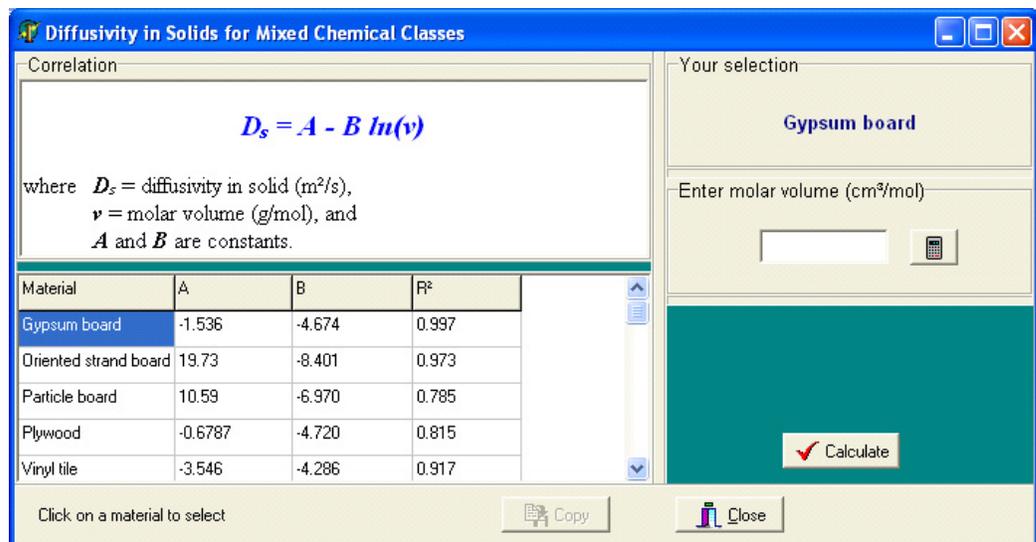United States
Environmental Protection
Agency

Program PARAMS User's Guide
Program Version: 1.0
Document Version: 1.0

Diffusivity in Solids for Mixed Chemical Classes

Correlation

$$D_s = A - B\ ln(v)$$

where D_s = diffusivity in solid (m²/s),
v = molar volume (g/mol), and
A and B are constants.

Material	A	B	R²
Gypsum board	-1.536	-4.674	0.997
Oriented strand board	19.73	-8.401	0.973
Particle board	10.59	-6.970	0.785
Plywood	-0.6787	-4.720	0.815
Vinyl tile	-3.546	-4.286	0.917

Click on a material to select

Your selection

Gypsum board

Enter molar volume (cm³/mol)

✓ Calculate

Copy   Close

Program PARAMS
User's Guide
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Document Version: 1.0

by

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Abstract

This Microsoft Windows-based computer program implements 30 methods for estimating the parameters in indoor emissions source models, which are an essential component of indoor air quality (IAQ) and exposure models. These methods fall into eight categories: (1) the properties of indoor air, (2) the first-order decay rate constants for solvent emissions from indoor coating materials, (3) gas-phase, liquid-phase, and overall mass transfer coefficients, (4) molar volume, (5) molecular diffusivity in air, liquid, and solid materials, (6) solid-air partition coefficient, (7) vapor pressure and volatility for pure organic compounds and petroleum-based solvents, and (8) the properties of water. Potential users include those who develop or use IAQ and exposure models and those who develop or use quantitative structure-activity relationship (QSAR) models. In addition, many calculations are useful to researchers in areas other than indoor air quality. Users can benefit from this program in two ways: first, it serves as a handy tool by putting commonly used parameter estimation methods in one place; second, it saves users time by taking over tedious calculations. It should be pointed out, however, that the methods implemented in this program cover only a fraction of the parameters that appear in the more than 50 indoor emission source models. Furthermore, the methods in the current version are mostly for gaseous pollutants; those for particulate matter are not included.

Foreword

The U.S. Environmental Protection Agency (EPA) is charged by Congress with protecting the Nation's land, air, and water resources. Under a mandate of national environmental laws, the Agency strives to formulate and implement actions leading to a compatible balance between human activities and the ability of natural systems to support and nurture life. To meet this mandate, EPA's research program is providing data and technical support for solving environmental problems today and building a science knowledge base necessary to manage our ecological resources wisely, understand how pollutants affect our health, and prevent or reduce environmental risks in the future.

The National Risk Management Research Laboratory (NRMRL) is the Agency's center for investigation of technological and management approaches for preventing and reducing risks from pollution that threaten human health and the environment. The focus of the Laboratory's research program is on methods and their cost-effectiveness for prevention and control of pollution to air, land, water, and subsurface resources; protection of water quality in public water systems; remediation of contaminated sites, sediments and ground water; prevention and control of indoor air pollution; and restoration of ecosystems. NRMRL collaborates with both public and private sector partners to foster technologies that reduce the cost of compliance and to anticipate emerging problems. NRMRL's research provides solutions to environmental problems by: developing and promoting technologies that protect and improve the environment; advancing scientific and engineering information to support regulatory and policy decisions; and providing the technical support and information transfer to ensure implementation of environmental regulations and strategies at the national, state, and community levels.

This publication has been produced as part of the Laboratory's strategic long-term research plan. It is published and made available by EPA's Office of Research and Development to assist the user community and to link researchers with their clients.

Sally Gutierrez, Acting Director
National Risk Management Research Laboratory

EPA Review Notice

This report has been peer and administratively reviewed by the U.S. Environmental Protection Agency and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

This document is available to the public through the National Technical Information Service, Springfield, Virginia 22161.

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1. Introduction

1.1 Purpose and Intended Users

Although over 50 indoor emission source models have been developed (Guo, 2002a), few are widely used in indoor exposure assessment. This imbalance is partially caused by the fact that many source models contain one or more parameters that are difficult to determine. This program is a step toward alleviating this problem by providing 30 methods for estimating some of the parameters in those source models. It is useful to those who develop or use indoor air quality (IAQ) and exposure models, and those who develop or use quantitative structure-activity relationship (QSAR) models. In addition, many methods in this program are useful to researchers in areas other than indoor air quality. Users can benefit from this program in two ways: (1) it serves as a handy tool by putting commonly used methods in one place, and (2) it saves users' time by taking over tedious calculations.

This program was developed based on the developer's review of existing parameter estimation methods for indoor emission source models (Guo, 2002b). Users are encouraged to read the review article for more detailed discussions and, more importantly, to consult with the original references.

The name of this program, PARAMS, is an abbreviation of parameters.

1.2 Limitations

Overall, development of parameter estimation methods has not progressed to the extent that IAQ modelers would like to see. Users are reminded that the number of parameters that can be estimated with this program is only a fraction of the total number of parameters in the existing indoor source models.

This program is intended to supplement, not to substitute for, experimentally determined model parameters. In other words, this program is most useful when experimentally determined values are not available.

Most methods implemented in this program are for gaseous pollutants. Methods for particulate matter are not included in the current version.

1.3 Parameter Estimation Methods Implemented

The methods implemented in this program are summarized in Table 1. Detailed discussions on each method is provided in Section 4. The References section gives a complete list of sources of these methods.

Table 1. List of Parameter Estimation Methods in PARAMS.

Method Group	Subgroup	No. of methods
	Density	1
Air properties	Moisture content	1
	Viscosity	1
	Petroleum-based paint	4
First-order decay rate constant	Latex paint	2
	Gas-phase	3
Mass transfer coefficient	Liquid-phase	2
	Overall	2
Molar volume	N/A	2
	Gas-phase	3
Molecular diffusivity	Liquid-phase	1
	Solid-phase	2
Solid-air partition coefficient	N/A	2
Volatility	N/A	2
	Vapor pressure	1
Water properties	Viscosity	1
Total		30

2. Installation and Technical Support

2.1 Minimum System Requirements
- Intel Pentium 90 or equivalent,
- Microsoft Windows 95 or later (see Section 2.4 for details),
- 16 Mb of RAM,
- 10 Mb free hard disk space,
- CD-ROM drive (for installation from CD),
- Software WinZip (for installation from zip file),
- Software Acrobat Reader 4.0 or later (for printing the User's Guide),
- VGA or higher resolution monitor, and
- Mouse or other pointing devices.

