



# Research and Development

SIMULATION TOOL KIT FOR  
INDOOR AIR QUALITY AND  
INHALATION EXPOSURE (IAQX)  
VERSION 1.0  
USER'S GUIDE

## Prepared for

National Risk Management Research Laboratory

## Prepared by

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## FOREWORD

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E. Timothy Oppelt, Director  
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**Simulation Tool Kit for  
Indoor Air Quality and Inhalation Exposure (IAQX)  
Version 1.0**

**User's Guide**

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## **ABSTRACT**

A Microsoft Windows-based indoor air quality (IAQ) simulation software package is presented. Named *Simulation Tool Kit for Indoor Air Quality and Inhalation Exposure*, or IAQX for short, this package complements and supplements existing IAQ simulation programs and is designed mainly for advanced users. IAQX version 1.0 consists of five stand-alone simulation programs. A general-purpose simulation program performs multi-zone, multi-pollutant simulations and allows gas-phase chemical reactions. The other four programs implement fundamentally based models, which are often excluded in the existing IAQ simulation programs. In addition to performing conventional IAQ simulations, which compute the time-concentration profile and inhalation exposure, IAQX can estimate the adequate ventilation rate when certain air quality criteria are provided by the user, a unique feature useful for product stewardship and risk management. IAQX will be developed in a cumulative manner and more special-purpose simulation programs will be added to the package in the future.

# TABLE OF CONTENTS

DISCLAIMER .....	-ii-
ABSTRACT .....	-ii-
LIST OF FIGURES .....	-vi-
LIST OF TABLES .....	-viii-
CHAPTER ONE. INTRODUCTION .....	-1-
1.1 What Is IAQX? .....	-1-
1.2 What's In IAQX? .....	-2-
1.3 Basic Framework .....	-3-
1.4 About This Guide .....	-4-
CHAPTER TWO. GETTING STARTED .....	-6-
2.1 System Requirements .....	-6-
2.2 Install IAQX .....	-6-
2.3 Uninstall IAQX .....	-6-
2.4 User-Interface Design .....	-6-
2.5 How to Start and Exit an IAQX Program .....	-7-
2.6 The Four-Step Procedure for a Simulation .....	-8-
2.7 Storage of IAQ Models .....	-8-
2.8 On-line Help .....	-8-
2.9 Contacting the Developer .....	-9-
CHAPTER THREE. THE GENERAL-PURPOSE SIMULATION PROGRAM (GPS.EXE) .....	-10-
3.1 Program Description .....	-10-
3.2 A Brief Tour of the Program .....	-10-
3.2.1 Start the Program .....	-11-
3.2.2 Define the IAQ Model .....	-11-
3.2.3 Compile the Model .....	-15-
3.2.4 Make the Simulation .....	-16-
3.2.5 Examine the Results .....	-16-
3.2.6 Calculate Inhalation Exposure .....	-16-
3.2.7 Calculate the Adequate Ventilation Rate .....	-16-

3.2.8 Save Your IAQ Model .....	-18-
3.3 More About the GPS Program .....	-18-
3.3.1. Define the Ventilation Rate .....	-18-
3.3.2 Add Pages .....	-23-
3.3.3 Source Models .....	-24-
3.3.4 Sink Models .....	-25-
3.3.5 Models for Air Cleaners .....	-26-
3.3.6 Chemical Reactions .....	-26-
3.3.7 Defining the HVAC System .....	-28-
3.3.8 Time-Varying Sources .....	-29-
3.3.9 Non-Zero Initial Concentrations .....	-29-
CHAPTER FOUR. MODELS FOR VOC EMISSIONS FROM SOLVENT-BASED INDOOR COATING PRODUCTS (VBX.EXE) .....	-31-
4.1 Model Description .....	-31-
4.1.1 Overview .....	-31-
4.1.2 The VB Model for TVOCs .....	-32-
4.1.3 The VBX Model for Individual VOCs .....	-32-
4.1.4 The First-Order Decay Model for Individual VOCs .....	-33-
4.1.5 Estimation of the Total Vapor Pressure and Average Molecular Weight for TVOCs Based on the VOC Contents in the Product .....	-33-
4.1.6 Model for Estimating Gas-Phase Mass Transfer Coefficient .....	-34-
4.2 A Brief Tour of the Program .....	-34-
4.3 More About the VBX Program .....	-41-
4.3.1 What If a VOC Does Not Exist in the VOC Database? .....	-41-
4.3.2 About the MSDS Option .....	-41-
4.3.3 Adding Sink Models .....	-43-
CHAPTER FIVE. MODELS FOR SMALL-SCALE SOLVENT SPILLS (SPILL.EXE) ...	-45-
5.1 Model Description .....	-45-
5.1.1 Model for Single-Component Solvent .....	-45-
5.1.2 Model for Solvent Mixture Whose Exact Composition Is Known .....	-45-
5.1.3 Model for Petroleum-Based Solvent .....	-46-
5.1.4 Estimation of the Spill Area .....	-47-
5.2 A Brief Tour of the Program .....	-47-
5.3 More About the SPILL Program .....	-50-
5.3.1 Adding Sink Models .....	-50-
5.3.2 Comparison of the Two Methods for Estimating the Gas-Phase Mass Transfer Coefficient .....	-50-
5.3.3 Dealing with the Temperature Drop .....	-51-
5.3.4 About the Short Circuiting Factor .....	-52-

CHAPTER SIX. A MODEL FOR VOC EMISSIONS FROM DIFFUSION-CONTROLLED HOMOGENEOUS SLABS (SLAB.EXE) .....	-53-
6.1 Model Description .....	-53-
6.2 A Brief Tour of the Program .....	-55-
6.3 More About the SLAB Program .....	-56-
6.3.1 Model Parameters for New Carpet Backing .....	-56-
6.3.2 Dealing with Zero Ventilation Rate .....	-56-
6.3.3 Source Reduction Simulation Mode .....	-56-
CHAPTER SEVEN. A MODEL FOR INDOOR PARTICULATE MATTER (PM.EXE) ..	-58-
7.1 Model Description .....	-58-
7.2 A Brief Tour of the Program .....	-59-
7.3 More About the PM Program .....	-63-
7.3.1 Calculation of PM Deposition Rate .....	-63-
7.3.2 PM Source Types .....	-64-
7.3.3 Adding Pages .....	-65-
7.3.4 HVAC Filters, Interzone Filters, and Free-Standing Filters .....	-65-
CHAPTER EIGHT. INSIDE IAQX .....	-67-
8.1 Programming Language .....	-67-
8.2 Method for Numeric Integration .....	-67-
8.3 Algorithm for Application-Phase Simulation .....	-67-
8.4 Algorithm for Estimating Adequate Ventilation Rate (AVR) .....	-69-
8.5 Handling of Time-varying Parameters .....	-69-
ACKNOWLEDGMENTS .....	-71-
REFERENCES .....	-72-

## LIST OF FIGURES

Figure 2.1 The user interface of the GPS program. ....	-7-
Figure 3.1 The main window of the GPS program. ....	-12-
Figure 3.2 The layout of the Sources page of the GPS program. ....	-13-
Figure 3.3 Layout of the model entry dialog box of the GPS program ....	-14-
Figure 3.4 The GPS' Sources page after adding a source model. ....	-15-
Figure 3.5 GPS dialog box for estimating the adequate ventilation rate. ....	-18-
Figure 3.6 Constant ventilation mode in the GPS program. ....	-19-
Figure 3.7 Cyclic ventilation mode in the GPS program. ....	-20-
Figure 3.8 Concentration profile generated by a constant source under the cyclic ventilation mode. ....	-21-
Figure 3.9 Comparison between the two time-varying flow modes. ....	-23-
Figure 3.10 Diagrammatic description of the air handling system. ....	-28-
Figure 3.11 The layout of the Input Data page of the GPS program. ....	-29-
Figure 3.12 Layout of the Conditions page of the GPS program ....	-30-
Figure 4.1 The main window of the VBX program (showing the Building page). ....	-35-
Figure 4.2 Layout of the Ventilation page of the VBX program: ....	-36-
Figure 4.3 Layout of the VOC Contents page of the VBX program ....	-37-
Figure 4.4 Dialog window for the built-in database of the VBX program ....	-39-
Figure 4.5 Layout of the VOC Contents page of the VBX program. ....	-40-
Figure 4.6 Layout of the Source page of the VBX program. ....	-41-



Figure 4.7 Layout of the VOC Contents page when the MSDS option is selected. . . . .	-42-
Figure 4.8 Defining the application-phase simulation in the Conditions page . . . . .	-43-
Figure 4.9 Layout of the Sink page of the VBX program. . . . .	-44-
Figure 5.1 Layout of the Solvent page of the SPILL program . . . . .	-48-
Figure 5.2 Layout of the Source page of the SPILL program. . . . .	-49-
Figure 5.3 Comparison of the gas-phase mass transfer coefficient for decane estimated by the two methods . . . . .	-51-
Figure 6.1 The main window of the SLAB program . . . . .	-55-
Figure 6.2 The SLAB dialog box for the Source Reduction simulation mode . . . . .	-57-
Figure 7.1 Layout of the Building page of the PM program . . . . .	-59-
Figure 7.2 Layout of the PM Properties page of the PM program. . . . .	-60-
Figure 7.3 Layout of the Outdoor Sources page of the PM program . . . . .	-61-
Figure 7.4 Layout of the Indoor Sources page of the PM program. . . . .	-62-
Figure 7.5 Layout of the Conditions page of the PM program. . . . .	-63-
Figure 7.6 Possible filter positions in three-zone (zone 1, zone 2, and HVAC) configuration. . . . .	-66-

## LIST OF TABLES

Table 1.1 Programs included in IAQX version 1. ....	-2-
Table 1.2 Candidate simulation programs for future inclusion in IAQX. ....	-3-
Table 2.1 Default file extensions for IAQX programs. ....	-8-
Table 3.1 Main features of the GPS program. ....	-10-
Table 3.2 Time-varying ventilation mode in the time/flow format (one zone). ....	-22-
Table 3.3 Time-varying ventilation mode in the duration/flow format (one zone). ....	-22-
Table 3.4 Source models available in the GPS program. ....	-25-
Table 3.5 Sink models available in the GPS program. ....	-26-
Table 3.6 Air cleaner/filter models available in the GPS program. ....	-26-
Table 4.1 User input required by the VBX program. ....	-32-
Table 4.2 Differences between the two VOC data options. ....	-38-
Table 7.1 An example data input for the on/off source type. ....	-65-
Table 7.2 An example data input for the time-varying source type. ....	-65-

# CHAPTER ONE

## INTRODUCTION

### 1.1 What Is IAQX?

IAQX is short for *Simulation Tool Kit for Indoor Air Quality and Inhalation Exposure*. It is a Microsoft Windows-based indoor air quality (IAQ) simulation package consisting of a general-purpose simulation program and a series of stand-alone, special-purpose programs.

Estimation of inhalation exposure to indoor air pollutants is an essential part of multi-pathway exposure assessment since most people spend a large portion of their time indoors. In the past two decades, a series of IAQ simulation programs have been developed. Insightful reviews of major software packages are given by Austin, et al. (1992) and Rector and Koontz (1993). More recent developments include several Microsoft Windows-based IAQ simulation programs such as RISK (Sparks, 1996), MEDB-IAQ (Zhang, et al., 1999), MCCEM (Koontz and Wilkes, 1999), and CONTAMW (Dols, et al., 2000). In-depth theoretical discussions on the framework of IAQ modeling and simulation have also been reported (Axley, 1995; Van Loy, et al., 1998).

IAQX is not intended to replace the existing IAQ simulation packages. Instead, it complements and supplements them by focusing on fundamentally based models. In recent years, modeling of indoor pollutant sources and sinks has gradually shifted from simple, empirical models to more complex, mass transfer models. While the latter have demonstrated improved accuracy, validity, and scalability, their usefulness has somewhat been overshadowed by their increased complexity. Potential users are often scared away at the sight of unfamiliar equations and tedious calculations. To a large extent, the newer models are excluded in the existing IAQ simulation packages. IAQX attempts to resolve this problem by shielding users from mathematical details, allowing them to concentrate on IAQ related issues. IAQX puts relatively simple mass transfer models in the general-purpose simulation program; more complex models are implemented as stand-alone, special-purpose simulation programs.

In addition to performing the conventional IAQ simulations, which calculate the pollutant concentration and/or personal exposure as a function of time, IAQX can estimate the adequate ventilation rate when certain air quality criteria need to be satisfied. This unique feature is useful for product stewardship and risk management.

IAQX is designed mainly for advanced users, those who are directly involved in exposure estimation, pollution control, risk assessment, and risk management. Users are encouraged to look into other available IAQ simulation programs to find ones that are most suitable to their specific needs.

## 1.2 What's In IAQX?

IAQX version 1 consists of five stand-alone programs: one is for general-purpose simulation, and four are for special-purpose simulation (see Table 1.1). This software package will be developed in a cumulative manner. More special-purpose programs will be added in the future. Table 1.2 lists five programs that are currently under consideration for future inclusion in IAQX.

Table 1.1 Programs included in IAQX version 1.

No.	Program	Purpose	Reference
1	GPS.EXE	A general-purpose simulation program	Guo (1996)
2	VBX.EXE	Models for predicting VOC emissions from solvent-based indoor coating materials based on product formulation	Guo, et al. (1999)
3	SPILL.EXE	Models for indoor solvent spills	Reinke and Brosseau (1997); Drivas (1982)
4	SLAB.EXE	A model for VOC emissions from diffusion-controlled homogeneous slabs such as new carpet backing	Little, et al. (1994)
5	PM.EXE	A model for indoor particulate matter	Nazaroff and Cass (1989)

Table 1.2 Candidate simulation programs for future inclusion in IAQX.

No.	Program	Purpose	Reference
6	PEST.EXE	Fugacity models for indoor application of pesticides	Matoba, et al. (1998)
7	WBC.EXE	Models for VOC emissions from indoor use of water-based cleaners.	To be determined
8	WATER.EXE	For VOC emissions from clean water use indoors (e.g., washing machine and dish washer)	Howard and Corsi (1998)
9	CHEM.EXE	A model shell for indoor air chemistry	Not applicable
10	LATEX.EXE	Models for VOC emissions from latex paint.	To be determined

### 1.3 Basic Framework

Like most IAQ models, the IAQX programs assume that a building is divided into air zones and that, within each zone, the air is well mixed. For a given air pollutant, its concentration in a given air zone  $i$  is determined by:

$$\begin{aligned}
 V_i \frac{dC_i}{dt} = & \sum_{j=1}^{n_R} R_j + p Q_{0i} C_0 + \sum_{k=1}^{n_i} Q_{ki} C_k - \sum_{k=0}^{n_i} Q_{ik} C_i - \sum_{L=1}^{n_i} S_L k_{aL} f(C_i) \\
 & + \sum_{L=1}^{n_i} S_L k_{aL} f(M_L) - \sum_{p=1}^{n_f} R_p Q_p C_i + V_i \sum_{g=1}^{n_x} X_g
 \end{aligned} \quad (1.1)$$

where  $V_i$  = volume of zone  $i$  ( $m^3$ );

$C_i$  = pollutant concentration in zone  $i$  ( $mg/m^3$ );

$t$  = time (h);

$n_R$  = number of indoor sources in zone  $i$ ;

$R_j$  = emission rate for indoor source  $j$  in zone  $i$  ( $mg/h$ );

$p$  = penetration factor for zone  $i$  (unitless);

$Q_{0i}$  = infiltration air flow rate from outdoors to zone  $i$  ( $m^3/h$ );

$C_0$  = pollutant concentration in ambient air ( $mg/m^3$ );

$n_z$  = number of air zones;  
 $Q_{ki}$  = air flow rate from zone k to zone i and  $k \neq i$  ( $m^3/h$ );  
 $C_k$  = pollutant concentration in zone k ( $mg/m^3$ );  
 $Q_{ik}$  = air flow rate from zone i to zone k and  $k \neq i$  ( $m^3/h$ );  
 $n_s$  = number of interior surface types;  
 $S_L$  = surface area for interior surface L in zone i ( $m^2$ );  
 $k_{aL}$  = adsorption rate constant for surface L, whose unit depends on  $f(C_i)$ ;  
 $f(C_i)$  = certain function of  $C_i$ ;  
 $k_{dL}$  = desorption rate constant for surface L, whose unit depends on  $f(M_L)$ ;  
 $M_L$  = amount of pollutant adsorbed on surface L ( $mg/m^2$ );  
 $f(M_L)$  = certain function of  $M_L$ ;  
 $n_f$  = number of air filters/cleaners associated with zone i;  
 $R_p$  = pollutant removal efficiency for air filter/cleaner p (unitless);  
 $Q_p$  = air flow rate passing through air filter/cleaner p ( $m^3/h$ );  
 $n_x$  = number of gas-phase chemical reactions which either consume or produce the pollutant; and  
 $X_q$  = rate of chemical reaction q ( $mg/m^3/h$  in Eq. 1.1; mole/ $m^3/h$  in simulation).

Eq. 1.1 represents a system of ordinary differential equations that, in most cases, require numerical solutions. The number of differential equations in the system depends on the complexity of the IAQ model and is limited to 100 or less in IAQX. The primary simulation output is a time-concentration table, from which personal inhalation exposure can be calculated:

$$I_x = R_B \sum_{i=1}^{n-1} \frac{(C_i + C_{i+1})(t_{i+1} - t_i)}{2} \quad (1.2)$$

where  $I_x$  = inhalation exposure (mg);  
 $R_B$  = breathing rate ( $m^3/h$ );  
 $n$  = number of data points in the time-concentration table;  
 $C_i$  = concentration at time  $t_i$  ( $mg/m^3$ ); and  
 $C_{i+1}$  = concentration at time  $t_{i+1}$  ( $mg/m^3$ ).

## 1.4 About This Guide

This User's Guide consists of eight chapters. Chapter 1 – *Introduction* – gives an overview of the software package. The user is urged to go through this chapter at least once. Chapter 2 -- *Getting Started* – contains information about software installation/uninstallation, descriptions of the user interface, and ways to contact the developer. Chapters 3 to 7 are detailed descriptions of individual IAQX programs. Each chapter is divided into three sections, an overview, a brief tour of the program, and discussions on more features. These five chapters are pretty much independent of each other. Thus, if you are interested in a particular program, go to

that chapter directly. However, you should go through Section 3.2 at least once because basic skills for using IAQX are introduced there. Chapter 8 – *Inside IAQX* – contains in-depth information about the development of IAQX including several key simulation techniques. Those who write IAQ simulation programs of their own may find this chapter useful.

IAQX implements published models only. A complete list of references is provided at the end of this Guide. The user is encouraged to read the original papers for more information about the models.

## **CHAPTER TWO GETTING STARTED**

### **2.1 System Requirements**

- Intel Pentium 90 or higher;
- Microsoft Windows 95, 98, or NT 4.0;
- 16 Mb of RAM;
- 5 Mb hard disk space;
- CD-ROM drive (for installation);
- VGA or higher resolution monitor; and
- Mouse or other pointing device.

### **2.2 Install IAQX**

Installing the IAQX programs to your computer is fairly easy. Simply insert the program CD in your CD-ROM drive. In some PC systems, the setup program will launch automatically. If not, you have two options: (1) go to the Windows' Control Panel, select Add/Remove Programs, and then click on the Install button or (2) use the Windows Explorer to find the SETUP.EXE file in the program CD and then double click on it.

### **2.3 Uninstall IAQX**

To uninstall IAQX programs, go to the Windows' Control Panel, select Add/Remove Programs, and then click on the Uninstall button. Select IAQX from the program list and click OK.

### **2.4 User-Interface Design**

All IAQX programs have similar user interfaces. The basic screen layout is based on multipage tabbed windows. Figure 2.1 shows the main window of the GPS program with five pages visible, identified by tabs. Be aware that most IAQX programs have one or more hidden pages, which are less commonly used and only become visible at the user's request. For example, program GPS has three hidden pages, designated to sink, air filter/cleaner, and gas-phase chemical reactions, respectively. They can be accessed by clicking the Add pages speed button (i.e., the one with a red # sign). For specific features of each program, see corresponding chapter for details.



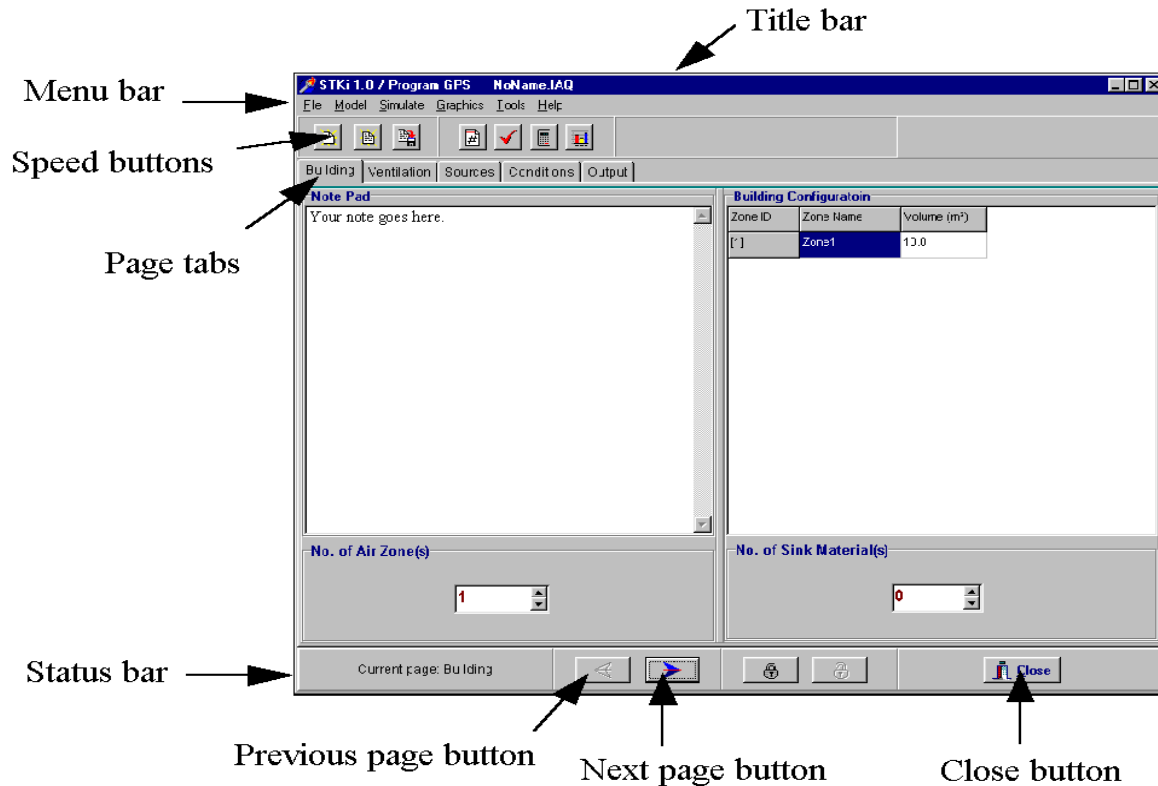


Figure 2.1 The user interface of the GPS program.

## 2.5 How to Start and Exit an IAQX Program

To start a program, select IAQX from the Windows' Programs list and then click on one of the program icons. After the welcome window is displayed, click the OK button to enter the main window.

There are three ways to exit a program: (1) select File/Exit from the main menu, (2) click the Close button near the bottom-right corner, or (3) click the Close Window button at the top-right corner (i.e., the one with a X sign).

Keep in mind that a simulation may go wrong from time to time. A relatively benign failure can be identified by unintelligent output. For instance, the output values look too large, too small, negative, or zigzagging. In most cases, it is caused by unrealistic model parameters. Check your input carefully and make changes if necessary. Sometimes, a program may fail to respond to your command, which is often an indication of more serious problems. To shut down the program, press Control-Alternate-Delete keys simultaneously. After the Close Program window appears, select the program you want to stop and then click the End Task button.

## 2.6 The Four-Step Procedure for a Simulation

With IAQX it takes four steps to make an IAQ simulation: define the IAQ model, compile the model, make the simulation, and examine the results. These steps are discussed in detail in Section 3.2 by using the general-purpose simulation program as an example. The user should go through Section 3.2 at least once because the basic skills apply to the rest of the programs as well.

## 2.7 Storage of IAQ Models

The user-created IAQ models can be saved to a disk file, which can be retrieved later. This feature allows the user to define a building environment only once. It is important to know that each IAQX program has its own default file extension (Table 2.1). An error-checking procedure prevents an IAQX program from opening a file created by other IAQX programs or other applications.

