RISK - An IAQ Model for Windows Leslie E. Sparks U. S. EPA National Risk Management Research Laboratory Air Pollution Prevention and Control Division Research Triangle Park, NC 27711

ABSTRACT

A computer model, called RISK, for calculating individual exposure to indoor air pollutants from sources is presented. The model is designed to calculate exposure due to individual, as opposed to population, activity patterns and exposure use. RISK is the third in a series of indoor air quality (IAQ) models developed by the Indoor Environment Management Branch of U. S. EPA's National Risk Management Research Laboratory. The model uses source emission and sink models developed as part of EPA's indoor source characterization research program. The source emissions models provided by the model include empirical first and second order decay models and mass-transfer models. The model allows for consideration of the effects of room-to-room airflows, air exchange with the outdoors, and air cleaners on the concentration/time history of pollutants. Comparisons of model predictions with data from experiments conducted in EPA's IAQ test house are discussed. The model predictions are generally in good agreement with the test house measurements.

INTRODUCTION

Indoor air quality (IAQ) is determined by the interactions of sources, sinks, and air movement between rooms and between the building and the outdoors. Sources may be located in rooms, in the heating, ventilation, and air-conditioning (HVAC) system, or outdoors. There may be sinks (i.e., materials that adsorb indoor pollutants) in the same locations. Sinks may also act as sources by reemitting the pollutants collected in them. Individual exposure to pollutants from indoor sources is determined by the combination of indoor pollutant concentrations and individual activity patterns. Several models have been developed to analyze the IAQ impacts of all these factors.

RISK (1) is the third in a series of IAQ models developed by the Indoor Environment Management Branch of U. S. EPA's National Risk Management Research Laboratory. The first model, INDOOR (2), was designed to calculate the indoor pollutant concentrations from indoor sources. The second model, EXPOSURE (3), extended INDOOR to allow calculation of individual exposure. **RISK** extends EXPOSURE to allow analysis of individual risk to indoor pollutant sources. The three models were all developed as tools to carry out the mission of the engineering portion of the EPA's indoor air research program, "To provide tools necessary to reduce individual exposure and risk to indoor air pollutants."

The three models reflect the status of EPA source and sink characterization research at the time the models were written. **RISK** includes new empirical source models and mass-transfer-based source models in addition to the common first order decay source models used in previous models. The mass-transfer-based source models are particularly useful for gas-phase-limited mass-transfer situations. **RISK** is the first version of the IAQ model designed for the Windows operating environment.

RELATIONSHIP BETWEEN MODELING AND SOURCE CHARACTERIZATION

The role of the model relative to source characterization can be seen in Figure 1. Data related to source characterization are developed as part of EPA's indoor air source characterization program. These data are used to develop source emission models that are used in this IAQ model. The source models are updated whenever the source characterization research program develops new information.

MODELING DECISIONS

Several decisions were made in designing the model. Some of the major decisions were:

- The emphasis was on model ease of use.
- The data requirements were minimized as much as possible.

- Data defaults would be provided as much as possible.
- Results of ongoing source and sink research would be incorporated into the model as soon as possible.
- User would be responsible for balancing flows.
- Room-to-room flows and ventilation rates were model inputs and would not be calculated from pressure/temperature data.

Most of these decisions were made to make the model easier to use. The requirement that the user balance the flows was designed to help the user understand the input data. The computer will determine if the flows balance, but it will not actually balance them. The purpose of this decision is to reinforce the idea that mass must be conserved. The user must determine where air is coming from and where it goes.

THEORY

Mass balance equations

RISK is a multi-room model based on earlier models, INDOOR (2) and EXPOSURE (3). **RISK** allows calculation of pollutant concentrations based on source emission rates, room-to-room air movement, air exchange with the outdoors, and indoor sink behavior.

Each room is considered to be a well mixed reactor. The validity of the well-mixed assumption was verified in several experiments in the EPA IAQ test house (3,4), and by data reported by Maldonado (5).

A mass balance for each room gives:

$$V_i dC_i / dt = C_{iIN} Q_{iIN} - C_{iOUT} Q_{iOUT} + S_i - R_i$$

where

 V_i = the volume of the room

C_i = the pollutant concentration in the room

C_{iIN} = the concentration entering the room

 Q_{iIN} = the air flow into the room

 C_{iOUT} = the concentration leaving the room

 Q_{iOUT} = the air flow leaving the room

 $S_i =$ the source term

 R_i = the removal term

and the subscript i refers to room i for a room in a set of multiple rooms, i = 1, 2, ... N where N is the number of rooms. The removal term, R_i , includes pollutant removal by air cleaners and sinks.

