cdot y(t)$$

Dishwasher:

Similar to the washing machine, the dishwasher is considered to be an independent source with its liquid and gas phase volumes represented as CMFMs (Corsi and Howard, 1998). The following sequence of cycles is employed for the dishwasher:

> Pre-rinse cycle (4 min) – Drain cycle (2 min) – Wash cycle (10 min) – Drain cycle (2 min) – Rinse cycle (6 min) – Drain cycle (2 min) – Rinse cycle (14 min) – Drain cycle (2 min)

The data used to compute the source emission rate for the dishwasher is presented in Table 4.

Table 4: Input Variables for the Dishwasher

Variable	Value
Henry's law constant for the base compound (chloroform), m_b (-)	0.541
Water flow rate into the dishwasher, Q_l (L/min)	13.8
Air flow rate in the dishwasher (average for all cycles), Q_g (L/min)	5.70
Volume of water in the dishwasher, V_l (L)	45.8
Volume of the dishwasher headspace, V_g (L)	181
Initial concentration of the contaminant in water, C_0(mg/L)	1.00
Initial concentration of the contaminant in the dishwasher air, y_0 (mg/L)	0.00
$K_{OL}A$ for the base compound (chloroform) – average for all cycles, (L/min)	38.0
K_G/K_L for the base compound (chloroform) – average for all cycles, (L/min)	160
Temperature of the water, t (^{0}C)	55.0

The steps followed to compute the source emission rate for the dishwasher are:

1. Obtain the $K_{OL}A$ for the contaminant of interest (explained in the first four steps for washing machine).
2. The liquid phase concentration in the dishwasher, after each cycle, is predicted by:

$$C(t) = C_0\left[\exp\left(-\frac{D}{2}t\right)\cosh\left(\sqrt{\left(\frac{D^2}{4}-E\right)}t\right)\right] +$$

$$\left(\frac{BF}{Z}+\frac{EC_0}{Z}-\frac{DC_0}{2}\right)\left[\frac{1}{\sqrt{\left(\frac{D^2}{4}-E\right)}}\exp\left(-\frac{D}{2}\cdot t\right)\sinh\left(\sqrt{\left(\frac{D^2}{4}-E\right)}t\right)\right]$$

where,

$D = Z + Y$

$Z = K_{OL}A / V_l$

$Y = Q_g / V_g + K_{OL}A / (V_g.m)$

$E = ZY - BX$

$B = K_{OL}A / (V_l.m)$

$X = K_{OL}A / V_g$

$F = Z.y_0 + X.C_0$

3. Similarly, the gas phase concentration for each cycle is predicted by the following equation:

$$y(t) = y_0\left[\exp\left(-\frac{D}{2}t\right)\cosh\left(\sqrt{\left(\frac{D^2}{4}-E\right)}t\right)\right] +$$

$$\left(F-\frac{D\cdot y_0}{2}\right)\left[\frac{1}{\sqrt{\left(\frac{D^2}{4}-E\right)}}\exp\left(-\frac{D}{2}\cdot t\right)\sinh\left(\sqrt{\left(\frac{D^2}{4}-E\right)}t\right)\right]$$

4. The ventilation decay rate between cycles is computed in a manner similar to that of the washing machine.

5. Mass emission rate as a function of time, is given by:

$$E_{dw} = Q_g \cdot y(t)$$

3.3.2 Ingestion

Ingestion exposure to a contaminant occurs when a person consumes water containing the contaminant. The parameters for ingestion exposure computation (EPA, 1995) are the volume of water ingested and the concentration of the contaminant in water at the time of ingestion, or

$$\text{Dose}_{ing} = C_w \cdot F_i \cdot V_I$$

where,

Dose_{ing} = Amount of contaminant i ingested (in mg/day)

C_w = Initial concentration of contaminant i in water (mg/L)

F_i = Fraction of contaminant i remaining in water at the time of ingestion (-)

V_I = Volume of water ingested per day (L).

Water used in the preparation of hot drinks like coffee and tea may have a lower concentration of the contaminant due to higher volatilization rates at elevated temperatures. The possible additional contamination loss has to be accounted for if V_I includes hot beverages and other fluids. Also, volume ingested may vary considerably for different age groups, climate, and activity patterns (Olin et al., 1998). Specific exposure analysis must take all these factors into account while establishing the value for V_I.

Assuming that the water is collected from the kitchen faucet (represented by a Plug Flow Model, PFM) and ingested immediately, the overall mass transfer coefficient of a contaminant for the kitchen faucet ($K_{OL}A$) can be used to compute the Volatilization Fraction, $K_{v,\,i}$ and then F for the contaminant as follows (Little, 1992):

$$F_i = 1 - K_{v,i/KF}$$

$$K_{v,i/KF} = 1 - \exp(-K_{OL} A_{i,KF})$$

where,

$K_{v,i/KF}$ = Volatilization fraction of the contaminant i from the kitchen faucet (-)

$K_{OL} A_{i,KF}$ = Overall mass tranfer coefficient of contaminant i for kitchen faucet (L/min)

F_i = Fraction of contaminant i in water at the time of ingestion (-)

3.3.3 Dermal Absorption

The primary function of the human skin is to protect the body from excessive loss of water (Olin et al., 1998). The skin's outermost layer, called the stratum corneum, consists of a tightly packed lipid protein matrix, which limits the movement of water (Olin et al., 1998). However, the stratum corneum is not a complete barrier and penetration of water and contaminant has been shown to occur (Jo et al, 1990 and Sheperd et al, 1994). Activities like showering, bathing and washing hands contribute significantly to the dermal absorption of the contaminant from water. Figure 3 illustrates the dermal sorption process. The different terminology in the figure is explained later in the section.

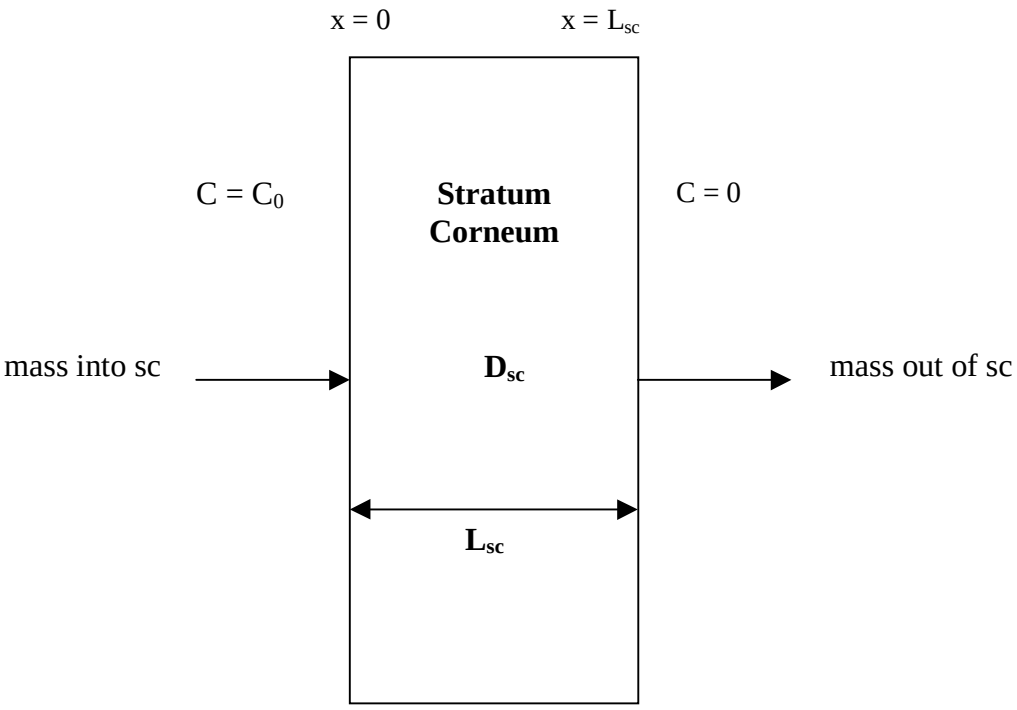

Figure 3: Schematic of Dermal Sorption Process

As described by Bunge (Olin et al., 1998), dermal absorption has been studied primarily in a pharmaceutical connection. Through many in vitro studies on both human and animal skin, it has been established that skin functions as a membrane and that the penetration rate becomes

steady after an initial lag time (t_{lag}). Consistent with descriptions of membrane behavior in other processes, the steady-state penetration rate of the chemical is defined as the product of the exposed area A and the mass-transfer flux J, where J is expressed in terms of a permeability coefficient for chemical transport across the stratum corneum (sc) and the concentration driving force ΔC. That is:

$$\frac{dM}{dt} = AJ \qquad \text{and} \qquad J = P_{sc}\Delta C$$

Typically, the chemical concentration in the receptor fluid is very low, and $\Delta C = C_w$, where C_w is the applied aqueous-phase concentration.

If the penetration rate is constant at the steady-state value from the beginning of the exposure, then the cumulative mass that will penetrate during an exposure of $t = t_{exp}$ is determined by integrating the above equation with respect to time to obtain:

$$M = AC_w P_{sc} t_{exp}$$

Note that equation ignores the existence of a lag time (t_{lag}), even though t_{lag} is rarely less than 15 minutes and often is much longer, sometimes several hours for chemicals of larger size (e.g., molecular weights larger than about 150-200). In reality, the cumulative mass which has penetrated across the skin is almost zero until $t \cong t_{lag}$. After that, the rate of penetration is described by the above equation

The amount of chemical which has penetrated across the skin during a chemical exposure lasting t_{exp} will be less than the total amount which has entered the body during that time. This is because the skin behaves as a chemical reservoir. After the chemical has been removed from the skin surface, the body will continue to absorb the chemical which is present in the skin when the exposure ended. Considering negligible desorption from outer skin layers, estimates of risk based on body burden should be calculated from the total amount which has entered into the skin during the exposure (and not the amount which has penetrated across the skin during the exposure). For a pseudo-homogeneous membrane, the total amount of chemical uptake into the skin can be calculated (Olin et al., 1998) as:

$$M_{in} = AC_w \sqrt{\frac{P_{sc} K_{sc/w} L_{sc} t_{exp}}{\pi}} \qquad \text{when } t_{exp} \le 2.4\, t_{lag,sc}$$

and

$$M_{in} = AC_w \left[P_{sc} t_{exp} + \frac{(K_{sc/w} L_{sc})}{3} \right] \qquad \text{when } t_{exp} > 2.4\, t_{lag,sc}$$

where the definitions of t_{lag} and the permeability coefficient P_{sc} are:

$$t_{lag} = \frac{L_{sc}^2}{6D_{sc}} \qquad P_{sc} = \frac{K_{sc/w} D_{sc}}{L_{sc}}$$

The time to reach steady state is approximated at 2.4 times the lag time (Bunge and Cleek, 1995). $K_{sc/w}$ is the equilibrium partition coefficient between the stratum corneum and water, D_{sc} is the effective diffusion coefficient for a chemical penetrating across the stratum corneum, and L_{sc} is the apparent thickness of the stratum corneum. It is typically assumed that $L_{sc} \approx 16 \mu m$.

To actually estimate dermal uptake, we must know the steady-state permeability coefficient for chemical transfer across the stratum corneum (P_{sc}) and either ($K_{sc/w}$ L_{sc}) or (D_{sc}/L_{sc}^2). For most chemicals of environmental concern, experimental measurements of these properties are not available (Bunge and McDougal, 1996). However, measurements for many other chemicals are reported in the literature (see for example, McKone and Howd, 1992). Consequently, several researchers have developed equations to estimate dermal uptake properties (P_{sc}, $K_{sc/w}$, and D_{sc}) using the available data. Generally, the input parameters utilized to establish the correlation of skin uptake properties are the octanol-water partition coefficient ($K_{o/w}$) and the molecular weight (Bunge and McDougal, 1996):

$$\log P_{sc} = -2.74 + 0.71 \cdot \log K_{o/w} - 0.0061 \cdot MW$$

$$\log K_{sc/w} = 0.74 \log K_{o/w}$$

The activities of showering, bathing and washing hands are considered for dermal sorption analysis. An individual being analyzed for dermal exposure, showers everyday, washes hands four times a day and bathes once a week.

3.3.4 Activity Pattern

To compute total exposure to an individual in a household, especially for inhalation and dermal exposure pathways, it is necessary to determine the occupancy pattern of the individual within the different compartments of the house, and the duration, frequency of usage and, in most cases, the flow rates of the different water devices. The human activity pattern and the water usage pattern considered by the model are outlined in the following sections.

3.3.4.1 Human Activity Pattern

Some of the important terms in tracking human activity through the house are (EPA, 1995):

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:

- There are N numbers of occupants in the house.
- All occupants of the house shower each morning.
- First shower starts at 7.00 a.m., i.e., SS_1 is 7.00 a.m. or 420 minutes.
  $ES_1 = 420 + Ts_1$
- The second shower starts after the first person finishes his shower and leaves the bathroom.
- The time spent in the bathroom (T_b) is assumed to be the same for all occupants of the house.
  $SS2 = ES1 + T_b$

The times of start and end of other showers are calculated similarly.

- Bathing event occurs every evening between 5.00 p.m. and 7.00 p.m. for the duration of 20 minutes.
- Each person takes a bath once every week.

An Occupancy Factor (OF) is utilized to characterize the time a person spends in the home (EPA, 1995). Based on the presence or absence of a person in a room (compartment), a value of one or zero is assigned to the occupancy factor.

3.3.4.2 Water Usage Pattern

The assumptions made on water usage are:

Shower (EPA, 1995):

- 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 (EPA, 1995):

- Water flow in the bathroom is assumed to be continuous, 24 hours a day.