Table 2.1 Default file extensions for IAQX programs.

Program	File Extension
GPS.EXE	.IAQ
VBX.EXE	.VBX
SPILL.EXE	.SPL
SLAB.EXE	.SLB
PM.EXE	.PM

User-specified file extensions are allowed, but not preferred. To open a model file with your own file extension, follow these steps: click the Open file speed button (or File/Open from the main menu); find the File Type box near the bottom; select “Any files”; select the model file by clicking on it; and click the Open button.

## 2.8 On-line Help

On-line help is available in all IAQX programs. It can be accessed by clicking Help from the main menu. Typical items in the Help submenu include “Model description,” “How-to’s,” “About IAQX,” and “About this program.” In addition, many pages have one or more Help buttons, which provide hints to specific items in that page.

## 2.9 Contacting the Developer

The user is encouraged to report bugs and other problems associated with this package. In return, the user will receive a copy of the programs and/or the User's Guide with errors corrected. The user will also be informed of any future developments of IAQX.

Limited technical support is available on a first-come-first-served basis. Be aware, however, that the developer does not guarantee, nor is he obligated, to answer all the user inquiries in a timely fashion.

In either case, the developer can be reached by mail, e-mail, or facsimile:

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## CHAPTER THREE

### THE GENERAL-PURPOSE SIMULATION PROGRAM (GPS.EXE)

#### 3.1 Program Description

Program GPS is a multizone, multipollutant simulation program, with which the user can develop and execute a wide range of IAQ models. Simple mass-transfer models are all implemented here. Program specifications are provided in Table 3.1.

Table 3.1 Main features of the GPS program.

Feature	Limit
Number of air zones	1 to 10
Number of sink materials	0 to 3 in each air zone
Ventilation modes	constant, cyclic, time/flow, and period/flow
Number of HVAC systems	1
Number of source models	26
Number of sink models	5
Number of air filter models	2
Maximum number of chemical reactions	5
Non-zero initial concentrations	allowed
Simulation period	user specified
Simulation output	concentration, inhalation exposure, and adequate ventilation rate

#### 3.2 A Brief Tour of the Program

This section gives you a first look at the program and introduces you to basic skills needed to work with the GPS program. Discussions on more advanced features are provided in

## Section 3.3.

### 3.2.1 Start the Program

To start the GPS program, select the IAQX folder from the Windows' Programs menu and then click the GPS icon. The first you see is a welcome window, in which the program title is displayed. To enter the program's main window, click the OK button. As you have seen in Figure 2.1, the main components of the window include (from top to bottom): the title bar, main menu, speed buttons, desk top area, and status bar.

The speed buttons provide quick access to frequently used menu items. Place the mouse cursor over a speed button and leave it there for a second, a small help window will appear to remind you of what the button does.

For clarity and easy access to all parts of the program, IAQX adopts a user-interface design called multipage tabbed windows. In GPS you can see five pages, identified by the tabs. They are: Building, Ventilation, Sources, Conditions, and Output. To turn to a page, simply click on the tab. You can also use the two arrow keys on the bottom to turn one page a time.

As mentioned in Chapter 2, it takes four steps to complete an IAQ simulation with the IAQX programs: define the IAQ model, compile the model, make the simulation, and examine the results. These steps and several more features are explained in Sections 3.2.2 to 3.2.8.

### 3.2.2 Define the IAQ Model

When defining an IAQ model, you should always start from the first page, where the basic structure of your model is laid out (Figure 3.1). The first thing you need to do is to specify the number of air zones in your model. You can have up to 10 air zones, although most IAQ models contain only one, two, or three zones. Click the up/down arrows to adjust the value. Note that, when you change the zone number, the size of the Building Configuration table changes accordingly. After the zone number is selected, move to the Building Configuration table, where the name and volume (m<sup>3</sup>) of each zone are defined. If you consider the heating, ventilation, and air-conditioning (HVAC) system as an air zone, define it as the last zone and name it either "HVAC" or "HAC." See Section 3.3.7 for more information about representation of the HVAC system.

An IAQ model is often considered inadequate nowadays without consideration of the sink effect. GPS allows each zone to have up to three sink materials. The default value is zero. When you change the number of sink materials, the Building Configuration table expands horizontally and the sink areas must be entered. In this brief tour, let's keep it simple by leaving alone the default value (zero) for the sink materials.

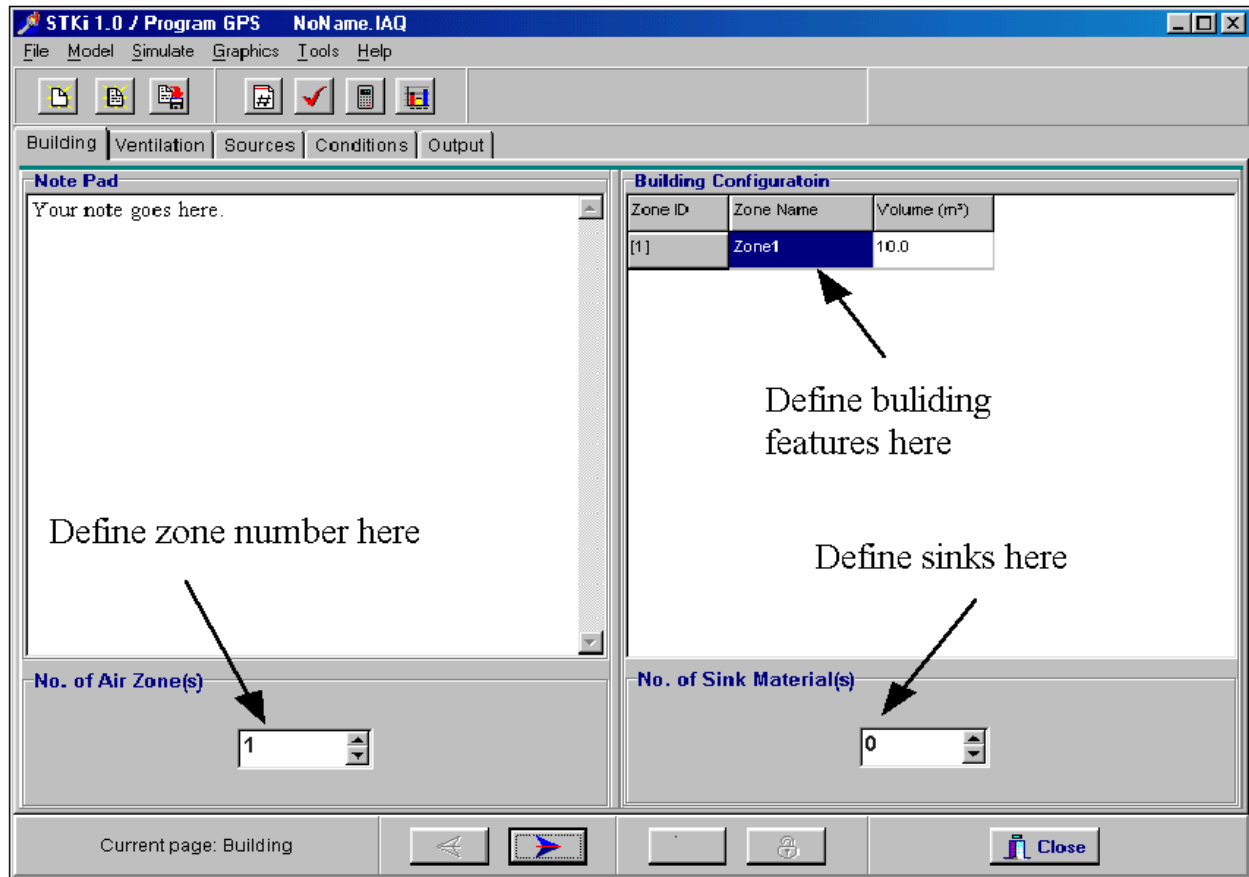


Figure 3.1 The main window of the GPS program.

The note pad on the left is a text editor where you can make notes. It is always a good practice to describe your IAQ by words, and perhaps to record the date and time as well. Delete the default text and add a few words of your own if you wish. You are now finished with the first page.

Click the Ventilation tab or click the Next Page button (the one with a right-arrow logo) to move to the next page. When you define the ventilation rate flow rates, remember that the outdoor air is always designated zone 0. IAQX allows four types of air exchange data: constant, cyclic, time-varying in time/flow format, and time-varying in period/flow format. See section 3.3.1 for more details about how to use these flow modes. The default setting is the constant flow mode, meaning that the ventilation rate does not change over time. Again, we'll use the default values for this demonstration.

Most IAQ models contain one or more emission sources. In GPS they are defined in the Sources page. As shown in Figure 3.2, there are four buttons on the right panel: Add, Delete,

Modify, and Help. To add a source, click the Add button. A dialog box will appear to show the categories of source models. Select a category then click the Select button. Or you can simply double-click on the selected item. If you want to add a first-order decay model to your IAQ model, select category 2 – “first-order & higher order models.” A new dialog box will appear to show all the models in this category. Select the first model (No. 21) by clicking on it and then click the Continue button to bring up the model entry window. As you can see in Figure 3.3, this dialog box contains all the information you need to define the source model.

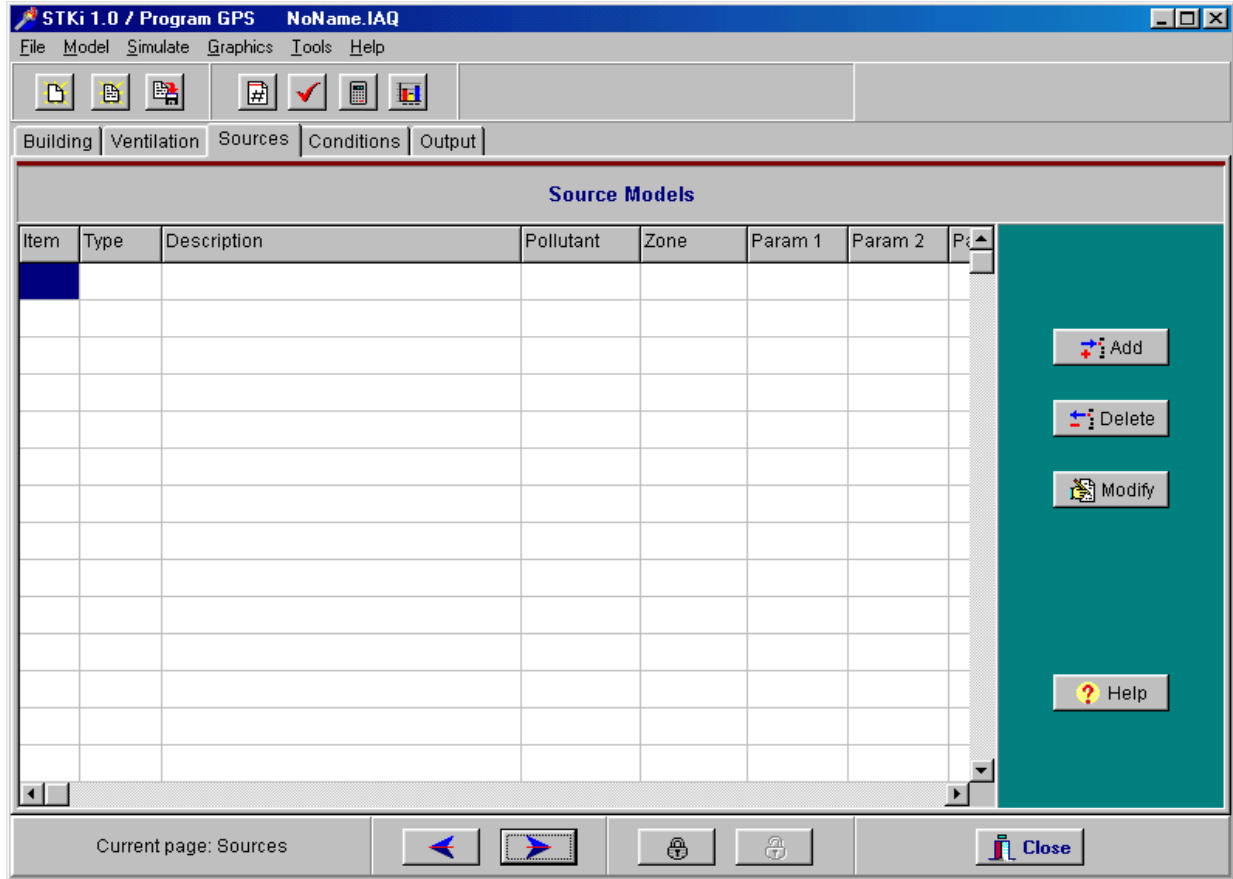


Figure 3.2 The layout of the Sources page of the GPS program. The source model table is empty.

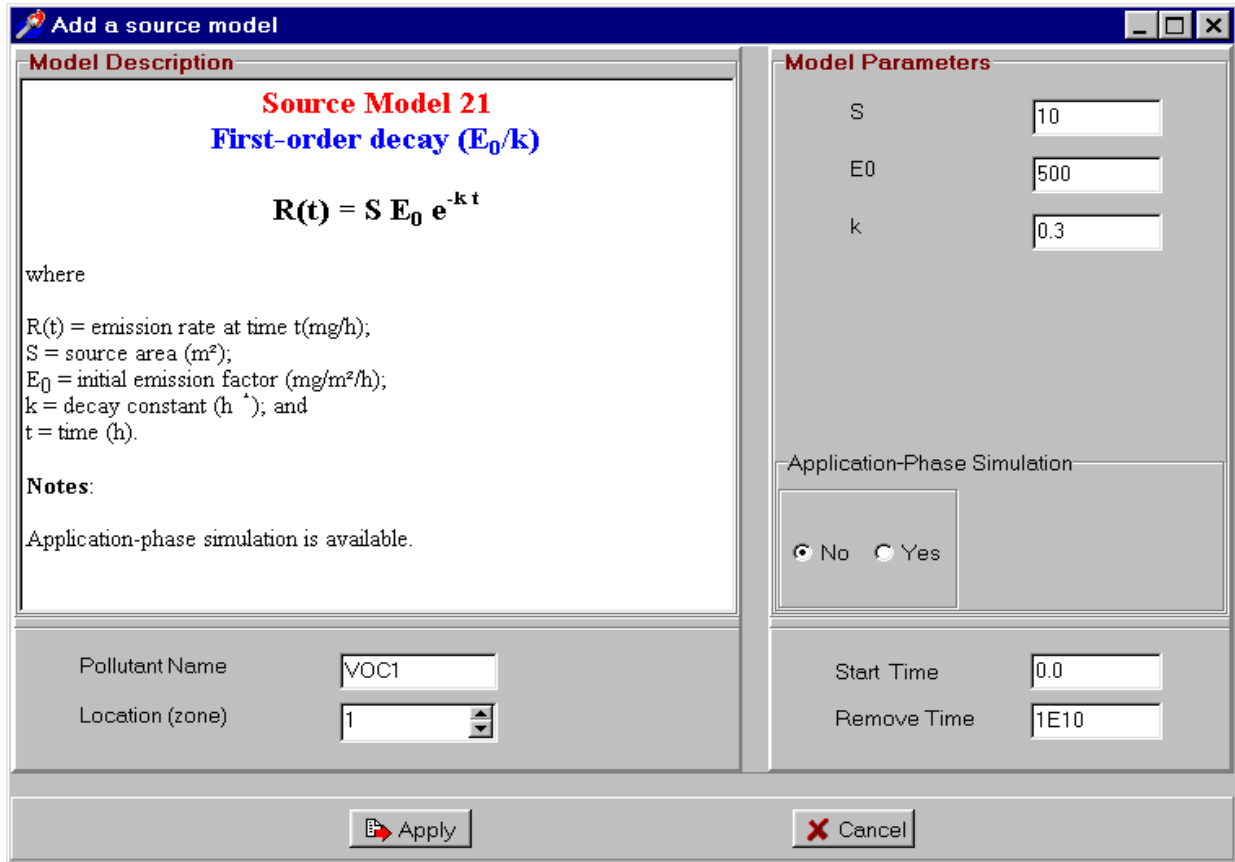


Figure 3.3 Layout of the model entry dialog box of the GPS program.

On the left is a text box containing the description of the model. Below it, the pollutant name and the source location are defined. Let's change the pollutant name from VOC1 to TVOC. Note that pollutant names are not case-sensitive. For instance, TVOC, Tvoc, and tvoc are considered identical by the program.

The next step is to enter the model parameters on the right panel. Be aware that the default values serve only as a starting point and that they do not represent the real source you are dealing with. It is your responsibility to enter the correct values.

After entering the parameters (S, E<sub>0</sub>, and k in this case), click the Apply button. The source model will be added to the Sources page (Figure 3.4). You can add a virtually unlimited number of sources to your IAQ model. Available source models in GPS are listed in Section 3.3.2.

To delete a source model from the table, click a cell in the row that you want to delete, and then click the Delete button. To modify or review a model in the table, select the item, then



click the Modify button (or simply double-click on the item) to bring back the model entry dialog box.

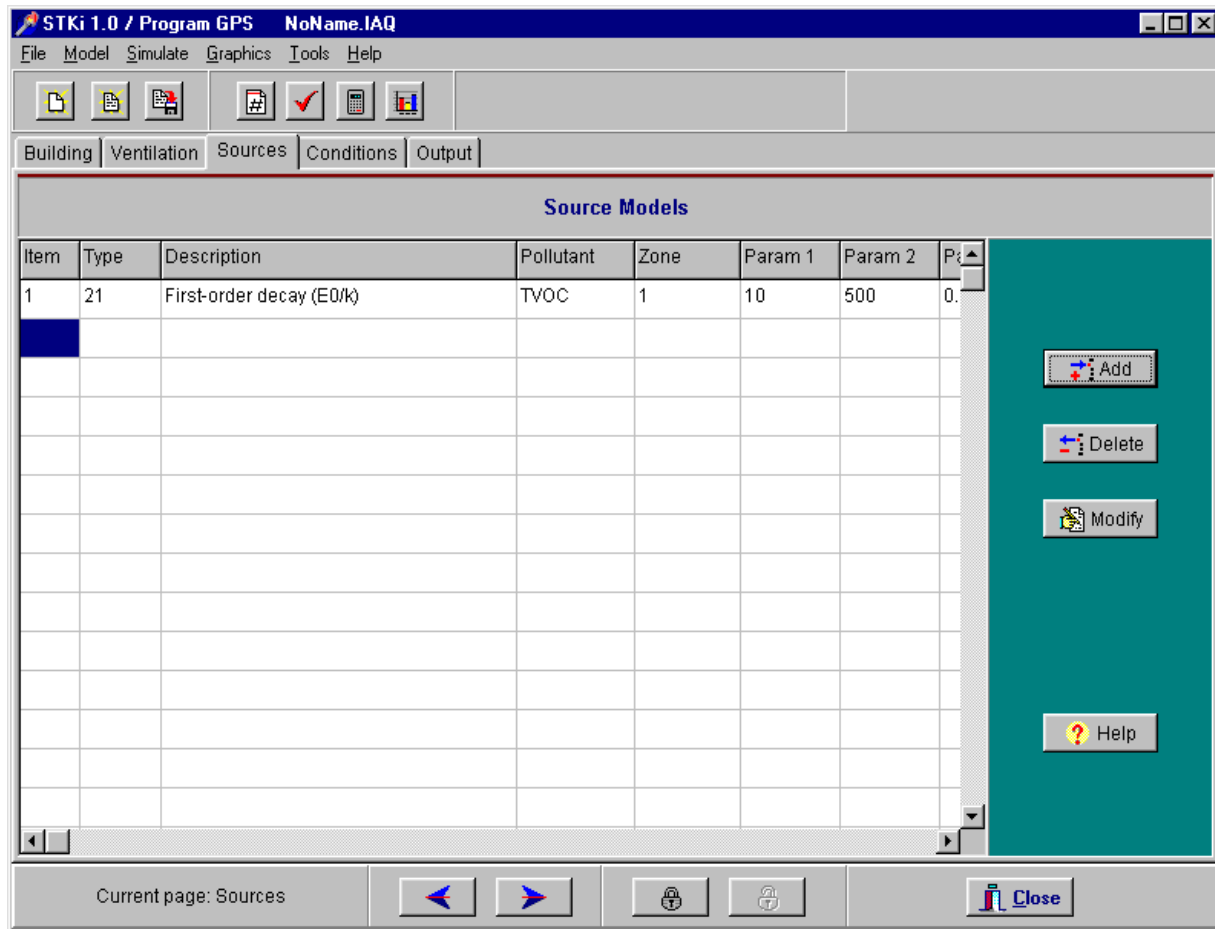


Figure 3.4 The GPS’ Sources page after adding a source model.

Let’s move to the Conditions page, where the user specifies the simulation period and number of data points in the output. If your model has non-zero initial concentrations, they should be entered here, too (see Section 3.3.9). For this demonstration, keep the default values.

### 3.2.3 Compile the Model

Now you have finished a simple but workable IAQ model. The next step is to let the program “compile” your model -- a process for the program to detect obvious errors in the user input and, if there are no errors, to read in all the parameters. Click the Compile speed button (i.e., the one with a red check sign). If you receive an error message, go to the corresponding

page and make corrections and compile again until the model is error free.

### 3.2.4 Make the Simulation

A successfully compiled model is ready to run. To start the simulation, click the Simulate speed button (i.e., the one with a calculator logo). Depending on the complexity of your model, the length of simulation period, and the speed of your computer, the time needed to complete a simulation may vary greatly, from a few seconds to a few minutes. During a simulation, the program keeps you informed of the simulation status by displaying a small message box. After the simulation is finished, click the OK button to go back to the main window. The resulting time-concentration data are displayed in the Output page (i.e., the last page).

### 3.2.5 Examine the Results

There are several ways to examine the results. The first thing you may want to do is to view a time-concentration plot. Click the Quick Plot speed button (the rightmost one with a bar-chart logo) to see an instant display of the x-y diagram. To print the diagram, click the Print button.

Often people want to export the data for further analysis. IAQX allows you to export the results to a spreadsheet, save them to an ASCII file, or print them to a hard copy. The five buttons in the Output page (Copy, Copy All, Help, Save, and Print) are self-explanatory. Both Copy and Copy All buttons can copy the data to the Windows clipboard but they work differently. If you would like to copy only part of the output data to the clipboard, you need to highlight the data section first and then click the Copy button. If you would like to copy all the data in the output table, you can click the Copy All button without having to highlight the data. Click the Help button in case you are confused. To paste the data to a spreadsheet, go to the spreadsheet application, move the cursor to a cell, and then click the Paste speed button.

### 3.2.6 Calculate Inhalation Exposure

Once the time-concentration data is generated, calculation of personal inhalation exposure is easy. Select Tool/Inhalation exposure from the main menu, enter the breathing rate and then click the OK button. The results will be displayed in a separate table next to the concentration table and there will be two tabs (“Concentration” and “Exposure”) near the bottom-left corner when you turn to the Output page. Like the concentration data, the inhalation exposure data can be viewed in a diagram or exported to a spreadsheet. For a quick plot, click the Quick plot speed button and then select Inhalation exposure. For more options, select Graphics/Select items from the main menu.

### 3.2.7 Calculate the Adequate Ventilation Rate

Conventional IAQ simulations take a set of parameters as the input and calculate the

indoor concentrations as the output. From time to time, the question may be raised in the opposite way: what is the adequate ventilation rate to keep the indoor pollution level below certain criteria? The IAQX programs can answer such a question by providing a special simulation mode. To utilize this feature, click Simulate/Adequate Vent from the main menu. In the Adequate Ventilation Rate dialog box (Figure 3.5), select peak concentration as the IAQ criterion. The simulation you have just finished gives a peak concentration of about 300 mg/m<sup>3</sup> if you did not change the default values. Assume the goal is to have the peak concentration below 100 mg/m<sup>3</sup>. Then enter 100 as the acceptable value. Leave other parameters unchanged, and then click the OK button. The simulation results show that the indoor concentration can be reduced to 103 mg/m<sup>3</sup> if the ventilation rate is increased to 3.95 air changes per hour.

Note that IAQX version 1 can estimate the adequate ventilation rate for single-zone models only and that you should always run a conventional simulation and examine the output before trying to estimate the adequate ventilation rate.