From the well-mixed assumption C_{iOUT} equals C_i. Equation (1) can be rewritten as:

$$V_i dCi/dt = C_{iIN}Q_{iIN} - C_i Q_{iOUT} + S_i - R_i$$
⁽²⁾

Equation (2) is one of a set of similar equations that must be solved simultaneously in a multiple room model. **RISK** uses a fast discrete time step algorithm developed by Yamamoto et al. (6) to solve the series of equations. The method is stable for all time steps and is accurate for sufficiently small time steps. (The size of the time step depends on how rapidly concentrations are changing. In general a time step of 1 minute is small enough when concentrations are changing rapidly, and time steps of several minutes to hours are adequate when concentrations are near steady state.) The time step must be small enough to capture the changing behavior of the ventilation system, the sources, the sinks, and the individual activity patterns.

(1)

Source terms

The ability of any model to predict indoor air pollutant concentrations depends on the accuracy of the source models incorporated into the model. **RISK** uses source models developed as a part of EPA's source characterization research program and source models provided in the literature. The model incorporates a wide range of emission characteristics to allow simulation of the range of sources encountered in indoor spaces. Several sources are allowed in each room.

The model includes a database of source emission rates for these various sources based on research conducted by the Indoor Environment Management Branch, National Risk Management Research Laboratory of EPA. The user can override the database emission rates.

Generally sources can be divided into the following categories:

- Long term steady state sources such as moth cakes.
- On/off sources such as heaters.
- Rapidly decaying sources such as painted surfaces.
- Long term slowly decaying sources such as pressed wood products.

Source behavior can be described by empirical source models or by source models based on mass transfer theory. The constants developed for empirical models are often affected by test conditions. For example, if gas-phase mass transfer limits the mass transfer rate, the empirical constants are affected by the air speed over the source. In general models based on mass transfer theory are easier to scale to new situations than are empirical models. **RISK** allows the user to use both types of source models. See References 7 and 8 for details of the mass transfer models.

Sink terms

Research in the EPA test house (2, 9, 10) and in the small chamber laboratory (10) has shown that sinks (i.e., surfaces that remove pollutants from indoor air) play a major role in determining indoor pollutant concentrations. These sinks may be reversible or irreversible. A reversible sink re-emits the material collected in it, and an irreversible sink does not. Sink behavior depends on the pollutant, on the nature of the sink, and on environmental factors such as temperature, air velocity, and humidity. Considerable research is necessary to define the behavior of sinks. Tichenor et al. (10) and Axley (11) have published sink models.

The sink model used in RISK is based on research of Tichenor et al.(10):

$$R_s = k_a C A_{sink} - k_d M_s {}^n A_{sink}$$

(3)

where

 R_s = the rate to the sink (mass per unit time)

 $k_a =$ the sink rate constant (length per time)

C = the in-room pollutant concentration (mass per length cubed)

 A_{sink} = the area of the sink (length squared)

 k_d = the re-emission or desorption rate constant (1/time if n = 1)

 M_s = the mass collected in the sink per unit area (mass per length squared)

n =an empirical constant. The recommended value of n, based on EPA research, is 1 (3). Experimental data in the EPA test house and small chambers show that, for many gaseous organic pollutants of interest in indoor air, k_a ranges from about 0.1 to 0.5 m/h, and the sink re-emission rate, k_d , is about 0.008/h for carpet and 0.1/h for most other materials. The model allows up to four sinks in a room.

The impact of sinks on individual exposure depends on the activity patterns. Sinks slightly reduce the peak exposure of individuals spending 24 h/day in a building and have no impact on their cumulative exposure. Sinks can have major impacts on the exposure of individuals with other activity patterns.

Exposure

The types of exposures of interest are instantaneous exposure and cumulative exposure. Instantaneous exposure is the exposure at any time, t, and cumulative exposure is the total or integrated exposure over the time of interest. The nature of the pollutant and the effects of the pollutant determine which type of exposure is more important.