2.2 Installing PARAMS from Compact Disk
- Insert the program CD;
- If the installation program does not start automatically, use Windows Explorer to find the CD-ROM drive, then click on file Setup.EXE; and
- Follow instructions to complete installation.

2.3 Installing PARAMS from Zip File
- If you received the zip file as an e-mail at-tachment, save the file (PARAMS.txt) to a temporary folder in your hard drive;
- Rename the file PARAMS.zip;
- Unzip (i.e., extract) the zip file with WinZip and run program Setup.EXE;
- Follow the instructions to complete installa-tion; and
- Delete installation files.

2.4 Installation Problems
This program has been tested for installation errors for Microsoft Windows 95, 98, 2000, ME, and XP Professional. It is not guaranteed that it will work under other versions of Windows. An independent quality assurance (QA) review revealed that this program could not be installed to Windows PC Home Edition.

Also note that, if your computer has Windows XP Professional and is connected to a network, you may receive an error message similar to the one shown in Figure 1. It means that you are not authorized to install any software on your computer, and you must ask a computer support technician to install the software for you.
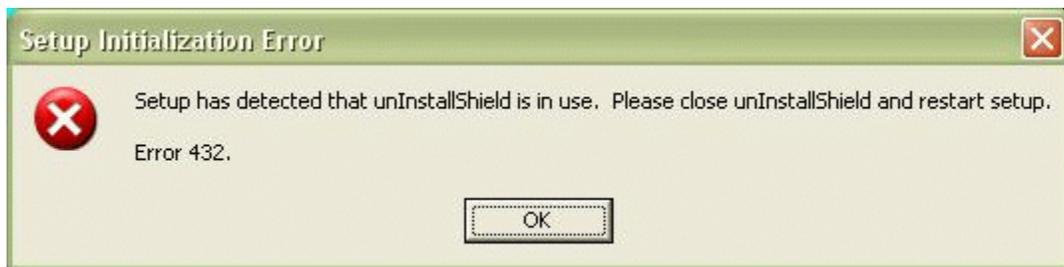
Figure 1. Error Message Encountered When Trying to Install PARAMS to a Network Computer with Security Restrictions.

2.5 Viewing and Printing the User's Guide

The User's Guide is provided in pdf file format, and requires Adobe Acrobat Reader (version 4 or higher) to read. There are two ways to access the document:

From Windows Start menu:

- Find the group name for program PARAMS by clicking on <Start>, <All Programs>,
- Click on the group name (The default name is "Params 1.0"),
- Click on "PARAMS Users Guide".

From the program CD:

- Place the program CD in the CD-ROM drive,
- Use the Windows Explorer to open folder \Manual,
- Double click on filename "PARAMS Users Guide.pdf".

2.6 Technical Support

For bug reporting, questions, comments, or suggestions, please contact the developer at the following address:

Dr. Zhishi Guo
U.S. EPA
Mail Code E305-03
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E-mail: guo.zhishi@epa.gov
Telephone: 919-541-0185
Fax: 919-541-2157

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3. A Brief Tour of the Program

3.1 User Interface

To start the program, choose Start Q> Programs Q> Params 1.0 Q> Params. This program has a fairly simple user interface. Figure 2 shows the main screen after the user launches the program under Windows XP. Note that, for other Windows operating systems, the appearance of the start screen may be slightly different. As shown in Figure 2, all the methods are organized in a tree list, very similar to the file list in Windows Explorer. To view more details in the list, simply click one of the plus (+) signs. There are two small buttons under the tree list. Clicking the one on the left (with an open book icon) makes the tree list fully expand; clicking the one on the right (with a closed book icon) makes the list collapse.

To select a parameter estimation method, click on one of the items in the tree list. The method selected will appear in the upper-right pane (Figure 3). The next step is to click the <Go> button to perform the calculation. Two examples are provided below.

3.2 Example 1: Calculating the density of air at 23 °C, 1 atm, and 65% RH

Move cursor to the tree list; click on the plus(+) sign in front of "Air properties" or double-click on "Air properties"; then click on "density." After the item you selected appears on the screen at the upper-right
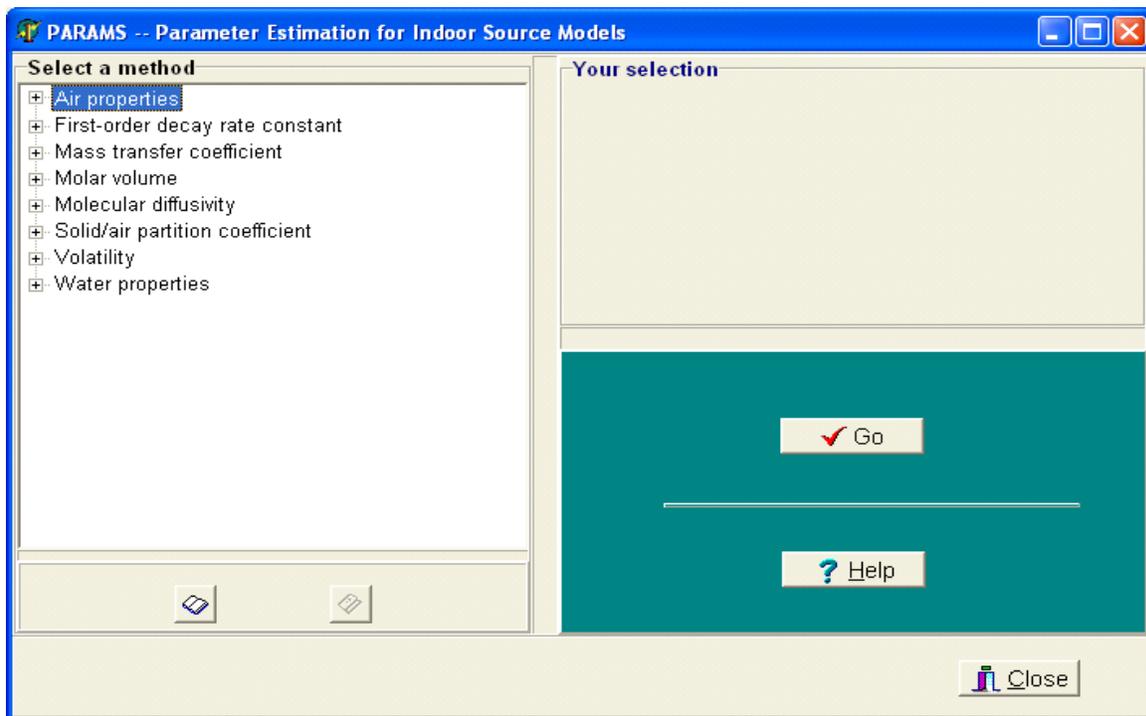
Figure 2. Layout of PARAMS' Main Screen, No Selected Method.
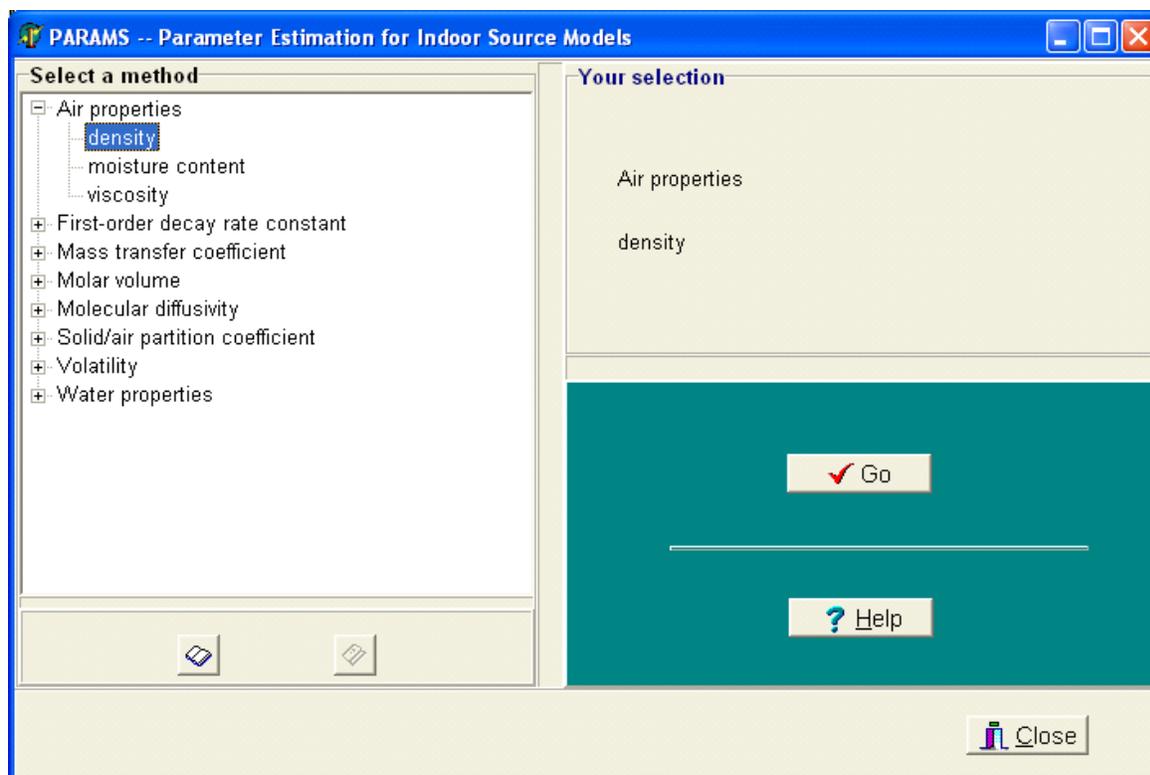
Figure 3. Layout of the Main Window after the Method for Air Density Is Selected.