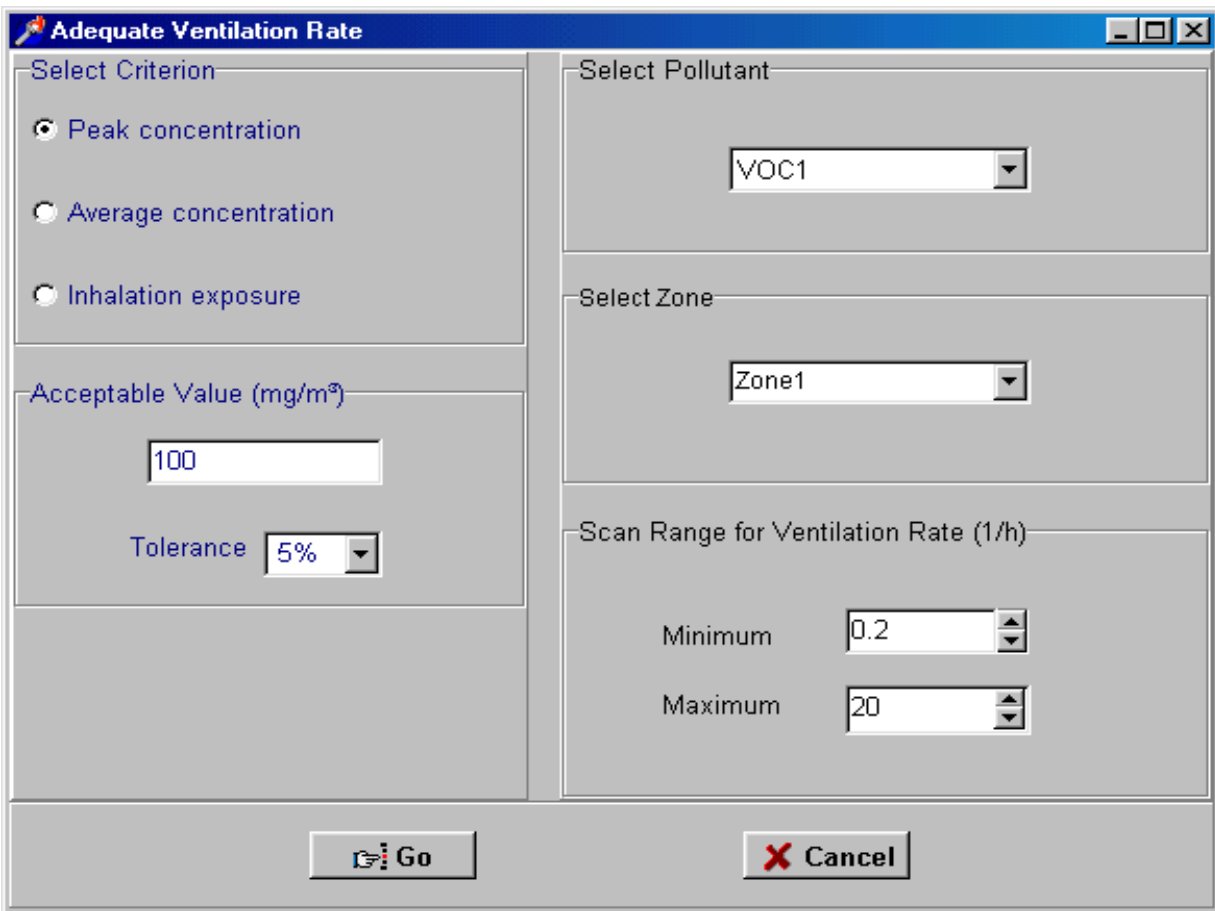


Figure 3.5 GPS dialog box for estimating the adequate ventilation rate.

### 3.2.8 Save Your IAQ Model

You can save your IAQ model to a disk file and retrieve it later. This feature is not only important for record-keeping, it also saves you time because, for a given scenario, the building configuration and ventilation rates do not change and you need to enter these parameters only once. To save an IAQ model, click the Save speed button (i.e., the one with a floppy disk logo) or select File/Save model from the main menu. Remember that each IAQX program has its own default file extension (see Table 2.1). The default file extension for this program is “.IAQ.”

## **3.3 More About the GPS Program**

### 3.3.1. Define the Ventilation Rate

#### *Four Ventilation Modes*

This program allows the user to choose from four ventilation modes:

- constant;
- cyclic;
- time-varying in time/flow format; and
- time-varying in period/flow format.

#### *Constant Mode*

The constant ventilation mode is the simplest, and the flow rates are entered in the form of a matrix (Figure 3.6). Note that the ambient air is always designated zone 0, and that the value in the *From [i]* row and *To [j]* column is the flow rate from zone i to zone j. The Flow Balance button checks and reports the balance of flow rates for each zone, a feature especially useful for a multizone flow matrix.

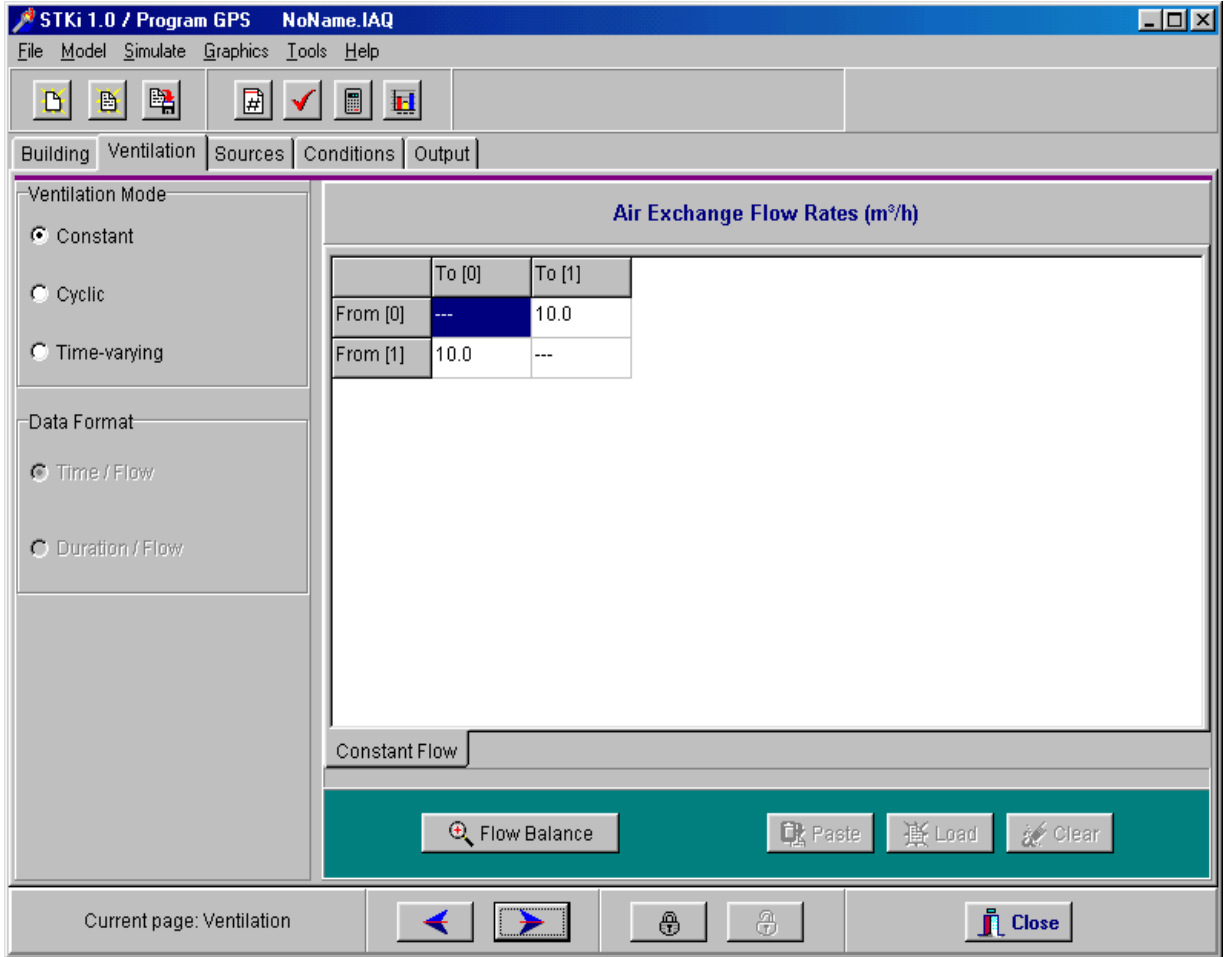


Figure 3.6 Constant ventilation mode in the GPS program. The matrix shown is for a single-zone model.

### *Cyclic Mode*

When the cyclic mode is selected, the user is asked to provide two air flow matrices and the cyclic periods for them. During the simulation, the two ventilation patterns will be used alternatively. For the data in Figure 3.7, the simulation will start by using flow matrix 1 for 2 hours, then shift to flow matrix 2 for 1 hour. This cycle will be repeated until the simulation is finished (Figure 3.8).

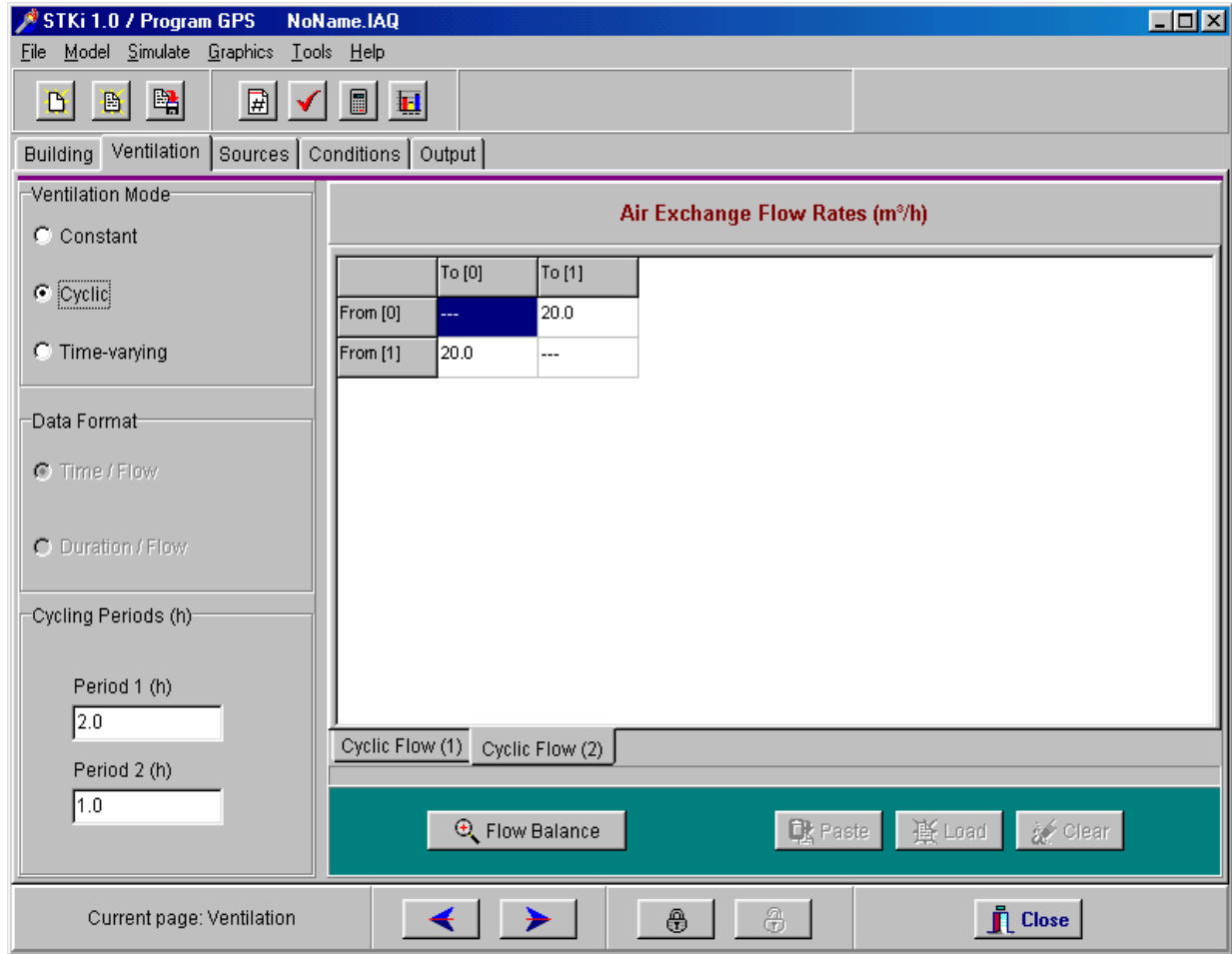


Figure 3.7 Cyclic ventilation mode in the GPS program. Note the two tabs near the bottom. The user is also prompted to enter the cycling periods (h) for the two ventilation patterns.

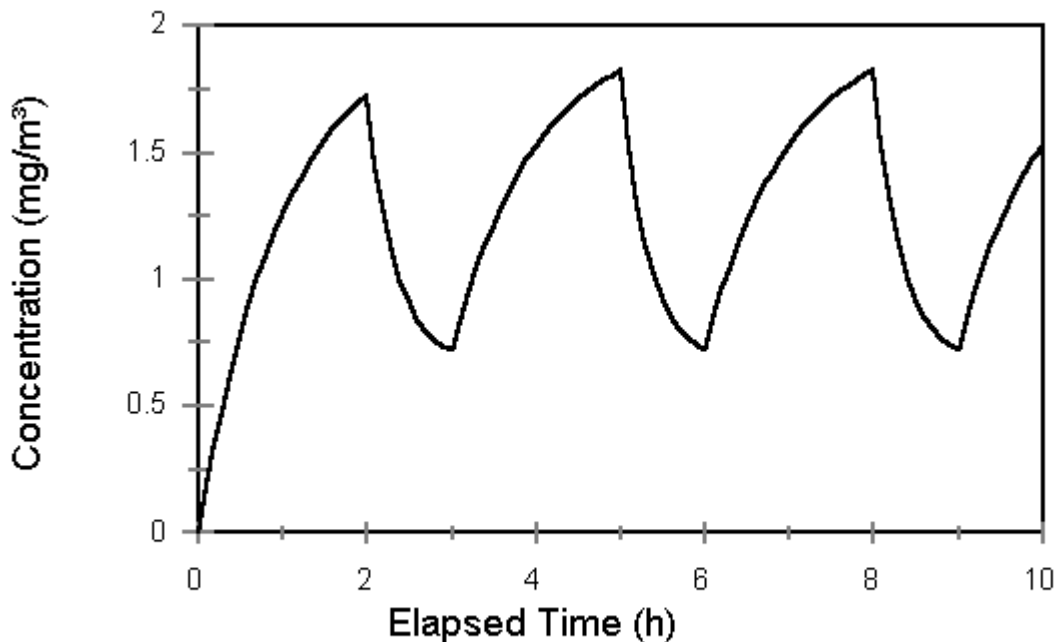


Figure 3.8 Concentration profile generated by a constant source under the cyclic ventilation mode.

### *Two Time-varying Modes*

The two time-varying modes – time/flow and period/flow – provide the user with more flexibility. When using these modes, be aware of the differences between them. In the time/flow format, the ventilation rates are given as a series of time/flow points. That is, the ventilation rates change from one point to another. The ventilation rates between two adjacent points are obtained by means of linear interpolation. This ventilation mode is useful when:

- The air flow rates are generated by a predictive infiltration/ventilation model; or
- The building has a variable air volume (VAV) air handling system.

In the period/time format, a series of constant ventilation rates are specified for different time periods. The important point is that, within each period, the ventilation rate remains constant. This ventilation mode is used when there are a limited number of ventilation patterns during a simulation.

The differences between these two modes are illustrated in Figure 3.9 by using data in Tables 3.2 and 3.3.

Table 3.2 Time-varying ventilation mode in the time/flow format (one zone).

Time (h)	Flow Rate (m <sup>3</sup> /h)
0	15
1	22
2	24
3	28
4	22
5	25
6	33
7	45
8	49
9	42
10	46

Table 3.3 Time-varying ventilation mode in the duration/flow format (one zone).

Duration (h)	Flow Rate (m <sup>3</sup> /h)
3	20
5	50
2	35



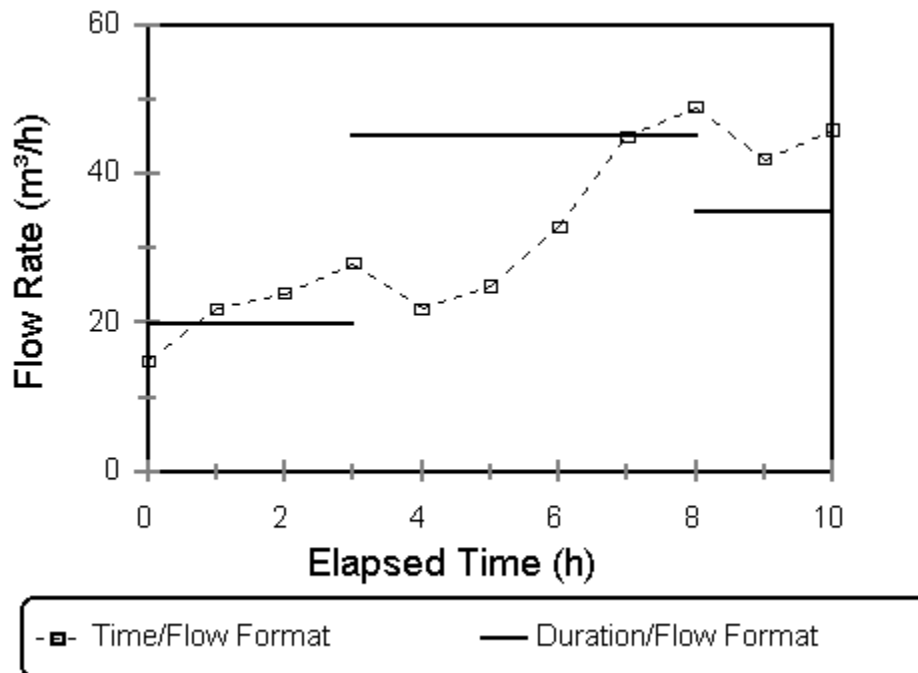


Figure 3.9 Comparison between the two time-varying flow modes. The plot was generated by using data in Tables 3.2 and 3.3.

### *Simplified Data Format for One-zone Models with the Time-varying Ventilation Mode*

If there are  $n$  air zones, the number of all possible air flows is  $n(n+1)$ . Thus, for a one-zone model, there are two flow rates, which are always equal. In this program, simplification is made for single-zone models with either time-varying ventilation mode: the user needs to enter only one flow rate in the time-varying flow table, like Tables 3.2 and 3.3. To minimize any potential confusion, the data table adjusts its size automatically.

### 3.3.2 Add Pages

In addition to the five pages that are permanently displayed, four more pages are available when you need them. They are labeled Sinks, Air cleaner/Filters, Reactions, and Input Data, respectively.

To add a page to your model, click on the Add Page speed button (i.e., the one with a red pound sign), select the page (or pages) you need, and then click the OK button. Adding models for sinks, air cleaning devices, or chemical reactions is similar to adding source models: go to the corresponding page, and then click on the Add button near the top-right corner.

The Input Data page is for accepting data for two time-varying sources: time-varying indoor sources and the ambient air as a time-varying source. For more information see Section 3.3.8.

Occasionally, you may add a page and then decide to remove it. To hide an added page, click the Add Page speed button again and uncheck the page you want to hide.

### 3.3.3 Source Models

Twenty-six source models are available in the GPS program. Some of them are mass transfer models. Table 3.4 lists all available models and references. Descriptions of each model can be found in the program by clicking the Add button in the Sources page. After you select a model, the model entry dialog box will appear with the model description on the upper-left corner. The user should consult with the original publications for more information about a specific model.

Table 3.4 Source models available in the GPS program.

Model Group	ID No.	Model Description	Reference
Constant & Instant	11	constant (as mass/time)	Dunn, 1987
	12	constant (as flow rate and concentration) <sup>1</sup>	Dunn, 1987
	13	constant (as mass/area/time)	ASTM, 1990
	15	ambient air as a constant source	Shair & Heitner, 1974
	16	instant pollutant release	Chang & Guo, 1992a
First-order & Higher-order	21	first-order (as $E_0$ and $k$ )	Dunn, 1987
	22	first-order (as $M_0$ and $k$ )	Clausen, 1993
	23	double first-order (+/+)	Chang & Guo, 1992b
	24	double first-order (+/-)	Chang & Guo, 1998
	25	second-order	Clausen, et al., 1993
	26	$n^{\text{th}}$ -order	Tichenor, et al., 1991
Solvent Evaporation	31	Evaporation from a solvent pool <sup>2</sup>	Chang & Krebs, 1992
	32	VB model for TVOCs	Tichenor, et al., 1993
	33	VBX model for individual VOCs	Guo, et al., 1998
Dry Sources	41	HCHO emission from particleboard	Hoetjer & Koerts, 1986
	42	VOC from PVC flooring (1)	Christiansson, et al., 1993
	43	VOC from PVC flooring (2)	Christiansson, et al., 1993
	44	biocide emissions from treated wood	Jayjock, et al., 1995
Emissions from Water	51	VOC from water w/ known $k_L$ <sup>3</sup>	Lyman, et al., 1990
	52	VOC from water w/ known $k_g$ <sup>4</sup>	Lyman, et al., 1990
Time-varying	61	time-varying indoor source	Koontz & Nagda, 1991
	62	ambient air as a time-varying source	Shair & Heitner, 1974
Combined <sup>5</sup> & Miscellaneous	71	VOC from latex paint and plaster during and after application	Zeh, et al., 1994
	72	power law model for building materials	Zhu, et al., 1998
	73	ambient air as a sine function	Shair & Heitner, 1974
	74	ambient air as a cosine function	Shair & Heitner, 1974

<sup>1</sup> This is a variant of source model 11.

<sup>2</sup> A similar model was first used for the outdoor environment (Mackay and Matsugu, 1973).

<sup>3</sup>  $k_L$  = overall liquid-phase mass transfer coefficient;

<sup>4</sup>  $k_g$  = overall gas-phase mass transfer coefficient;

<sup>5</sup> Combined models are those with two or more distinctive terms.

### 3.3.4 Sink Models

Five sink models are available in the GPS program (Table 3.5). As for source models, model descriptions can be found in the program. Note that, when you select a non-zero value for the sink materials in the Building page, the Sinks page becomes visible automatically. Always

remember to enter the sink areas in the Building Configuration table. To add a sink model, click the Sinks page tab, then click the “Add” button on the right. After you select a model, the model entry window will appear with the description on the upper-left corner.

Table 3.5 Sink models available in the GPS program.

ID Number	Model Description	Reference
1	first-order deposition (irreversible)	Nazaroff & Cass, 1986
2	first-order reversible	Tichenor, et al., 1991
3	higher-order reversible	Sparks, 1991
4	reversible w/ pollutant degradation	Jayjock, et al., 1995
5	two-node model	Jørgensen, et al., 2000

### 3.3.5 Models for Air Cleaners

Models for air filters and air cleaners are still rare. Two models are available in the GPS program, one for constant removal rate and the other for declining removal rate. Depending on whether the filter/cleaner is stand-alone or in the HVAC system, each model has two different forms (Table 3.6). The on-line description of these models can be found the same way as for the source and sink models. By default, the Filters & Cleaners page is hidden. Use the Add Page speed button to bring it up.

Table 3.6 Air cleaner/filter models available in the GPS program.

ID Number	Cleaner/Filter Type	Model Description	Reference
11	stand-alone	constant removal rate	Sparks, 1996
12	stand-alone	declining removal rate	None
21	in HVAC system	constant removal rate	Sparks, 1996
22	in HVAC system	declining removal rate	None

### 3.3.6 Chemical Reactions

The user needs to remember two things when dealing with gas-phase chemical reactions. First, this program is not designed to run indoor photochemical models, which will be taken care of by a special-purpose simulation program in IAQX. Second, the concentration units used in chemical reactions are incompatible with those commonly used in conventional IAQ simulations. Chemical reactions take place on a molecule-to-molecule basis. The most commonly used concentration units in atmospheric chemistry are molecules/cm<sup>3</sup> and parts per million (ppm).

This program has several features that help the user ease the unit conflict problem. However, it is ultimately the user's responsibility to keep different parts of the model in harmony.

The GPS program requires that concentrations be given in **mole/m<sup>3</sup>** whenever chemical reactions are involved in an IAQ model. Consequently, the emission rate will be **mole/h**, instead of mg/h. Conversion between mg/m<sup>3</sup> and mole/m<sup>3</sup> is easy:

$$\frac{(mg / m^3)}{1000 \text{ mw}} = (mole / m^3) \quad (3.1)$$

where mw = molecular weight (g/mole).