Individual exposure is determined by the time spent at a given pollutant concentration. Therefore, it is a function of both the building concentration/time history and the individual activity pattern--that is, where the individual is located at what time. Different activity patterns, for example, entering and leaving a building at different times or moving from one room to another, result in different exposures to the same building pollutant concentration/time history. Sparks (12) discusses exposure modeling.

Calculation of exposure requires the pollutant concentration, the time exposed to the concentration, and (for inhalation exposure) the breathing rate and the volume per breath. The time exposed to the concentration depends on the individual activity pattern.

An activity pattern, in the context of the model, is defined by providing the time a person enters and leaves the various rooms of the building, or leaves the building for the outdoors. The model allows up to 10 room changes per day. The model is based on a 24-hour day. The activity patterns in the model repeat from day to day.

The model provides instantaneous exposure time plots and cumulative exposure time plots for individual activity patterns. Instantaneous exposure allows identification of high exposure situations and of peak exposure.

While the model was designed to allow assessment of the impact of indoor air pollution sources and sinks and IAQ control options on individual exposure from specific activities, it can also be used to help estimate population exposures if data on population activity patterns are available. The model can be run for each activity pattern and then the results can be weighted according to the population statistics.

Risk assessment

Risk assessment is a general term that includes four components: hazard identification, exposure assessment, dose/response evaluation, and risk characterization. A risk assessment can be quantitative or qualitative depending on the data available and the requirements for the assessment. **RISK** uses a risk calculation scheme described in References 13, 14, 15, and 16. The calculation scheme developed by these authors provides a systematic way for estimating risk.

Risk estimates based on currently available data are projections containing a great deal of uncertainty. This is particularly true when using a model such as this one to calculate risk estimates for individuals, because such numbers as carcinogenic potency, upon which the model depends for calculating individual and population cancer risk, are projections of population risks based upon a variety of extrapolations and assumptions. Risk estimates generated by models such as this one are useful mainly for the purpose of comparing scenarios rather than for determining absolute risks to individuals or populations.

Mølhave et al. (17) present an example of using an IAQ model to carry out a risk assessment. This paper demonstrates the steps necessary to carry out a risk assessment. Mølhave et al. show the importance of obtaining the right data from source testing to carry out the risk assessment. They also demonstrate the effects of the assumptions involved in risk assessment by providing examples of the range of answers possible depending on the assumptions used. Sparks et al. (18) discuss source testing necessary to obtain data required for conducting risk assessment.

Risk characterization framework

The predictive risk equation developed by Naugle and co-workers (13, 14, 15) is based on four general equations. These equations relate source factors, activity patterns, dose factors, and dose response to risk. The equations are:

Exposure

Concentration x Duration = Exposure

Dose

Exposure x Dosimetry factors = Dose (note that biological effects are included in the dosimetry factors and are not part of the exposure calculation)

Individual Risk

Dose x Dose/response relationship = Individual risk

Population Risk

Individual risk x Exposed population = Population risk

The framework subdivides the four components of the risk assessment process into 10 elements to provide a refined and systematic way of describing the risk estimation process. These elements are:

• Source factors

The starting point for the risk analysis. The estimation of risk can be based on the study of a single source emitting one or more pollutants of concern or the study of a pollutant or mixture that is emitted from one or more sources.

• Pollutant concentration

The pollutant concentration of interest depends on the effect that is of interest. The concentration may be the peak concentration, the average concentration, or some threshold concentration.

• Exposure duration and setting

The exposure duration and setting combines the setting in which exposure occurs and an estimation of the time spent in that environment.

• Exposure

The outcome of exposure duration and setting is individual exposure.

• Dosimetry factor

The dosimetry factor addresses factors which influence how much of the exposure to a pollutant is available to the body. For many air pollutants the major factor is inhalation rate.

• Dose

Dose represents the amount of a substance available for interaction with metabolic processes or biologically significant receptors.

• Response factor

Response factor describes the magnitude of the response of an individual to a given dose of the substance.

• Individual risk

Individual risk represents the risk of an individual exposed at the given concentration, duration, etc. For cancer risk the individual risk is expressed as lifetime individual risk.

• Exposed population

Exposed population is the number of individuals who are exposed to the conditions covered by the risk assessment.

• Risk to exposed population (Population risk)

The risk calculation framework can be placed in a spreadsheet format for ease of calculation. **RISK** uses the spreadsheet format shown in Figure 2. The IAQ model calculates the concentration, duration, and exposure. The user must independently provide the dosimetry factors, the response factors, and the population.

