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AIR QUALITY MODEL FOR VOLATILE CONSTITUENTS FROM INDOOR USES OF WATER

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An indoor-air quality model, MAVRIQ, has been developed to simulate the air concentration of organic compounds due to volatilization of chemicals originating in the domestic water supply. MAVRIQ can also simulate the inhalation exposure to an individual. An application of MAVRIQ, presented in this paper, demonstrates the effect of various water uses on the air concentrations in a test house.

INTRODUCTION

Human exposure to many organic compounds has been suspected of causing negative health effects ranging from fatigue to cancer. Hundreds of volatile organic compounds (VOCs) have been detected in tap water throughout the United States in surveys conducted by the EPA (1). In the past, public health officials have considered ingestion as the primary route of exposure. When contamination of the water supply occurs, residents are routinely advised to stop drinking the tap water. Our research has shown that inhalation exposures (the amount of the contaminant entering the lungs) resulting from volatilization of VOCs during other water uses, such as showering, can lead to overall doses as large or larger than those which occur from drinking the water. A predictive mass balance model which considers the physical processes of chemical volatilization from water use in the home has been developed to address the issue of whether residents should also be advised to restrict their use of water for these other, non-consumptive purposes. An overview and sample application of the model, MAVRIQ (Model for Analysis of Volatiles and Residential Indoor-Air Quality), is presented in this paper.

Numerous models currently exist for predicting indoor air quality. A model by Sparks (2), INDOOR, is a multi-room mass-balance model directed primarily at modeling the effects of combustion-type sources. CONTAM (3) is a very flexible, general mass-balance model based on idealizing a building as assemblages of flow elements connecting well-mixed system nodes. PAQM (4) simulates personal exposure by moving an individual between various micro-environments based on activity patterns. In addition, many other models with similar capabilities are available.

MAVRIQ has the capability to simulate contaminant generation due to volatilization of chemicals and the subsequent inhalation exposure resulting from indoor uses of water.

MAVRIQ is a very flexible model with no limitations on the number of compartments, species, flow elements, contaminant sources, or individuals being modeled.

THE MAVRIQ MODEL

MAVRIQ implements a deterministic, pollutant mass-balance calculation for indoor pollutant concentrations. The building is idealized as a collection of well-mixed compartments interconnected by *flow elements*. The compartments are typically determined by physical boundaries in the building. Usually, each room, or group of rooms with similar characteristics is idealized as a compartment, however, a room which is not well-mixed may be idealized as multiple compartments. Flow elements represent the air transport process from one compartment to another. The contaminants are transported between compartments by the air flows. The air flows may be constant, based on short-term conditions of interest. The air flows may also be variable, responding to changing conditions in the model, such as the opening and closing of windows or doors, or responding to changing environmental conditions, such as the ambient wind speed or temperature.

Volatilization

MAVRIQ utilizes the following equation for the volatilization of VOCs from showers based on modifications of the two-film theory (5):

$$S = f \cdot F_w (C_w - C_A/H) \qquad (1)$$

where S is the volatilization source term (mg/min), f is the fractional volatilization, F_W is the flowrate of the water (m^3/min),, C_W is the concentration of the contaminant in the water prior to volatilization (mg/m^3),. C_A is the concentration in the air (mg/m^3), and H is the dimensionless Henry's Constant. Each of the above parameters is assumed constant for a specific shower and contaminant, with the exception of the air concentration, C_A. The coefficient, f, is a function of the characteristics of the chemical and the shower system, and ranges from zero to unity. The effect of volatilization from the pool of water around the drain is also included in f. The shower characteristics such as the drop size distribution, residence time, flowrate, and water temperature are specific to each individual shower. The relevant chemical characteristics include the solubility, vapor pressure, and diffusion properties. This equation is also valid for other water uses.

Solution Methods

The differential equations are solved by the fourth-order Runge-Kutta method (also referred to as the Kutta-Simpson formula) for temporal integration. Although this method is not as computationally efficient as other methods, it is very stable, self-starting, and accurate. Typical modeling problems require only a few minutes of computer time on a PC, and therefore, the computational efficiency is not a limiting factor.

Model Validation

Several validations of MAVRIQ have been performed. The first involved an analytical validation based on a one-compartment system with a volatilization source. MAVRIQ predictions matched the analytical solution to the last calculated decimal place. The second was a comparison of MAVRIQ's results and those of CONTAM with identical inputs. The results of the two models were within 2%. The last involved modeling an actual case study in a community where the water supply (groundwater) was contaminated. Both tracer gas (SF_6) and TCE concentration data were collected while the shower was running. MAVRIQ was calibrated using the tracer gas data, and then its predictions for TCE concentrations were compared with the actual data. The results of this validation are presented elsewhere (5).

ILLUSTRATIVE APPLICATION

The following sample application is used to demonstrate the capabilities and potential uses of MAVRIQ. This application uses a modified version of the National Swedish Institute for Building Research (IBR) test house along with the calibrated air flow patterns presented by Axley (3). The test house, modified to include water sources, is presented in Figure 1. The system idealization used in this application is shown in Figure 2.