More conversion factors are provided in the program. Just select Tool/Conversion factor from the main menu.

### *Add Chemical Reactions*

To add chemical reactions, make the Chem Rex (for chemical reaction) page visible: click the page tab, click the Add button near the top-right corner, and then follow instructions.

### *Reaction Orders*

Most chemical reactions that may occur in the indoor air are either of first or second order. The following reactions are of first order:



The following reactions are of second order:



### *Add Reactions with Unknown Products*

When the products of a chemical reaction are unknown, you can leave the right-hand side of the reaction equation empty. The following equations are all valid:



### 3.3.7 Defining the HVAC System

In IAQX, the heating, ventilation, and air-conditioning (HVAC) system is treated as a special air zone with all the properties (such as volume and sink areas) and functions (such as air exchanges with outdoor air and other zones) that a regular zone has, plus several special functions. For instance, the mixing pattern is different from that of a regular zone, and the air filters can be placed in three possible locations: recirculation, makeup, or supply air streams (Figure 3.10).

This program recognizes the existence of an HVAC system if the last zone is named either HVAC or HAC. The volume of the HVAC system is often difficult to estimate. However, since the flow-to-volume ratio is much greater for the HVAC than for regular air zones, it is not necessary to accurately determine the total volume of the HVAC system. A rough estimation will not affect the accuracy of the simulation. Use the Filters & Cleaner page to add models for HVAC filters.

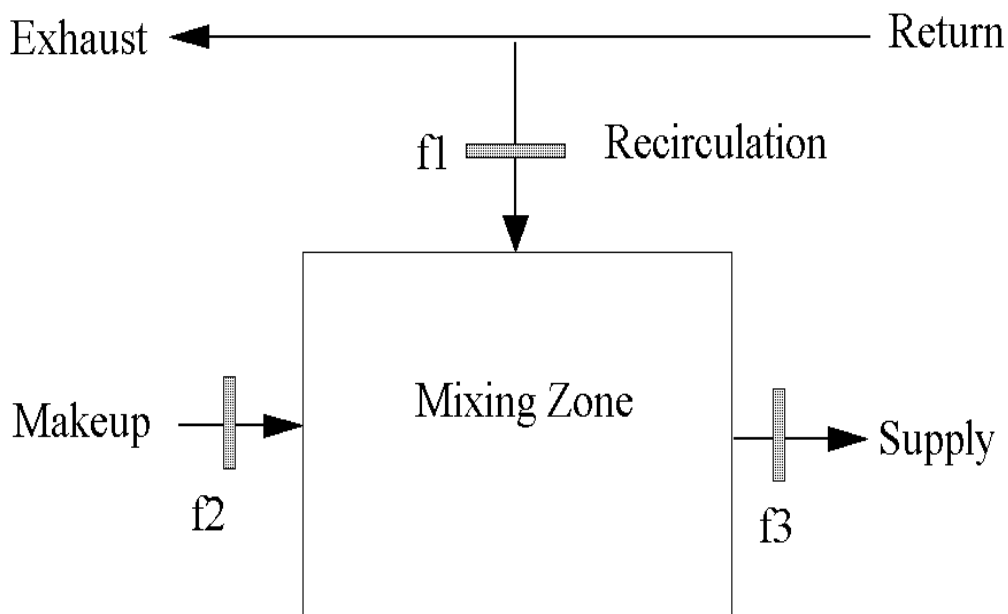


Figure 3.10 Diagrammatic description of the air handling system. Three possible positions for the air filter are marked f1, f2, and f3.

### 3.3.8 Time-Varying Sources

This program accepts two types of time-varying sources: time-varying indoor source (source No. 61) and ambient air as a time-varying source (source No. 62). Like other source models, they are defined in the Sources page. However, the user is required to provide the time-varying emission rate or outdoor concentration in the form of a data table. Two data tables are available in the Input Data page (Figure 3.11). The data formats are slightly different for these two models. Make sure you enter the data in the right place. There is a Data Format button in each page. Click on it to display the data format before you enter the data.

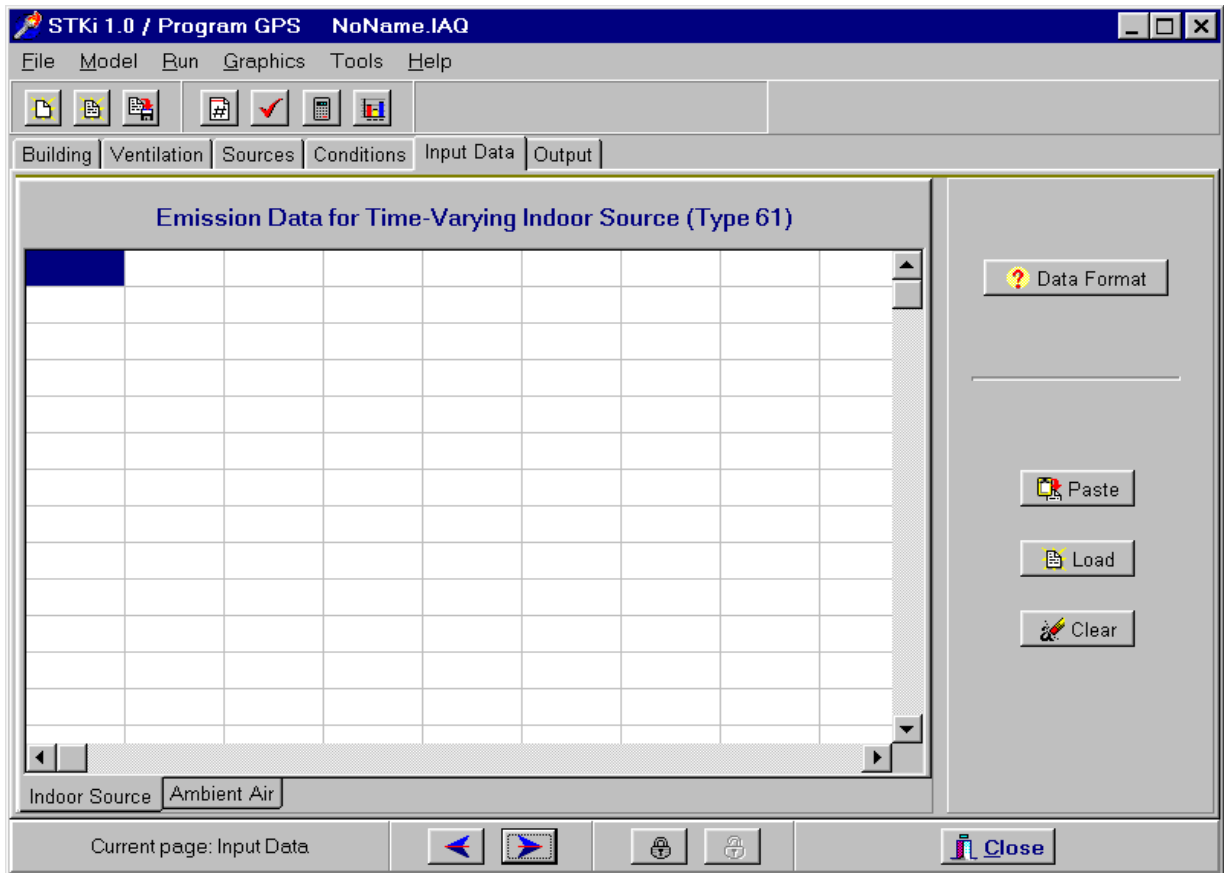


Figure 3.11 The layout of the Input Data page of the GPS program. Note the two tabs near the bottom-left corner and the Data Format button near the top-right corner.

### 3.3.9 Non-Zero Initial Concentrations

Non-zero initial concentrations are entered in the Conditions page. You should do this after you finish with all other pages.

There are two radio buttons in the selection box near the bottom-left corner labeled “Are

there non-zero initial air concentrations?” Select Yes to make the table on the right visible (Figure 3.12). When you click the Scan button, the program will search different parts of your model to find all the pollutant names and put them in the table. The only thing you need to do is to enter the concentration values. If a pollutant name does not exist in the other parts of your model, you can always add it to the table manually.

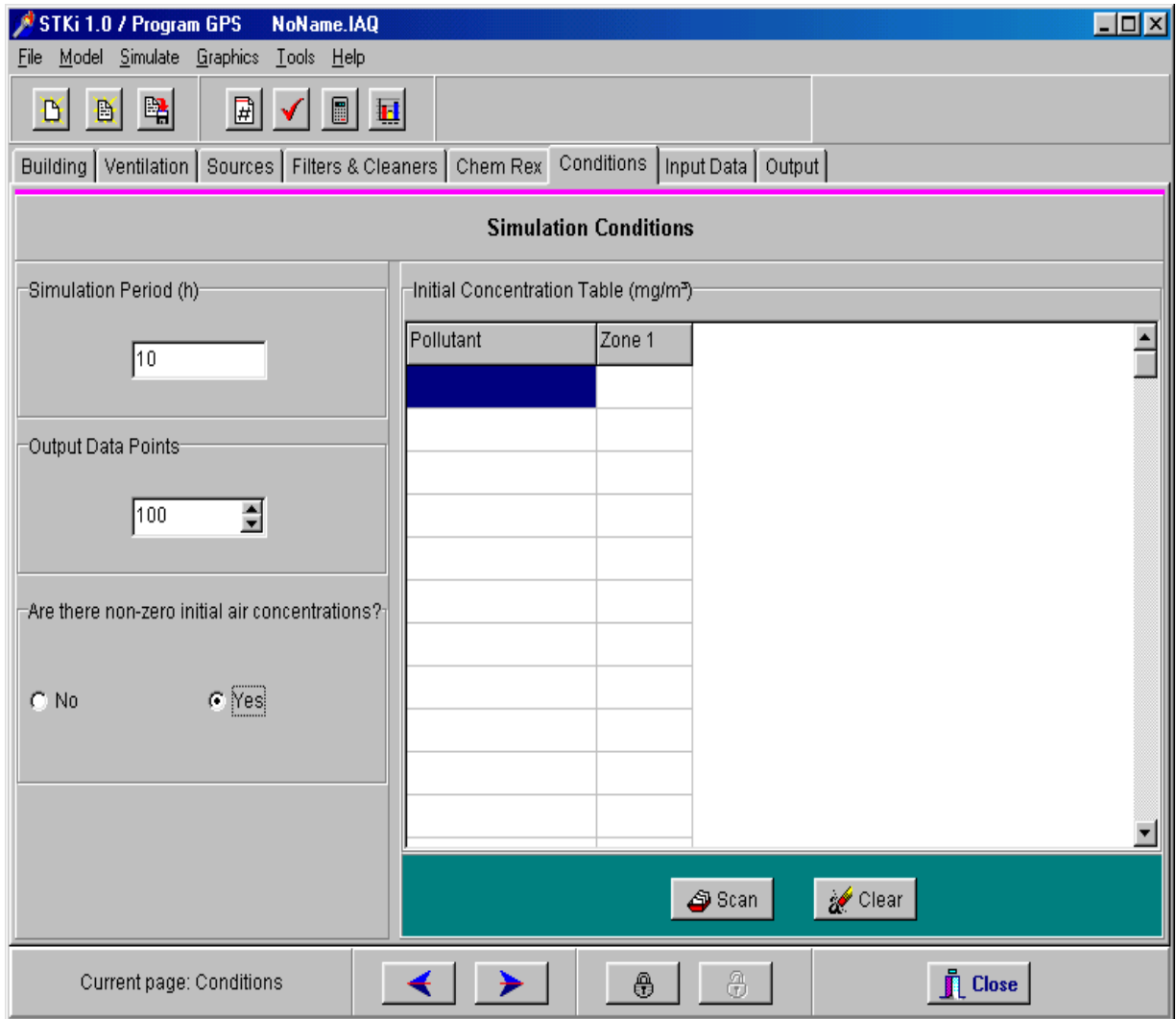


Figure 3.12 Layout of the Conditions page of the GPS program. The Initial Concentration Table is visible.



## **CHAPTER FOUR**

### **MODELS FOR VOC EMISSIONS FROM SOLVENT-BASED INDOOR COATING PRODUCTS (VBX.EXE)**

#### **4.1 Model Description**

##### 4.1.1 Overview

The VBX program utilizes three source models to predict the emissions of total volatile organic compounds (TVOCs) and/or individual volatile organic compounds (VOCs) from solvent-based indoor coating materials based on product formulation (Guo et al., 1999). Depending on the user's knowledge of the VOC contents in the product, this program offers two options for data entry: "Bulk analysis" and "MSDS."

The "Bulk analysis" option utilizes two mass transfer models (see Sections 4.1.2 and 4.1.3) and requires the user to provide the contents of major VOCs in the liquid product. A dozen or so major VOCs are usually sufficient, and the minimum number allowed is five.

The "MSDS" option is useful when information about the contents of major VOCs is not available. In this option, the first-order decay model is used (Section 4.1.4) and its parameters are estimated based on the information that can be found in the Material Safety Data Sheet (MSDS).

The required user input for the source is listed in Table 4.1. Note that similar source models are available in the general-purpose simulation program (GPS.EXE). However, GPS does not have the capability to estimate the model parameters based on the product formulation.

Table 4.1 User input required by the VBX program.

	VOC Data Option		
	Bulk Analysis		MSDS
Pollutant	TVOC	Individual VOC	Individual VOC
Model Implemented	VB	VBX	1st-order decay
Source area	X	X	X
Wet film thickness	X	X	X
Product density	X	X	X
Contents of major VOCs	X	X	
Content of VOC of interest		X	X
Most abundant VOC			X
Room temperature	X	X	X

#### 4.1.2 The VB Model for TVOCs

The rate of TVOC emissions is estimated by using the VB model:

$$E(t) = k_m (1.32 P_0 \frac{\bar{m}}{v_m} \frac{M_T}{M_{T0}} - C) \quad (4.1)$$

where  $E(t)$  = emission factor (mg/m<sup>2</sup>/h);

$k_m$  = gas-phase mass transfer coefficient (m/h);

$P_0$  = total vapor pressure for TVOCs (mmHg);

$\bar{m}$  = average molecular weight for TVOCs (g/mole);

$v_m$  = mole volume (m<sup>3</sup>);  $v_m = 0.0243$  m<sup>3</sup> at 1atm and 23°C;

$M_T$  = amount of TVOCs remaining in the source (mg/m<sup>2</sup>);

$M_{T0}$  = amount of TVOCs applied (mg/m<sup>2</sup>); and

$C$  = indoor TVOC concentration (mg/m<sup>3</sup>).

The coefficient 1.32 in Eq. 4.1 is for converting the total vapor pressure to the saturated concentration. Methods for estimating the total vapor pressure, average molecular weight, and gas-phase mass transfer coefficient are described in Sections 4.1.4 and 4.1.5.

#### 4.1.3 The VBX Model for Individual VOCs

The emission rate of an individual VOC is estimated by the VBX model:

$$E_i(t) = k_m (1.32 P_i \frac{\bar{m}}{v_m} \frac{M_i}{M_T} - C_i) \quad (4.2)$$

where  $E_i(t)$  = emission factor for compound i (mg/m<sup>2</sup>/h);  
 $P_i$  = vapor pressure for pure compound i (mm Hg);  
 $M_i$  = amount of compound i remaining in the source (mg/m<sup>2</sup>); and  
 $C_i$  = concentration of compound i in indoor air (mg/m<sup>3</sup>).

#### 4.1.4 The First-Order Decay Model for Individual VOCs

If you do not know the contents of major VOCs in the product, but you know the TVOC content and the contents of individual VOCs in which you are interested, the emission factor can be estimated from:

$$E(t) = E_0 e^{-kt} \quad (4.3)$$

$$E_0 = 1.32 k_m P_i \frac{\bar{m}}{v_m} \frac{y_i}{y_0} \quad (4.4)$$

$$k = \frac{E_0}{z d y_i} \quad (4.5)$$

where  $E_0$  = initial emission factor (mg/m<sup>2</sup>/h);  
 $k$  = first-order decay rate constant (h<sup>-1</sup>);  
 $t$  = time (h);  
 $\bar{m}$  = average molecular weight for TVOCs (g/mole), represented by the molecular weight for the most abundant VOC in the product;  
 $m_i$  = molecular weight for component i (g/mole);  
 $y_i$  = content of an individual VOC in the product (mg/g);  
 $y_0$  = content of TVOCs in the product (mg/g);  
 $z$  = wet film thickness (μm); and  
 $d$  = product density (g/mL).

This model requires less information from the user, and the application-phase simulation can be easily implemented. However, it is less accurate than the VBX model and works only for individual VOCs.

#### 4.1.5 Estimation of the Total Vapor Pressure and Average Molecular Weight for TVOCs Based on the VOC Contents in the Product

The two parameters  $P_0$  and  $\bar{m}$  in the VB model (Eq. 4.1) can be estimated from the contents of major VOCs in the product.

$$P_0 = \frac{\sum_{i=1}^n \frac{P_i y_i}{m_i}}{\sum_{i=1}^n \frac{y_i}{m_i}} \quad (4.6)$$

$$\bar{m} = \frac{\sum_{i=1}^n y_i}{\sum_{i=1}^n \frac{y_i}{m_i}} \quad (4.7)$$

where  $P_i$  = vapor pressure for compound  $i$  (mm Hg);  
 $y_i$  = content of compound  $i$  in the liquid product (mg/g); and  
 $m_i$  = molecular weight for compound  $i$  (g/mole).

#### 4.1.6 Model for Estimating Gas-Phase Mass Transfer Coefficient

A model developed by Sparks, et al. (1996) is used to estimate the gas-phase mass transfer coefficient ( $k_m$ ):

$$k_m = 0.33 D L_c^{-\frac{1}{3}} \left( \frac{v d}{\mu} \right)^{\frac{2}{3}} \quad (4.8)$$

where  $D$  = diffusivity of the VOC in air ( $m^2/h$ );  
 $L_c$  = characteristic length of the source, equal to the square root of the source area (m);  
 $v$  = air velocity over the source, (m/h);  
 $d$  = density of the air ( $g/m^3$ ); and  
 $\mu$  = viscosity of the air (g/h/m).

## **4.2 A Brief Tour of the Program**

Click on the VBX icon to launch the program. You will find that the main window (Figure 4.1) is very similar to that for the GPS program. In fact, all IAQX programs have similar user interfaces.

Six tabbed pages are permanently displayed: Building, Ventilation, VOC Contents, Source, Conditions, and Output. The Building page is almost identical to that in the GPS program. However, the zone number is limited to 3 instead of 10 and the number of sink materials is limited to 2.

The Ventilation page is simpler than its counterpart in the GPS program. Currently, special-purpose models allow only constant flow rates. For single-zone models, only the left panel is visible (Figure 4.2a), and the user can enter either the air exchange rate or the flow rate. For multizone models, the right panel is visible, and the flow table is identical to those in the GPS program (Figure 4.2b). The display changes automatically (no user intervention is needed).

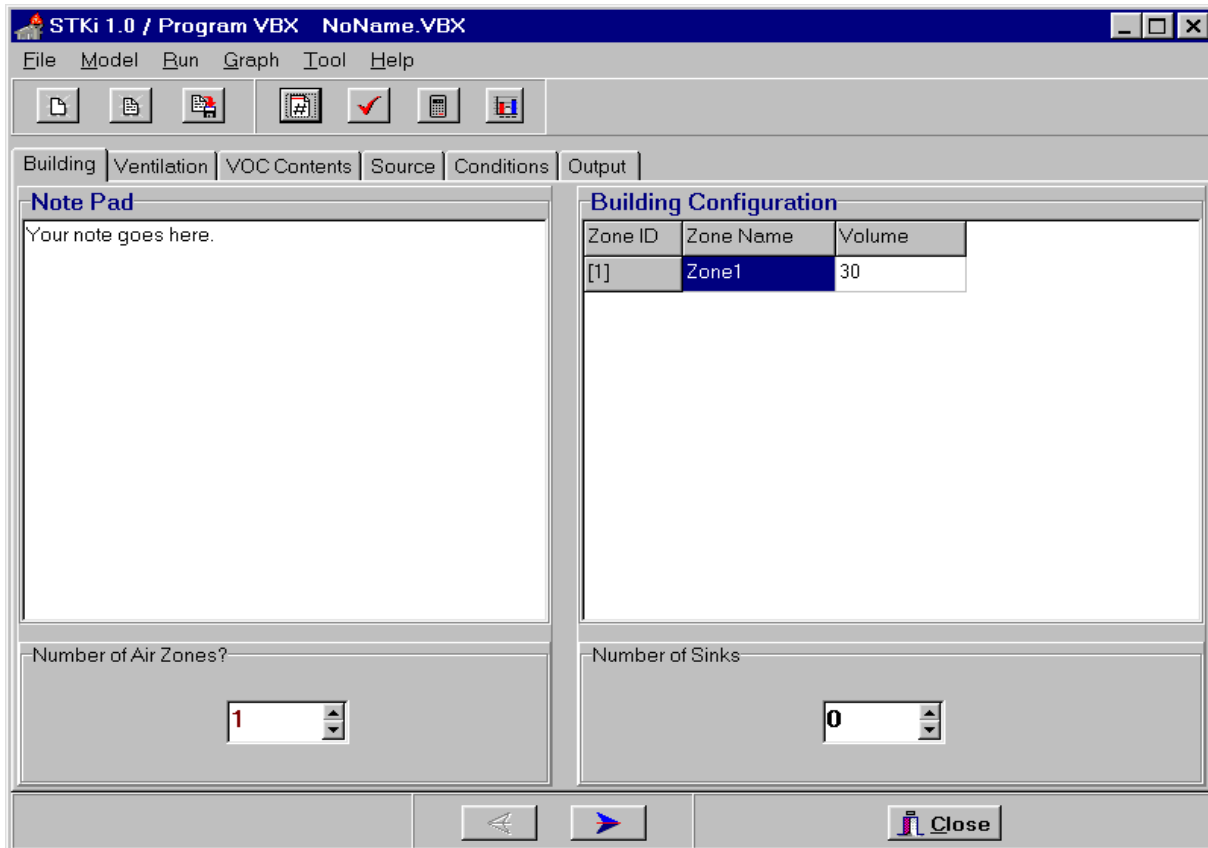


Figure 4.1 The main window of the VBX program (showing the Building page).

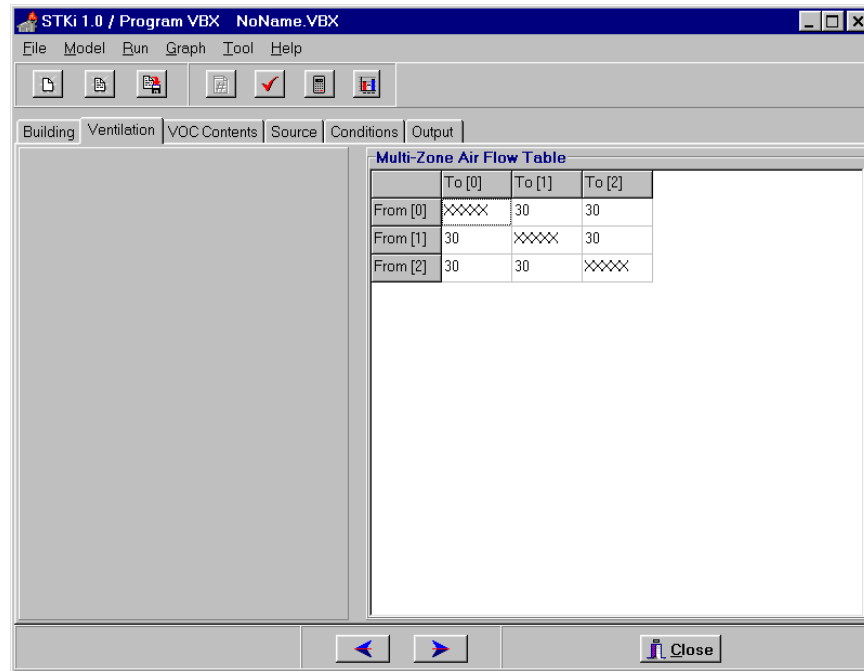
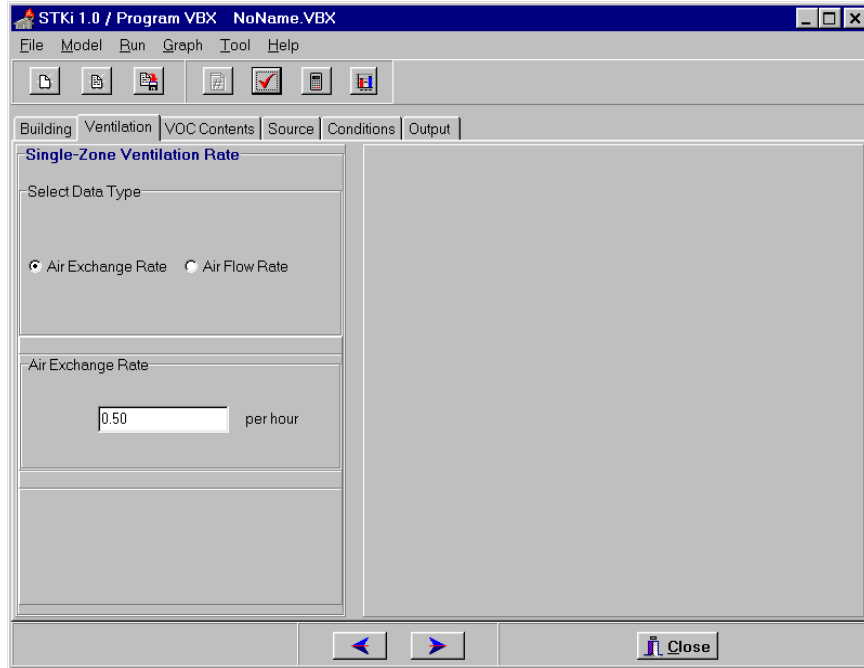


Figure 4.2 Layout of the Ventilation page of the VBX program: single zone (top); multi-zone (bottom)

Now turn to the VOC Contents page (Figure 4.3). The first thing you need to do with this page is to determine what kind of VOC content data you want to use. In the upper-left corner, there two radio buttons in a selection box labeled “VOC Data Options.” As mentioned in Section 4.1.1, you can choose either “Bulk analysis” or “MSDS” depending on whether or not you know the content of major VOCs in the product. Table 4.2 compares these two options with more details. For this demonstration, select “Bulk analysis.”