corner (see Figure 3), click on the <Go> button to open the calculation sheet. Note that PARAMS can compute the density for either dry or wet air, and that the default setting is for dry air. To switch to moist air, select "moist air" from below the temperature entry box. Change the temperature to 23; adjust the RH value to 65; and, finally, click the <Calculate> button. The result should be 0.0011843 g/cm³ (See Figure 4). If you would like to use the result in a different application (such as a spreadsheet), click the <Copy> button to copy the result to Windows clipboard. You can latter paste the result to the application. Use of the <Paste & Exit> button, which is dimmed in Figure 4, will be explained in the next example.

3.3 Example 2: Calculating the Gas-Phase Mass Transfer Coefficient for n-Decane ($C_{10}H_{22}$) at 23 °C and 50% RH from Sherwood Number

From the tree list, select "Mass transfer coefficient"

-> "gas phase" -> "from Sherwood number;" click the <Go> button to display the calculation screen (Figure 5).

This method requires five parameters: (1) density of air, (2) viscosity of air, (3) velocity of air in the room, (4) diffusivity of the compound in room air, and (5) characteristic length of the source. If you know all of their values, you can enter them manually. You can also use the built-in calculators for air density and viscosity and for diffusivity of the compound. In other words, you can calculate these values without leaving the program.

To calculate the density of air, click the calculator button next to the entry box; the calculation screen for air density will appear (see Figure 4); enter or adjust the required parameters; click the <Calculate> button; then click the <Paste & Exit> button to paste the result to the calculation screen for the gas-phase mass transfer coefficient.

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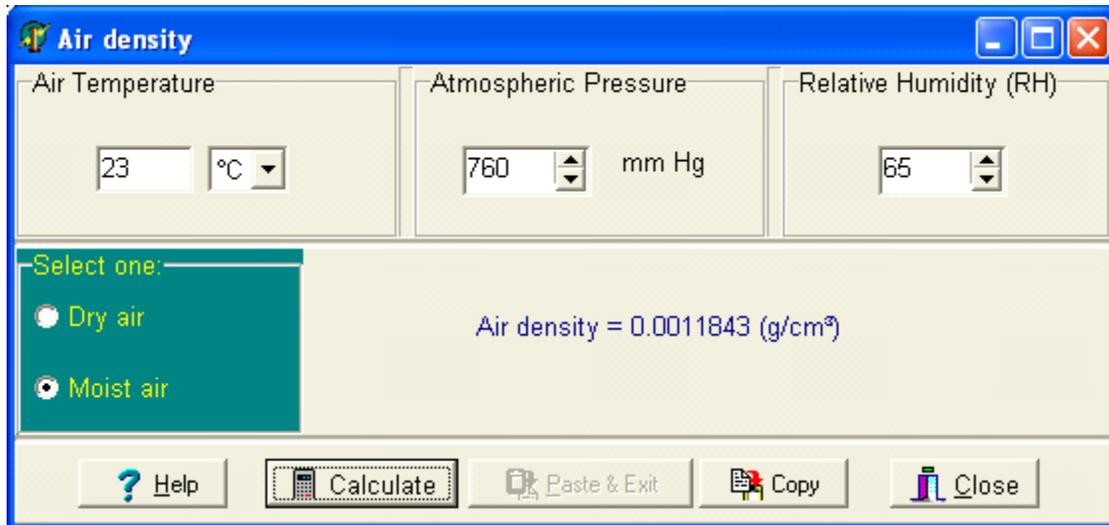
Figure 4. Calculation Screen for Air Density.
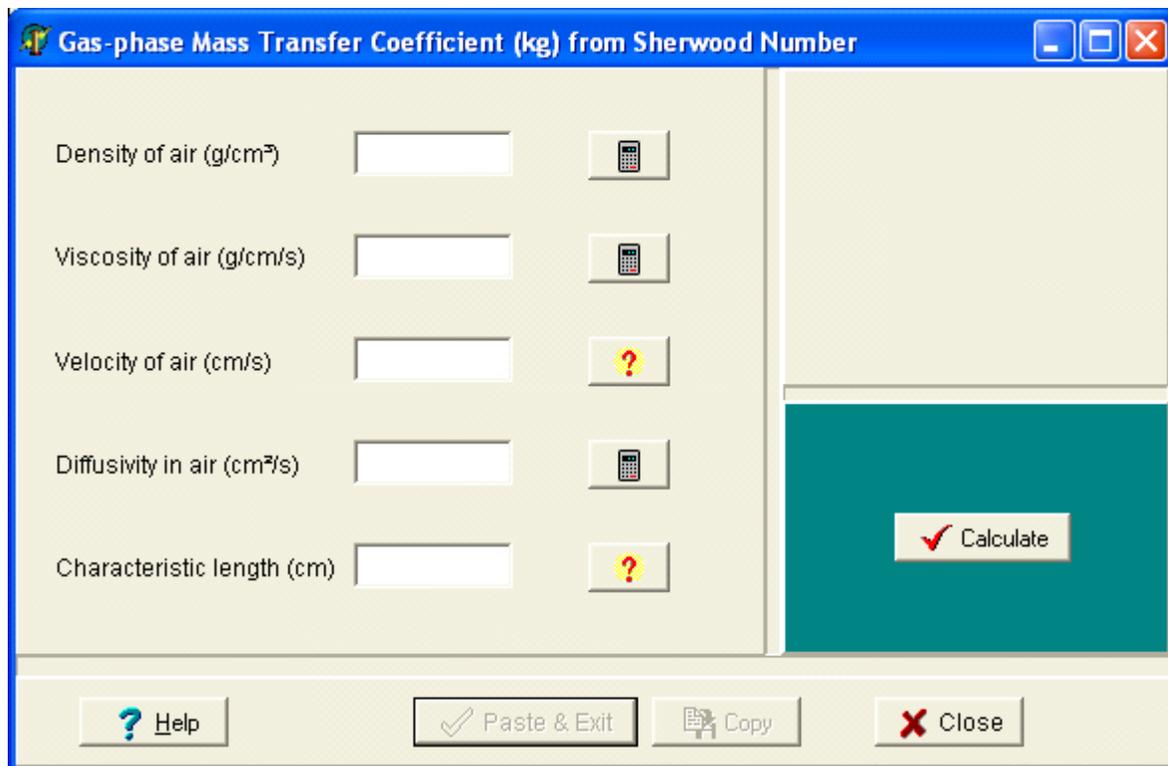
Figure 5. Calculation Screen for Gas-Phase Mass Transfer Coefficient Based on Sherwood Number. The Arrow Points to the Built-in Calculator for Air Density.