Contaminant generation takes place through volatilization of chemicals during water-using events. The volume, flowrate, duration, and frequency data for water consumption used as input for the model have been obtained primarily from a U.S. Department of Housing and Urban Development (HUD) survey of 200 households (6). The model inputs, presented in Table 1, reflect the survey results for a household of three people. Each event uses the average amount of water for that event type reported in the survey, but the number of events has been adjusted to the nearest whole number. The contaminant modeled in this application has characteristics similar to trichloroethylene. The model input for the chemical concentration in the water was 20 mg/m^3.

Currently, MAVRIQ does not contain a method for modeling the contaminant generation rate for water use events characterized by non-continuous flows, such as toilets and dishwashers. These events were approximated as events with a constant flowrate over the event duration. Although this is not entirely accurate, it is a reasonable approximation. The model was run with the same inputs for several consecutive days until the concentration profiles began repeating. This occurred after the second day. The resulting concentration profiles are presented in Figures 3-5.

CONCLUSIONS

The results demonstrate large temporal and spatial variations in the concentration profiles. The contaminant concentration in the source room rose quickly as expected, but the other rooms also exhibited significant concentrations. The resulting inhalation exposure to a particular individual is affected primarily by his/her location within the home. This suggests the need for modeling the behavioral aspects of the individual for an accurate estimate of the potential for exposure.

MAVRIQ can be utilized to assess the severity of a water pollution incident. The user may vary the input parameters to evaluate the effectiveness of different mitigation measures, such as the installation of a fan in the bathroom. The results can be used to determine whether residents should be advised to restrict their water use, or to choose the most efficient and cost effective corrective strategy.

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Table I: Model Inputs for Daily Water Uses

Water Source	f	H	Event Duration (min)	Start[a] Time (hr)	Flowrate (L/min)	Daily Water Use (L)
Shower	0.63	0.87	7.7	7.0	7.95	61.2
			7.7	7.5	7.95	61.2
Bath	0.47	0.87	30.0	20.0	2.21	66.3
Toilet	0.30	0.40	continuous	---	0.17	251.1
Dishwasher	0.90	0.87	30.0	18.5	1.04	31.2
Clothes Washer	0.90	0.87	30.0	12.0	5.30	159.0
Faucet (Kitchen)	0.50	0.40	10.0	8.5	1.55	15.5
			10.0	12.0	1.55	15.5
			10.0	18.2	1.55	15.5
Faucet (Bathroom)	0.50	0.40	5.0	7.2	1.55	7.8
			5.0	7.8	1.55	7.8
			5.0	11.0	1.55	7.8
			5.0	18.0	1.55	7.8
			5.0	22.0	1.55	7.8
Faucet (Laundry)	0.50	0.40	5.0	11.9	1.55	7.8
TOTAL						**723**

[a] Start time of an event based on 24 hours with midnight as 0

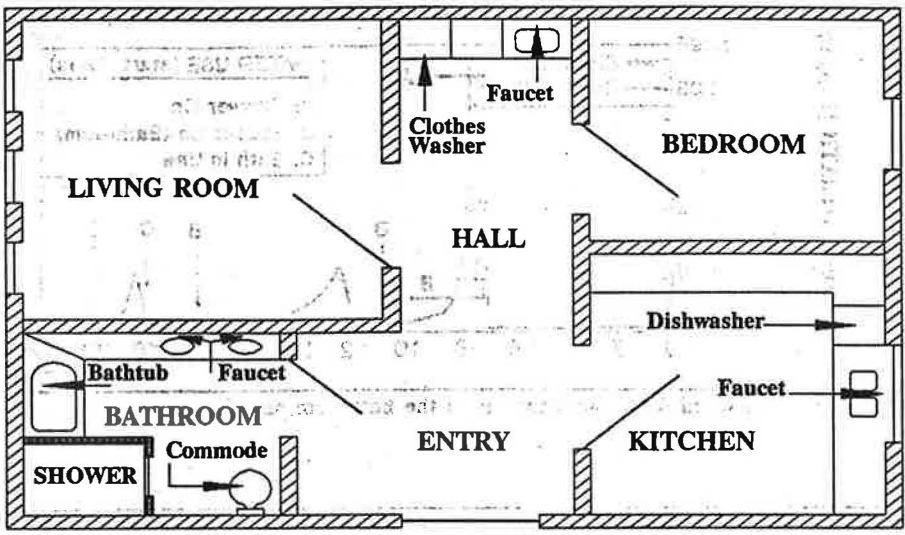

Figure 1: The IBR Five-Room Test House (After Axley, 1988)
The water sources have been added for this application