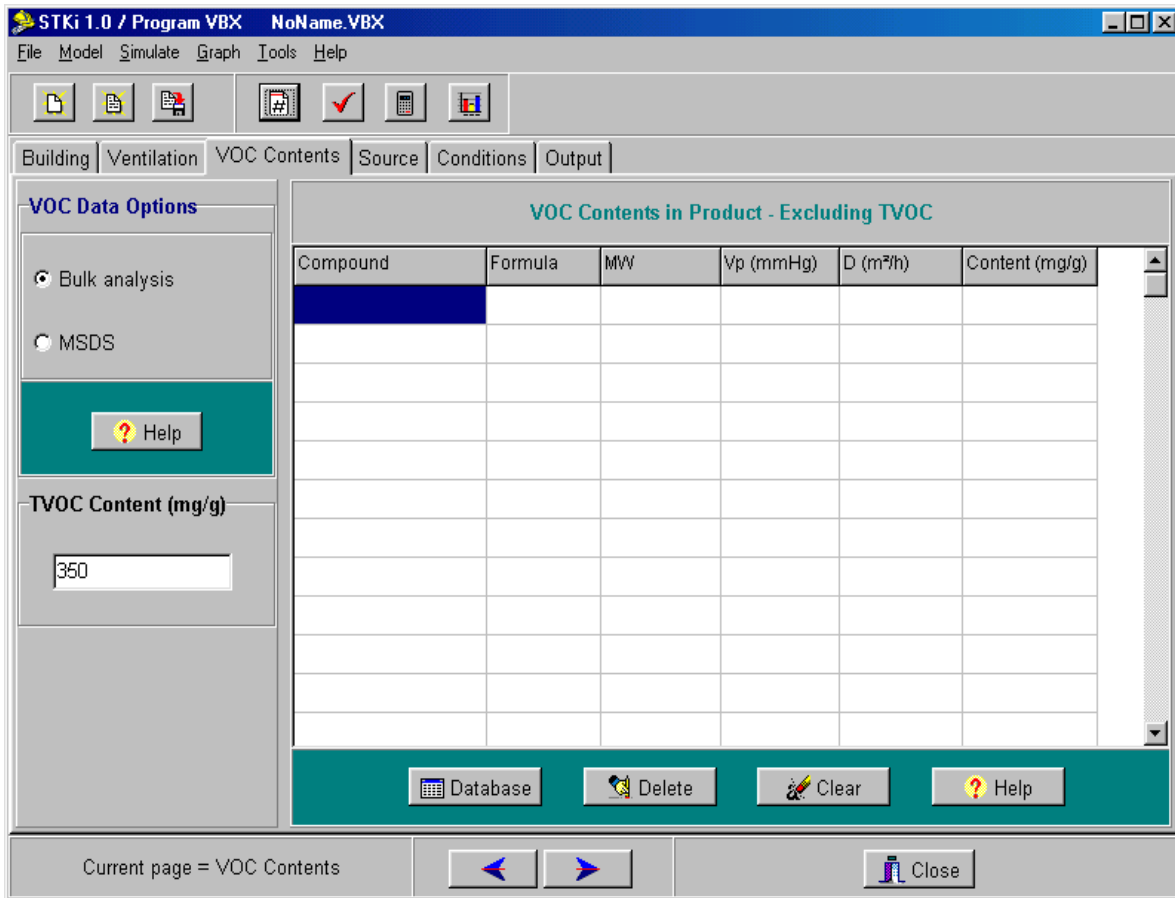


Figure 4.3 Layout of the VOC Contents page of the VBX program.

Table 4.2 Differences between the two VOC data options.

VOC Data Option	Bulk Analysis	MSDS
Data required from user	Contents of TVOCs and major VOCs	Contents of TVOCs and VOCs of interest
Typical data source	GC analysis for VOC content in product	MSDS
Minimum number of VOCs required	5	1
Model used	VB/VBX	First-order decay

Now, move to the bottom-left corner of the window, where you give the TVOC content in (mg/g product). For this demonstration, enter 500.

Move to the VOC content table on the right. The required information for each compound is:

- compound name;
- molecular weight;
- vapor pressure;
- diffusivity in air; and
- content in product.

Entering these parameters for a dozen or so compounds is tedious. This program simplifies the data entry by providing the user with a mini-database.

Click the Database button below the table. A dialog window will display the available VOC names in the database (Figure 4.4).



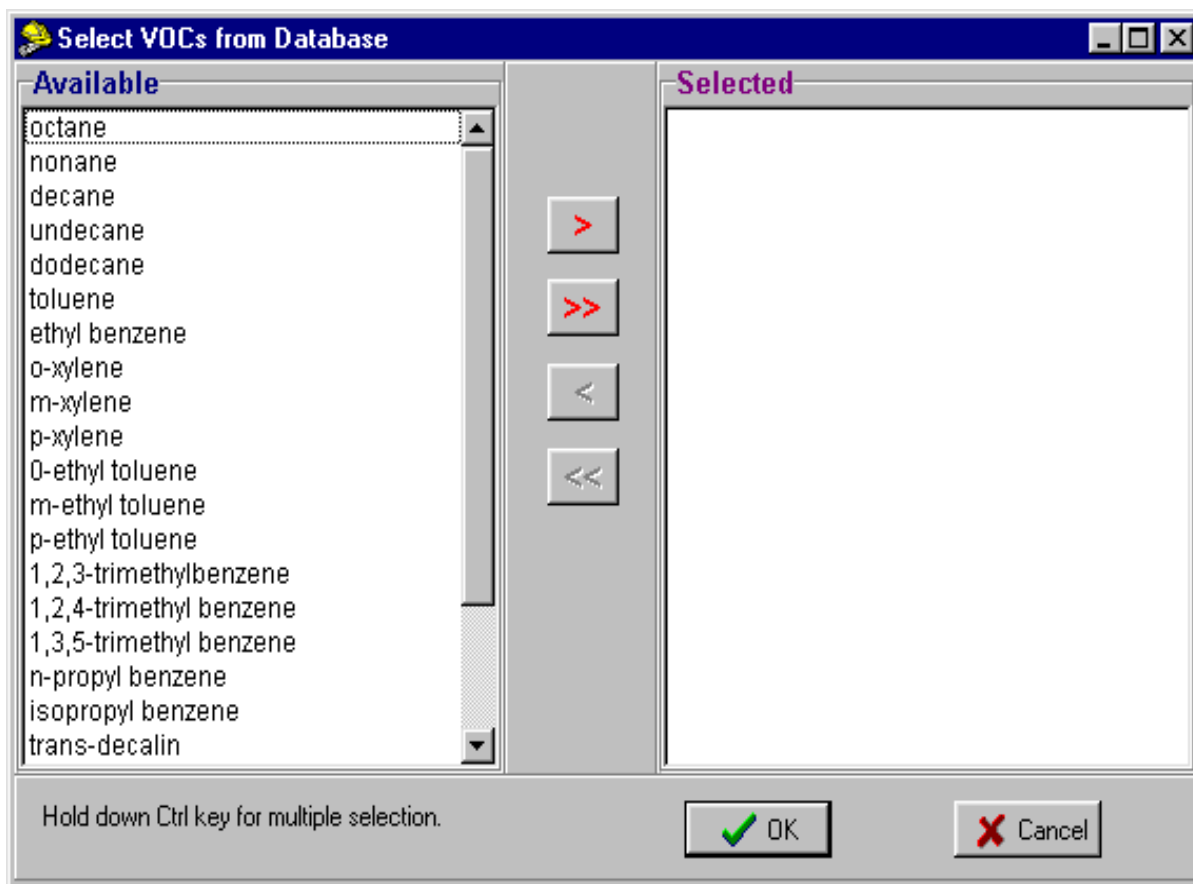


Figure 4.4 Dialog window for the built-in database of the VBX program.

Select VOCs from the left panel, then click the right arrow to copy selected compounds to the right panel. For multiple selection, hold down the Control key while you select. As an example, let's select the first five compounds. After you finish, click OK. As you can see, all the parameters are entered to the VOC table except VOC contents (Figure 4.5). Let's enter 20, 50, 100, 50, and 20 (mg/g) for the five compounds, respectively. Note that, for real coating products, the sum of the contents for individual VOCs is always less than the TVOC content because routine GC analysis cannot identify and quantify all the compounds in petroleum-based solvents. See the demonstration model file "BULK.VBX" for an example.

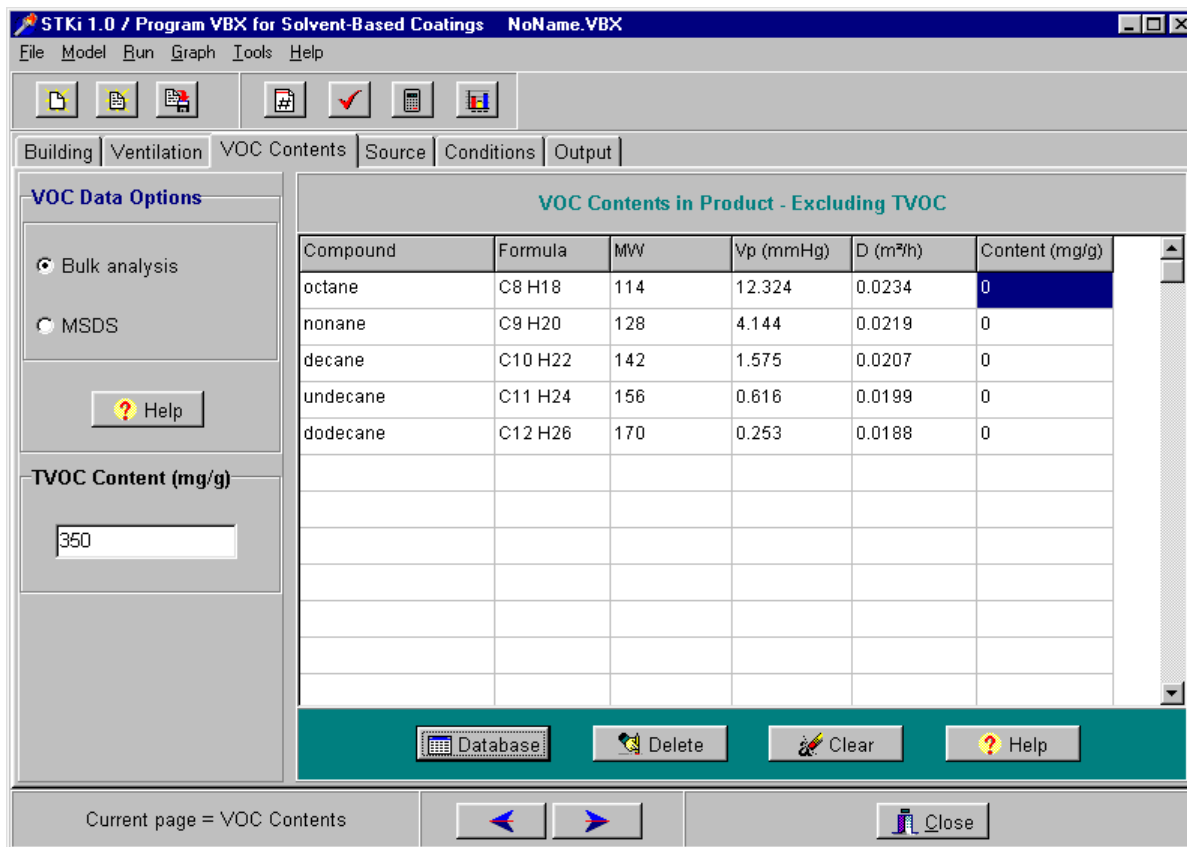


Figure 4.5 Layout of the VOC Contents page of the VBX program. Five VOCs have been entered by using the built-in mini-database.

Next, turn to the Source page, in which you specify four parameters for the source and select the VOCs for output (Figure 4.6). The source parameters are: product density (g/mL), wet film thickness ( $\mu\text{m}$ ), coated area ( $\text{m}^2$ ), and source location (zone ID). The recommended wet film thickness can be found in the product label. For alkyd paint, the typical value is in the 75-100  $\mu\text{m}$  range. For this demonstration, enter 75  $\mu\text{m}$  for the wet film thickness.

With the “Bulk analysis” option, often you do not need to simulate all the VOCs you enter. This program allows you to select the species in which you are interested. There are two list boxes on the right. To choose TVOCs and decane for output, select them from the Available Species box and then click the Select button to make them appear in the Selected Species box. Note that if a compound name does not appear in the Selected Species box, its simulation results will be ignored in the output data table.

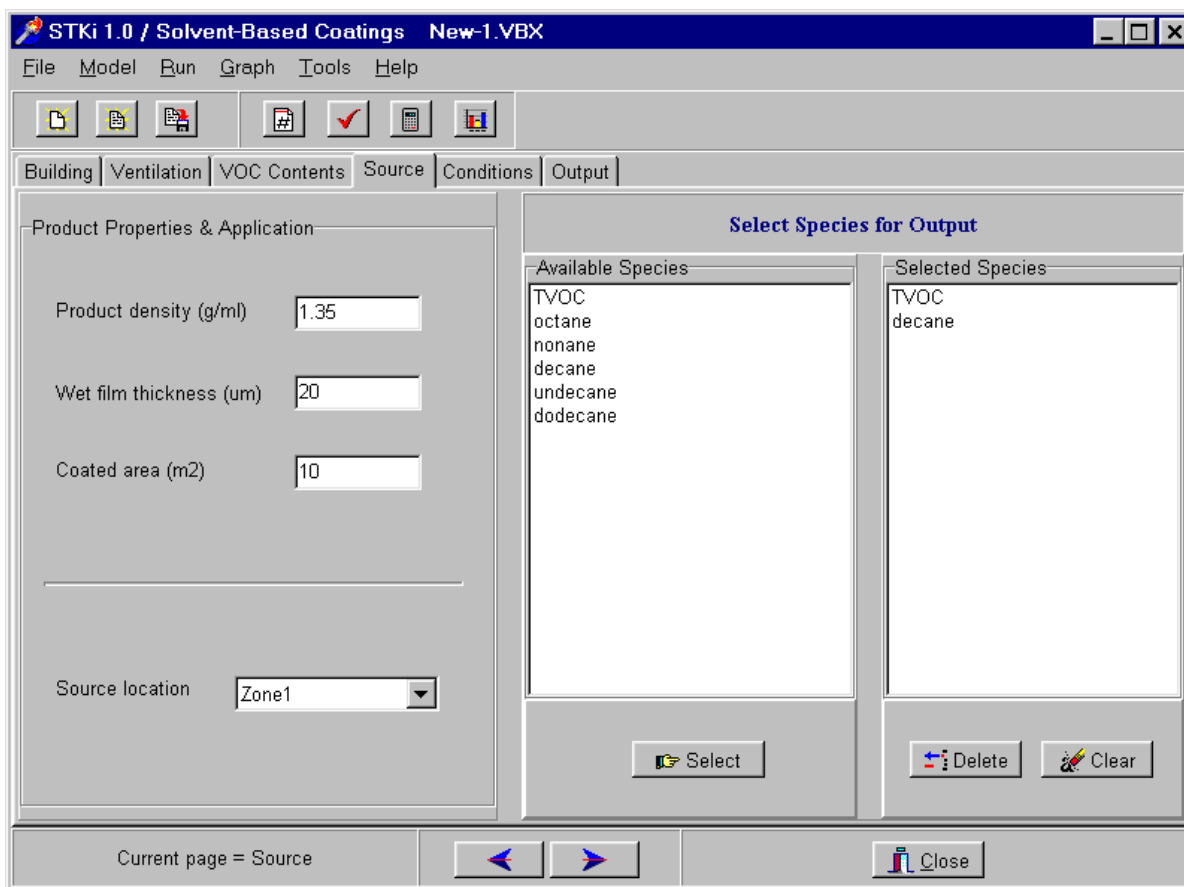


Figure 4.6 Layout of the Source page of the VBX program.

To finish this IAQ model, turn to the Conditions page to enter several more parameters – all are self-explanatory. Now compile and run the program the same way you did with the GPS program.

### 4.3 More About the VBX Program

#### 4.3.1 What If a VOC Does Not Exist in the VOC Database?

If a VOC does not exist in the database, go to the last row of the table in the VOC Contents page and enter the parameters manually. In addition, this program has tools to help the user compute the molecular weight, diffusivity, etc. Simply select Tools from the main menu and find the tool you need.

#### 4.3.2 About the MSDS Option

With the MSDS option, the user can enter only one compound in the VOC content table.

The user is also required to specify the most abundant VOC in the solvent (Figure 4.7). This information will be used to estimate the average molecular weight for TVOCs. In most cases it is decane. In rare cases, it can be undecane (in some alkyd paint) or xylene (in some conversion varnish). Also note that the MSDS option allows for the application-phase simulation (Section 8.3) and that the related parameters are entered in the Conditions page (Figure 4.8).

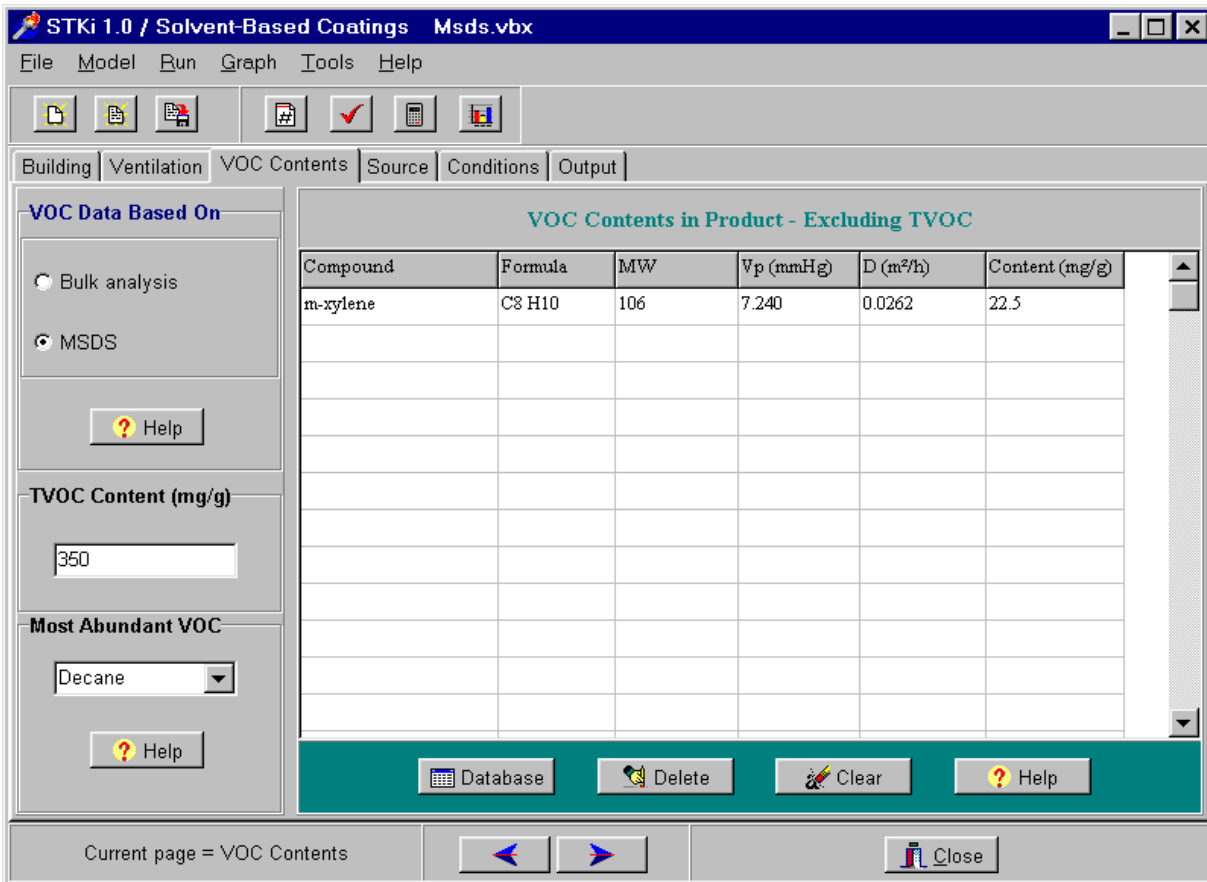


Figure 4.7 Layout of the VOC Contents page when the MSDS option is selected. The selection box labeled “Most Abundant VOC” becomes visible.

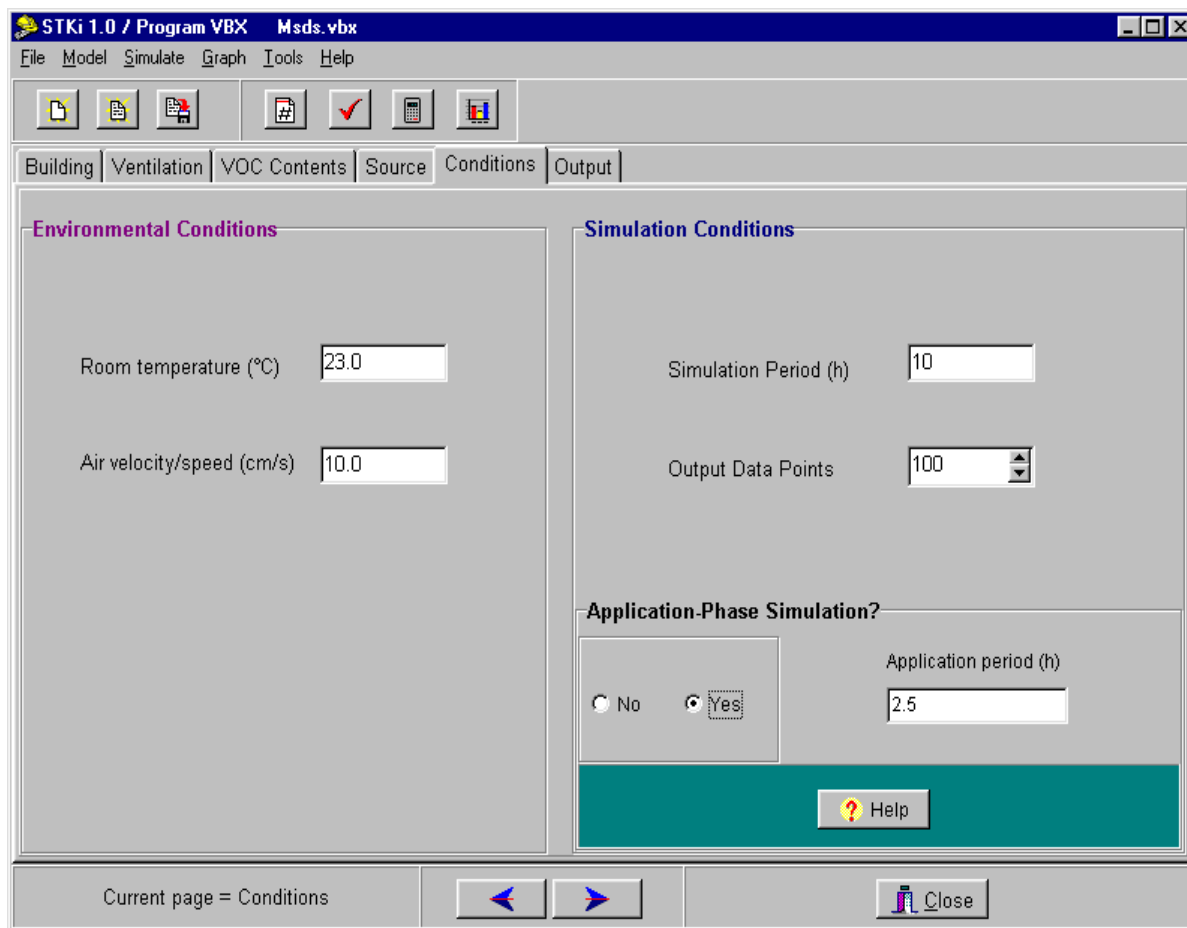


Figure 4.8 Defining the application-phase simulation in the Conditions page.