Main House:

- The kitchen faucet is used four times per person per day (Olin et al., 1998). Duration of each use is assumed to be one minute. The kitchen faucet can be operated anytime between 6.00 a.m. and 12.00 p.m.
- The washing machine is operated once a week. The duration of the operation of the washing machine is 32 minutes (Corsi and Howard, 1998) and it can be operated anytime between 10.00 a.m. and 10.00 p.m.
- The dishwasher is operated every evening between 7.00 p.m. and 9.00 p.m. The duration of its operation is of 42 minutes (Corsi and Howard, 1998).

In order to account for episodic water usage, a function $H\left(t, \tau_i^0, \tau_i^*\right)$ is utilized to essentially switch the water flow / emission rate on or off depending upon whether the device is in use or not.

It is assumed that the water is used in the bathroom throughout the day. Hence the value of H for the bathroom is 1 for the entire day. Similarly, the dishwasher is operated every evening for 42 minutes. The value of H for the dishwasher is 1 for the duration of its operation and 0 for the rest of the time.

In addition, to account for once weekly use of the washing machine, a check function, which works with the probability of 1/7 for the washing machine event to occur for each day of the model run, is utilized. A similar check function is also used to check whether the person taking a bath in any given day is the individual being tracked for exposure analysis.

3.3.5 Exposure Computations

For inhalation analysis, the basic outputs from the model are the concentrations of a given contaminant in each compartment as a function of time. In order to calculate exposure to the contaminant, it is necessary to specify the location of an individual as a function of time during the day. OF is utilized to track the occupancy of the individual in the different compartments.

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

$$ID_{t,con} = \left[\overline{C_{s,t}}OF_{s,t} + \overline{C_{b,t}}OF_{b,t} + \overline{C_{a,t}}OF_{a,t}\right]\Delta t$$

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 total dose are (mg/L)(min/day).

$$Dose_{inh} = \int_0^{1440} ID_t$$

Then, the total inhalation exposure to the contaminant (E_{inh}) is expressed in mg per year. This is calculated from the average daily dose (Dose/1440) as follows:

$$E_{inh}\left(\frac{mg}{year}\right)=\left(\frac{Dose_{inh}}{1440}\right).\left(\frac{mg}{L}\right).\left(\frac{min}{day}\right).\text{Breathing Rate}\left(\frac{L}{min}\right).\frac{365\,days}{yr}$$

The total exposure via ingestion to a contaminant (E_{ing}) can be obtained by:

$$E_{ing}\left(\frac{mg}{year}\right)=\text{Dose}_{ing}\left(\frac{mg}{day}\right).\frac{365\,days}{year}$$

Similarly, total dermal exposure to a contaminant (E_{der}) is calculated from:

$$E_{der}\left(\frac{mg}{year}\right)=M_{in}\left(\frac{mg}{day}\right).\frac{365\,days}{year}$$

The total exposure to a contaminant (E_{tot}) is the sum of the three exposures:

$$E_{tot}=E_{inh}+E_{ing}+E_{der}$$

3.3 Uncertainty Analysis

Exposure to contaminants, through different pathways, is calculated by multiplying together a series of relevant terms. Most of these terms have an associated uncertainty. The uncertainty is of two basic types: natural variability due to heterogeneity among different members of a given population and uncertainty resulting from lack of knowledge about the value 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 a specific value or range of values (EPA, 1995). There are many different types of PDFs, for example normal, lognormal, uniform, triangular, and beta. Each PDF is specified by one or more parameters. For example, a mean and a standard deviation specify a normal PDF. The different PDFs used in this analysis are explained in Appendix B.

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.

An effective exposure analysis must account for correlation among different input variables. Some correlation (like the total volume of the house depending on the number of occupants) considered by the EPA model (1995) is incorporated in this study.

The uncertainty analysis used by the model is based upon a two-dimensional or nested Monte-Carlo method. In the nested approach, the model run consists of two sets of loops, the inner and the outerloops. A set of predetermined number innerloops is completed before the outerloop is incremented by a step. 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).

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. The process is repeated for the rest of the outer loops. Figure 4 presents a flowchart explaining the use of the two-dimensional Monte-Carlo approach in the extended model.

The model variables and the PDFs associated with them are explained and summarized in Appendix C. However, the PDFs for the additional parameters incorporated in the extended model are not available. An effort has been made to quantify the uncertainty of the parameters using the available data. For example, determining the mass transfer coefficient for the kitchen faucet, ten sets of data from Corsi's (1998) experiments are available. A function randomly

selects a single set of data to be used in the analysis for each model run. Hence, every run of the model maybe using a different data set for its computations. Table 20 in Appendix C gives the list of the experimental values used for the different water using devices.

The total model run consists of 2000 inner x 250 outerloops. After each outerloop (i.e. after the first 2000 inner loops) a range of percentiles (from 5^{th} to the 95^{th}) of exposure to each of the exposure pathway is computed. This set of data characterizes the uncertainty in the output. In order determine the bounds of percentiles (the variability in the output) for each exposure pathway, the median value of exposure, across all the outerloops, is tracked. The outerloops with the lowest and the highest median values (for each exposure pathway) is identified and the data set associated with the particular outerloop (i.e. the summary statistics of the 2000 innerloops associated with the outerloop) is reported as either the lower or the upper bounds of exposure as the case maybe. This lower and upper bounds of exposure, represented graphically, can help us determine both the ranges of uncertainty about exposure for a given percentile as well as the uncertainty about a percentile for a given exposure value (Macintosh et al, 1995).

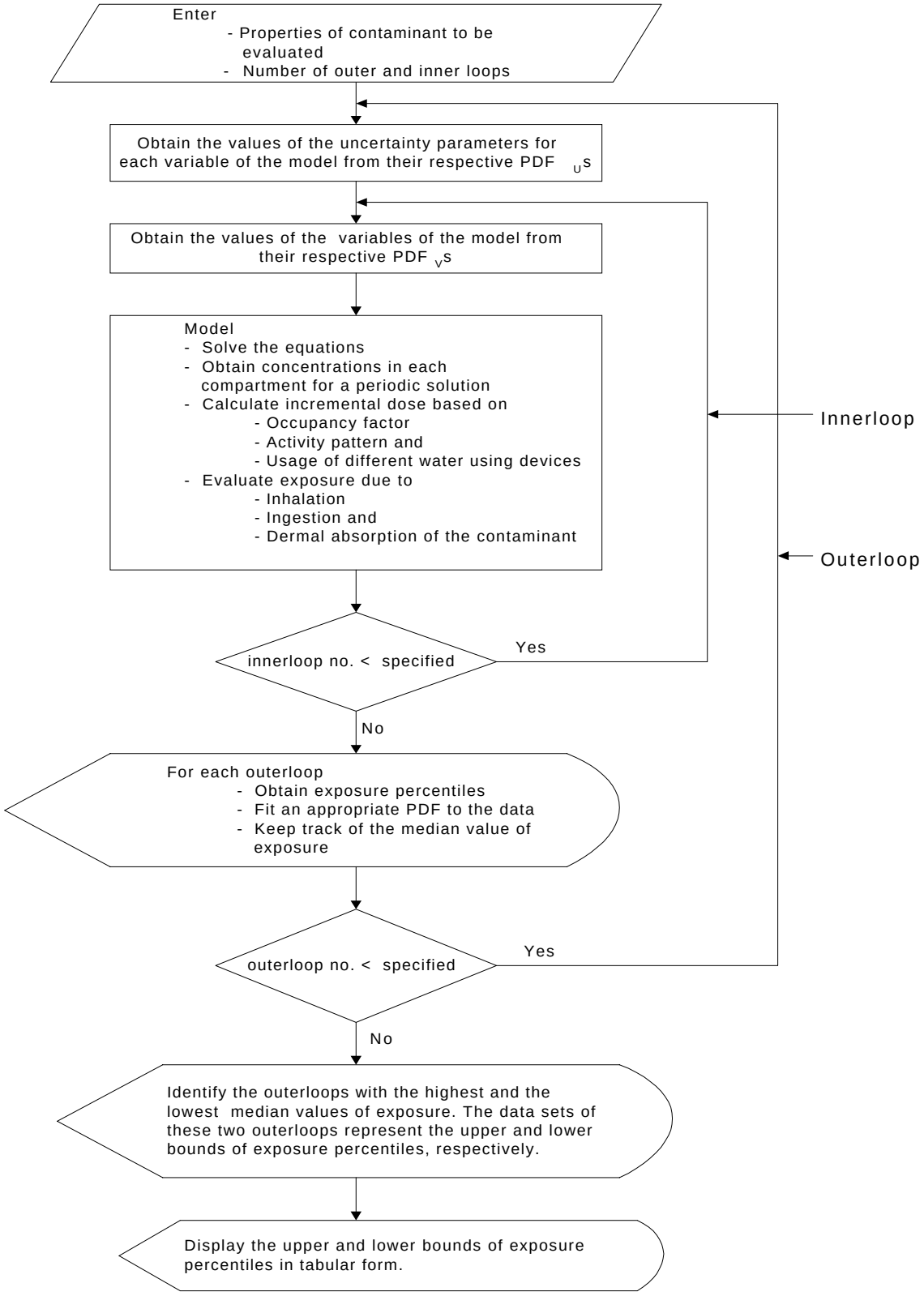

Figure 4: Flow Chart for the Computer Program

3.3 Default Computation

In addition to performing uncertainty analysis, the model estimates point value of inhalation, ingestion, dermal and total exposure to an entire range of chemical contaminants found in water. The default values of the model variables used and the method by which they were obtained is explained in detail in the section on sensitivity analysis

3.4 Visually Based Computer Package

A windows based visual front end to the model has been developed. Microsoft Visual C++ (Version 5.0) Builder was employed to create a dialog box based interactive window to ease the execution and comprehension of the model. The output data of a model run can be imported to a spreadsheet program like Excel with ease for further data analysis. Effort has been made to structure the computer program in an object-oriented format. This structured format should prove useful while considering addition of new components to the model during the process of its development.

4. VERIFICATION OF THE MODEL

4.1 Extended Three Compartment Model

4.1.1 Numerical Solution

The differential equations representing the mass balances for the chemical contaminant were solved simultaneously using the fourth order Runge-Kutta Method. There are four simultaneous differential equations in the model, one for each of the compartments and the fourth to account for the change in contaminant concentration during surface volatilization from bath water.

4.1.2 Analytical Solution

The model utilizes the Runge Kutta numerical method to develop the concentration profiles of the contaminant in the three compartments. The first version of the model (Little et al., 1998) was verified with the help of analytical solution using Mathematica. For inhalation exposure analysis, the current model employs similar numerical solution technique to generate the concentration profiles of contaminants. Dermal and ingestion exposure calculations are based on algebraic equations and their computational verification is presented later in the section.

4.2 Exposure Model

The exposure model was verified through calculations in an Excel spreadsheet identical to the ones used in the program. Three representative contaminants: chloroform, chromium and methyl parathion, were evaluated. A comparison of the exposure results for two cases: with and without the operation of the washing machine, given by the program and by the Excel spreadsheet is shown in Table 5.

Table 5: Comparison of Exposure Results from Program and Excel

Description	Chloroform (mg/yr per mg/l)		Chromium (mg/yr per mg/l)		Methyl parathion (mg/yr per mg/l)	
Case I: Washing machine off	Program	Excel	Program	Excel	Program	Excel
Inhalation exposure						
Shower/Bath	250	250	0.00	0.00	0.16	0.16
Bathroom	69.2	69.2	0.00	0.00	0.06	0.06
Main House	81.8	81.8	0.00	0.00	0.08	0.08
Inhalation total	401	401	0.00	0.00	0.30	0.30
Ingestion exposure	132	132	365	365	365	365
Dermal exposure	125	125	7.10	7.11	208	209
Total exposure	658	658	372	372	574	574
Case II: Washing machine on						
Inhalation exposure						
Shower/Bath	251	251	0.00	0.00	0.16	0.16
Bathroom	69.2	69.2	0.00	0.00	0.06	0.06
Main House	89.2	89.2	0.00	0.00	0.08	0.08
Inhalation total	409	409	0.00	0.00	0.30	0.30
Ingestion exposure	132	132	365	365	365	365
Dermal exposure	125	125	7.10	7.11	208	209
Total exposure	666	666	372	372	574	574

4.3 Comparison of PDFs with Excel Functions

In the following 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. The program employs the IMSL C Numerical Libraries version 2 to evaluate these functions. Samples from this comparison are shown in the tables.

4.3.1 Truncated Normal Distribution

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

Var = NORMSINV(p, m, sd)

where

p = Probability

m = Mean

sd = Standard deviation

Table 6: Comparison of Truncated Normal Variable Values

p	m	sd	Variable from Program	Variable from Excel	% Difference in Variable values
0.147	10.0	2.39	7.52	7.52	0.00
0.278	8.55	2.55	7.05	7.05	0.00
0.950	10.7	2.15	14.3	14.3	0.00
0.237	9.32	2.60	7.45	7.45	0.00
0.229	8.14	2.43	6.33	6.33	0.00
0.454	8.12	3.25	7.75	7.75	0.00
0.225	9.13	2.24	7.44	7.44	0.00
0.184	8.52	1.63	7.05	7.05	0.001
0.382	9.58	3.39	8.56	8.56	0.001
0.030	9.52	1.95	5.84	5.84	0.001

Figure 5 shows a plot of the comparison between Normal variable values from the program and those from Excel.