Similarly, you can calculate the viscosity of air by clicking on the second calculator button.

Air velocity inside a room varies from case to case. For this exercise, enter 5. For hints, click the button with a question mark. It will tell you that the typical range air velocity in the indoor environments is from 5 to 10 cm/s.

To calculate the diffusivity of n-decane in air, click the calculator button next to the entry box for diffusivity; the program will ask you to select one from three available methods. If you are unfamiliar with these methods, click on the <Help> button. For this practice, select FSG method 1. In the calculation screen for diffusivity in air, enter the molecular formula for n-decane by changing the carbon number to 10 and hydrogen number to 22; click the <Calculate> button; then click the <Paste & exit> button (Figure 6).

Characteristic length is a measure of source size. For this exercise, enter 20. Note that hints are available for this input parameter.

Finally click the <Calculate> button to get the result.
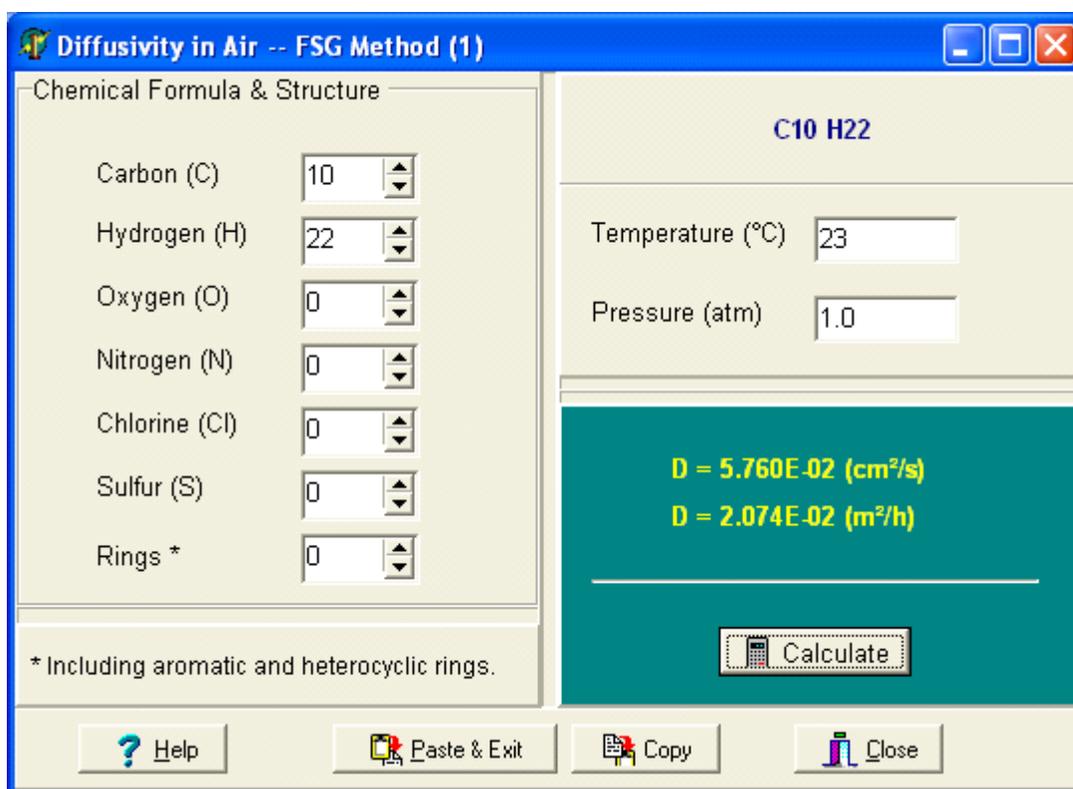
Figure 6. Calculation Screen for Diffusivity in Air (FSG Method 1).

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4. Method Descriptions

4.1 Properties of Air

The properties of air calculated by this program are density, moisture content, and viscosity.

4.1.1 Density of Dry and Moist Air

The density of dry or moist air is calculated from Equations. 1 and 2 (Weast, 1973, page F-9), respectively.

$$d_{dry} = d_0 \frac{T_0}{T} \frac{P}{P_0} \tag{1}$$

$$d_{moist} = d_0 \frac{T_0}{T} \frac{P - 0.3783 \, p_w}{P_0} \tag{2}$$

where d_{dry} = density of dry air at temperature T and pressure P, in grams per cubic meter,

d_{moist} = density of moist air at temperature T and pressure P, in grams per cubic meter,

d_0 = density of dry air at temperature T_0 and pressure P_0, in grams per cubic meter,

T_0 = standard temperature = 273.2 K,

T = temperature of air in Kelvin,

P_0 = standard atmospheric pressure = 760 mm Hg,

P = atmospheric pressure in millimeters mercury (Hg), and

p_w = partial pressure of moisture in air in millimeters Hg.

In this program, d_0 = 0.0012929 g/cm³ at 0 °C and 760 mmHg is from Weast (1973, page F-9).

The user input for moisture content is in relative humidity, which is then converted to partial pressure (millimeters Hg) by using Equation 3.

$$p_w = \frac{RH}{100} \times P_{w0} \tag{3}$$

where RH = relative humidity, and
P_{w0} = water vapor pressure at given temperature in millimeters Hg.

The method used to estimate the water vapor pressure (P_{w0}) is described in Section 4.8.1. The calculation screen is shown in Figure 4 in the previous section.

4.1.2 Moisture Content in Air

This program computes the moisture content in room air—either saturated or unsaturated—in parts per million and grams per cubic meter. Information required from the user includes room temperature, atmospheric pressure, and for unsaturated air, relative humidity. Figure 7 shows the calculation screen.

Calculation of moisture content in air involves three steps:

Step 1: Calculating water vapor pressure by using Equation 44 in Section 4.8.1;

Step 2: Calculating the partial pressure by using Equation 3;

Step 3: Converting partial pressure to concentration units by Equations 4 and 5.

$$C_{w1} = 10^6 \, P_w / P_0 \tag{4}$$

where C_{w1} = water content in air in parts per million,
P_0 = atmospheric pressure in millimeters Hg.

$$C_{w2} = 10^{-3} \, C_{w1} \, M_w / v_T \tag{5}$$

where Cw_2 is in grams per cubic meter,
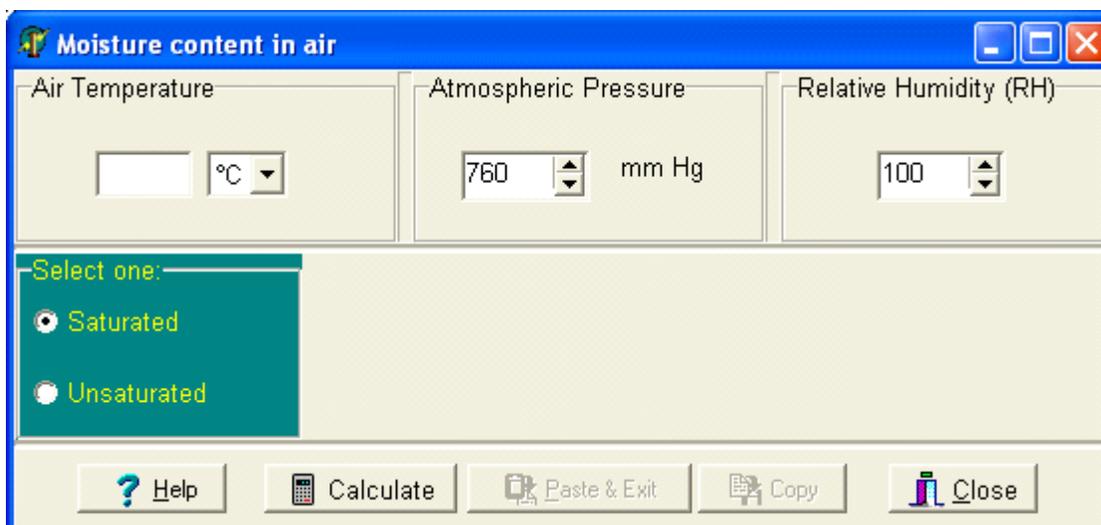
Figure 7. Calculation Screen for Moisture Content in Air.