### 4.3.3 Adding Sink Models

The Sink page (Figure 4.9) is hidden when you start the program. To add a sink model, make the Sink page visible by clicking on the Add Page speed button (the one with a pound sign). Five sink models are available in this program, and different sink materials can be represented by different sink models. There is a button below the table labeled “Update VOC Names.” Click on it: all selected VOCs will show up in the table.

To learn more about the sink models, see the on-line help by clicking the Detail button. Remember that the number of sink materials is specified in the Building page.

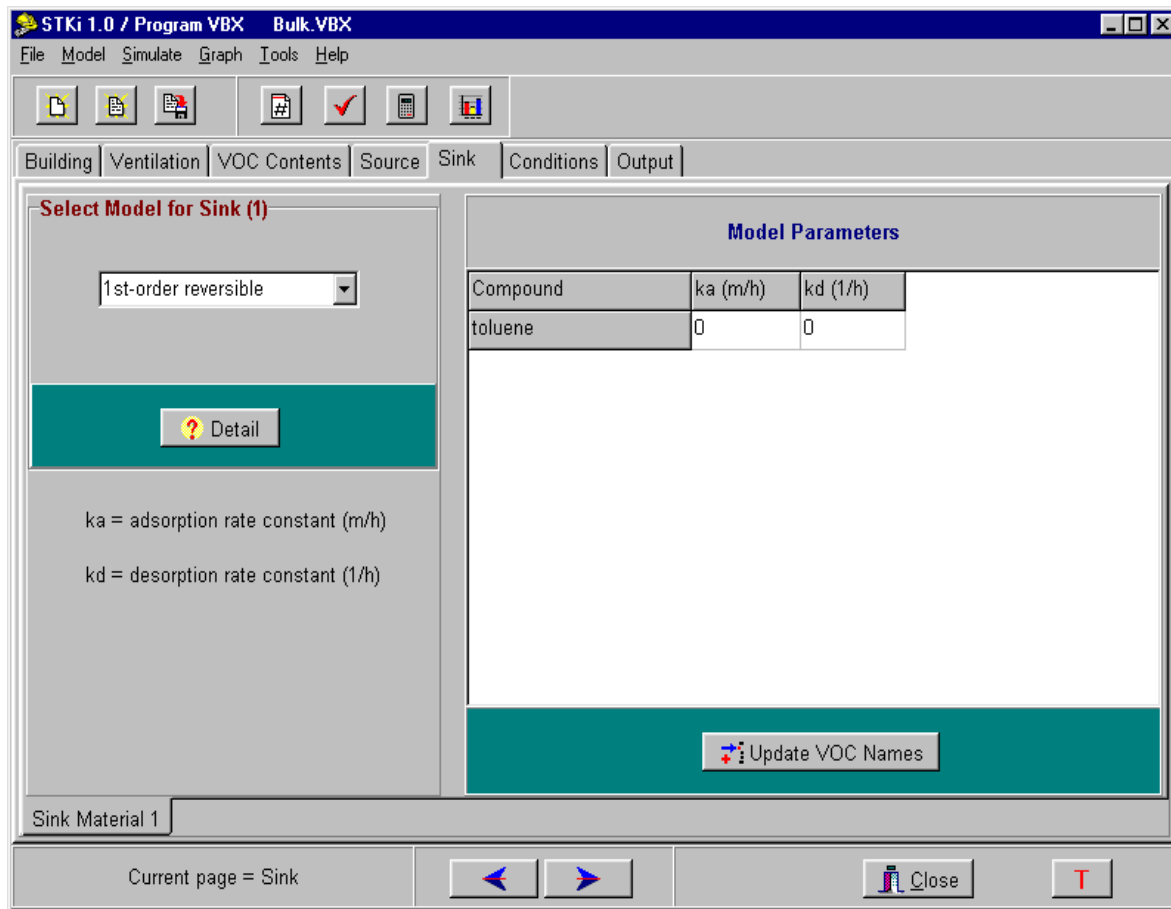


Figure 4.9 Layout of the Sink page of the VBX program.

## CHAPTER FIVE

### MODELS FOR SMALL-SCALE SOLVENT SPILLS (SPILL.EXE)

#### 5.1 Model Description

Program SPILL contains three mass transfer models for estimating the indoor VOC concentrations following unstrained, small-scale solvent spills on hard flooring.

##### 5.1.1 Model for Single-Component Solvent

Reinke and Brosseau (1997) evaluated several methods for predicting the indoor VOC concentrations following spills of pure solvent and concluded that the Penetration Theory or the Mackay and Matsugu Method under the isothermal assumption performed better than the rest of the methods. This program uses the latter method, which estimates the emission factor from:

$$N_A = 2.778 \times 10^{-7} \frac{k_m (y_{A^*} - y_{A_{room}})}{V_{spill}} \quad (5.1)$$

where  $N_A$  = molar flux of compound A (kg-mol A / m<sup>2</sup> / s);  
 $k_m$  = gas-phase mass transfer coefficient (m/s);  
 $y_{A^*}$  = mole fraction of A at saturation (kg-mol A / kg-mol gas);  
 $y_{A_{room}}$  = mole fraction of A in well-mixed air (kg-mol A / kg-mol gas); and  
 $V_{spill}$  = gas molar volume at solvent pool temperature (m<sup>3</sup> / kg-mol);

The authors recommend that the mass transfer coefficient ( $k_m$ ) be calculated from a method proposed by Mackay and Mastugu (1973):

$$k_m = 0.0292 u^{0.78} X^{-0.11} Sc^{-0.67} \quad (5.2)$$

where  $u$  = velocity of air flowing across the solvent pool (m/s);  
 $X$  = pool diameter (m), approximated by the square root of the spill area; and  
 $Sc$  = Schmidt number (unitless).

More discussion on calculating the mass transfer coefficient is provided in Section 5.3.2.

##### 5.1.2 Model for Solvent Mixture Whose Exact Composition Is Known

For a solvent mixture with  $n$  components, a model developed by Drivas (1982) is used to

predict the emission of an individual component i:

$$E(t) = k_m \left( C_{oi} \frac{W_i}{\sum_{j=1}^n W_j} - C_i \right) \quad (5.3)$$

Where  $W_i$  = amount of component i remaining in the pool (mol);  
 $W_j$  = amount of component j remaining in the pool (mol);  
 $C_{oi}$  = saturation concentration of component i (mol/m<sup>3</sup>); and  
 $C_i$  = air concentration of component i (mol/m<sup>3</sup>).

Note, however, that Drivas's original model ignores the effect of air concentration  $C_i$ , which is valid under the outdoor environmental conditions.

### 5.1.3 Model for Petroleum-Based Solvent

If the solvent of concern is a petroleum product, such as mineral spirits, it is difficult, if not impossible, to determine its exact composition because it may contain hundreds of compounds. Routine GC analysis can easily quantify 10 to 20 major VOCs. If we assume that the properties of the imaginary solvent consisting of all the major VOCs identified by the GC analysis resemble those of the original solvent (Guo, et al., 1999), the emissions of TVOCs or individual VOCs from the spill can be estimated from Eqs. 5.4 and 5.5, respectively:

$$E(t) = k_m (C_v - C) \quad (5.4)$$

$$E(t) = k_m \left( C_v \frac{w_i}{w_T} \frac{m_T}{m_i} - C_i \right) \quad (5.5)$$

where  $C_v$  = total vapor pressure for TVOCs converted to concentration units (mg/m<sup>3</sup>);  
 $C$  = TVOC concentration in indoor air (mg/m<sup>3</sup>);  
 $C_{vi}$  = vapor pressure for pure component i converted to concentration units (mg/m<sup>3</sup>);  
 $C_i$  = indoor concentration of component i (mg/m<sup>3</sup>);  
 $w_i$  = amount of component i remaining on the floor (mg);  
 $w_T$  = amount of TVOCs remaining on the floor (mg);  
 $m_T$  = average molecular weight of TVOCs (g/mol); and  
 $m_i$  = molecular weight of component i (g/mol).

The two parameters for TVOCs --  $C_v$  and  $m_T$  -- can be estimated from the properties and contents of identified major VOCs (see Eqs. 4.6 and 4.7).



### 5.1.4 Estimation of the Spill Area

The emission rate is the product of the emission factor and source area:

$$R(t) = A(t) E(t) \quad (5.6)$$

where  $R(t)$  = emission rate (mg/h);  
 $A(t)$  = spill area (m<sup>2</sup>); and  
 $E(t)$  = emission factor (mg/m<sup>2</sup>/h).

A special problem associated with solvent spills is that the spill area decreases with time. According to Drivas (1982) and Reinke and Brosseau (1997), the spill area at any time ( $A$ ) can be approximated by:

$$A(t) = A_0 \frac{W(t)}{W_0} \quad (5.7)$$

where  $A_0$  = initial spill area (m<sup>2</sup>);  
 $W(t)$  = amount of solvent remaining on the floor (mol); and  
 $W_0$  = initial amount of solvent spilled (mol).

Eq. 5.7 assumes that an unrestrained small spill maintains a constant depth and decreases only in area and not in depth, as it evaporates.

## 5.2 A Brief Tour of the Program

The user interface for this program is very similar to that for the VBX program. The first two pages (Building and Ventilation) are identical to those in the VBX program. The next four pages relate to: Solvent, Source, Conditions, and Output, respectively. In this demonstration, we will use the default values in the first two pages. Now, move to the Solvent page (Figure 5.1) by clicking its tab.

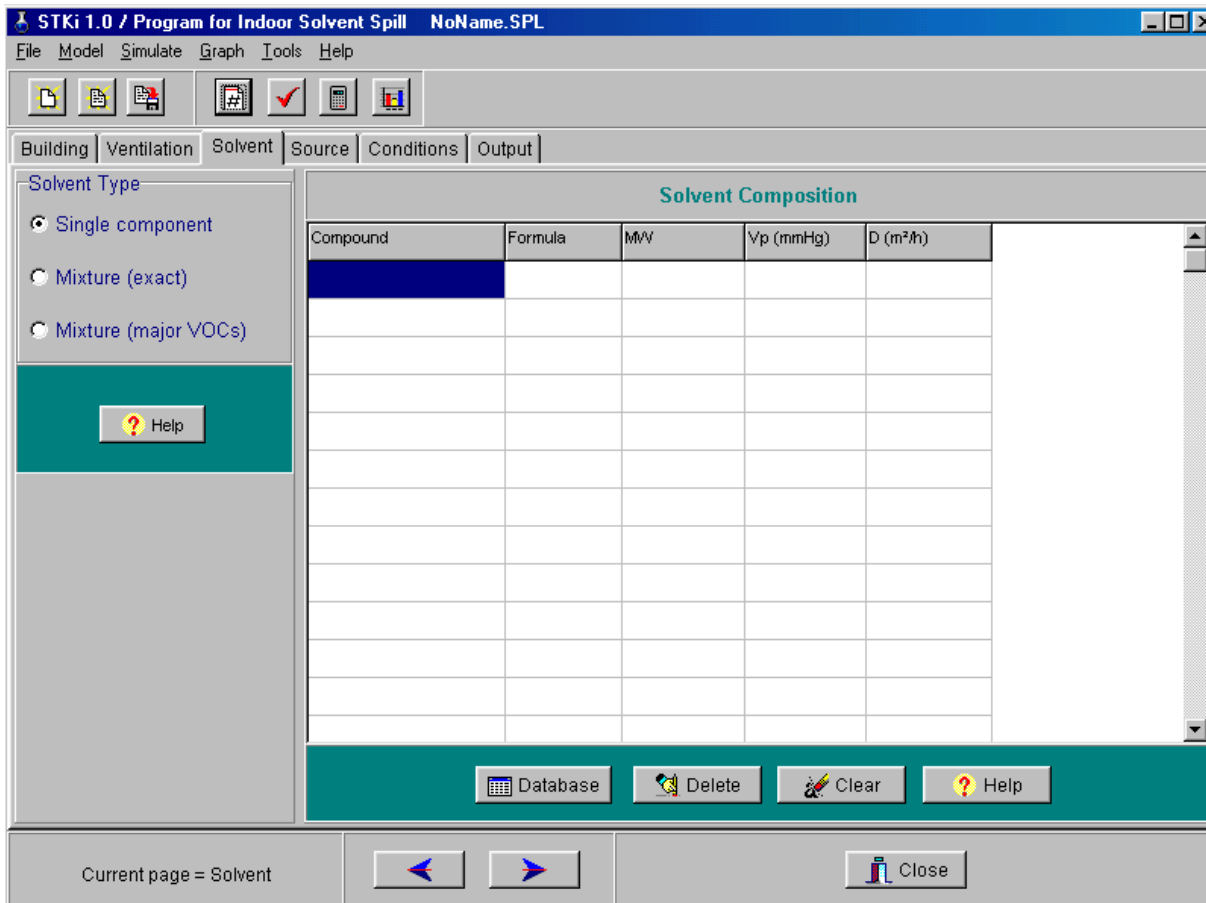


Figure 5.1 Layout of the Solvent page of the SPILL program.

The first thing you need to determine is the solvent type. There are three choices:

- Single component: for single-component solvent;
- Mixture (exact): for multicomponent solvent whose exact composition is known;  
or
- Mixture (major VOCs): for petroleum-based solvent, whose major components are known.

These choices are discussed in Sections 5.1.1 - 5.1.3. There is also a Help button in the Solvent page. Click on it to find more information about how to select the solvent type. For this demonstration, select type I -- single component.

The next step is to enter the properties of the solvent components. The required parameters for each component include: component name, molecular formula, molecular weight,

molecular diffusivity in air, and vapor pressure. Although you can enter these parameters manually, it will save you time to use the built-in VOC database. Click the Database button, select a compound from the list in the left panel (toluene, for example), then click the right arrow (>) to copy it to the right panel. Click OK to close the database. Now look at the Solvent page. All required physical properties for toluene (formula, molecular weight, vapor pressure, and diffusivity in air) are copied to the table. Note that, if you are dealing with a multiple component solvent, the content of each component (in mg/g) is also required.

Now move to the Source page by clicking its tab. In addition to the VOC content data entered in the previous page, four more parameters are needed to define the source: solvent density, amount of solvent spilled, spill area, and the cleanup time. The first three parameters are fairly straightforward. If you have no idea about how to estimate the spill area, click the button with a question mark for help.

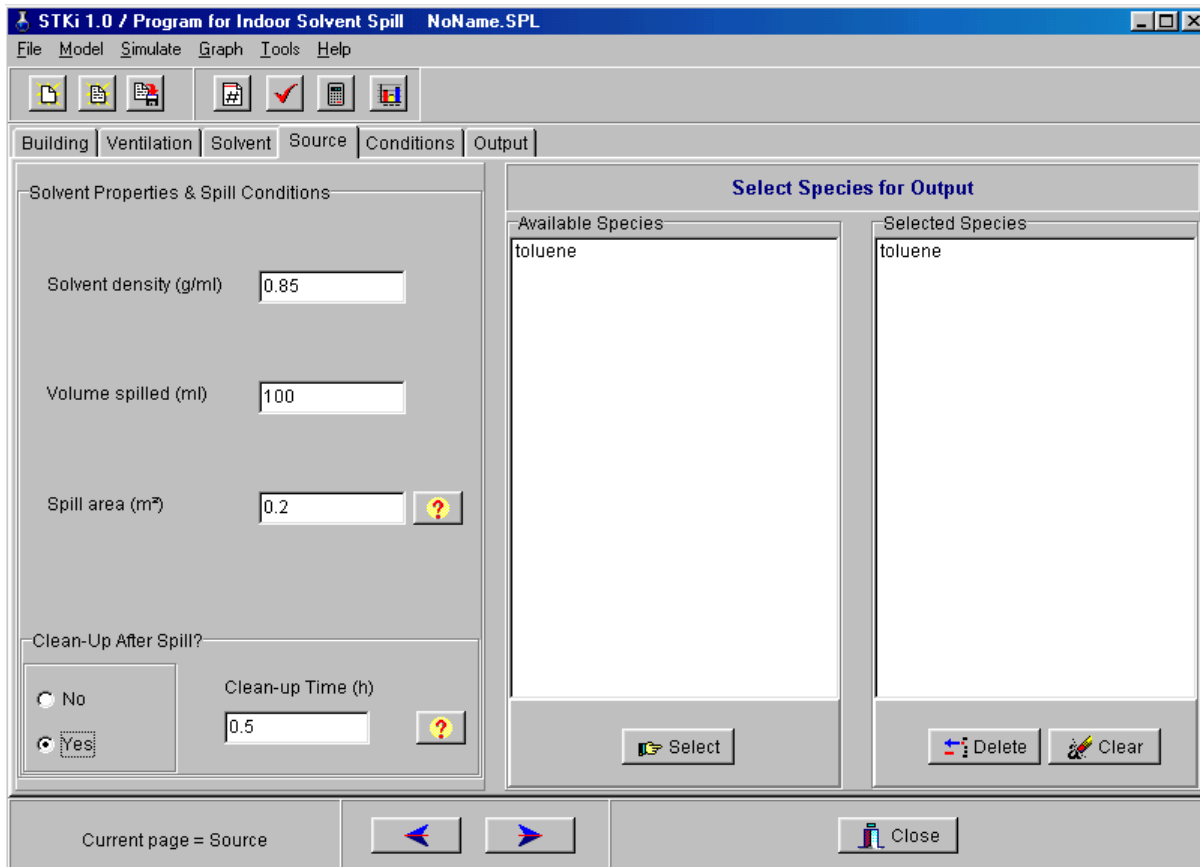


Figure 5.2 Layout of the Source page of the SPILL program.

In real life, a solvent spill is often followed by some cleanup actions. This program allows the user to specify a time to shut off the source. The cleanup time is the elapsed time when the source is removed as a result of any cleanup actions. To use this feature, click Yes near the bottom-left corner and then enter the cleanup time.

On the right side of the Sources page, there are two list boxes. The one on the left shows all available VOCs in the solvent, and the one on the right is for selected compounds for the simulation output. This feature is useful when the solvent contains many compounds and you do not want simulations for every one of them. For a single-component solvent, the selection is done automatically. Otherwise, the user can select compounds from the left box and then click the Select button.

Turn to the Conditions page, where the user specifies the environmental and simulation conditions. In most part, this page is self-explanatory except for the selection box at the bottom-right corner, labeled “How to estimate gas-phase mass transfer coefficient?” By default, the Mackay & Matsugu method (Mackay & Matsugu, 1973) is used for solvent types I and II; and the Sparks method (Sparks, et al., 1996) for solvent type III. The user does have the option to choose either of them, however. See Section 5.3.2 for more discussions on this matter.

Now compile and run the model as you do in other IAQX programs. There are two demonstration files in the “demo” folder: “solvent-2.spl” and “solvent-3.spl.” They are example cases using the other two models. They can be loaded into the program by clicking File/Open from the main menu, or clicking the Open File speed button.

## **5.3 More About the SPILL Program**

### 5.3.1 Adding Sink Models

Adding a sink model in this program is the same as in the VBX program. See Section 4.3.5 for details.

### 5.3.2 Comparison of the Two Methods for Estimating the Gas-Phase Mass Transfer Coefficient

This program provides two methods for calculating the gas-phase mass transfer coefficient: the Mackay and Matsugu method (Eq. 5.2) and the Sparks method (Eq. 4.8). The default selections are the Mackay and Matsugu method for the first two models (i.e., Eqs. 5.1 and 5.3) and the Sparks method for the third model (Eqs. 5.4 and 5.5). Both selections are recommended by the authors of the emission models.

The user should be aware that the two methods differ significantly in the air velocity range commonly found in indoor environments (Figure 5.3). Currently, there are no reported data to determine which of the two methods is more accurate for solvent spills. Thus, if you are unfamiliar with gas-phase mass transfer theories, using the default method is probably the better choice. This program does, however, give advanced users the option to choose either method for

any of the three models.

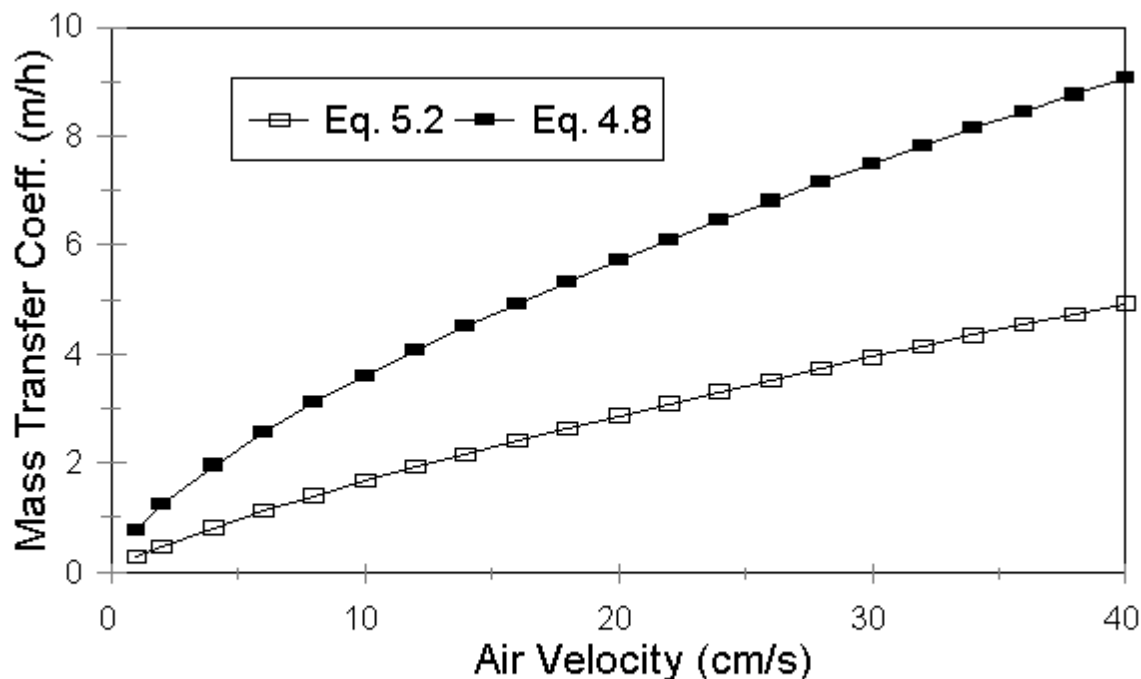


Figure 5.3 Comparison of the gas-phase mass transfer coefficient for decane estimated by the two methods.

### 5.3.3 Dealing with the Temperature Drop

Solvent evaporation is an endothermic process. Consequently, the temperature of spilled solvent is often lower than its surroundings. Reinke and Brosseau (1997) evaluated models that take this factor into consideration and found that adding the heat transfer term does not seem to improve the model performance.

Very limited data suggest that the temperature drop can be 2 to 4 °C depending on the volatility of the solvent and the properties of the flooring. Practically, this factor can be taken into consideration by using the vapor pressure at a lower temperature. This is an area that needs more experimental data.

#### 5.3.4 About the Short Circuiting Factor

The original model proposed by Reinke and Brosseau (1997) has a short circuiting factor to adjust for the short circuiting of the air exchange flow in a room. This program does not include this feature. In other words, each air zone is considered well-mixed. If short circuiting is an important factor, the user can divide the room into multiple air zones.