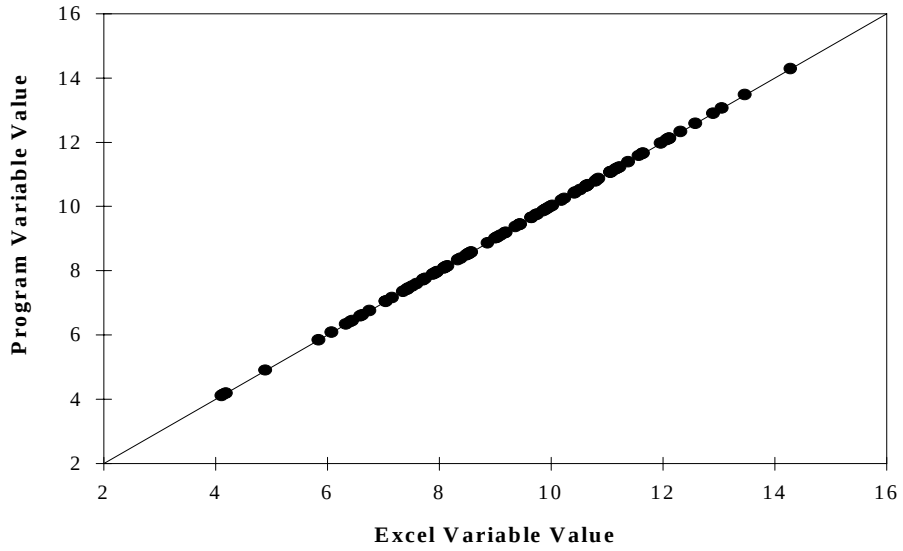

Figure 5: Comparison of Normal Variable Values from the Program and Excel

4.3.2 Truncated Lognormal Distribution

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

Var = LOGINV(p, gm, gsd)

where

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

Table 7: Comparison of Truncated Lognormal Variable Values

p	gm	gsd	Variable from Program	Variable from Excel	% Difference in Variable values
0.891	9.51	0.469	24000	24000	0.00
0.704	9.57	0.586	19500	19500	0.001
0.540	9.45	0.420	13300	13300	0.001
0.871	9.73	0.455	28100	28100	0.001
0.594	9.46	0.680	15100	15100	0.001
0.383	9.71	0.467	14400	14400	0.001
0.784	9.52	0.457	19600	19600	0.001
0.704	9.65	0.422	19500	19500	0.001
0.131	9.36	0.441	7090	7090	0.001
0.807	9.63	0.603	25600	25600	0.001

Figure 6 shows a plot of the comparison between Lognormal variable values from the program and those from Excel.

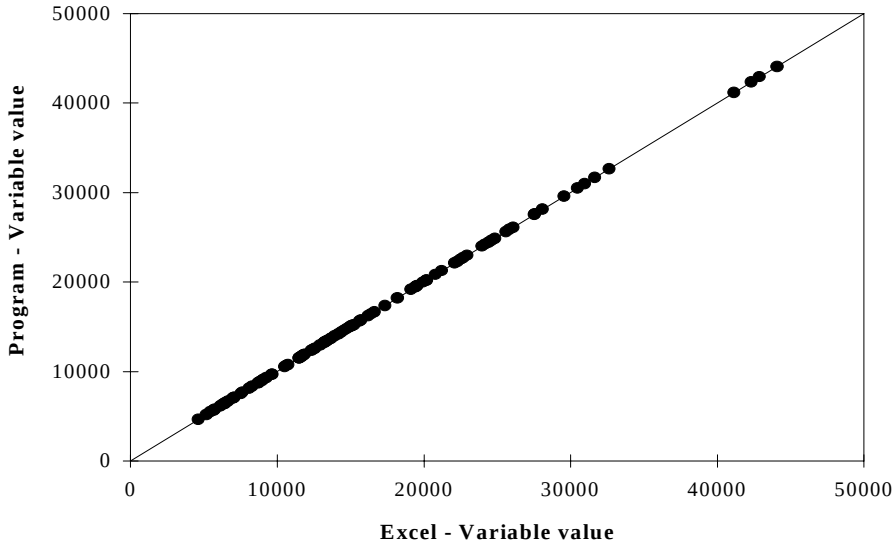

Figure 6: Comparison of Lognormal Variable Values from the Program and Excel

4.3.3 Beta Distribution

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

Var = BETAINV(p, alpha, beta, min, max)

where

p	=	Probability
alpha	=	Parameter 1 for Beta Distribution
beta	=	Parameter 2 for Beta Distribution

Table 8: Comparison of Beta Variable Values

p	a	b	Variable from Program	Variable from Excel	% Difference in Variable values
0.571	1.18	1.08	0.729	0.729	0.00
0.453	1.28	1.03	0.685	0.685	0.00
0.857	1.34	1.08	0.915	0.915	0.00
0.611	2.02	1.10	0.838	0.838	0.0001
0.415	2.81	1.40	0.761	0.761	0.0001
0.419	2.62	1.68	0.716	0.716	0.0001
0.298	1.43	1.07	0.605	0.605	0.0009
0.314	1.26	1.07	0.585	0.585	0.0009
0.211	1.19	1.04	0.51	0.506	0.001
0.182	1.68	1.48	0.516	0.516	0.001

Figure 7 shows a plot of the comparison between Beta variable values from the program and those from Excel.

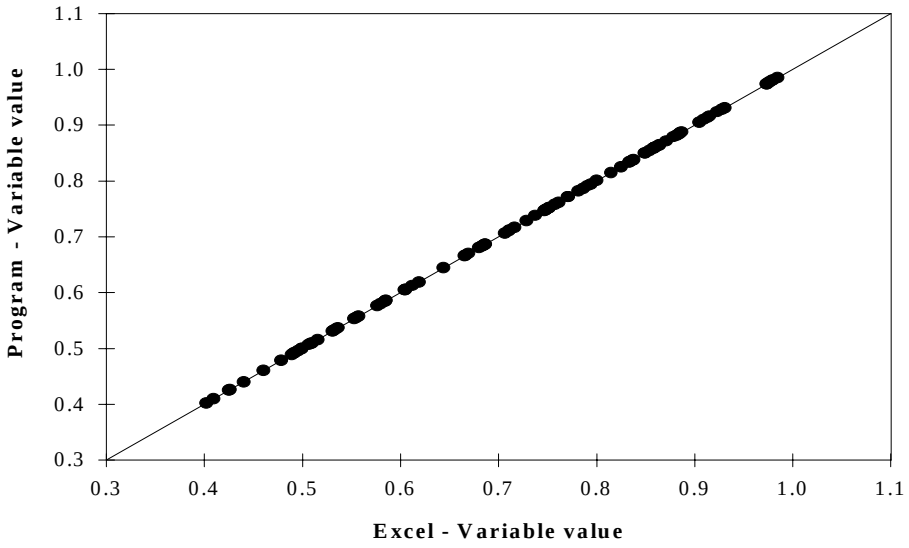

Figure 7: Comparison of Beta Variable Values from the Program and Excel

4.3.4 Student's-t Distribution

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

Var = TINV(p, df)

where

p = Probability

df = Degrees of freedom

Table 9: Comparison of Student's t Variable Values

p	qf	Variable from Program	Variable from Excel	% Difference in Variable values
0.30	24.0	-0.533	-0.533	0.0023
0.314	24.0	-0.491	-0.491	0.0013
0.316	24.0	-0.486	-0.486	0.0010
0.333	24.0	-0.436	-0.436	0.0030
0.494	24.0	-0.017	-0.0166	0.0691
0.498	24.0	-0.005	-0.0051	0.0812
0.512	24.0	0.03	0.0297	0.0333
0.957	24.0	1.79	1.79	0.0003
0.973	24.0	2.03	2.03	0.0036

Figure 8 shows a plot of the comparison between Student's t variable values from the program and those from Excel.

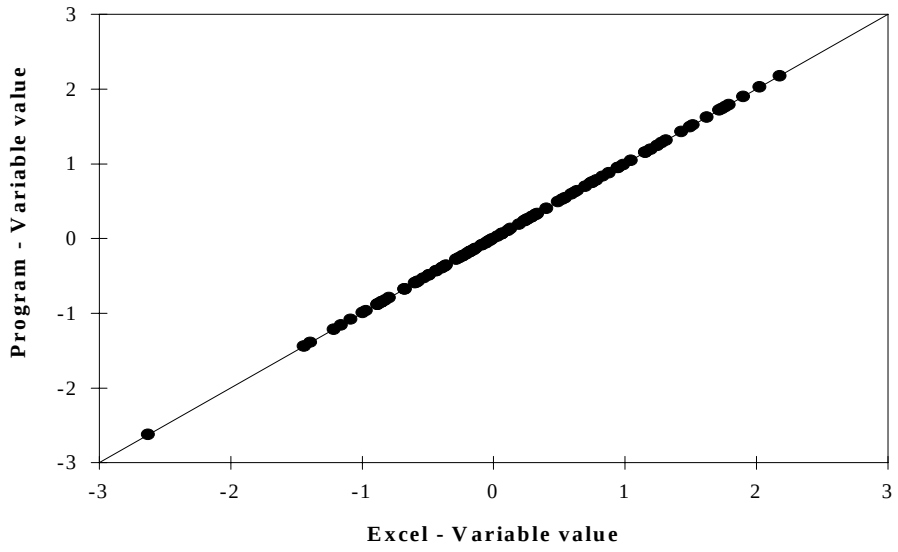

Figure 8: Comparison of Student's-t Variable Values from the Program and Excel

4.3.5 Chi-squared Distribution

In Excel the variable with chi-squared distribution is calculated as follows:

Var = CHIINV(1 - p, df)

where

p = Probability

df = Degrees of freedom

Table 10: Comparison of Chi-squared Variable Values

p	qf	Variable from Program	Variable from Excel	% Difference in Variable values
0.169	24.0	17.4	17.4	0.0004
0.193	24.0	17.9	17.9	0.0001
0.201	24.0	18.1	18.1	0.0005
0.203	24.0	18.1	18.1	0.0003
0.398	24.0	21.6	21.6	0.0001
0.412	24.0	21.9	21.9	0.0002
0.419	24.0	22.0	22.0	0.0002
0.694	24.0	27.0	27.0	0.0003
0.704	24.0	27.1	27.2	0.0001
0.709	24.0	27.3	27.3	0.0003

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

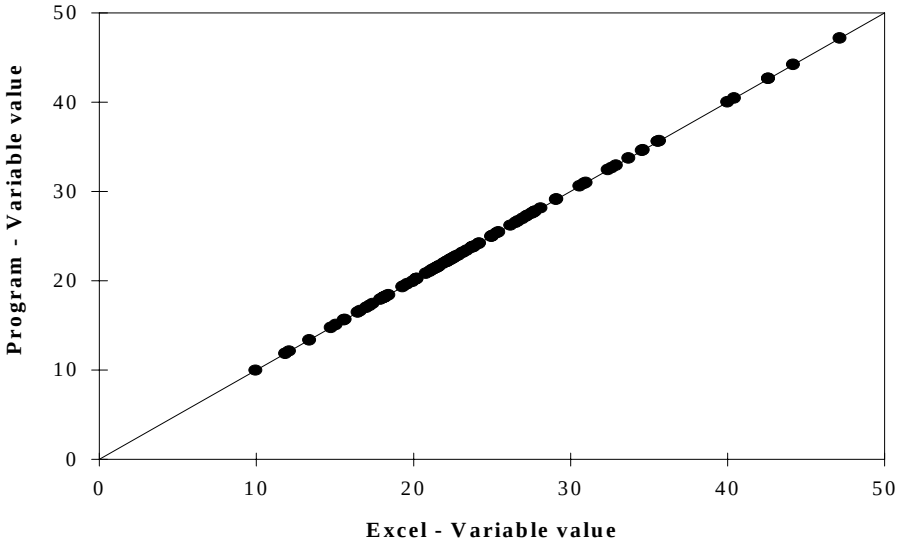

Figure 9: Comparison of Chi-Squared Variable Values from the Program and Excel

4.4 Conclusions

The exposure calculations were checked by comparing those calculated by the program with an identical computation using an Excel spreadsheet. The results of the two independent procedures were essentially the same. The accuracy of the IMSL computer sub-routines used to evaluate the probability distributions were also checked against the equivalent Excel functions. No difference was found. These independent tests of the computer program, in addition to the analytical verification of its previous version, are a good demonstration of the model's reliability.

5. RESULTS AND DISCUSSION

5.1 The Model Output

The output variables from the extended model are exposures from the three major pathways of ingestion, inhalation and dermal sorption. Ingestion exposure is primarily the function of the volume of water ingested. For inhalation pathway, exposure is evaluated from the concentrations of chemical contaminants in the air of the different compartments and the human activity pattern. The magnitude of dermal exposure depends upon the duration of exposure to the contaminated water and the surface area of the exposed skin. 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). For most of the model variables, the uncertain parameters are selected in the outer Monte Carlo loop, and with these values held constant, a number of iterations are performed within the inner Monte Carlo loop to characterize the variability of the exposure predictions. As explained in the previous section, the variability of the output is expressed by two PDFs, which represent the lower and upper bounds of exposure.

This study considered three representative compounds: chloroform, methyl parathion, and chromium for detailed analysis. The contaminants were selected for their significant variations in chemical properties.

A contaminant's concentration in the different compartments of a house, as a function of time, is a primary requirement for inhalation exposure computations. The concentration profile of the contaminants in the compartment air for chloroform and methyl parathion is presented in Figures 10 and 11. As the volatility of chromium is negligible, its concentration profile in the compartment air is zero. Default set of values of the model variables was used to develop the profile in the three compartments for a typical day. Development of the default variables for the model is explained in greater detail in the section on sensitivity analysis. Two cases, one in which the washing machine is operated on the day under consideration and the other when it is not in operation, are presented.