M_w = molecular weight for water in grams per mole,

v_T = molar volume of gas at temperature T in liters.

4.1.3 Viscosity of Air

This program calculates the absolute viscosity of air between 0 and 74 °C by using experimental data found in the literature. Figure 8 shows the calculation screen, and Table 2 the viscosity data.

Table 2. Absolute Viscosity of Air from the Literature[a]

Temperature (°C)	Viscosity	
	(μPoise)	(g/s/cm)
0	170.8	1.708×10^{-4}
18	182.7	1.827×10^{-4}
40	190.4	1.904×10^{-4}
54	195.8	1.958×10^{-4}
74	210.2	2.102×10^{-4}

[a] Source: Weast, 1973; page F-43.

A third-order polynomial (Equation 6) is used to calculate the viscosity at any temperature between 0 and 74 °C under the standard atmospheric pressure. The coefficients in Equation 6 were determined by least square with $r^2 = 0.999999998$, where r is the correlation coefficient.

$$\mu = 170.80 + 0.915439\,T - 0.0170441\,T^2 + 1.60383 \times 10^{-4}\,T^3 \tag{6}$$

where μ = absolute viscosity in microPoise (1 Poise = 1 gram per centimeters per second), and

T = temperature in degrees Celsius.

Note that some indoor source models require kinematic viscosity, which is the ratio of the absolute viscosity and air density. Kinematic viscosity has the unit of Stokes or, equivalently, square centimeters per second.

4.2 First-Order Decay Rate Constant for Emissions from Paint

The software contains methods for calculating the first-order decay rate constant for both latex and petroleum-based paints. The decay rate constant for petroleum-based paint can be calculated by four methods.

Figure 8. Calculation Screen for Air Viscosity.
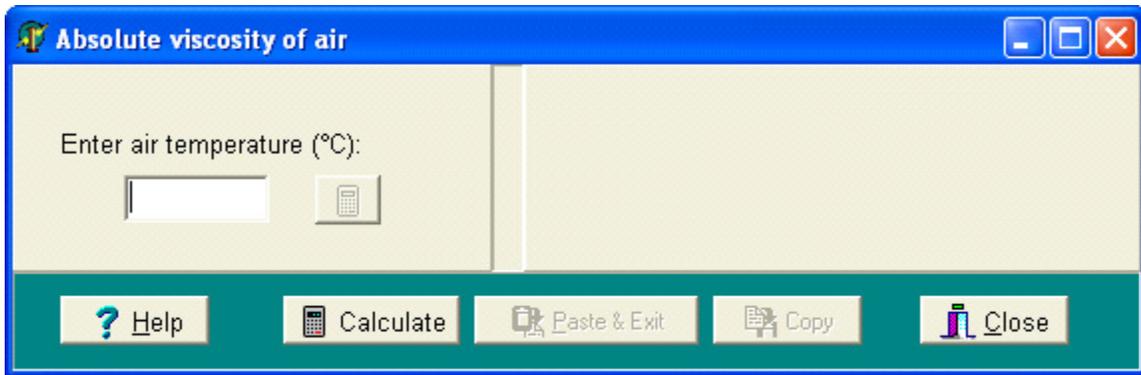
4.2.1 Methods for Petroleum-Based Paint

The first-order decay emission model has two forms (Equation 7), and they are equivalent because of the relationship in Equation 8 (Guo, 2000a).

$$E = E_0\, e^{-kt} = M_0\, k\, e^{-kt} \tag{7}$$

$$M_0 = E_0 / k \tag{8}$$

where E = emission factor in milligrams per square meter per hour,
E_0 = initial emission rate in milligrams per square meter per hour,
M_0 = initial pollutant mass in the source in milligrams per square meter,
k = first-order decay rate constant (h^{-1}), and
t = time in hours.

When the initial pollutant mass (M_0) is known, the decay constant (k) becomes the only parameter to be determined, and this program provides four methods for estimating k for emissions of volatile organic compounds (VOCs) and total VOCs (TVOCs) from petroleum-based paint. These methods are the Chinn-Evans and Guo methods for TVOCs and the Guo and Koontz methods for individual VOCs.

Chinn-Evans Method
Evans (1994) proposed to estimate k from the 90% drying time ($t_{0.9}$) for solvent evaporations from petroleum-based paint (Equation 9).

$$k = \frac{\ln 10}{t_{0.9}} \tag{9}$$

where $t_{0.9}$ is calculated from Equations 10 and 11 (Chinn, 1981).

$$\log_{10} t_{0.9} = 7.3698 - 0.9546 \log_{10} C_v \tag{10}$$

$$C_v = \frac{16040\, m\, P}{T} \tag{11}$$

where C_v = solvent volatility in milligrams per cubic meter,
m = molecular weight of solvent in grams per mole,
P = vapor pressure of solvent in millimeters Hg, and
T = temperature in Kelvin.

Input parameters include vapor pressure, molecular weight, and temperature. Built-in calculators are available for the first two parameters (Figure 9). If this method is used to estimate k for TVOC emissions for a solvent mixture, parameter P in Equation 11 should be replaced by the total vapor pressure for the solvent. The total vapor pressure can be (1) experimentally determined, (2) estimated based on the contents of the major VOCs (see Section 4.7.2), or (3) approximated by the vapor pressure of the most abundant VOC in the mixture—a calculator is avail-
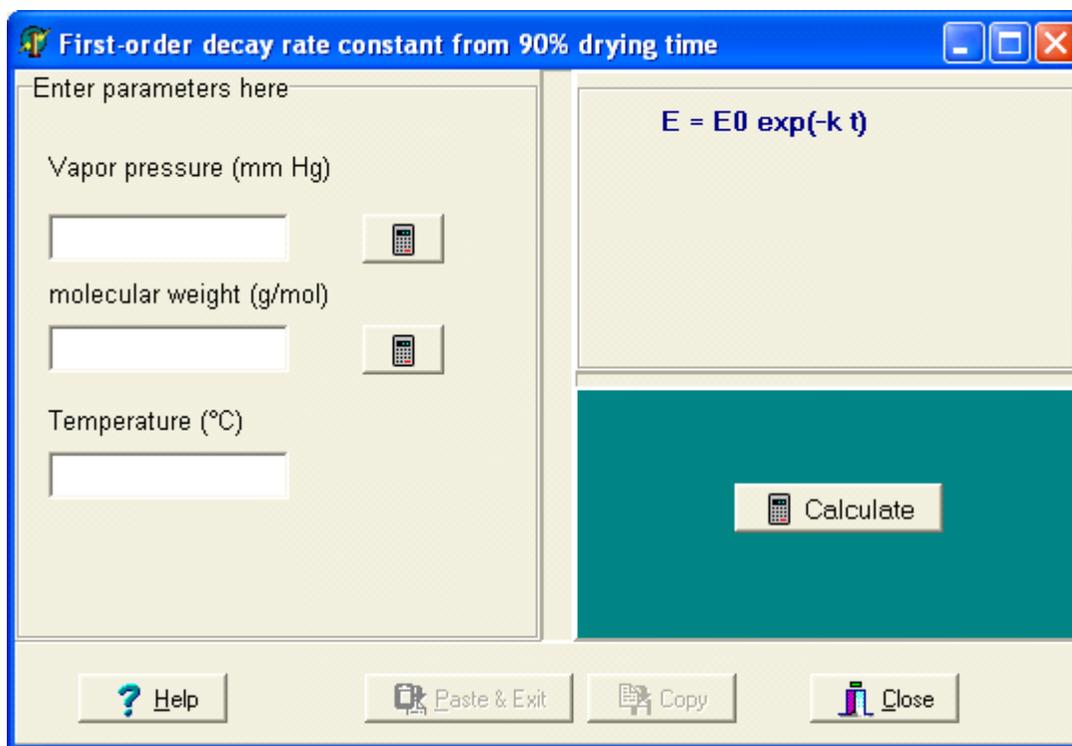
Figure 9. Calculation Screen for First-Order Decay Rate Constant with the Chinn Method.

ble in the data entry window. The average molecular weight for TVOCs can be (1) estimated based on the contents of the major VOCs (see Section 4.7.2) or (2) approximated by the molecular weight of the most abundant VOC in the mixture.