## CHAPTER SIX

### A MODEL FOR VOC EMISSIONS FROM DIFFUSION-CONTROLLED HOMOGENEOUS SLABS (SLAB.EXE)

#### 6.1 Model Description

Program SLAB implements an emission model developed by J. C. Little, A. T. Hodgson, and A. J. Gadgil (Little, et al., 1994) for predicting the VOC emissions from diffusion-controlled homogeneous slabs. This model was initially developed based on the experimental data for new carpet backing. It can be used for other similar sources, however. The mathematical expressions for this model are fairly long. The user is encouraged to go through the original paper for more details. A brief description is provided below.

This model was derived based on the standard diffusion equation:

$$\frac{\partial C(x,t)}{\partial t} = D \frac{\partial^2 C(x,t)}{\partial x^2} \quad (6.1)$$

where  $C(x,t)$  = pollutant concentration in the slab ( $\text{mg}/\text{m}^3$ );  
 $D$  = diffusion coefficient in the slab ( $\text{m}^2/\text{h}$ );  
 $x$  = linear distance from the bottom of the slab (m); and  
 $t$  = time (h).

The actual model is an approximate solution to the above diffusion model applied to a one-zone environment with a constant air exchange rate. Calculation of indoor air concentration involves five steps:

Step 1: calculate coefficient  $h$  from

$$h = \frac{Q}{A D K_v} \quad (6.2)$$

where  $Q$  = air exchange flow rate ( $\text{m}^3/\text{h}$ );  
 $A$  = area of the slab ( $\text{m}^2$ );  
 $K_v$  = partition coefficient (unitless).

Step 2: calculate coefficient  $k$  from

$$k = \frac{V}{A K_v} \quad (6.3)$$

where  $V$  = volume of the room or test chamber ( $m^3$ ).

Step 3: calculate coefficient  $q_n$  by finding  $n$  smallest positive roots ( $n = 1, 2, \dots$  up to 200) of the following non-linear equation:

$$q_n \tan(q_n L) = h - k q_n \quad (6.4)$$

where  $L$  = thickness of the slab (m).

Step 4: calculate the pollutant concentration at the top surface of the slab,  $C(L,t)$ , from:

$$C(x,t) = 2 C_0 \sum_{n=1}^{\infty} \frac{e^{-Dq_n^2 t} (h - k q_n^2) \cos(q_n^2 x)}{[L(h - k q_n^2)^2 + q_n^2 (L + k) + h] \cos(q_n L)} \quad (6.5)$$

where  $x$  = linear distance from the bottom of the slab,  $x = L$  at the slab surface (m);  
 $C_0$  = initial concentration in the slab ( $mg/m^3$ ); and  
 $n = 1$  to  $\infty$  is the number of terms for the summation and, practically,  $n < 200$ .

Step 5: calculate the air concentration from:

$$y(t) = \frac{C|_{x=L}(t)}{K_v} \quad (6.6)$$

where  $y$  = pollutant concentration in the air ( $mg/m^3$ ); and  
 $C|_{x=L}$  = pollutant concentration at the top surface of the slab ( $mg/m^3$ ).

\_\_\_\_\_ In this model, the source is described with four parameters: source area  $S$ , initial pollutant concentration in the slab ( $C_0$ ), molecular diffusivity of the pollutant in the slab ( $D$ ), and the thickness of the slab ( $L$ ). Discussions on estimation these parameters are provided in Section 6.3.

There are two reasons why IAQX implements this model with a stand-alone program. First, it requires special numerical treatment to compute the indoor concentration. Second, since the authors give the indoor concentration directly without an expression for the emission factor,



this model, in its current form, can be applied only to a one-zone environment; it cannot coexist with models for indoor sinks and air cleaners, which are available in other IAQX programs.

## 6.2 A Brief Tour of the Program

Click the SLAB.EXE logo to start the program. As shown in Figure 6.1, there are only two tabbed pages in this program: Model and Output. All the parameters are entered in the Model page. The source is described by five parameters: the area ( $m^2$ ), the VOC content in the slab ( $g/m^3$ ); the molecular diffusivity of the VOC in the slab ( $m^2/s$  or  $m^2/h$ ), the air/solid partition coefficient (unitless), and the thickness of the slab (m). There are already default values in each input box. The user needs to replace them by proper values for a given VOC in a given product.

After entering all the parameters, click the Compile speed button (the one with a red check sign). After successful compilation, click the Simulation speed button. Like in other IAQX programs, the output results can be viewed graphically or exported to a spreadsheet.

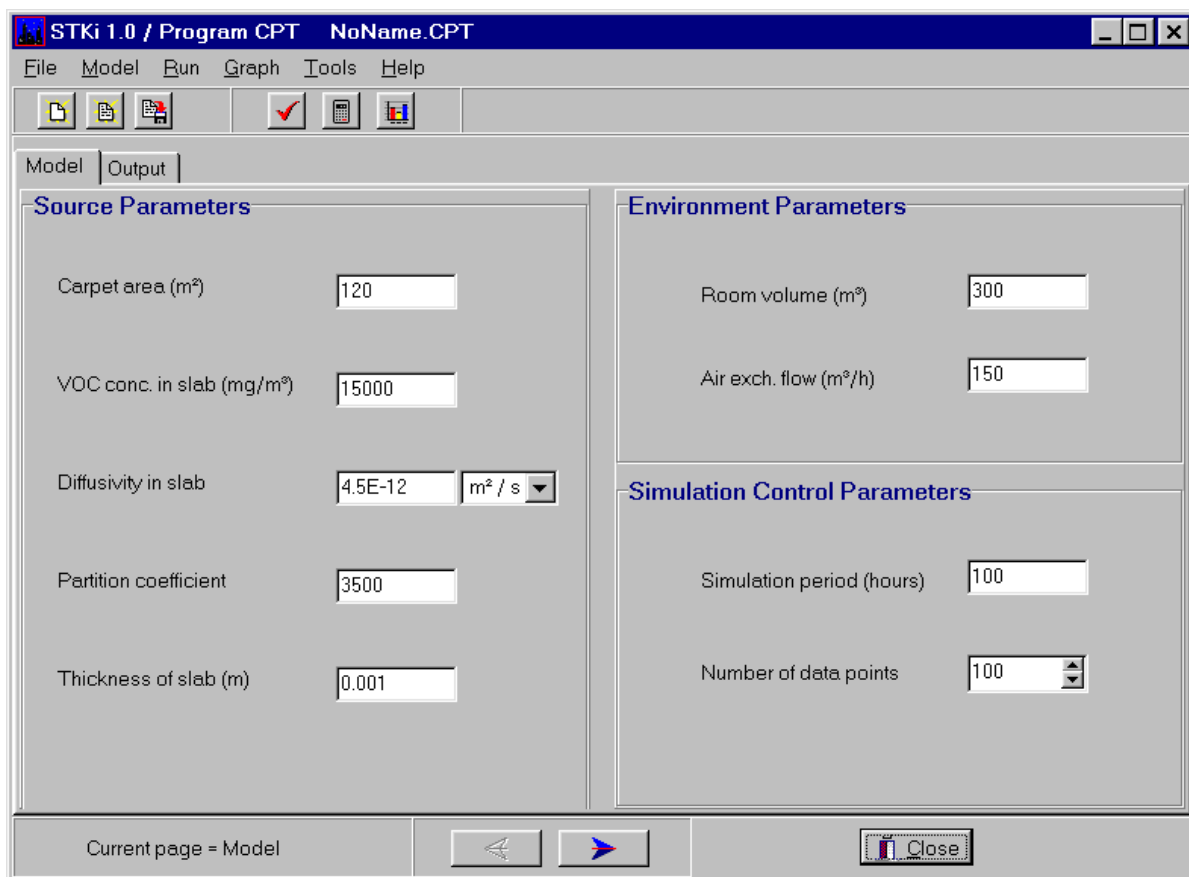


Figure 6.1 The main window of the SLAB program.

## 6.3 More About the SLAB Program

### 6.3.1 Model Parameters for New Carpet Backing

Among the five parameters that describe the source, the area and thickness of the slab are easy to determine. The other three parameters are usually obtained from experiments. According to the authors, these parameters vary significantly from compound to compound and from carpet to carpet. The following ranges are reported by the authors:

VOC content in slab:	from 340 to 255000 mg/m <sup>3</sup> ;
Partition coefficient:	from 1 to 450000;
Diffusivity in slab:	from $6 \times 10^{-14}$ to $1 \times 10^{-11}$ m <sup>2</sup> /s ( $2.2 \times 10^{-14}$ to $3.6 \times 10^{-8}$ m <sup>2</sup> /h);
Thickness of slab:	from 1 to 2 mm.

Several recent articles (Bodalal, et al., 2000, for instance) have reported the experimentally determined molecular diffusivities for common indoor VOCs in various substrates. Certain empirical correlations have also been developed .

### 6.3.2 Dealing with Zero Ventilation Rate

For some reason, this model does not allow a zero ventilation flow rate. Sometimes, one may want to calculate the upper limit of the indoor concentrations by setting the ventilation flow rate to zero. In such cases, the SLAB program will display an error message and prompt the user to enter a small positive value (e.g., 1E-4).

### 6.3.3 Source Reduction Simulation Mode

In addition to the two simulation modes that other IAQX program have (i.e., the conventional simulation and the adequate ventilation rate), program SLAB has a third simulation mode called Source Reduction. This simulation mode allows the user to estimate the degree of pollutant reduction in the source needed to satisfy certain IAQ criteria. As shown in Figure 6.2, the dialog box is very similar to that for the adequate ventilation mode. To choose this mode, select Simulate/Source reduction from the main menu.

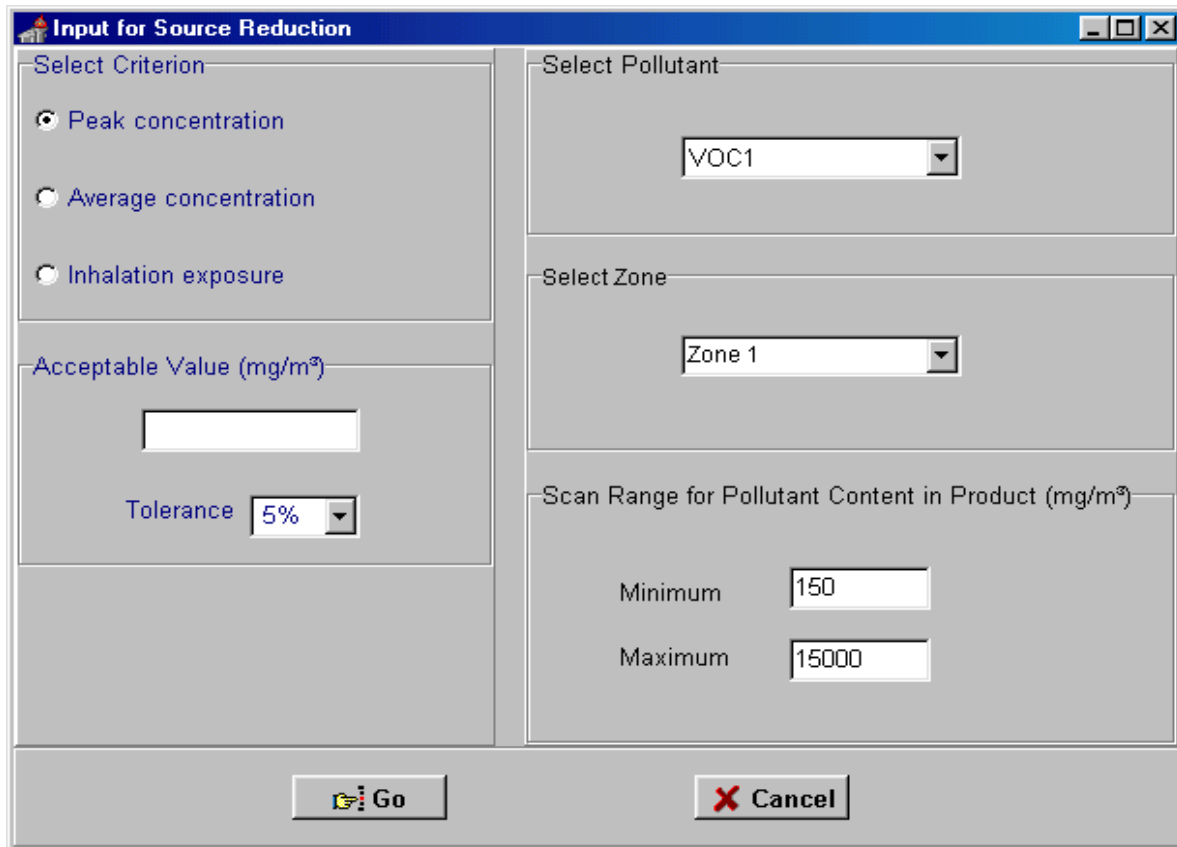


Figure 6.2 The SLAB dialog box for the Source Reduction simulation mode.

## CHAPTER SEVEN

### A MODEL FOR INDOOR PARTICULATE MATTER (PM.EXE)

#### 7.1 Model Description

Program PM.EXE implements a generic model for indoor particulate matter (PM) developed by W. W. Nazaroff and G. R. Cass (Nazaroff and Cass, 1989). The model takes into consideration: infiltration of ambient PM, interzone air movement, indoor sources, deposition, filtration, and coagulation. Coagulation is not implemented in this program, however.

The authors describe their model with several equations. See the reference for more details. Briefly, for a given size group (or section, or bin), its mass concentration in zone i is calculated from:

$$V_i \frac{dC_i}{dt} = p Q_{oi} C_0 + \sum_{j=0}^n (1 - f_{ji}) Q_{ji} C_j - \sum_{j=0}^n Q_{ij} C_i + \sum_{k=1}^m R_k - k_D V_i C_i - C_i \sum_{l=1}^q Q_l (1 - f_l) \quad (7.1)$$

where  $V_i$  = volume of zone i ( $m^3$ );  
 $C_i$  = concentration in zone i ( $\mu g/m^3$ );  
 $t$  = time (h);  
 $p$  = penetration factor (unitless);  
 $Q_{oi}$  = air flow from outside to zone i ( $m^3/h$ );  
 $C_0$  = concentration in the ambient air ( $\mu g/m^3$ );  
 $f_{ji}$  = filter's removal efficiency for air flow from zone j to zone i and  $j \neq i$  (unitless);  
 $Q_{ji}$  = air flow rate from zone j to zone i and  $j \neq i$  ( $m^3/h$ );  
 $C_j$  = concentration in zone j ( $\mu g/m^3$ );  
 $Q_{ij}$  = air flow rate from zone i to zone j and  $j \neq i$  ( $m^3/h$ );  
 $R_k$  = emission rate for indoor source k ( $\mu g/h$ );  
 $k_D$  = first-order deposition rate constant ( $h^{-1}$ );  
 $Q_l$  = air flow rate passing through the free-standing air filter l ( $m^3/h$ );  
 $f$  = removal efficiency for the free-standing air filter l (unitless);  
 $n$  = number of air zones;  
 $m$  = number of indoor sources in zone i; and  
 $q$  = number of free-standing air filter/cleaners in zone i.

The HVAC system is handled as a special air zone (see Section 7.3.4). For PM deposition, this program accepts either the first-order deposition rate constant (shown in Eq. 7.1) or the deposition velocity (not shown in Eq. 7.1). See Section 7.3.1 for more details.

## 7.2 A Brief Tour of the Program

NOTE: In this program, the PM concentration is expressed in ( $\mu\text{g}/\text{m}^3$ ), while all other IAQX programs use ( $\text{mg}/\text{m}^3$ ) for pollutant concentrations.

As shown in Figure 7.1, seven pages are permanently displayed in this program: Building, Ventilation, PM Properties, Outdoor Sources, Indoor Sources, Conditions, and Output. Three more pages are hidden and available on demand (see Section 7.3.1).

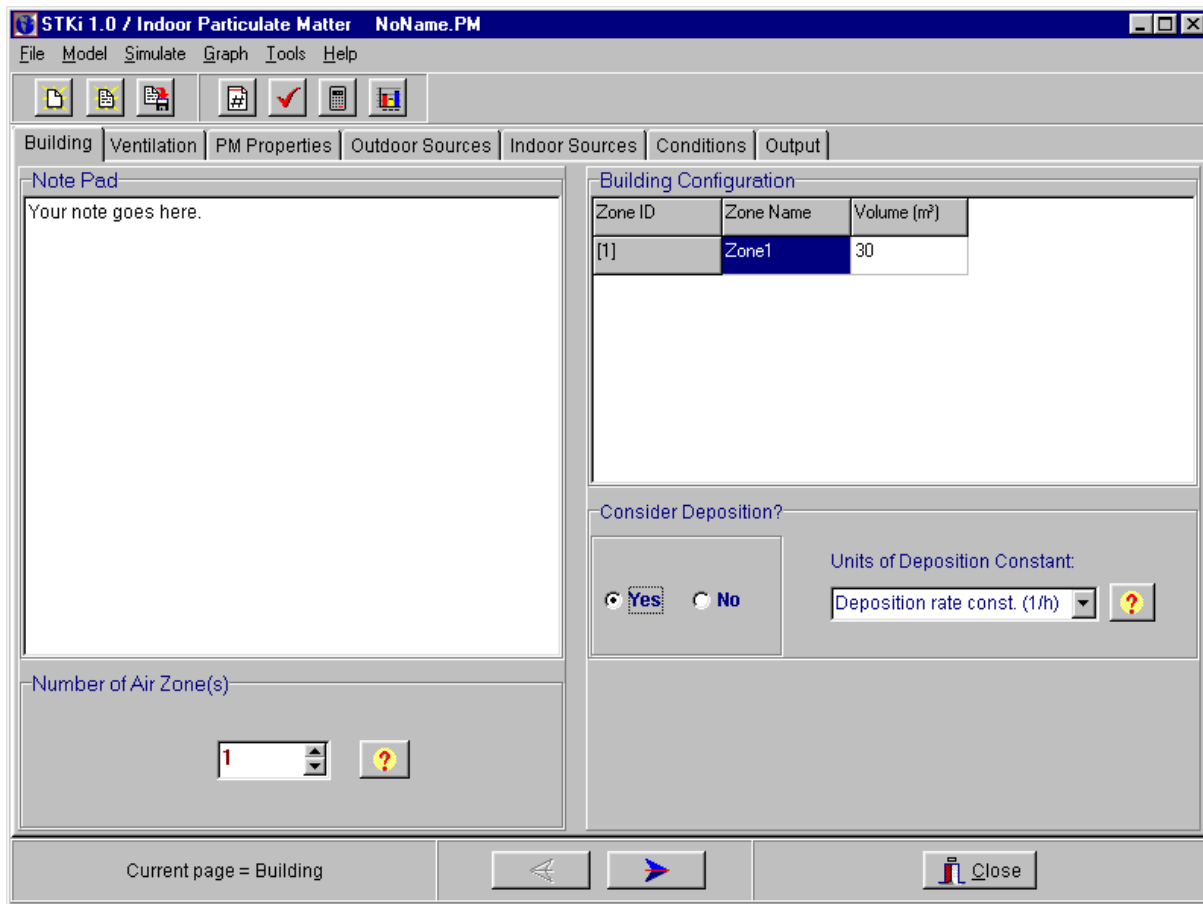


Figure 7.1 Layout of the Building page of the PM program. Note that the user has selected “Deposition rate const. (1/h)” for calculating deposition rate.

The first page of this program is slightly different from those in other special-purpose programs. First, unlike other special-purpose programs, this program allows the user to define an HVAC system in the Building Configuration table. This feature is necessary because air filters are most likely to be found in the HVAC system. Second, this program allows the user to define

three types of sink surfaces instead of two. Unlike gas-phase air pollutants, the PM deposition rate has to do with the orientation of the surfaces. For example, the surface types can be: floor, ceiling, and walls. The characteristic constant for PM deposition in the indoor environment is reported in the literature as either deposition velocity or deposition rate constant. This program accepts either description. See Section 7.3.3 for more details. There are three Help buttons in this page, two of which are shown in Figure 7.1 The third will appear when you select deposition velocity rather than deposition rate constant. Click on those buttons for more information about how to define the HVAC system, deposition rate, and sink types.

The Ventilation page is identical to those in VBX.EXE and SPILLEXE. You should have no problem entering ventilation parameters. The PM Properties page (Figure 7.2) is used to define the particle size groups and their deposition velocities or rate constants, depending on your selection in the Building page. Use the spin editor above the Help button to specify the number of PM size groups. The minimum value is 1 and the maximum 10. Give each size group a name that you understand (such as “PM10,” “PM2.5,” “2-5 μm,” and “<1”) and then enter the deposition velocity or rate constant for each size group.

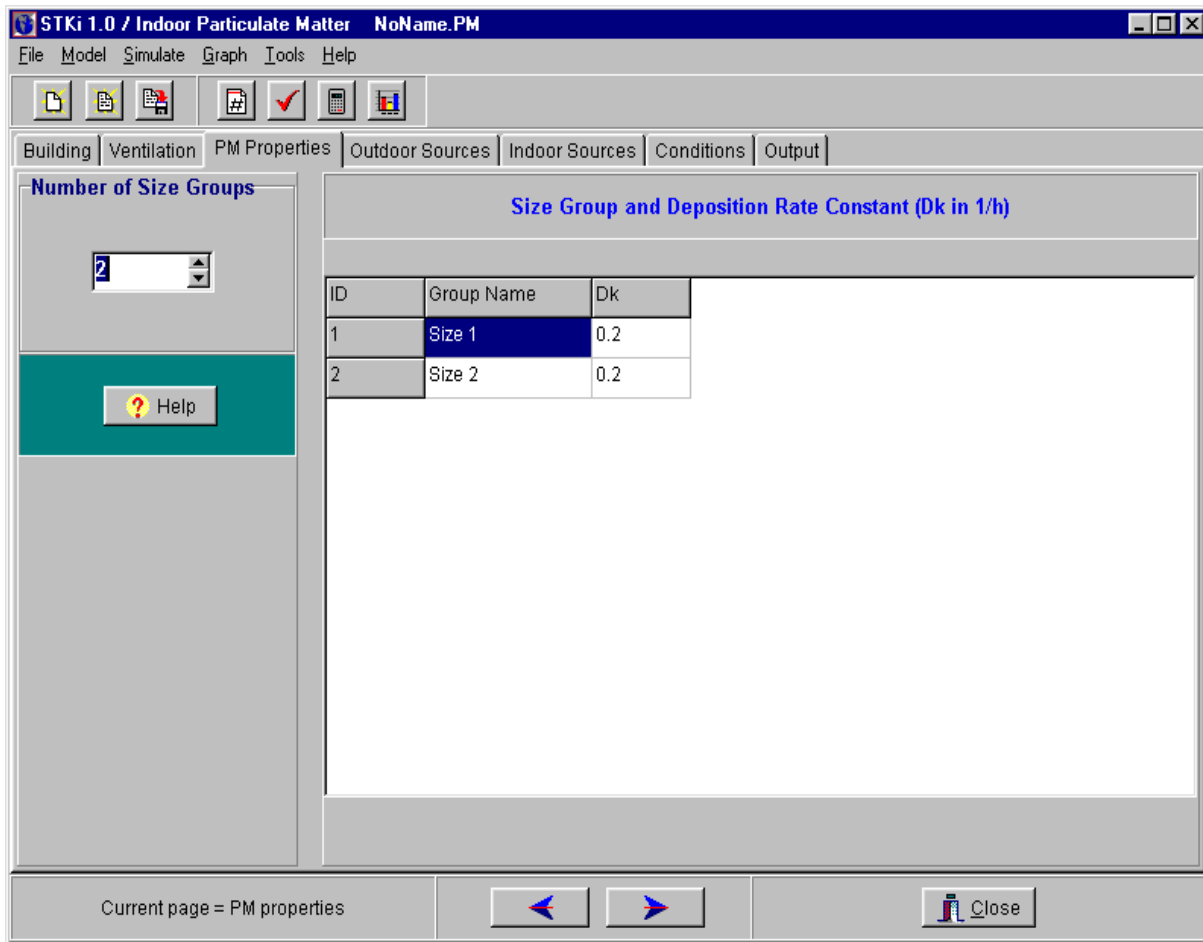


Figure 7.2 Layout of the PM Properties page of the PM program.

Penetration of the outdoor PM is defined in the Outdoor Sources page (Figure 7.3), where the user is asked to provide the following information:

- type of outdoor PM concentration data;
- infiltration factor; and
- outdoor PM concentrations.

The outdoor PM concentrations can be either constant or time-varying. A demonstration file called “ambient.pm” shows how to define the time-varying outdoor sources.