TYPES OF RISK

Cancer risk

Most risk characterization studies of environmental pollutants have concentrated on cancer risk. Cancer risk is typically expressed as lifetime risk--the probability of developing cancer over a lifetime for the average individual in a defined population and for a defined exposure scenario.

Non-cancer risk

Non-cancer risks have received less attention than cancer risks. Pierson et al. (15) recommend that many of the mathematical operations used in the risk framework be dropped when it is applied to non-cancer risks. Individual risk may be estimated as the probability of a response (adverse health effect) or the degree to which exposure or dose exceeds a threshold for adverse health effects.

Irritant risk

An irritant response to a substance often occurs when the concentration exceeds some threshold value. Examples of irritant effects include eye irritation, odor, and nasal irritation. The concentration required to produce an irritant effect may depend on individual susceptibility. The duration of the irritant exposure is often important. **RISK** provides information on the time spent above a user specified irritant threshold concentration.

The avoidance of irritant risk is a major consideration in IAQ. For example, the American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) ventilation rate standard (19) is designed to ensure that no more than 20% of the occupants of a building express displeasure with the IAQ. A major consideration in developing the standard was to provide sufficient outdoor air to avoid complaints due to human body odor.

Chronic risk

Chronic risk is usually associated with long term exposure to a pollutant. Chronic risk is also often associated with threshold-based doses. Little research has been published to quantify the chronic risk of common indoor pollutants. Seifert (20) includes chronic risk as a factor in his ranking of sources. **RISK** provides information on the time spent above a user specified threshold concentration.

MODEL VERIFICATION

Several experiments have been conducted to verify the model predictions. Most of these tests have been conducted in the EPA IAQ test house. A full description of the test house can be found in Reference 3. The floor plan of the IAQ test house is shown in Figure 3.

Two types of experiments have been conducted in the IAQ test house. One type of experiment used tracer gas with known emission rates. These experiments test the model's ability to track pollutant transport in the building and to respond to changes in factors such as room-to-room airflows [due for example to heating and air-conditioning (HAC) system operation] and air exchange with the outdoors. The second type of experiment uses real sources and tests the source and sink models as well as the transport portions of the model. The results of the two types of experiments will be briefly discussed.

The American Society for Testing and Materials (ASTM) (21) has developed guidelines for comparing model predictions with data. The ASTM criteria include:

• The slope and intercept of the best fit line between measured and predicted values. The ideal is an intercept of 0 and a slope of 1. The ASTM guidelines recommend that the intercept be within 25% of the average and the slope be between 0.75 and 1.25.

• The correlation coefficient between measured and predicted concentrations. The recommended value is 0.9 or greater.

• The normalized mean square error (NMSE) given by:

$$NMSE = \frac{\left(\overline{C_p - C_m}\right)^2}{\overline{C}_p * \overline{C}_m}$$
(4)

where

 C_p = the predicted concentration

 C_m = the measured concentration

The bars indicate average; e.g., $\overline{C_p}$ is the average of all the predicted concentrations. The NMSE has a value of 0 when there is perfect agreement for all pairs of measured and predicted concentrations.

NMSE is near 0.25 for differences between measured and predicted of about 50%. ASTM recommends that the value of NMSE for an adequate model be less than or equal to 0.25.

• The fractional bias, FB, is used to measure bias. The fractional bias is given by:

$$FB = \frac{2(\overline{C_p} - \overline{C_m})}{\overline{C_p} + \overline{C_m}}$$
(5)

FB ranges from -2 to +2 with a value of 0 indicating perfect agreement. ASTM recommends that the absolute value of FB for an adequate model be less than or equal to 0.25. ASTM recommends that the model be judged based on all the criteria. It is possible to have an adequate model even if all the criteria are not met.

Tracer gas experiments

Several tracer gas experiments have been conducted in the EPA IAQ test house. These experiments were conducted under a range of house operating conditions such as HAC on continuously, HAC off, HAC on an on/off cycle, and windows open. Comparison of model predictions with these data can be used to verify model assumptions regarding air flow in the house and model response to changing conditions independent of the source and sink effects. The ASTM criteria are given in Table 1. The agreement between the model predictions and the measured data is excellent. These results demonstrate that the model is able to capture the dynamics of air movement in the test house. A plot of predicated versus measured tracer gas concentrations is shown in Figure 4.