This method tends to overestimate k for an individual VOC in a mixture. One should also be aware that the correlation (Equation 10) was found with the 90% evaporation time being determined on paper filters with dry air flowing through (ASTM, 1977). Apparently, the experimental conditions (e.g., film thickness and ventilation rate) are far from realistic. Besides, this method ignores the effect of film thickness. Despite these limitations, it is very useful for rough estimations because all the parameters in Equations. 10 and 11 are easily obtained.

Guo Method for TVOCs
This method (Equation 12) was obtained by simplify-

ing a mass transfer model (Guo, 1999). It also provides an estimate of the initial emission factor (Equation 13). Information required from the user is shown in Figure 10.

$$k = \frac{k_g C_T}{\theta d\, y_T} \tag{12}$$

$$E_0 = k_g C_T \tag{13}$$

where k is in h^{-1},
k_g = gas-phase mass transfer coefficient in meters per hour,
C_T = TVOC saturation concentration converted from total vapor pressure in milligrams per cubic meter,
θ = thickness of paint film in meters,
d = density of paint in grams per cubic meter,
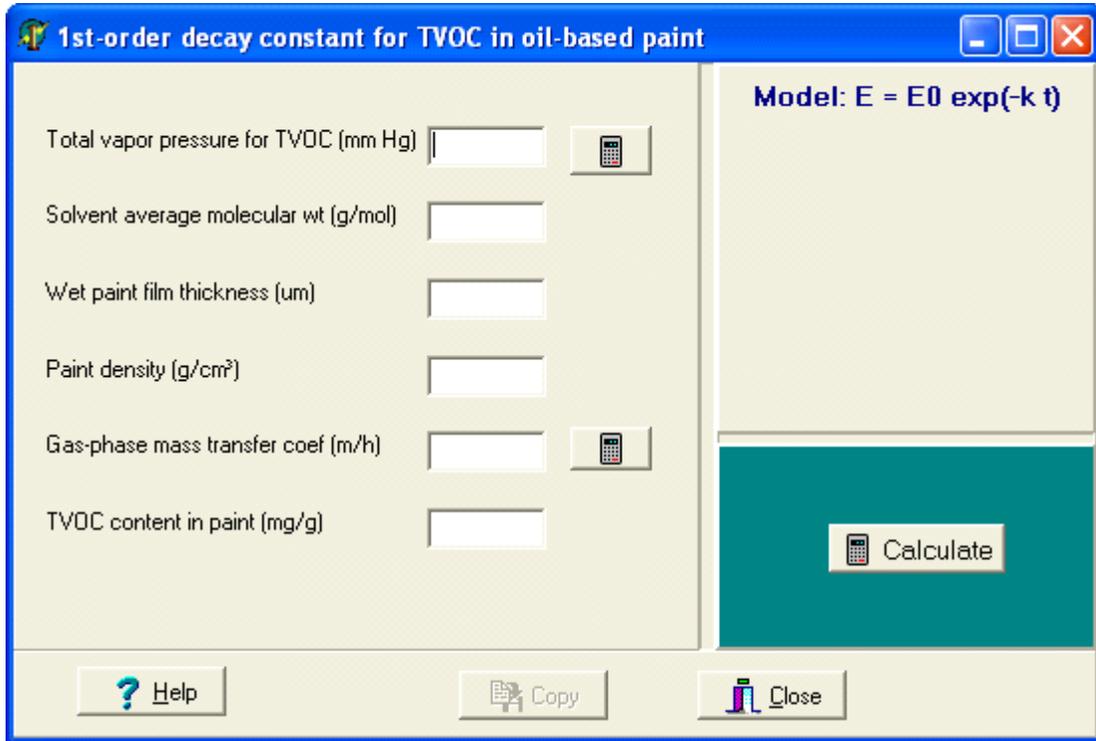y_T = TVOC content in paint in milligrams per gram, and

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**Figure 10. Calculation Screen for First-order Decay Rate Constant for
TVOC Emissions from Oil-Based Indoor Coating Materials.**

E_0 = initial emission factor in milligrams per square meter per hour.

If the user calculates the mass transfer coefficient (k_g), the molecular formula of the most abundant component in the solvent should be used. As previously described, the total vapor pressure (C_T) can be (1) experimentally determined, (2) estimated based on the contents of the major VOCs (see Section 4.7.2), or (3) approximated by the vapor pressure of the most abundant VOC in the mixture. The calculator button next to the total vapor pressure in the data entry window is for option (2). The method described in Section 4.7.1 can be used for option (3)

Guo Method for Individual VOCs
Equations 14 and 15 (Guo, 1999) are used to estimate the first-order decay rate constant (k) and the initial emission rate (E_0) for individual VOCs from oil-based indoor coating materials. Seven input parame-

ters are required from the user (Figure 11).

$$k = \frac{k_g \, C_v \, m_T}{\theta d \, y_T \, m_i} \quad (14)$$

$$E_0 = k_g \, C_v \, \frac{y_i \, m_T}{y_T \, m_i} \quad (15)$$

where k is in hr^{-1},

C_v = VOC saturation concentration converted from vapor pressure in milligrams per cubic meter,

y_i = VOC content of the paint in milligrams per gram,

m_T = average molecular weight for TVOCs in grams per mole, and

m_i = molecular weight for the VOC of interest in grams per mole.

Koontz Method for Individual VOCs
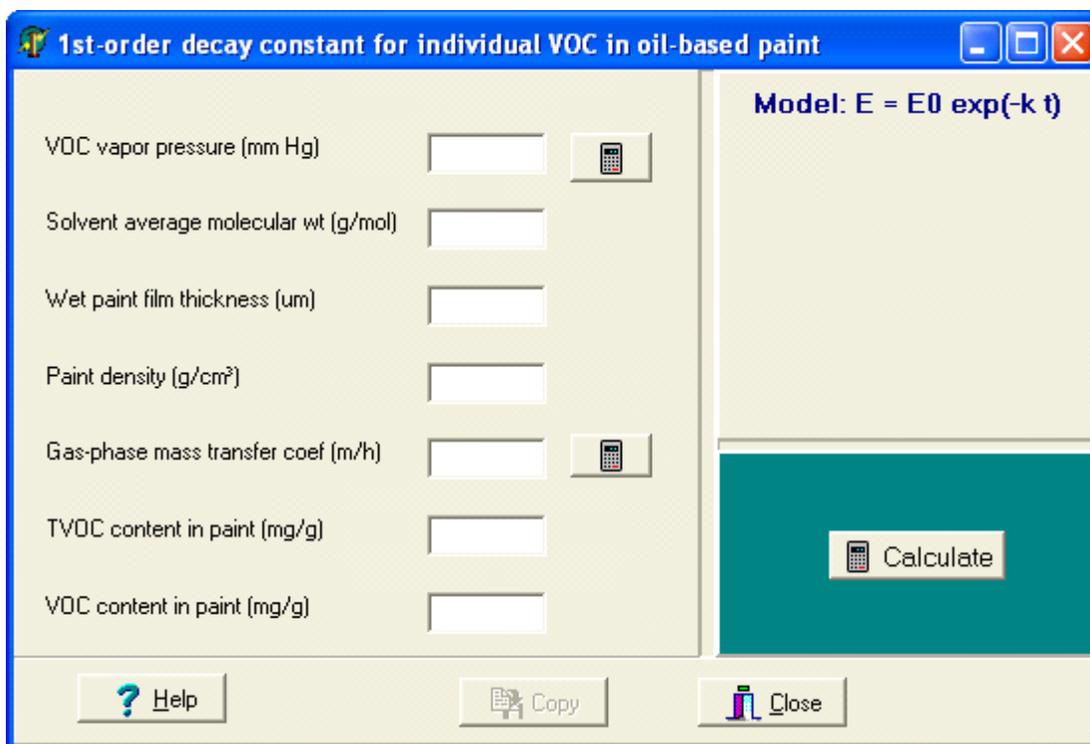The Koontz correlation (Equation 16) was found