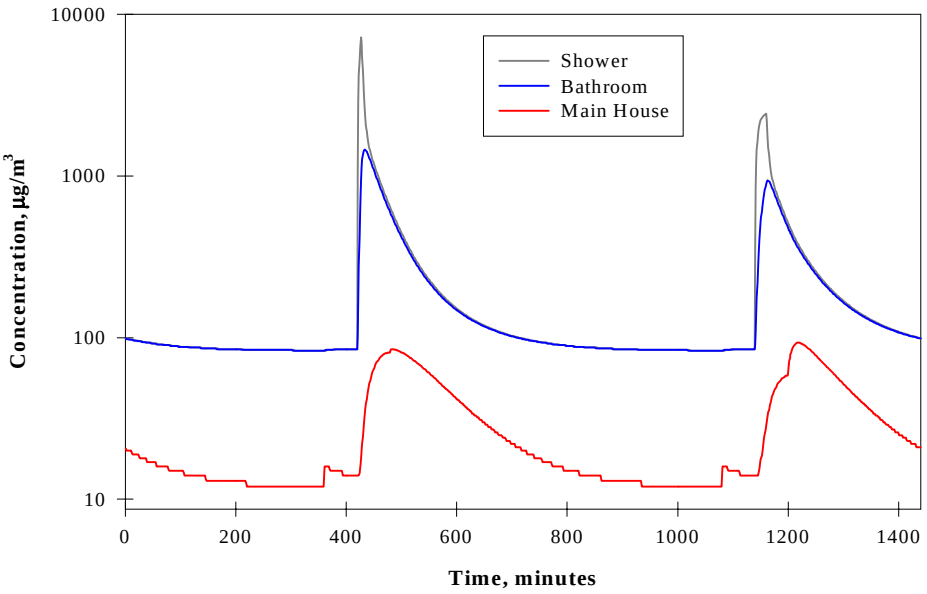

Figure 10 a: Concentration Profile of Chloroform – Washing Machine Off

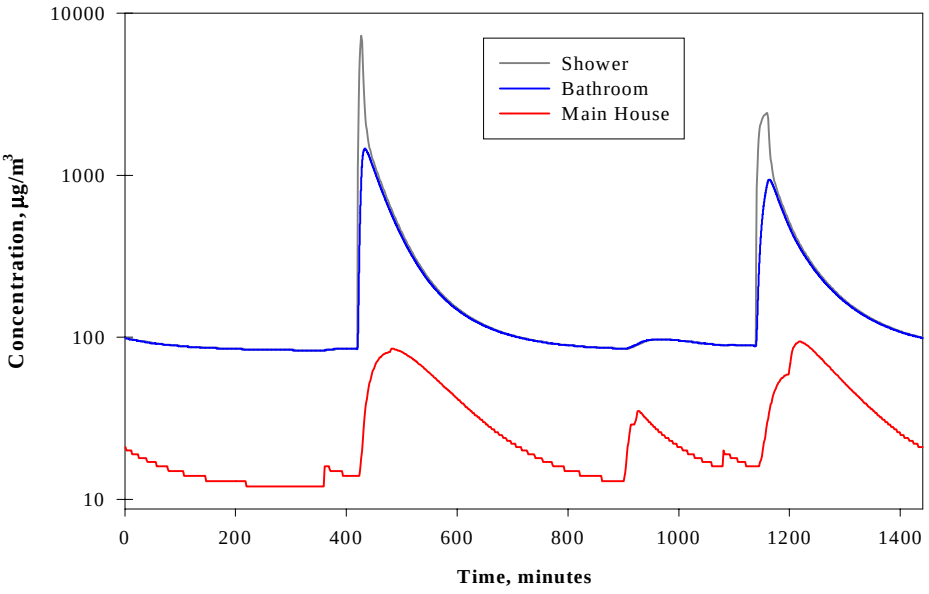

Figure 10 b: Concentration Profile of Chloroform – Washing Machine On

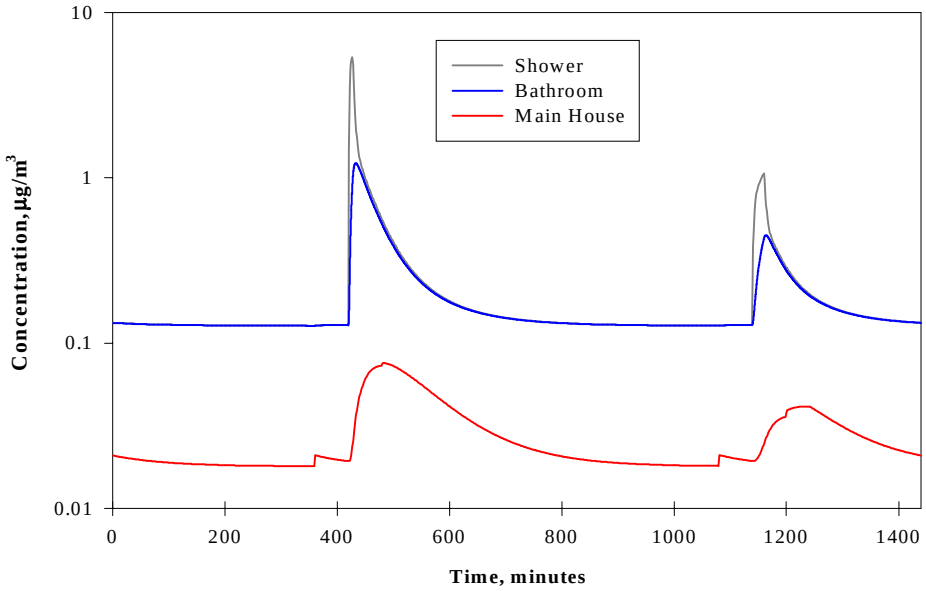

Figure 11 a: Concentration Profile of Methyl Parathion – Washing Machine Off

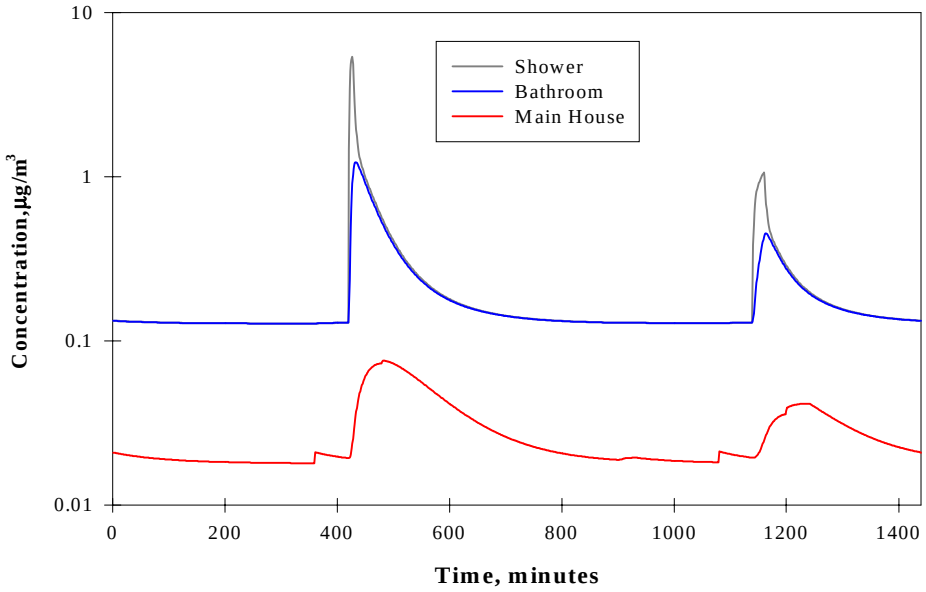

Figure 11 b: Concentration Profile of Methyl Parathion – Washing Machine On

The relative contribution of each exposure pathway to total exposure for the three contaminants is presented in Figures 12, 13 and 14. The average of the lowest and the highest median values of exposure for each of the pathways were taken for the purpose. Figure 15 compares the absolute magnitude of the exposure pathways for the three contaminants.

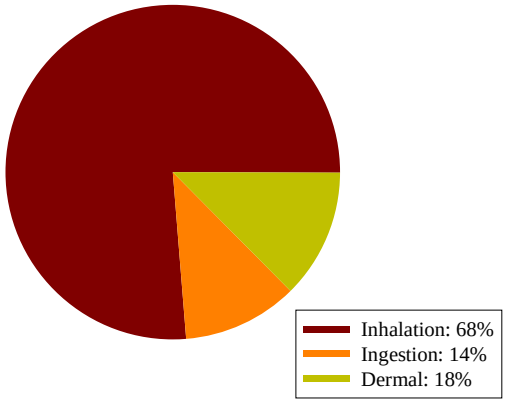

Figure 12: Impact of Each Exposure Pathway for Chloroform

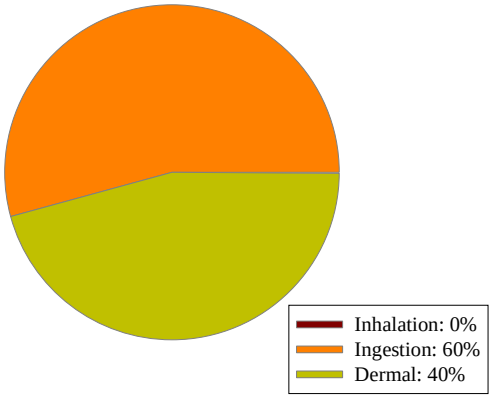

Figure 13: Impact of Each Exposure Pathways for Methyl Parathion

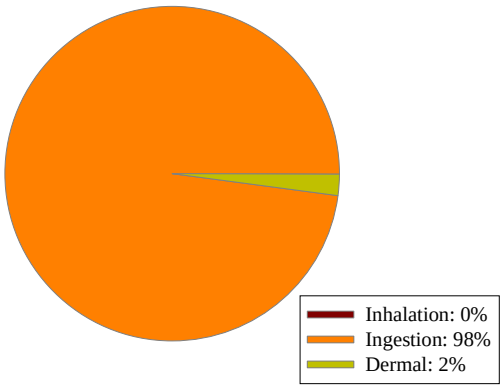

Figure 14: Impact of Each Exposure Pathway for Chromium

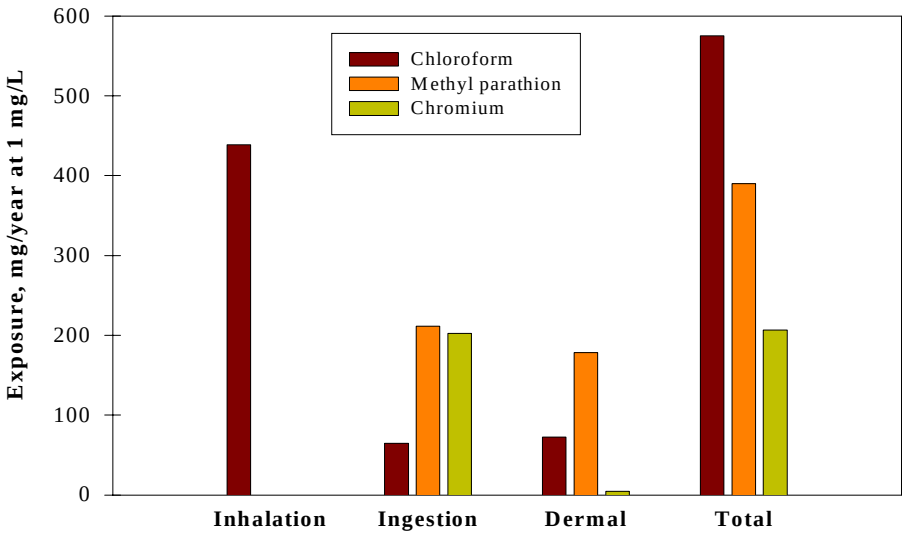

Figure 15: Median Values of Exposures to the Three Contaminants

A total model run of 2000 inner x 250 outer loops was employed to perform uncertainty analysis of exposure for each contaminant. The median values of exposure, for each pathway and total exposure, are tracked for all the outer loops of the model run. The set of data associated with the lowest and the highest median values represent the lower and the upper bounds of exposure.

Figures 16, 17 and 18 present the bounds of total exposure to the three contaminants. Statistical analysis using SAS software shows that the exposure distributions are well represented by the lognormal distribution. P value for the hypothesis assuming lognormal distribution and its parameters for the three contaminants are presented in Table 11.