Source sink experiments

When actual sources are used in the test house, the modeling must include the effects of sources and sinks. Disagreement between the predictions and the measurements in these experiments is most likely due to inadequacies in the source and or sink models. The ASTM criteria for the model for several test house experiments using real sources are given in Table 2. Most of the experiments shown in Table 2 are discussed in Reference 4.

CONCLUSIONS

A new easy-to-use IAQ model has been developed. The model includes the results of ongoing research on sources and sinks. The model predictions meet the ASTM criteria for IAQ models.

MODEL AVAILABILITY

The model, including disks for Windows computers and the manual, is available from the National Technical Information Service (NTIS) in Springfield, VA.

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Figures

Risk analysis process

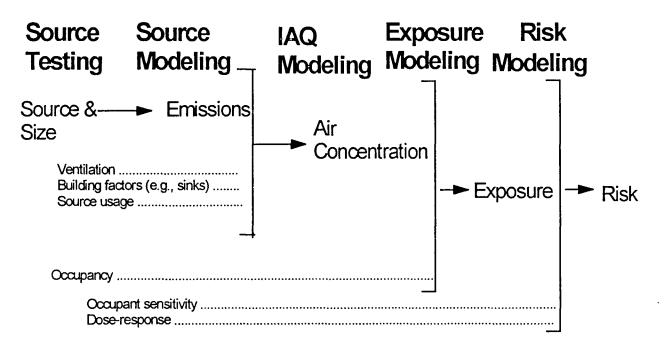


Figure 1. Risk Analysis process.

Concentration	Duration	1 .			1 .	1		Population Risk
C	t	E=C x t	factors, F	D=ExF	Res	LR=ResXD	P	PR = PxLR
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Figure 2. Risk calculation framework.

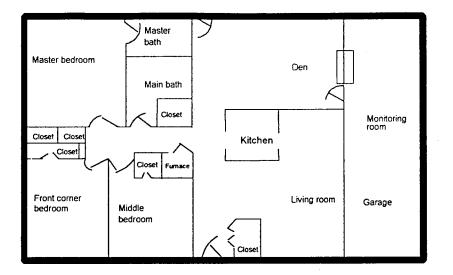


Figure 3. Floor plan of EPA IAQ test house.

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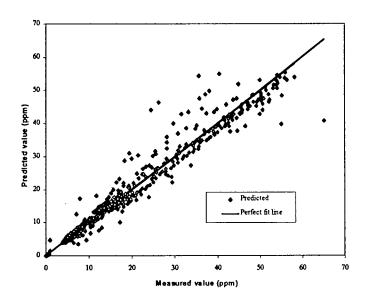


Figure 4. Comparison of predicted and measured tracer gas concentrations in EPA IAQ test house.

Table I. ASTM model criteria for tracer gas experiments

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Criterion	Value	Recommended value
NMSE	0.038	<0.25
Correlation coefficient	0.99	>0.9
Fractional bias	0.01	Absolute value <0.25
Regression intercept	0.3	25% of average value of the measurements
Regression slope	0.98	0.75 to 1.25

Table 2. ASTM model criteria for experiments using sources.

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Source	NMSE	Fractional bias	Correlation coefficient
Aerosol	0.05	0.094	0.99
Floor wax	0.19	-0.07	0.96
Polyurethane	0.28	0.12	0.96
Wood stain	0.16	0.03	0.95
Latex paint (Ethylene glycol)	0.08	0.04	0.97
Latex paint (Texanol)	0.21	-0.25	0.98

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4. TITLE AND SUBJULE RISKAn IAQ Model for Windows	5. REPORT DATE	5. REPORT DATE		
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Research Triangle Park, NC 27711		EPA/600/13		
15. SUPPLEMENTARY NOTES Author Sparks' phone nu 54. Presented at EPA/AWMA Meeting, Eng July 21-23, 1997, Research Triangle Park, 16. ABSTRACT The paper presents a computer m	gineering Solutions to IA	Q Problems.		
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17. KEY WORDS AND DO a. DESCRIPTORS	CUMENT ANALYSIS	5 c. COSATI Field/Group		
a. DESCRIPTORS Air Pollution	Air Pollution Control	13B		
Mathematical Models	Stationary Sources	13B 12A		
Decay	Indoor Air Quality	14G		
Mass Transfer	RISK			
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