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Figure 11. Calculation Screen for *k* and *E* for Emissions of Individual VOCs from Oil-Based Coating Materials.

from experimentally determined k's for alkyd paint (Koontz, 2001),

$$k = 2.95 \times 10^9 \frac{P^{0.27}}{m^{4.02}\, \theta^{0.58}};\ \ (r^2 = 0.86) \tag{16}$$

where k is in h^{-1},

   P = vapor pressure in millimeters Hg,
   m = molecular weight in grams per mole,
   θ = thickness of paint film in mils, and
   r = correlation coefficient.

User inputs are vapor pressure, molecular weight, and wet film thickness (Figure 12).

4.2.2 Methods for Latex Paint

The dual exponential decay model (Equation 17) is often used for glycol emissions from latex paint. Wilkes, et al. (1996) proposed Equations 18 and 19 for estimating k_1 and k_2, respectively. This method does not estimate E_1 and E_2.

$$E = E_1\, e^{-k_1 t} + E_2\, e^{-k_2 t} \tag{17}$$

$$k_1 = 233.25\, P;\ \ \ (r^2 = 0.92) \tag{18}$$

$$k_2 = 5.839 \times 10^{-5} m;\ \ \left(r^2 = 0.96\right) \tag{19}$$

where E_1 = initial emission factor for "fast" emis-
       sions in milligrams per square meter per
       hour,
   E_2 = initial emission factor for "slow" emis-
       sions in milligrams per square meter per
       hour,
   k_1 = first-order decay rate constant for "fast"
       emissions (h^{-1}),
   k_2 = first-order decay rate constant for "slow"
       emissions (h^{-1}),
   P = vapor pressure in millimeters Hg,
   m = molecular weight in grams per mole, and
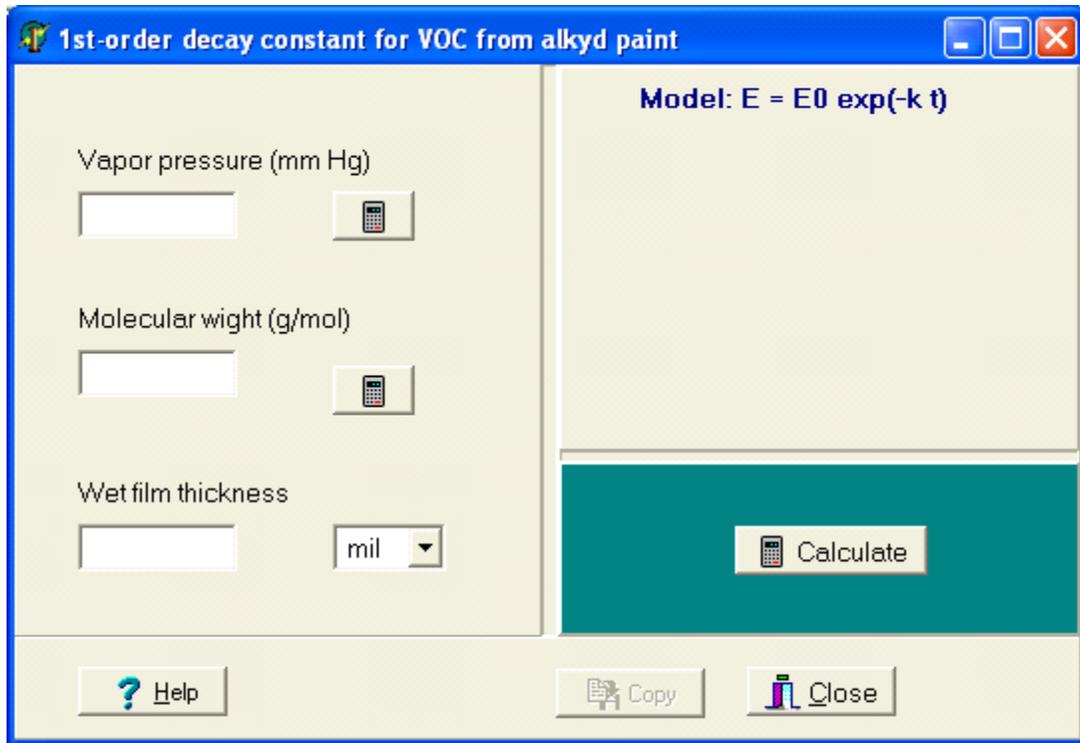 r = correlation coefficient.

Figure 12. Calculation Screen for Estimating the First-Order Decay Rate Constant for VOC Emissions from Alkyd Paint with the Koontz Method.

hese two parameters are calculated with two separate calculation screens (Figure 13).

4.3 Mass Transfer Coefficient

The software can calculate the gas-phase mass transfer coefficient by either the Sherwood, the Sparks, or the Mackay-Matsugu method. The liquid-phase mass transfer coefficient can be calculated either for still water pools and films or for moving water. The overall mass transfer coefficient can be calculated on a generic basis or for still water pools and films.

4.3.1 Gas-Phase Mass Transfer Coefficient

Three methods are provided for calculating the gas-phase mass transfer coefficient: Sherwood method, Sparks method, and Mackay-Matsugu method. Since all three methods require the same user input, they share the same calculation screen (Figure 14).

Sherwood Method

This method (Bennet and Myers, 1982) is based on correlations between three dimensionless numbers: Sherwood number (Sh), Schmidt number (S_c), and Reynolds number (R_e).