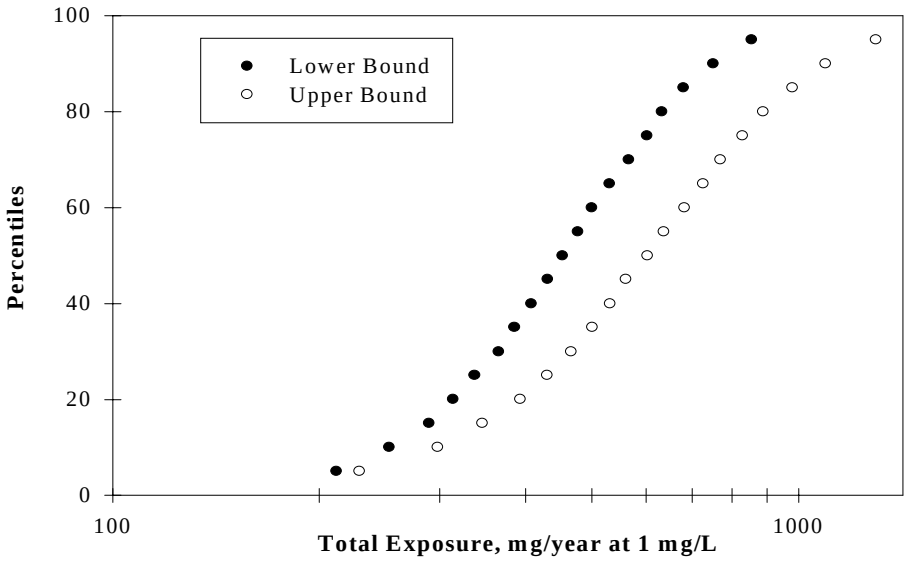

Figure 16: Bounds of Total Exposure for Chloroform

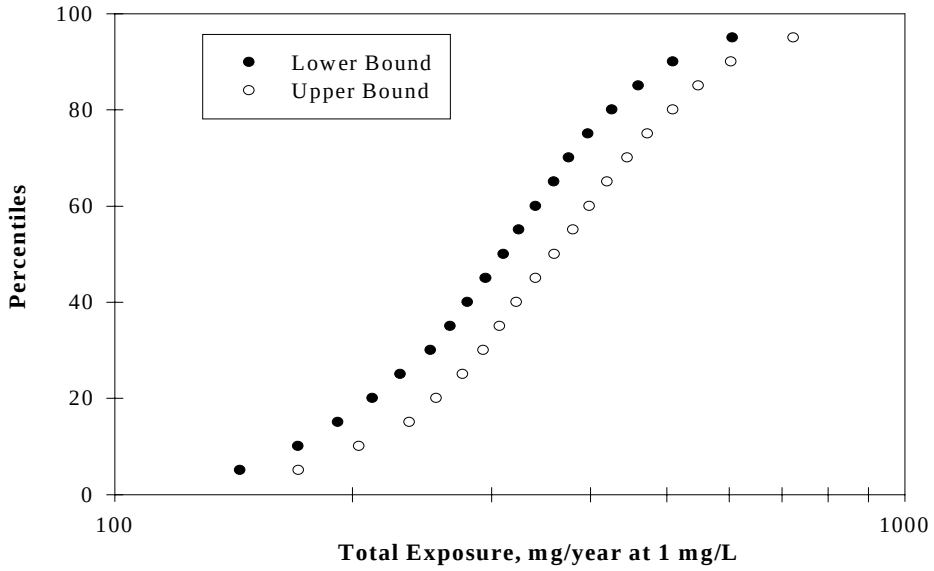

Figure 17: Bounds of Total Exposure for Methyl Parathion

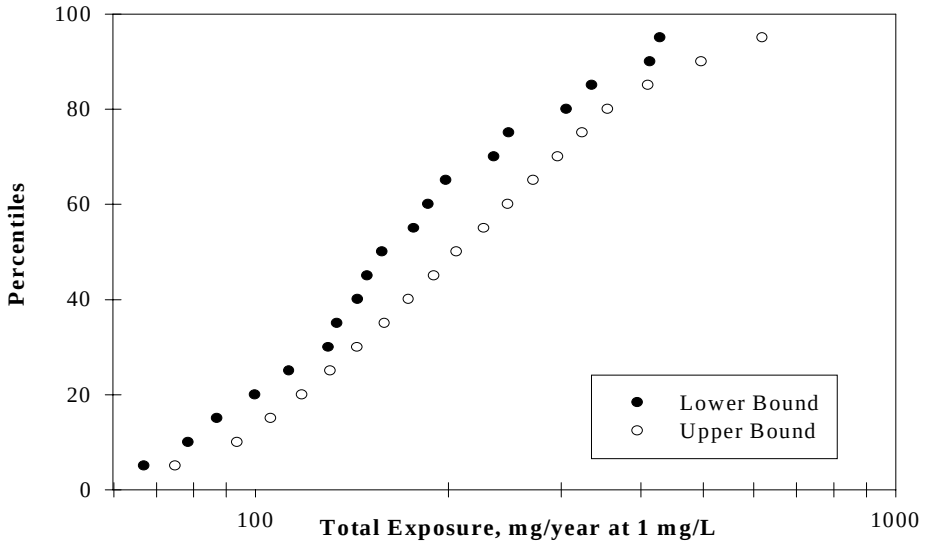

Figure 18: Bounds of Total Exposure for Chromium

Table 11: Parameters of the PDFs for Total Exposure

		Statistical Properties		
Contaminant	Bounds	Geometric mean, gm	Geometric standard deviation, gsd	P value
Chloroform	Lower	2.65	0.163	0.997
	Upper	2.77	0.197	0.999
Methyl	Lower	2.48	0.164	0.999
parathion	Upper	2.55	0.163	1.00
Chromium	Lower	2.23	0.235	0.831
	Upper	2.32	0.252	0.994

As expected, the inhalation pathway is a major contributor to total exposure for chloroform due to the high Henry's law constant (m) associated with it. Conversely, because of its high volatility, chloroform's impact on ingestion exposure is relatively low. Although the KOW value for chloroform is fairly high, the relative contribution of dermal exposure to total exposure is small (18%) due to the greater impact of inhalation exposure. The total exposure to chloroform is the highest among the three contaminants studied.

For methyl parathion, the low value of Henry's constant (8.0x10-6) makes its contribution to inhalation exposure negligibly small. The major exposure pathway for methyl parathion is ingestion due to the low volatility of the contaminant. The high Kow for methyl parathion makes the contribution of dermal exposure very significant (40%).

Impact via inhalation of gas phase chromium is negligible. Exposure via dermal sorption is also very small (2%) due to the contaminant's low Psc and Ksc/w values. The major exposure pathway for chromium is ingestion (98%). The total exposure to chromium is the least among the three compounds studied.

5.2 Comparison with the Previous Model

The previous version of the model, based on the EPA model (Little et al., 1998), evaluated inhalation exposure to radon and its progeny. The model utilizes the concept of transfer efficiency of radon. The model does not consider individual water devices in the main

house and utilizes a generalized water flow rate model for main house. Further, the model does not account for the bathing event.

Figure 19 compares the bounds of inhalation exposure for radon for the EPA model and the current model.

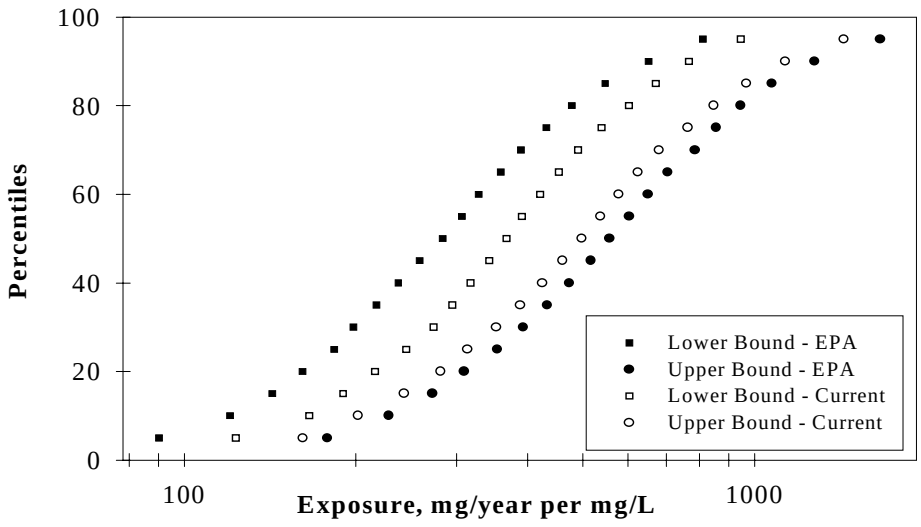

Figure 19: Bounds of Inhalation Exposure to Radon

The marked reduction in the width of the uncertainty band between the lower and the upper bounds of exposure in the new model may be explained by the fact that the model now utilizes specific water using devices, in contrast to the EPA model's generalized water usage, especially in the main house. In the absence of PDFs for the new input variables, the model uses the numerical values obtained from experimental data (Corsi and Howard, 1998, Olin et al., 1998). The relatively narrow range of values of the new variables could have contributed to the reduction of uncertainty in the model, thereby, limiting the magnitude of exposures to a lower range during Monte Carlo simulation.

5.3 Sensitivity Analysis

The two-dimensional Monte Carlo analysis provides a range of exposure values for the chemical contaminants. This does not provide any information on the relative importance of each variable in the calculations, nor does it indicate 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 mathematical model is assessed by calculating the percent change in the output variable per unit increase (1%) in an input variable. The rate of change of the output variable depends on the values selected for each of the model inputs. The inputs to the model are varied. Usually output changes on the scale of +1% or -1% are observed for variables that are important in determining exposure. Variables that have little impact on the output have a rate of change close to zero.

To obtain default values of the variables with a known Probability Density Function (PDF) (EPA, 1995), the program was modified to give as an output, each value of the variable for each of the innerloop for the program's total run of 2000 inner times 250 outer loops. From each outer loop (i.e. 2000 innerloops and hence, 2000 values for each variable) a mean value of the variable is calculated. Finally, the median of the 250 mean values was established as the default value of the variable. These default values and those of other input variables, which were acquired either from literature or calculated based on established formula, are presented in Table 12.

Table 12: Default Values of the Input Variables in the Model

Variable	Units	Values
Occupancy factor (OF)$^+$	-	0.726
Volume of main house (V_a)$^+$	L	219000
Volume of bathroom (V_b)$^+$	L	15700
Volume of shower (V_s)$^+$	L	2000
Total water use in bathroom (I_b)$^+$	L/day	47.3
Time in shower (t_s)$^+$	min	7.45
Transfer efficiency in bathroom (P_b)$^+$	-	0.301
Shower flow rate (SFR)$^+$	L/min	6.10
Time in bathroom (t_b)$^+$	min	15.1
Time leave home (LH)$^+$	minutes	453
Time return home (RH)$^+$	Minutes	847
Breathing rate (BR)$^+$	L/min	9.24
Volume of water ingested (V_I)$^+$	L/day	0.79
Time in bath (t_{bath})	min	20.0
K_G/K_L for shower ($K_GK_{L,sh}$)	-	200
Temperature in the shower (T_s)	C	21.0
Volume of the bath water (V_{bath})	L	73.0
K_G/K_L for bath ($K_GK_{L,bath}$)	-	54.0
Temperature of the bath water (T_{bath})	C	24.0
Kitchen Faucet flow rate (KFFR)	L/min	4.80
K_G/K_L for Kitchen Faucet ($K_GK_{L,KF}$)	-	104
Temperature of the Kitchen Faucet water (T_{KF})	C	24.0
Exposed surface area of the body (A_{body})	cm^2	18000
Exposed surface area of the skin (A_{hands})	cm^2	720

$^+$ Values determined from PDF curves

The effect on exposure for each model variable depends primarily upon the nature of the contaminant. For a volatile compound, for example, breathing rate (BR) would have significant impact on inhalation exposure. The Henry's constant and the mass transfer coefficients for a contaminant would have notable effects on inhalation and ingestion exposures. The volume of

water ingested (VI) would affect ingestion exposure the most if the contaminant has a low Henry's law constant. The skin surface area of the exposed body (Abody), especially for compounds with low molecular weight and high permeability coefficient, would significantly affect dermal sorption.

A sensitivity analysis of each model variable for the three exposure pathways was performed for the three representative contaminants. Table 13 lists the most influential variables for each contaminant and exposure pathway.

Table 13: Rate of Change of Exposure

	% Change in Exposure per % increase in Variable Value		
Exposure Pathway / Variable	Chloroform	Methyl Parathion	Chromium
Inhalation			
Breathing rate (BR)	1.00	1.00	-
Time in shower (t_s)	0.60	0.55	-
Volume of the shower (V_s)	- 0.53	- 0.34	-
$K_{OL}A$ for bath	0.28	0.17	-
$K_{OL}A$ for shower	0.20	0.15	-
Residence time in Main house (R_a)	0.24	0.00	-
Time in bath (t_{bath})	0.47	0.39	-
Total water use in bathroom (I_b)	0.24	0.00	-
Volume of the main house (V_a)	-0.23	-0.34	-
Volume of the bathroom (V_b)	-0.21	-0.34	-
Shower flow rate (SFR)	0.17	0.00	-
Time in bathroom (t_b)	0.13	0.15	-
Henry's constant (m)	0.09	1.02	-
Occupancy factor (OF)	0.06	0.00	-
Volume of the bath water (V_{bath})	0.06	0.00	-
Temperature of bath water (t_{bath})	0.05	0.00	-
$K_{OL}A$ for washing machine	0.02	-	-
Ingestion			
Volume of water ingested (V_I)	1.26	1.26	1.27
$K_{OL}A$ for kitchen faucet	-0.64	-0.0007	-
K_G/K_L for kitchen faucet	-0.05	-0.0007	0.00
Dermal sorption			
Octanol-water partition coefficient (K_{ow})	2.86	4.48	0.96
Skin surface area - body (A_{body})	0.98	0.98	0.99
Time in bath (t_{bath})	0.25	0.25	0.65
Time in shower(t_s)	0.15	0.15	0.24
Skin surface area – hands (A_{hands})	0.02	0.02	0.01

Summary

The current exposure model is based upon a previously developed EPA model which evaluated inhalation and ingestion exposure to radon and daughter products originating in drinking water. The extended model performs an integrated exposure analysis, incorporating inhalation, ingestion and dermal sorption exposure pathways, for the entire range of chemical contaminants found in drinking water. Water using devices like shower, bath, bathroom, kitchen faucet, washing machine and dishwasher are included as sources in the model. 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 in each of the three compartments, usage pattern of the water devices and human activity pattern, 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. A sensitivity analysis was conducted to identify the most important variables that affect the individual exposure pathways. Finally, the model considered three representative contaminants: chloroform, methyl parathion and chromium, in a detailed analysis. As expected, the overall mass transfer coefficient, especially for showers and baths, is the major determinant of the magnitude of inhalation exposure. The overall mass transfer coefficient for the kitchen faucet, for volatile compounds, substantially affects ingestion exposure. The role of Henry's constant is significant for inhalation exposure. The octanol-water partition of the compound has a considerable effect on the extent of dermal sorption. In addition, human activity pattern, in terms of usage of the water devices and the occupancy of different compartments, and a person's individual characteristics (breathing rate, amount of water consumed, body surface area), have a significant impact on the magnitude of total exposure to a given chemical contaminant.