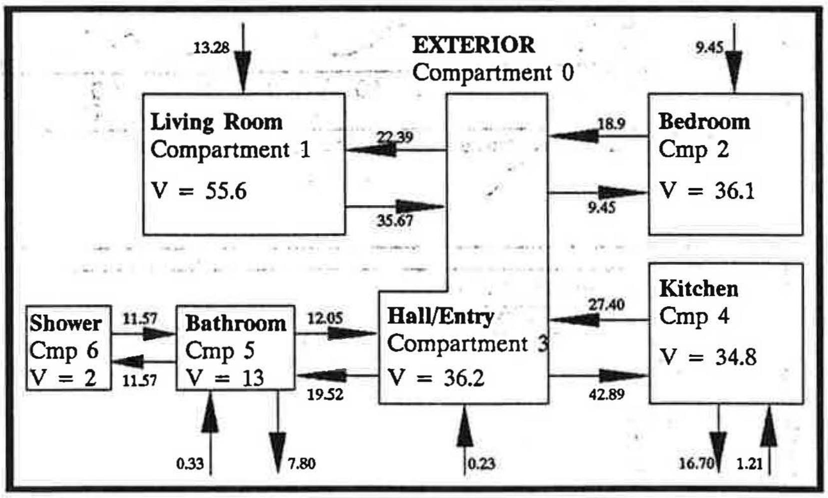

Figure 2: Idealization of IBR Test House (After Axley, 1988)
Flows are in L/s, volumes are in m^3, initial concentrations = 0

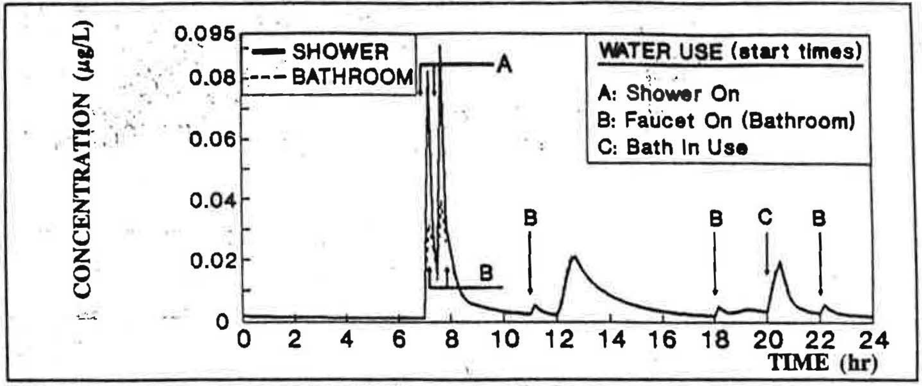

Figure 3: Modeled Air Concentrations in the Bathroom and Shower

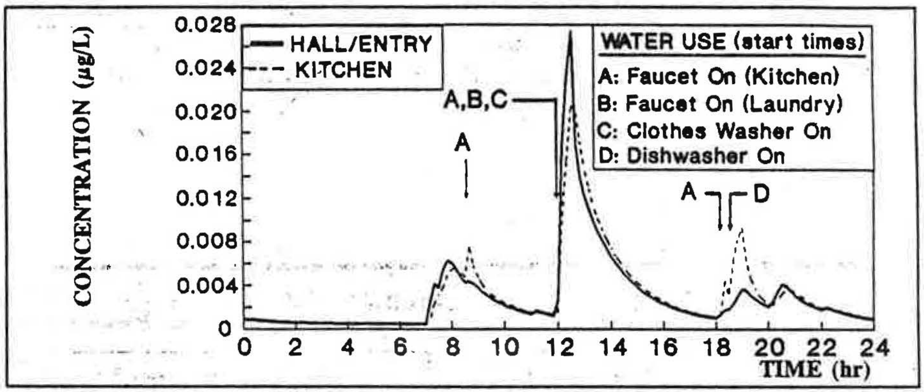

Figure 4: Modeled Air Concentration in the Kitchen and Hall/Entry

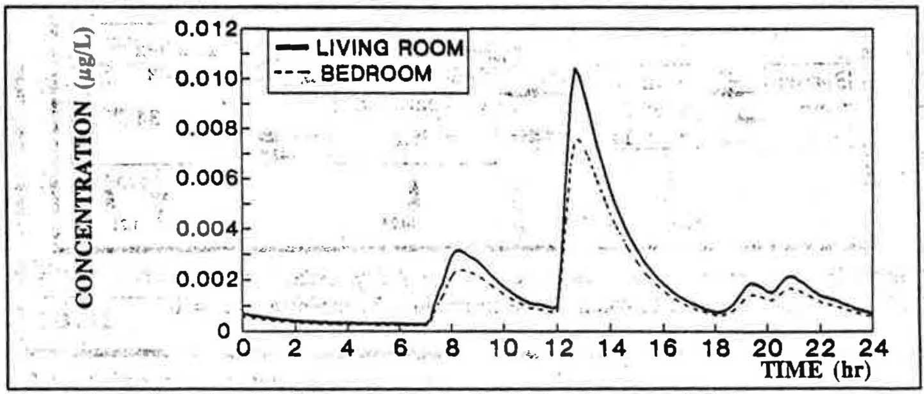

Figure 5: Modeled Air Concentration in the Living Room and Bedroom