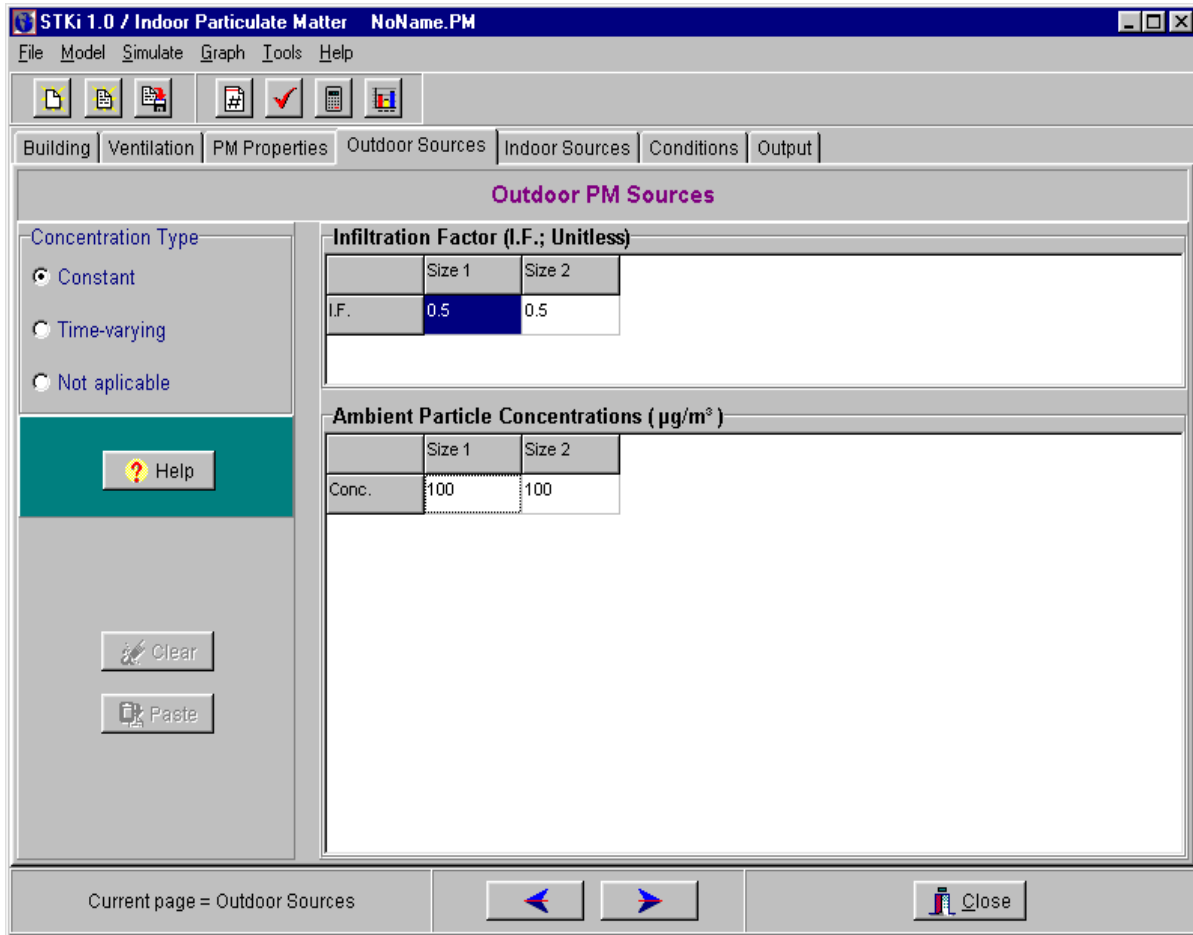


Figure 7.3 Layout of the Outdoor Sources page of the PM program.

In the Indoor Sources page (Figure 7.4), the user can define up to five indoor PM sources: the number is controlled by the spin editor near the top-left corner. If there is more than one source, you can navigate from one to another by clicking the tabs near the bottom (labeled “Source (1),” “Source (2),”...).

Parameters for each source are: (1) source location, (2) emission type, and (3) emission rate. Currently, you can choose from three emission types: constant, on/off, and time-varying. See Section 7.3.2 for more information about these emission types.

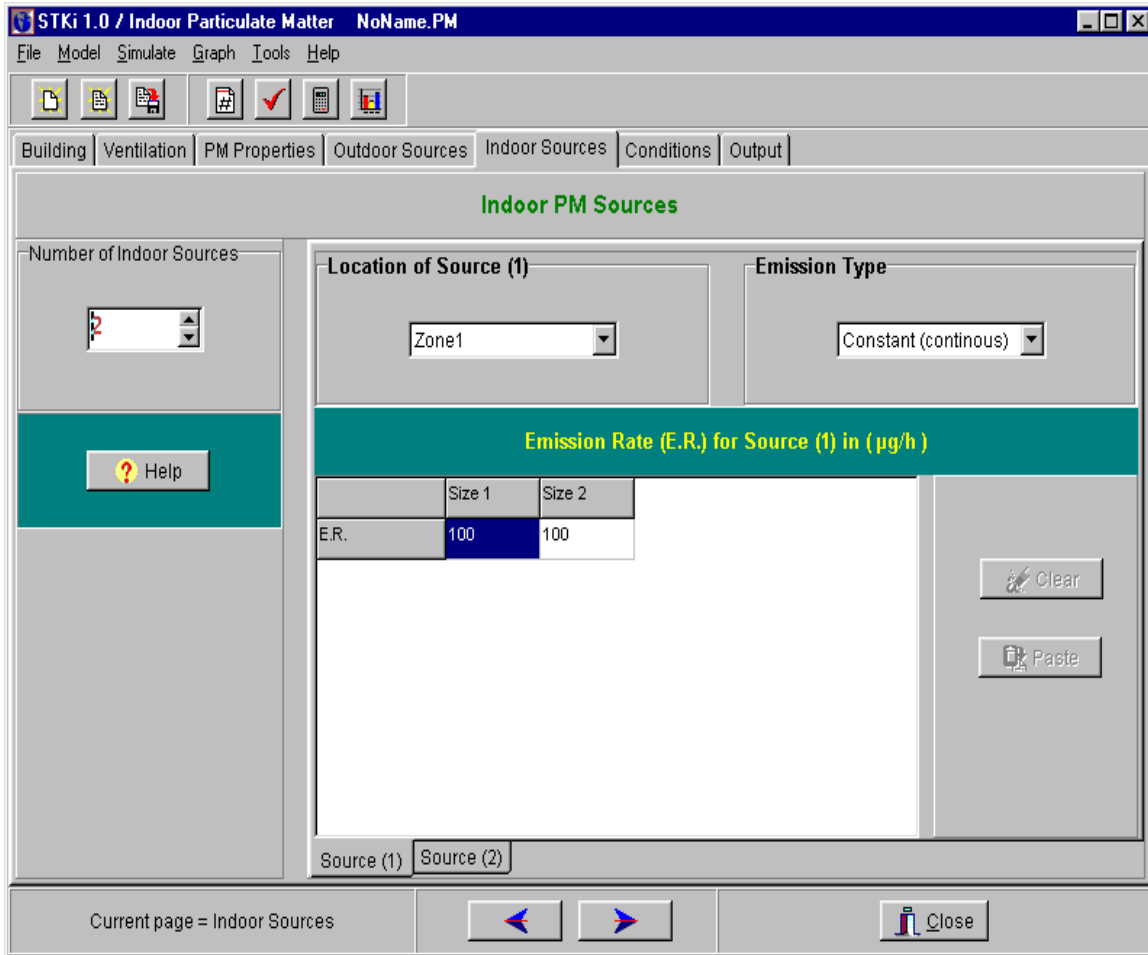


Figure 7.4 Layout of the Indoor Sources page of the PM program.

In the Conditions page (Figure 7.5), the user enters the simulation period, output data points, and non-zero initial concentrations. To define non-zero initial concentrations, click “Yes” in the selection box labeled “Are There Any Non-Zero Initial Concentrations?” and then enter the initial concentrations in the table below. The table for initial concentrations will become invisible if the user clicks “No” in the selection box. The default setting is “No.” After you finish entering all the parameters, compile and then run the model.



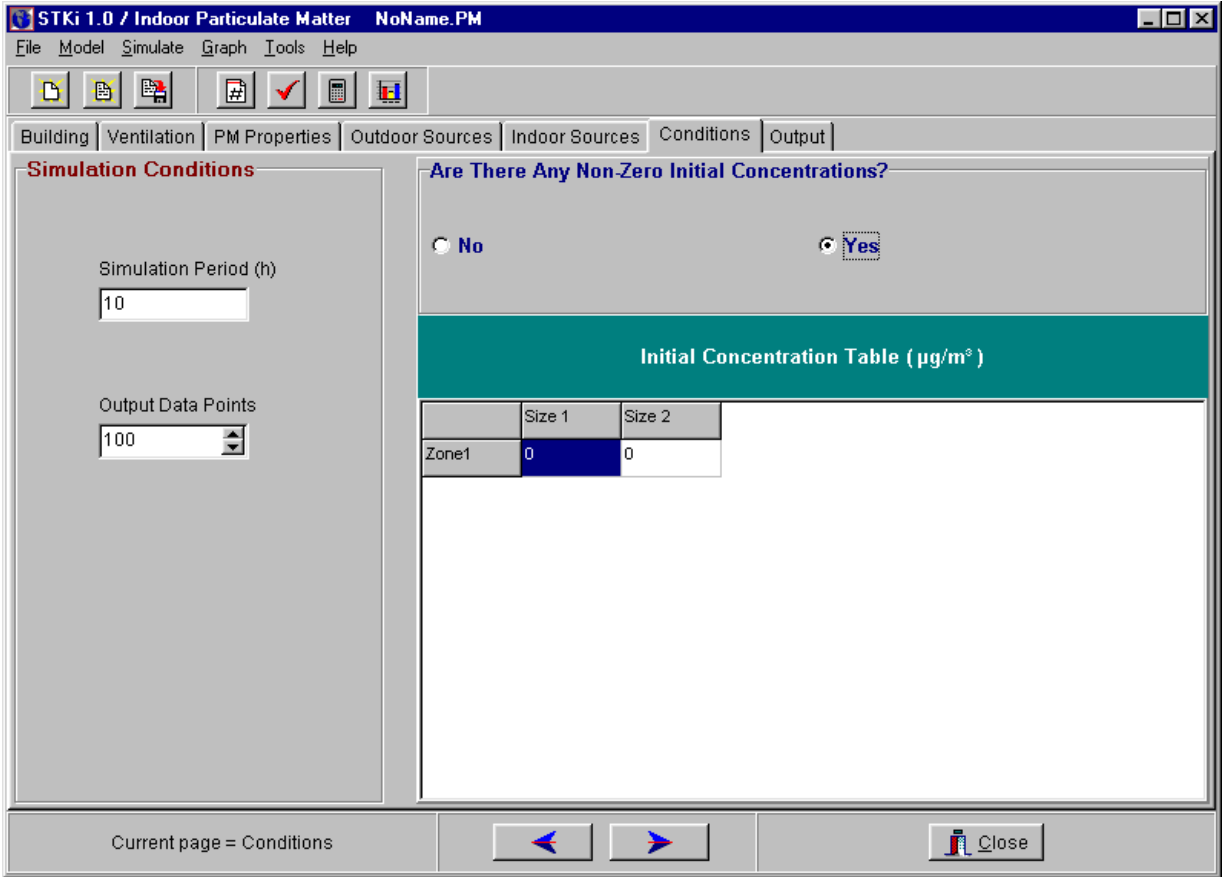


Figure 7.5 Layout of the Conditions page of the PM program.

### 7.3 More About the PM Program

#### 7.3.1 Calculation of PM Deposition Rate

The PM deposition rate is size dependent. The first-order deposition rate can be expressed in two ways:

$$R = C \sum_{i=1}^n (D_{v_i} S_i) \quad (7.2)$$

$$R = D_k V C \quad (7.3)$$

where  $R$  = deposition rate ( $\mu\text{g}/\text{h}$ );  
 $C$  = indoor concentration of PM in certain size ( $\mu\text{g}/\text{m}^3$ );  
 $D_{vi}$  = deposition velocity for surface  $i$  ( $\text{m}/\text{h}$ );  
 $S_i$  = area for surface  $i$  ( $\text{m}^2$ );  
 $n$  = number of surface materials;  
 $D_k$  = first-order deposition rate constant ( $\text{h}^{-1}$ ); and  
 $V$  = room volume ( $\text{m}^3$ ).

Since both  $D_{vi}$  and  $D_k$  can be found in the literature, this program allows the user to select either equation to compute the deposition rate. When you choose Eq. 7.2, you can specify more than one surface type in each zone. On the other hand,  $D_k$  in Eq. 7.3 is more of a lumped constant and the user does not need to know the surface areas. Conversion between the two constants is fairly straightforward:

$$D_k = \frac{\sum_{i=1}^n (D_{vi} S_i)}{V} \quad (7.4)$$

There are a number of theoretical models in the literature for estimating the PM deposition velocity in the indoor environment. An article by Lai and Nazaroff (2000) represents the most recent development in this research area at the time this Guide was prepared. This article contains a brief review of the previously published deposition models.

### 7.3.2 PM Source Types

In this program, the PM emission rate from an indoor source can be represented by three emission types: constant, on/off, and time-varying. For the constant type, the emission rate remains constant during the entire simulation period, and the emission rate for each size group is represented by a single value. The on/off type allows the user to define a source that is active only in a user-specified time period. Examples of such sources are cigarette smoking and carpet vacuuming. This source type requires the user to provide the source start time, end time, and the emission rates at the start and end times (Table 7.1). Note that the two emission rates do not have to be the same (see PM10 in Table 7.1). When the two values are different, the emission rate at any time during the active period is calculated by linear interpolation.

Table 7.1 An example data input for the on/off source type.  
(The user enters values in the unshaded area.)

Time (h)	PM2.5	PM10
2.0	25000	80000
2.5	25000	120000

When the time-varying source type is selected, the user needs to provide a data table such as the one shown in Table 7.2. Up to 1000 rows of data are allowed. If the emissions data are stored in a spreadsheet, you can use the Windows clipboard to copy and paste the data from the spreadsheet by clicking the Paste button.

Table 7.2 An example data input for the time-varying source type.  
(The user enters values in the unshaded area.)

Time (h)	PM2.5	PM10
0	55000	150000
1	25000	80000
2.5	20000	65000
5	20000	65000
10	1200	6700

### 7.3.3 Adding Pages

There are three hidden pages in this program. You need them to define PM filters. To add pages, click on the Add Page speed button (i.e., the one with a red pound sign) or select Model/Add page from the main menu.

### 7.3.4 HVAC Filters, Interzone Filters, and Free-Standing Filters

For convenience, this program lists all filters in three groups: HVAC filters, interzone filters, and free-standing filters ( Figure 7.6 ). The HVAC filters are in-line and are considered part of the HVAC system. The interzone filters treat the air flow between two zones, one of which can be the HVAC system. Examples of this type of filter are those located in air registers. Interzone filters can also be used to represent the PM removal process between two zones due to

restricted air passage (such as a door seam or windows). Free-standing filters are self-explanatory and require the user to specify the passing air flow rate.

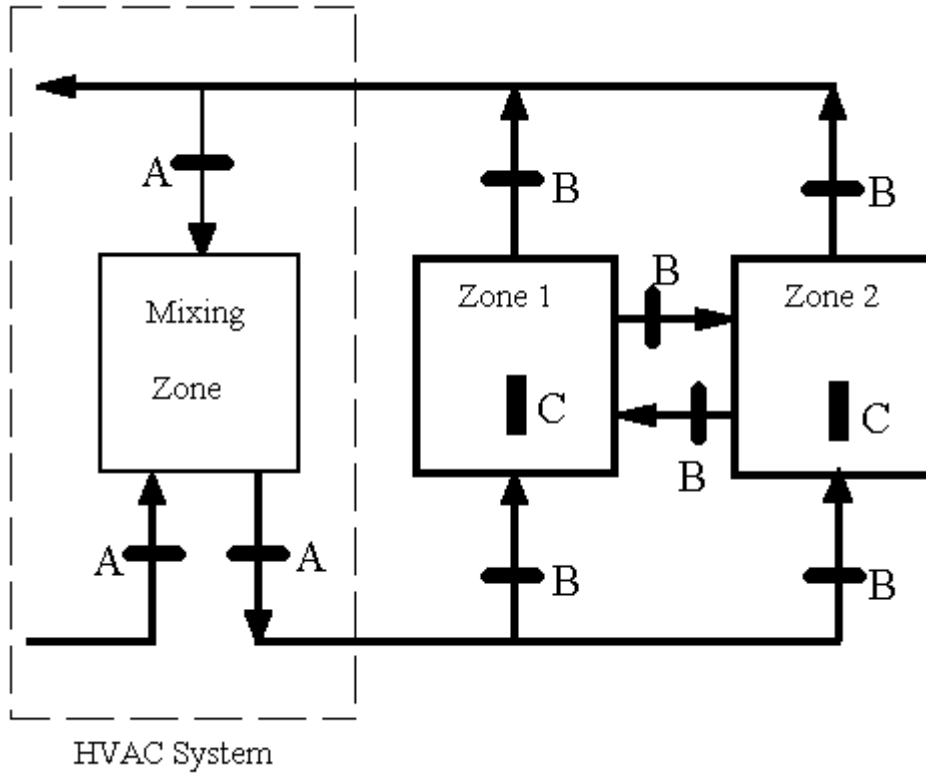


Figure 7.6 Possible filter positions in three-zone (zone 1, zone 2, and HVAC) configuration. A = HVAC filter, B = interzone filter, and C = free-standing filter.

## **CHAPTER EIGHT INSIDE IAQX**

### **8.1 Programming Language**

All the programs in IAQX version 1.0 are written in Delphi 5 (Professional Edition), a Microsoft Windows-based Object Pascal compiler developed by Inprise Corporation, 100 Enterprise Way, Scotts Valley, CA 95066-3249, U.S.A.

### **8.2 Method for Numeric Integration**

Except for SLAB.EXE which does not require an integration algorithm, all other IAQX programs use a fourth-order/fifth-order Runge-Kutta-Fehlberg method (Cheney and Kincaid, 1980) to integrate the system of differential equations that represents the IAQ model. The method makes six function evaluations at each step and computes simultaneously a fourth- and a fifth-order approximation, from which an error estimation is made and the step size adjusted. Computer implementation of this method was originally developed in Fortran by Watts and Shampine (Forsythe, et al., 1977). This algorithm is fairly effective and does a reasonable job for non-stiff and moderately stiff systems, but can not handle very stiff situations. The developer made several minor changes to the code to improve its stability. The local error control was set to  $5 \times 10^{-6}$  (relative error).

### **8.3 Algorithm for Application-Phase Simulation**

Indoor sources with large areas and decaying emission rates, such as newly painted walls, require special treatment to estimate the emission rate during the application period because the source area is changing. This is sometimes called application-phase simulation. The algorithm used in IAQX is based on a method reported by Zeh, et al. (1994). Since the authors did not provide any proof of the validity of the method, brief derivations are given below.

The most commonly used model for decaying sources is the first-order decay model. Eq. 8.1 (Clausen, 1993) is one of its forms:

$$R = S M_0 k e^{-kt} \quad (8.1)$$

where  $R$  = emission rate ( $\text{mg}/\text{m}^3$ );  
 $S$  = source area ( $\text{m}^2$ );  
 $M_0$  = amount of pollutant applied to a unit area of surface ( $\text{mg}/\text{m}^2$ );  
 $k$  = first-order decay rate constant ( $\text{h}^{-1}$ ); and

$t$  = elapsed time (h).

Eq. 8.1 can be rewritten as:

$$R = S M k = k W \quad (8.2)$$

where  $M = M_0 e^{-kt}$  is the amount of pollutant remaining in a unit area at time  $t$  (mg/m<sup>2</sup>); and  
 $W = S M$  is the total amount of pollutant remaining in the source (mg).

If we divide a large source into  $n$  small increments, then the total emission rate at any time can be expressed as:

$$R_T = k \sum_{i=1}^m W_i = k W_T \quad (8.3)$$

where  $R_T$  = the total emission rate for the source (mg/h);  
 $m$  = number of incremental areas;  $m < n$  during the application and  $m = n$  after the application;  
 $W_i$  = amount of pollutant remaining in increment  $i$  (mg); and  
 $W_T$  = total amount of pollutant remaining in the source (mg).

Thus, in order to compute the total emission rate, one needs to keep tracking the total amount of pollutant remaining in the source ( $W_T$ ):

$$\frac{dW_T}{dt} = \frac{W_0}{t_A} - k W_T \quad (\text{if } t > t_A) \quad (8.4)$$

$$\frac{dW_T}{dt} = -k W_T \quad (\text{if } t > t_A) \quad (8.5)$$

where  $W_0$  = total amount of the pollutant in the coating material to be applied (mg); and  
 $t_A$  = duration of the application phase (h).

IAQX adds Eqs. 8.4 and 8.5 to the system of differential equations when the user chooses to include the application-phase simulation.

## 8.4 Algorithm for Estimating Adequate Ventilation Rate (AVR)

Mathematically, this task is similar to the root-trapping process for a non-linear equation, which involves solving the equation iteratively with different values of the independent variable until a certain tolerance is met. However, this method requires many iterations and is too time-consuming for a system of differential equations. IAQX minimizes the number of simulations by using the third-order Lagrange interpolation.

The user input includes: (1) selection of an air quality criterion, which can be peak concentration, time-averaged concentration, or cumulative inhalation exposure; (2) a search range for the ventilation rate, defined by the minimum value  $N_{\min}$  and the maximum value  $N_{\max}$  (the default values are 0.1 to 20 air exchanges per hour); and (3) a tolerance level (the default value is 5%). IAQX then performs two simulations at  $N_{\min}$  and  $N_{\max}$ , respectively, followed by two more simulations at air exchange rates between  $N_{\min}$  and  $N_{\max}$ . Using the four data points, a third-degree polynomial can be established between the ventilation rate and the indoor pollution level:

$$\ln N = a + b C_R + c C_R^2 + d C_R^3 \quad (8.6)$$

where  $N$  = trial ventilation rate ( $\text{h}^{-1}$ ); and

$C_R$  = an indicator of indoor air pollution level (e.g., the peak concentration).

The barycentric form of Lagrange interpolation (Pizer and Wallace, 1983) was used to estimate coefficients  $a$ ,  $b$ ,  $c$ , and  $d$  in Eq. 8.6. Substituting the desired level of  $C_R$  into Eq. 8.6 provides an estimate of AVR (i.e.,  $N$  in Eq. 8.6). A fifth simulation is then performed at the estimated AVR to check if the tolerance level is met. If not, the new data point ( $C_R$ ,  $N$ ) is inserted into the data array, and the coefficients in Eq. 8.6 are recalculated. This checking process is repeated until the tolerance is met. With this method, six simulations are usually required to find the AVR at the tolerance level of 5%.

## 8.5 Handling of Time-varying Parameters

Time-varying parameters are those given as a data table. Examples are the time-varying ventilation rate, ambient air as a time-varying pollutant source, and time-varying indoor sources. If the data points are  $(t_1, x_1)$ ,  $(t_2, x_2)$ , ...  $(t_n, x_n)$ , IAQX calculates the value for  $x$  and any time  $t$  during the simulation by means of linear interpolation. Eqs. 8.7 to 8.9 represent the actual algorithm used.

$$x = 0 \quad \text{if } t < t_1 \quad \text{or} \quad t > t_n \quad (8.7)$$

$$x = x_i \quad \text{if } t = t_i \quad (8.8)$$

$$x = x_i + \frac{(x_{i+1} - x_i)(t - t_i)}{t_{i+1} - t_i} \quad \text{if } t_i \leq t \leq t_{i+1} \quad (8.9)$$



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16. ABSTRACT The User's Guide describes a Microsoft Windows-based indoor air quality (IAQ) simulation software package designed Simulation Tool Kit for Indoor Air Quality and Inhalation Exposure, or IAQX for short. This software complements and supplements existing IAQ simulation programs and is designed mainly for advanced users. The package consists of a general-purpose simulation program and four stand-alone, special-purpose simulation programs. The general-purpose program performs multizone, multipollutant simulations and allows gas-phase chemical reactions. The special-purpose programs implement fundamentally based models, which are often excluded in existing IAQ simulation programs. In addition to performing conventional IAQ simulations, which compute the time-concentration profile and inhalation exposure, IAQX can estimate the adequate ventilation rate when certain air quality criteria are provided by the user, a unique feature useful for product stewardship and risk management. IAQX will be developed in a cumulative manner, and more special-purpose simulation programs will be added to the package in the future.		
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