6. FUTURE WORK

6.1 Recommendations on Additional Data and Uncertainty Analysis

The input variables of the EPA model (EPA, 1995) are described with probability density functions (PDFs). In addition, to account for knowledge uncertainty (EPA, 1995), the parameters of the PDFs for the input variables are described by unique PDFs of their own. The statistical fit of the variables in the EPA model was based on extensive survey of residential households across the United States. Let us take an example of volume of the bathroom, V_b.

EPA utilized the survey data collected by National Kitchen and Bath Association on the size of bathrooms in households. The data was well fit by the truncated log normal distribution. To account for knowledge uncertainty, the parameters of the lognormal distribution for the bathroom, the geometric mean (gm) and the geometric standard deviation (gsd) were described with the student's t and chi-squared distributions, respectively.

The extension of the EPA model required additional input variables to calculate exposure values from additional exposure pathways and water devices. Most of the values of the new variables used by the model are based on experimental results (Corsi and Howard, 1998) and some on survey data (Olin et al., 1998). None of the new input variables, however, are described in terms of PDFs.

Wherever possible, the model utilizes a random function to select a different set of experimental data for each loop of the model run. Some element of variability, therefore, exists between different loops of the model run. However, to make the uncertainty analysis of the model complete and more relevant, each input variable should be described statistically with the help of a PDF.

The values of the new input variables are based on a very limited set of data. Sensitivity analysis of these preliminary values would identify more critical model variables. An extensive process of data collection and statistical fitting of these variables and their incorporation in the model would contribute significantly to the refinement of the model, specifically in its ability to perform uncertainty analysis of exposure.

Table 14 lists important variables that require further analysis and data collection.

Table 14: Variables Requiring Additional Data

Volume of the bath water (or different types of bathtubs)
Duration and frequency of use of the bathtub
Patterns of usage and types of:
Toilets
Wash basins
Kitchen faucets
Washing machines
Dishwashers
Mass transfer coefficients for water devices for a range of:
Temperatures
Flow conditions
Sequence and duration of cycles (wash, rinse) for washing machine and dishwasher (or by model type)
Skin surface areas of:
Body
Hands
Occupancy patterns of the different compartments

The lower and upper bounds of exposure in this study is determined by CDF curves representing the lowest and the highest median values in the outerloops. In future, additional statistical analysis of the median values followed by expressing the exposure bounds by, say, the 5^{th} and the 95^{th} percentile of the median, instead of the two extreme medians, can make the results more representative.

6.2 Additional Sources

One component the present model does not consider is the impact of aerosols. ILSI report (Olin et al., 1998) defines aerosol as airborne particles sufficiently small (diameter $Dp \leq 10\mu m$) that it does not rapidly settle out of air. Aerosols are directly formed from activities like showering and using humidifiers. Aerosols are also formed when the water droplets evaporate. Hence, water droplets from activities like showering, bathing, washing (hands, face, clothes, and dishes), toilet use, humidifier use, cleaning, cooking and outdoor water use are also potential sources of aerosols (Olin et al., 1998). Exposure to aerosol occurs primarily from inhalation and their subsequent absorption in the human respiratory system including the surface of the lung. The primary factor that determines the relative magnitude of deposition in different regions of the

respiratory tract (nose, airways and alveolar) is the particle size distribution of the aerosol (Olin et al., 1998). Hence, the nature of the source is very significant in aerosol exposure analysis. Another potential source of exposure from aerosols is via dermal sorption when the aerosols are deposited on the exposed skin surface during different water use activities.

In order to incorporate exposure via aerosols into the model, major sources of aerosols, particularly showering and humidifier use (Olin et al., 1998), should be considered. Data on the magnitude of aerosol formation, droplet size distribution and deposition rates and the usage pattern of showers and humidifiers will be required.

For volatile contaminants in water, humidifiers can also be a significant source for inhalation exposure via the vapor phase.

6.3 Lung-Deposition Model

Inhalation is an important route of uptake for gaseous and volatile chemicals as well as for aerosols. In order to evaluate contaminant exposure via inhalation of aerosols and their subsequent deposition in the respiratory system (primarily the surface of the lung), a simplified lung deposition model (Miller et al., 1985) can be utilized. The model considers the lower respiratory tract to be sequential sets of parallel cylinders, the interior of which represent the lumen as shown in Figure 20. The airways of the lung are represented by these concentric cylinders, such that the dimensions of the rigid inner cylinder correspond to the airway itself, and the dimensions of the outer cylinder correspond to the alveoli around the airway (Georgopoulos et al., 1997). Axial transport occurs only through the inner cylinder via advection and dispersion, both of which are computed as functions of the average air flow velocity, which is calculated assuming a sinusoidally varying alveolar volume. Radial flux is evaluated by assuming local equilibrium between the concentration in the airway and the airway walls (Georgopoulos et al., 1997).

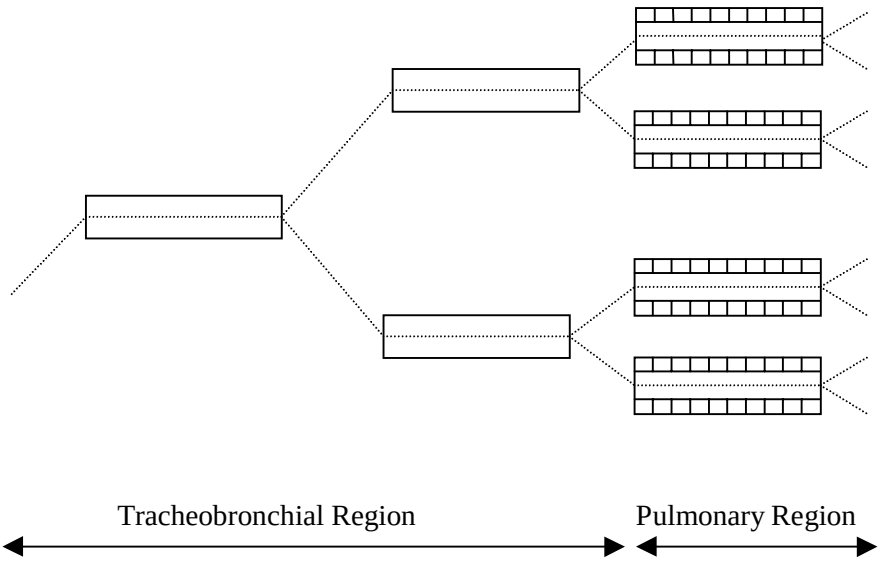

Figure 20: Schematic Representation of Lung Model

6.4 Non Residential Environments

The present model considers a household with three compartments with water devices and human activity pattern specific to a residential environment. However, a person spends a significant amount of his time away from home. Time spent in offices, schools and hospitals involve use of water devices specific to these environments which may result in significant exposures. Hence, a complete exposure analysis from indoor water sources must consider the non residential environments as well.

The present model can be modified to represent non-residential environments. The exposure analysis for the non-residential model would follow a computational procedure very similar to the current model but would require an entirely new set of data for the model parameters. The reformulation of the model would essentially require an extensive study and data collection on:

- The type, orientation, interaction (for ventilation between compartments) and sizes of the compartments,
- Water using devices specific to the environment (water fountain, shower stall, bathroom facility)

- Water utilization rates, and
- Activity pattern and personal characteristics of different categories of people (staff/teachers, patient/students).

6.5 Multi-Compartment Model

The extensive collection of information, as recommended in the previous sections, on different water using devices, ventilation, sizes and interaction of compartments and human activity patterns in both residential and non-residential environments would make it possible for the development of a generalized, user-defined multi-compartment model as shown in Figure 21.

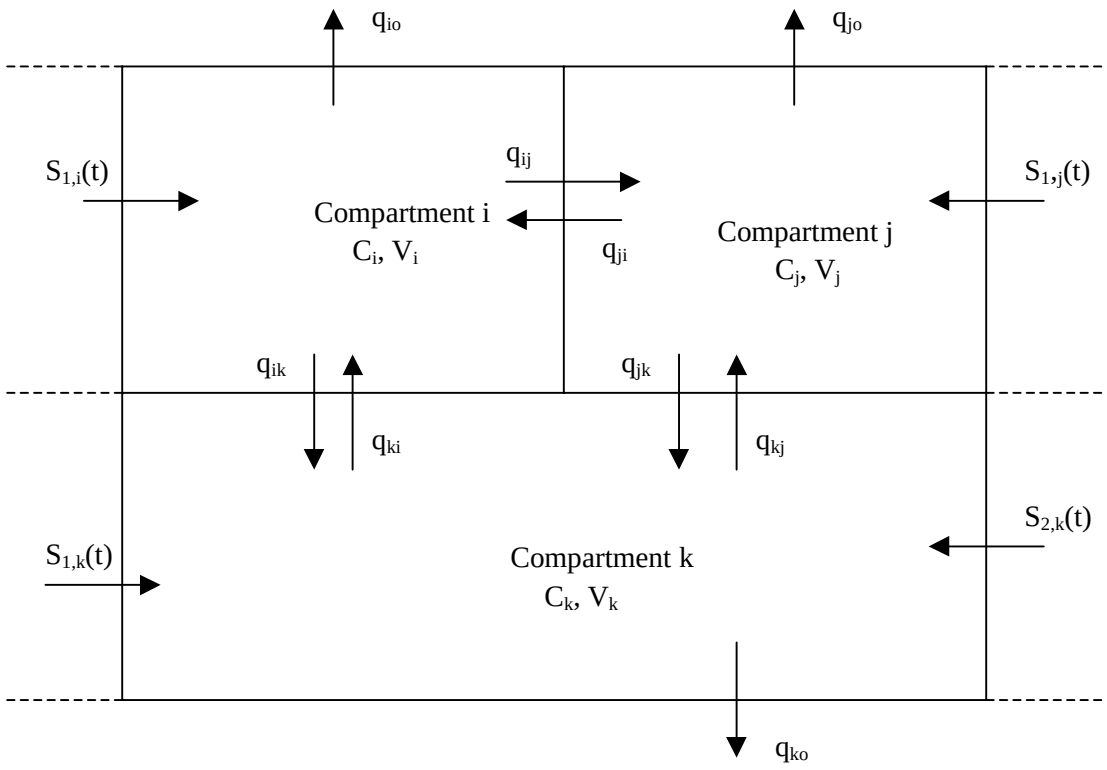

Figure 21: User defined Multi-Compartment Model

Each compartment in the model can have can have more than one water using device. $S_{i,k}$ refers to source number i in compartment k. Similarly, q_{kl} refers to air exchange rate from compartment k to compartment l and q_{k0} refers to ventilation from compartment K to the outside air.

When analyzing inhalation exposure, the water flow regime for each device (Source) can be characterized into either a plug flow model (PFM) or completely mixed flow model (CMFM). Note that CMFM with no flow is usually referred to as a batch reactor. The source term for devices that approximate PFMs can typically be incorporated using a pseudo steady-state assumption as has been done for shower (Little, 1992). When the water within a device approximates a CMFM (for example, dishwasher, bath), an additional compartment that holds water, as opposed to air, but that is nevertheless well mixed, can be specified. These water compartments exchange volatile contaminants with the gas phase in the compartment where they are located.

Dermal exposure computation requires information on the duration of the use of the device, concentration profile of the contaminant in the water pool and the skin surface area exposed to water during the operation of the device.

6.6 Coupling with PBPK Model

After an individual's exposure to a contaminant is estimated, the next step involves understanding the contaminant transport within a human body. Pharmacokinetic techniques, which refer to the prediction of time dependent concentration of a substance in a living system, are employed to describe this uptake (Gerlowski and Jain, 1983). The physiologically based pharmacokinetic approach separates the body into a series of anatomical compartment interconnected by the body's fluid system. A contaminant may, for example, show high affinity for certain organs or maybe toxic to some tissue. The multi compartment approach enables the estimation of contaminant concentration in different organs of the human body. Hence, the biologically effective dose estimated by the physiologically-based pharmacokinetic (PBPK) model provides a link between exposure assessment and risk assessment (Georgopoulos et al., 1997).

The generalized integrated exposure model envisaged by this study can be re-structured so that it can be easily coupled to a PBPK model such as that described by Georgopoulos et al. (1997).

REFERENCES

American Water Works Association (AWWA), Water Quality and Treatment: A Handbook of Community Water Supplies, 4rth ed., McGraw Hill Inc., 1990.

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.

Andelman, J. B., Human exposure to volatile halogenated organic chemicals in indoor and outdoor air, *Environmental Health Perspectives*, 62, 313-318, 1985.

Andelman, J. B., Total exposure to volatile organic compounds in potable water, *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.

Bogen, K. T., and Spear, R. C., Integrating uncertainty and interindividual variability in environmental risk assessment, *Risk Analysis*, 7, 427-436, 1987.

Bogen, K. T., Colston, B. W. Jr., and Machicao, L. K., Dermal absorption of dilute aqueous chloroform, trichloroethylene, and tetrachloroethylene in hairless guinea pigs, *Fundamental and Applied Toxicology*, 18, 30-39, 1992.

Brown, H. S., Bishop, D. R., and Rowan, C. A., The role of skin absorption as a route of exposure for Volatile Organic Compounds (VOCs) in drinking water, *American Journal of Public Health*, 74, 479-484, 1984.

Bunge A.,and McDougal, J., Dermal uptake, Chapter 6 in Estimation of dermal and inhalational exposures to drinking water contaminants. Draft document, ILSI Risk Science Institute, 1996.

Bunge, A. L., and Cleek, R. L., A new method for estimating dermal absorption from chemical exposure. 2. Effect of molecular weight and octanol-water partitioning. *Pharmacological Research*, 12, 88-95, 1995.

Cleek, R. L., and Bunge, A. L., A new method for estimating dermal absorption from chemical exposure. 1. General approach. *Pharmacological Research*, 10, 497-506, 1993.

Corsi, Richard, and Howard, Cynthia, Volatilization Rates from Water to Indoor Air, Phase II, USEPA Office of Research and Development, Report, Washington D.C., 1998.

Crank J, The Mathematics of Diffusion, Oxford University Press, Oxford, 1975.

EPA 1983, National revised Primary Drinking Water Regulations; Advance Notice of Proposed Rulemaking. Federal Register 48 (194, 45502-45521).

EPA 1989, Exposure Factors Handbook. Washington D.C.: U.S. Environmental Protection Agency , Office of Health and Environmental Assessment, EPA 600/8-89/043.

EPA 1995, Uncertainty Analysis of Risks Associated with Exposure to Radon in Drinking Water. EPA Report, EPA-822-R-96-005, March 1995.

DOE/EIA. 1991, Commercial Building Characteristics 1989. Washington D.C. U.S. Department of Energy, Energy Information Administration. DOE/EIA. 0249(89).

Georgopoulos et al., Integrated Exposure and Dose Modeling and Analysis System. 1. Formulation and Testing of Microenvironmental and Pharmacokinetic Components. *Environmental Science & Technology*, 31, 17-27, 1997.

Gerlowski, L. E., and Jain, R. K., Physiologically Based Pharmacokinetic Modeling: Principles and Applications. *Journal of Pharmaceutical Sciences,* 72, 1103-1127, 1983.

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.

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.

Giardino, N. J., and Andelman, J. B., Characterization of the emissions of trichloroethylene, chloroform and 1,2-dibromo-3-chloropropane in a full-size, experimental shower, *Journal of Exposure Analysis and Environmental Epidemiology*, 6, 413-423, 1996.

Howard, Cynthia, and Corsi, Richard, Volatilization of Chemicals from Water to Indoor Air: Role of the Kitchen Sink, *Journal of Air and Waste Management Association*, 46, 830-837, 1996.

Jo, W. K., Weisel, C. P., and Lioy, P. J., Routes of chloroform exposure and body burden from showering with chlorinated tap water, *Risk Analysis*, 10, 575-580, 1990.

Jo, W. K., Weisel, C. P., and Lioy, P. J., Chloroform exposure and the health risk associated with multiple uses of chlorinated tap water, *Risk Analysis*, 10, 581-585, 1990.

Leabo, A. L., Basic Statistics, Richard D. Irwin Inc., 1972.

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.

Little, J. C., Applying the two-resistance theory to contaminant volatilization in showers, *Environmental Science & Technology*, 26, 1341-1349, 1992.

Little, John C., Khanal, Rajesh, and Sankaran, Karpagam Uncertainty Analysis of Risk Associated with Exposure to Volatile Compounds in Drinking Water, USEPA Office of Water, Washington D.C., 1998.

Macintosh, David L., Xue, Jianping, Ozakaynak, Haluk, Spengler, John D., and Ryan, P. B., A Population Based Exposure Model for Benzene, *Journal of Exposure Analysis and Environmental Epidemiology*, 5, 375-403, 1995.

McBean, E. A., and Rovers, F. A., Statistical procedure for analysis of environmental monitoring data and risk assessment, Perntice Hall PTR, New Jersey, 1998.

McKone, T. E., Human exposure to volatile organic compounds in household tap water: The indoor inhalation pathway. *Environmental Science & Technology*, 21, 1194-1201, 1987.

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.

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.

Miller et al., A Model of the Regional Uptake of Gaseous Pollutants in the Lung. Toxicology and Applied Pharmacology, 79, 11-27, 1985.

Nazaroff, W. W., Doyle, S. M., Nero, A. V., and Sextro, R. G., Potable Water as a source of airborne ^{222}Rn in U.S. Dwellings: A review and assessment, *Health Physics*, 52, 281-295, 1987.

Nazaroff, W. W., and Nero, A. V., Radon and its decay products in indoor air, John Wiley & Sons, 1988.

Olin, Stephen S., Ed., Exposure to Contaminants in Drinking Water: Estimating Uptake Through Skin and by Inhalation, ILSI Press, Washington D.C., 1998.

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.

Selleck, R. E., Mariñas, B. J., and Diyamandoglu, V., Sanitary Engineering and Environmental Health Research Laboratory, UCB/SEEHRL Report No. 88-3/1, University of California, Berkeley, California, 1988.

Shepherd, J., Kemp, J., and Corsi, R. L., Residential washing machines as sources of indoor air pollution - chloroform formation, mass transfer, and emission dynamics, presented in the proceedings of AWMA Annual Meeting, Cincinnati, Ohio, 1994.

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.

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.

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 in the Model

Table 15: Source/Sink Terms in the Mathematical Model

		Source Terms		Sink Term
Compartment	Water Devices	Q	Air inflow	Air outflow
Shower	Shower	$\left(1-e^{\left(\frac{K_{OL}A}{SFR}\right)}\right)\cdot\left(C_0-\frac{y_s}{m}\right)$	$q_{bs}\ y_b$	$q_{sb}\ y_s$
	Bath	$K_{OL}A\cdot\left(C_0-\frac{y_s}{m}\right)$		
Bathroom		$\left(1-e^{\left(-\frac{K_{OL}A}{WFR_b}\right)}\right)\cdot\left(C_0-\frac{y_s}{m}\right)^{+}$	$q_{sb}\ y_s+q_{ab}\ y_a$	$\left(q_{bs}+q_{bo}+q_{ba}\right)y_b$
Main House	Kitchen Faucet	$\left(1-e^{\left(-\frac{K_{OL}A}{WFR_{kf}}\right)}\right)\cdot\left(C_0-\frac{y_a}{m}\right)$	$q_{bs}\ y_b$	$\left(q_{ab}+q_{ao}\right)y_a$
	Washing machine	E_{wm}		
	Dishwasher	E_{dw}		

[+]$K_{OL}A$ for the bathroom is computed on the basis of transfer efficiency of radon.

The mass balance for the gas phase concentration of a contaminant in the three compartments of the model is expressed as:

$$V_s \cdot \frac{dy_s(t)}{dt} = Q_s(t) + [q_{bs} \cdot y_b(t)] - [q_{sb} \cdot y_s(t)]$$

$$V_b \cdot \frac{dy_b(t)}{dt} = Q_b(t) + [q_{sb} \cdot y_s(t) + q_{ab} \cdot y_a(t)] - [(q_{bs} + q_{b0} + q_{ba}) \cdot y_b(t)]$$

$$V_a \cdot \frac{dy_a(t)}{dt} = Q_{kf}(t) + Q_{wm}(t) + Q_{dw}(t) + [q_{ba} \cdot y_b(t)] - [(q_{ab} + q_{a0}) \cdot y_a(t)]$$

Appendix B
Probability Distribution

In a graphical representation of a PDF (Figure 22), 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 (Leabo, 1972). Hence, if an arbitrary vertical strip under the PDF curve is selected, the probability that the variable will have a value which lies 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 under the curve.

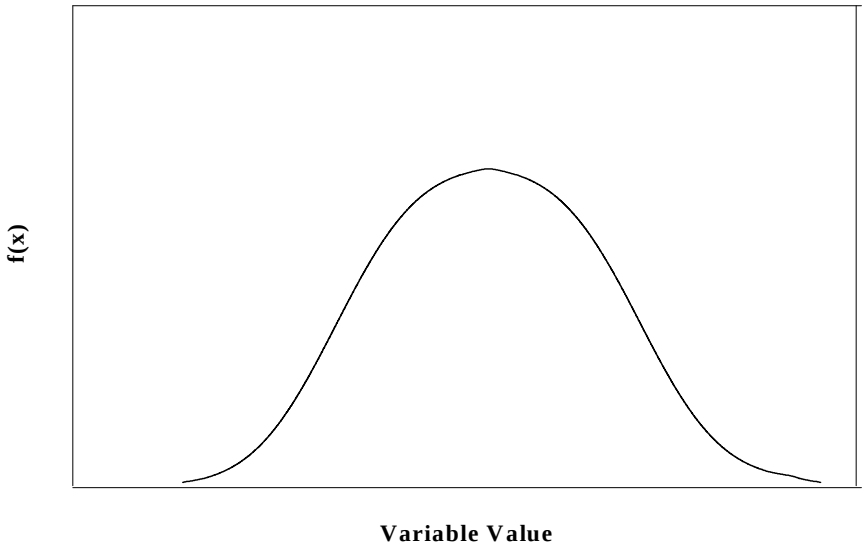

Figure 22: PDF Curve

A probability distribution can also be represented by a Cumulative Distribution Function (CDF), F(x) (McBean et al., 1998). The CDF (Figure 23) 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,

$$F(x) = \mathrm{Prob}[X \le x] = \int_{-\infty}^{x} f(x)dx$$

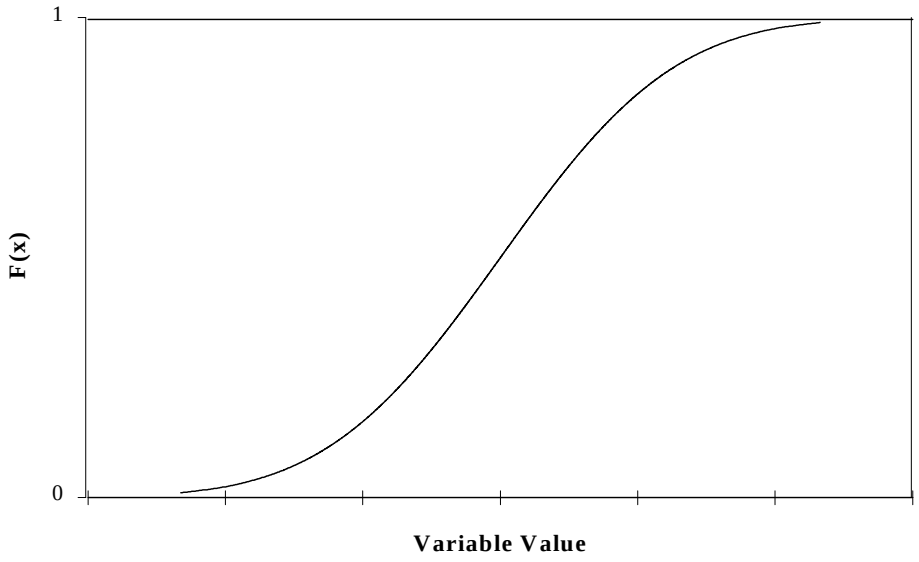

Figure 23: CDF Curve

To assign a value to a given variable described by a particular distribution and its parameter(s), a random number from that distribution and bounded by those parameters, has to be generated. The normal procedure followed to accomplish this is to utilize the inverse of the Cumulative Distribution Functions.

The program employs library functions IMSL C Numerical Libraries version 2.0 to compute the inverse CDF of distributions. A probability number is generated with the help of a random number generator and the values of the variables associated with that number are obtained from the inverse CDFs.

1. Uniform Distribution

There are two parameters to the uniform distribution (U): 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:

PDF: $f(x) = \frac{1}{b-a}$ $\qquad a \le x \le b$

CDF: $F(x) = \int_a^x f(x)dx = \int_a^x \frac{dx}{b-a} = \frac{x-a}{b-a}$ $a \le x \le b$

The uncertainty in the parameters is again distributed uniformly. The parameter min assumes values between a and b. The parameter max assumes values between c and d.

2. Triangular Distribution

The PDF for the triangular distribution (TRI) is:

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

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

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).
The CDF for the triangular distribution is given by:

$$F(x) = \int_a^x f(x)dx = \int_a^x \frac{2(x-a)}{(b-a)(c-a)}dx \qquad a \le x \le c$$

$$F(x) = \int_c^x f(x)dx = \int_c^x \frac{2(x-a)}{(b-a)(c-a)}dx \qquad c \le x \le b$$

Solving the above equations, the following exact solutions were obtained for the value of the variables:

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

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

3. Normal Distribution

For variables such as Breathing Rate the most appropriate distribution was found (EPA, 1995) 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:

PDF: $$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma} \right)^2 \right] \qquad -\infty < x < \infty$$

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 (TS) and chi-squared (CH) distributions respectively. The PDFs for student's-t and chi-squared distributions will be discussed in later sections.

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

CDF: $$F(x) = \int_{-\infty}^{x} \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma} \right)^2 \right] dx \qquad -\infty < x < \infty$$

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

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 (EPA, 1995). Data of this type was found to be represented well by a lognormal distribution (LN). In some cases, however, the values were found to lie within an interval. For these cases, a 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:

PDF: $$f(x) = \frac{1}{x\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\ln x - \mu}{\sigma}\right)^2\right] \qquad 0 < x < \infty$$

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 variables 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 the minimum and the maximum.

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.

$$gm = e^{\mu}$$
$$gsd = e^{\sigma}$$

Since there is uncertainty associated with this approximation, the uncertainty about μ and σ were modeled using student's t and chi-squared distributions respectively.

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

CDF: $$F(x) = \int_0^x \frac{1}{x\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\ln x - \mu}{\sigma}\right)^2\right] dx \qquad 0 < x < \infty$$

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

5. Beta Distribution

Many variables in the EPA model are evaluated as fractions and assume values over a narrow range (for example, between zero and one). The occupancy factor and the fraction ingested 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. Limited information

was 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:

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

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:

$$a = \frac{(\text{mean} - \text{min})(2.\,\text{mode} - \text{min} - \text{max})}{(\text{mode} - \text{mean})(\text{max} - \text{min})} \qquad a > 1$$

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

Uncertainty about the mean was usually modeled as uniform and uncertainty about the mode was usually modeled as uniform or triangular.

6. Student's-t Distribution

The student's t distribution and the chi-squared 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 variable 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 (EPA, 1995).

$$\frac{m - \mu}{s/\sqrt{n}} = TS_{n-1}$$

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

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

$$TS_{qf-1} = \frac{m-\mu}{s/\sqrt{qf}}$$

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 TS is calculated. Since m, s, qf are known, μ can be calculated.

7. Chi-squared Distribution

The important parameters of a chi-squared distribution are m and qf. The χ^2 variate with qf-1 degrees of freedom is expressed as,

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

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, and qf are known, σ can be calculated directly.

Appendix C
The Model Variables

This section presents the description of the variables used by the model. The variables with known PDFs are described in terms of both their variability (PDF_v) and uncertainty (PDF_u). Wherever applicable, the procedure for computing a value of a variable for a given contaminant on the basis of the known value of the variable for the base contaminant, is also explained.

1. Number of People per House (PNUM)

The information collected by U.S. DOE (1982) in a survey of 6051 randomly selected U.S. residences was used by the EPA (EPA, 1995) to determine the relative frequency of homes as a function of number of residents (PNUM).

Table 16: 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 16. Since this distribution is based on over 6000 observations, PNUM was not treated as an uncertain variable (EPA, 1995).

2. Compartment Volumes

2.1 Volume of Shower (V_s)

Since limited information was available on shower volume,V_s, it was modeled as a uniform distribution with uncertain minimum and maximum values (EPA, 1995).

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

PDF_u (min) ~ U(1000, 1500)

PDF_u (max) ~ U(2500, 3000)

The same value of volume is considered for bathing as the event occurs in the same compartment.

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) ~ TLN(gm, gsd, min, max)

PDF_u (ln(gm)) ~ TS(m, s, qf)

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

m = ln(14000)

s = ln(1.66)

qf = 25

min = 4000

max = 60000

2.3 Volume of the Main House (V_a)

The EPA report used house volume data based on a U.S. DOE survey (1982) 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.

The report follows the procedure developed by Nazaroff et al. (1987) to estimate house volume from the floor area by assuming a wall height of 2.4 m (8 ft). Per capita volume (V_t) is obtained by dividing the house volume by the number of people in the house (PNUM). The resulting distributions were found to be well fit by lognormal PDFs and hence, the value of V_t was modeled as a set of truncated lognormal distributions, based on the number of people in the house.

Table 17: 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 17 are approximately equal to the 99th and the 1st percentile values, estimated from graphs of data presented by the original authors (Nazaroff et al. 1987). Since the study involved a large number of homes from different cities across the U.S. a qf of 100 was assigned (EPA, 1995).

Using the distributions formulated by Nazaroff et al. (1987), 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 PDF for total volume per capita (V_t). 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 value 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 (EPA, 1995).

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 (PNUM · 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. Water Usage

3.1 Shower/Bath Flow Rate

The value of the shower flow rate is based on the experimental data from Corsi's experiments (1998). The flow rate considered by the model depends upon the experimental data set selected for a given model run. The values of the variables for ten different sets of experiments are presented in Table 19.

The volume of the water used for bathing event is 76.0 L/event (Corsi and Howard, 1998). As the model considers only the surface volatilization portion of the event, the bath flow rate is not relevant to the present model.

3.2 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.

$I_b = PNUM \cdot WU_b$

$PDF_v(WU_b)$ ~ U(min, max)
$PDF_u(min)$ ~ U(15, 20)
$PDF_u(max)$ ~ U(75, 85)

3.3 Water Use in Main House

The main house water use is the sum total of the water used in the kitchen faucet, the washing machine and the dishwasher. The data used by the model for all of these devices is based on the data used by Corsi (1998) in his experiments. The numerical values of the data used by the model are presented in Table 19.

3.4 Volume of Water Ingested (V_I)

The amount of water ingested by a person per day was modeled as a beta distribution (EPA, 1995) as follows:

$PDF_v(V_I)$ ~ BETA(mean, mode, min, max)

PDF_u (mean) ~ U(0.70, 0.90)

PDF_u (mode) ~ U(min, mean) if (mean < 0.5 · (min + max))

~ U(mean, max) if (mean > 0.5 · (min + max))

min = 0.50

max = 1.00

3.5 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 by the EPA as:

$PDF_v(VR_a)$ ~ TLN(gm, gsd, min, max)

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

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

m = ln(0.68)

s = ln(2.01)

qf = 25

min = 0.1/hr

max = 3.5/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 EPA modeled the ventilation rate as independent of house size.

3.6 Bathroom Residence Time (R_b)

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

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

Normal exhaust rates for fans supplied by different manufacturers range from about 40 to 160 ft^3/min with most mid-range fans discharging about 70 to 90 ft^3/min. Based on these data, the EPA modeled the air flow rates into and out of the bathroom separately for three different conditions.

Table 18: PDFs for R_b Based on Cases of Bathroom Ventilation

Case	Description	PDFs	Values
1	Door open, fan off	R_{b1} ~ U(min, max)	min ~ U(20, 30)
			max ~ U(40, 50)
2	Door closed, fan off	R_{b2} ~ U(min, max)	min ~ U(20, 30)
			max ~ U(150, 250)
3	Door closed, fan on	$R_{b3} = V_b/EXFR$	mode ~ U(2000, 2500)
		EXFR ~ TRI(min, max, mode)	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 (EPA, 1995).

3.7 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 and the study by Wilkes et al. (1992) which suggested that the residence time in the shower is relatively brief, the EPA modeled the value of R_s as:

$PDF_v(R_s)$ ~ U(min, max)

$PDF_u(min)$ ~ U(2, 3)

$PDF_u(max)$ ~ U(4, 6)

4. Human Activity Patterns

4.1 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:

$PDF_v(T_s)$ ~ TLN(gm, gsd, min, max)

$PDF_u(ln(gm))$ ~ TS(m, s, qf)

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

m = ln(6.8)

s = ln(1.6)

qf = 100

min = 1

max = 30

4.2 Time in Bathroom After Shower (t_b)

EPA's exposure assessment predicts the time a person spends in the bathroom to be about 4 to 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 to 20 minutes, with a range of 1 to 30 minutes. Hence, T_b was modeled as:

$PDF_v(T_b)$ ~ U(min, max)

PDF_u (min) ~ U(1, 10)

PDF_u (max) ~ U(20, 30)

4.3 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:

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

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

4.4 Time Return Home (RH)

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

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

4.5. Occupancy Factor (OF)

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:

PDF_v (OF) ~ BETA(mean, mode, min, max)

PDF_u (mean) ~ U(0.65, 0.80)

PDF_u (mode) ~ U(min, mean) if (mean < $0.5 \cdot$ (min + max))

~ U(mean, max) if (mean > $0.5 \cdot$ (min + 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)
$OF_{min} = LH_{min}/1440$

4.6 Breathing Rate (BR)

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) ~ TN(mean, std, min, max)
PDF_u (mean) ~ TS(m, s, qf)
PDF_u (std^2) ~ INVCH(s, qf)

m = 9.1
s = 2.0
qf = 10
min = 2.6
max = 46.6

The model variables with known PDFs are summarized in Table 19 and the experimental data used by the model is presented in Table 20.

Table 19: Summary of Model Variables with Known PDFs

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	Vb ~ 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)	max = 60
			qf = 25	
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)	max = 1,100,000
			qf = 100	
	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)	max = 700,000
			qf = 100	
	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)	max = 450,000
			qf = 100	

	Vt4 ~ TLN(gm, gsd, min, max)	ln_2(gm) ~ TS(m, s, qf) ln(gsd) ~ INVCH(m, qf)	m = ln(89,000) s = ln(1.67) qf = 100	min = 20,000 max = 400,000
	Vt5 ~ TLN(gm, gsd, min, max)	ln_2(gm) ~ TS(m, s, qf) ln(gsd) ~ INVCH(m, qf)	m = ln(75,000) s = ln(1.70) qf = 100	min = 15,000 max = 350,000
	Vt6 ~ TLN(gm, gsd, min, max)	ln_2(gm) ~ TS(m, s, qf) ln(gsd) ~ INVCH(m, qf)	m = ln(54,000) s = ln(1.78) qf = 100	min = 10,000 max = 300,000
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
Shower air residence time	Ra ~ U(min, max)	min ~ U(a, b) max ~ U(c, d)	a = 2 c = 4	b = 3 d = 6
Bathroom air residence time (door open)	Rb1 ~ U(min, max)	min ~ U(a, b) max ~ U(c, d)	a = 20 c = 40	b = 30 d = 50
Bathroom air residence time (door closed)	Rb2 ~ U(min, max)	min ~ U(a, b) max ~ U(c, d)	a = 20 c = 150	b = 30 d = 250
Bathroom fan exhaust rate	EXFR ~ TRI(min, max, mode)	mode ~ U(a, b)	min = 1000 max = 5000	a = 2000 b = 2500

Main house ventilation rate	VRa ~ TLN(gm, gsd, min, max)	ln_2(gm) ~ TS(m, s, qf) ln(gsd) ~ INVCH(m, qf)	m = ln(0.68) s = ln(2.01) qf = 25	min = 0.1 max = 2
Radon transfer efficiency in Bathroom	Pb ~ U(min, max)	min ~ U(a, b) max ~ U(c, d)	a = 0.15 c = 0.35	b = 0.25 d = 0.45
Volume of water ingested	V_I ~ B(mean, mode, min, max)	mean ~ U(a, b) mode ~ U(mean, max) or U(min, mean)	a = 0.70 b = 0.90	min = 0.5 max = 1.0
Time in shower	t_s ~ TLN(gm, gsd, min, max)	ln_2(gm) ~ TS(m, s, qf) ln(gsd) ~ INVCH(m, qf)	m = ln(6.8) s = ln(1.6) qf = 100	min = 1 max = 30
Time in bathroom	t_b ~ U(min, max)	min ~ U(a, b) max ~ U(c, d)	a = 1 b = 10	c = 20 d = 30
Breathing rate	BR ~ TN(mean, std, min, max)	mean ~ TS(m, s, qf) std^2 ~ INVCH(m, qf)	m = 9.1 s = 2.0 qf = 10	min = 2.6 max = 46.6
Occupancy factor	OF ~ B(mean, mode, min, max)	mean ~ U(a, b) mode ~ U(mean, max) or U(min, mean)	a = 0.65 b = 0.80	min = 0.33 max = 1.0

Table 20: Experimental Data Used by the Model

Device/ Experiment no.		Variables						
		m_b (-)	Q_l (L/s)	Q_g (L/s)	$K_{OL}A_b$ (L/s)	K_g/K_l (-)	T (^oC)	V_l (L)
Shower	1	0.126	6.1	360.0	6.62	200.0	21	-
	2	0.132	6.1	360.0	6.83	195.0	22	-
	3	0.250	6.1	364.0	9.02	110.0	36	-
	4	0.239	6.1	371.0	8.72	143.0	35	-
	5	0.229	6.1	367.0	9.89	138.0	34	-
	6	0.126	9.1	370.0	9.34	153.0	21	-
	7	0.132	9.1	343.0	11.77	223.0	22	-
	8	0.239	9.1	379.0	11.80	111.0	35	-
	9	0.229	9.1	354.0	13.97	131.0	34	-
	10	0.229	9.1	373.0	12.91	153.0	34	-
Bath	1	0.145	-	373.0	1.24	54.0	24	73.0
	2	0.219	-	379.0	1.25	35.0	33	73.0
	3	0.239	-	373	1.28	78.0	35	73.0
Kitchen Faucet	1	0.139	4.8	-	1.05	104.0	23	-
	2	0.139	7.9	-	1.33	51.0	23	-
	3	0.139	4.8	-	0.66	43.0	23	-
	4	0.139	7.9	-	1.18	27.0	23	-
	5	0.139	4.8	-	1.04	18.0	23	-
	6	0.139	6.3	-	1.32	18.0	23	-
	7	0.139	7.9	-	1.80	18.0	23	-
	8	0.139	4.8	-	1.10	14.0	23	-
	9	0.139	6.3	-	8.16	38.0	23	-

VITA

Rajesh Khanal was born in April 1966 in Kathmandu, Nepal. He graduated with a Bachelor's degree in Civil Engineering from Bangladesh University of Engineering and Technology, Dhaka, Bangladesh, in 1992. He worked for different consulting services, primarily in the water supply sector, for nearly five years before joining the Masters program at Virginia Tech from the fall semester of 1997. Rajesh will be working as Information Technology Associate for Capital One Services in Richmond, Virginia, from June of 1999.