$$Sh = \frac{k_g L}{D_a} \tag{20}$$

$$R_e = \frac{L u \rho}{\mu} \tag{21}$$

$$S_c = \frac{\mu}{\rho D_a} \tag{22}$$

where k_g = gas-phase mass transfer coefficient in meters per hour,

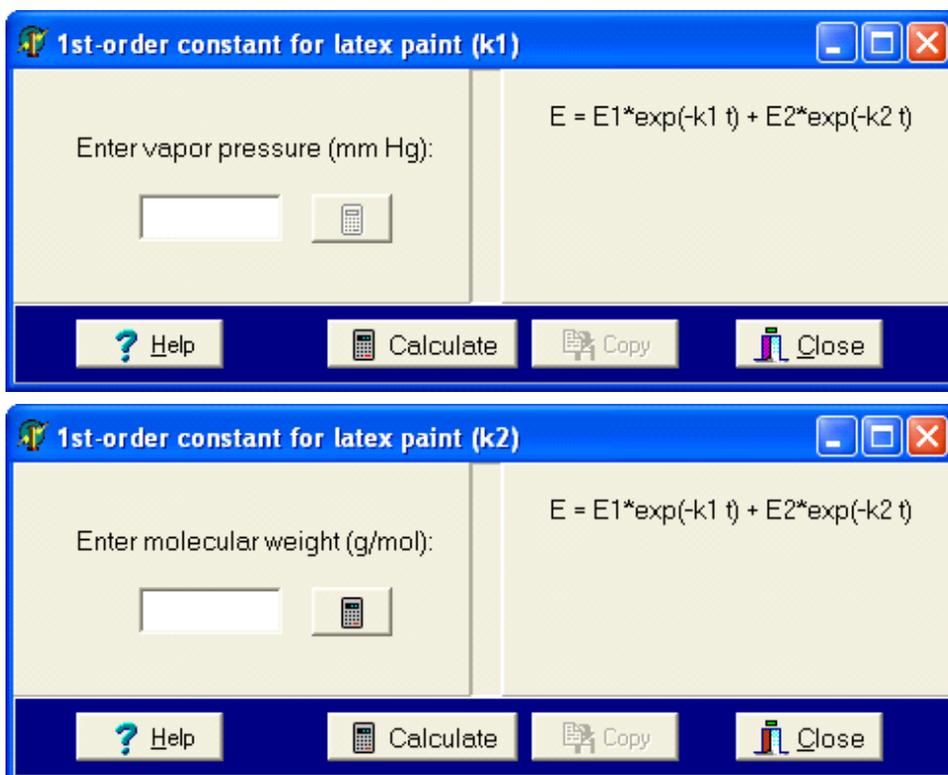L = characteristic length of the source in meters,

15

Figure 13. Calculation Screens for Estimating the First-Order Decay Rate Constants for VOC Emissions From Latex Paint. The Screen on Top Is for k_1 and the One on Bottom for k_2.
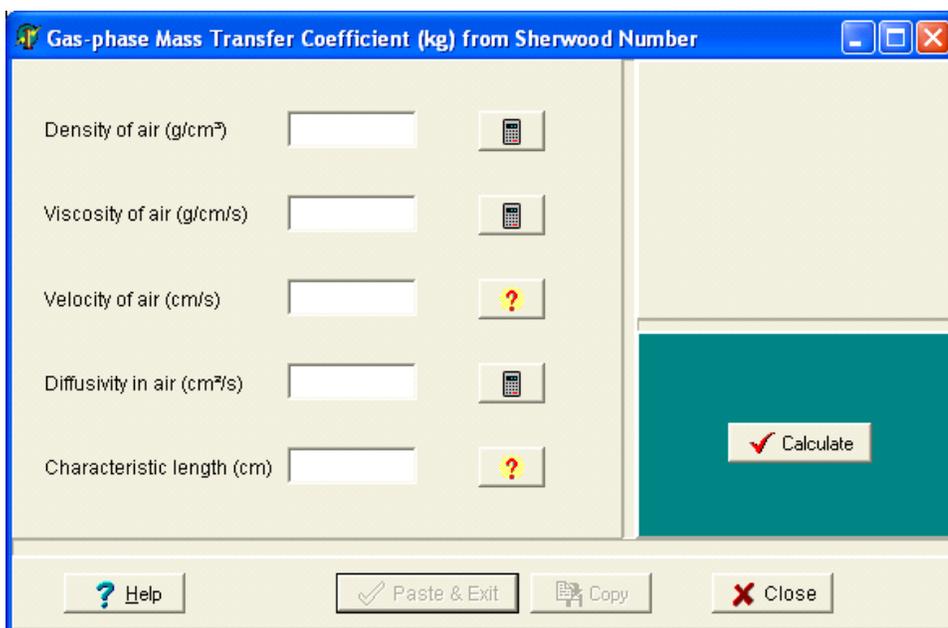

Figure 14. Calculation Screen for Gas-Phase Mass Transfer Coefficient.

D_a = diffusivity in air in square meters per hour,
u = air velocity in meters per hour,
ρ = density of air in grams per cubic meter, and
μ = viscosity of air in grams per meter per hour.

A series of correlations have been developed between Sh, S_c, and R_e (Bennett & Myers, 1982; White, 1991). For example, Equation 23 applies to laminar flow conditions and is used in this program.

$$Sh = 0.664 \, S_c^{\frac{1}{3}} \, R_e^{\frac{1}{2}} \tag{23}$$

The calculation involves four steps.
Step 1. Calculate the Reynolds number (Equation 21);
Step 2. Calculate the Schmidt number (Equation 22);
Step 3. Calculate the Sherwood number (Equation 23); and
Step 4. Calculate the gas-phase mass transfer coefficient (k) from Equation 20.

Sparks Method
Sparks, et al (1996) proposed a simpler method based on experimental data obtained from small chambers and a test house (Equation 24), and is used in several emission source models for interior paint.

$$k_g = 0.33 \, D_a \, L^{-1} \, R_e^{\frac{2}{3}} \tag{24}$$

Mackay-Matsugu Method
This method was based on experimental data for water evaporation (Mackay and Matsugu, 1973) and has been used mostly for solvent spills.

$$k_g = 0.0292 \, u^{0.78} \, L^{-0.11} \, S_c^{-0.67} \tag{25}$$

where k_g, u, and L are in meters per hour, meters per hour, and meters, respectively.

These three methods require the same user input. Currently there are not sufficient experimental data to discriminate one method from the others. This developer suggests the following "rules-of-thumb" for method selection: (1) choose the method that is recommended by the source model; (2) if the source model does not recommend a specific method, use the Sherwood method.

4.3.2 Liquid-Phase Mass Transfer Coefficient
The software can calculate the liquid-phase mass transfer coefficient for still water pools and films and for moving water.

Still Water Pools and Films
For still, shallow water pools and films, Guo and Roache (2003) proposed to use Equation 26 to estimate the liquid-phase mass transfer coefficient.

$$k_L(X) = 2.99 \times \sqrt{D_L(X)} \tag{26}$$

where $k_L(X)$ = liquid-phase mass transfer coefficient for compound X in meters per hour,
$D_L(X)$ = diffusivity of compound X in water in square meters per hour.

A calculator is provided in the calculation screen for the diffusivity in water (Figure 15), and the method is discussed in Section 4.5.2.

Moving Water
This method (Equation 27) is for ambient water bodies (Southworth, 1992) and is included in this program because there are no similar methods for indoor conditions. User inputs are molecular weight, velocity of water flow, and water depth (Figure 16.). Use this method with caution.

$$k_L = 23.51 \frac{u_c^{0.969}}{Z^{0.673}} \sqrt{\frac{32}{m}} \tag{27}$$

where k_L is in centimeters per hour,
u_c = velocity of water current in meters per second,
Z = water depth in meters, and
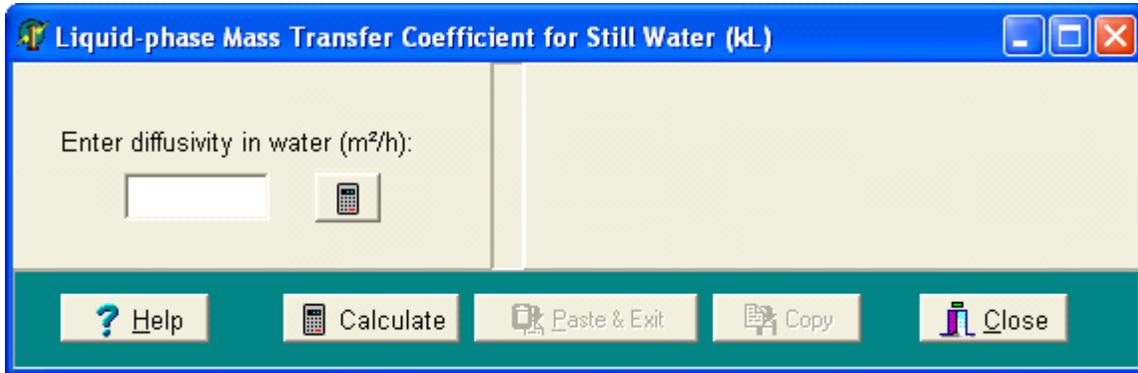m = molecular weight in grams per mole.

17

Figure 15. Calculation Screen for Liquid-Phase Mass Transfer Coefficient for Still Water.
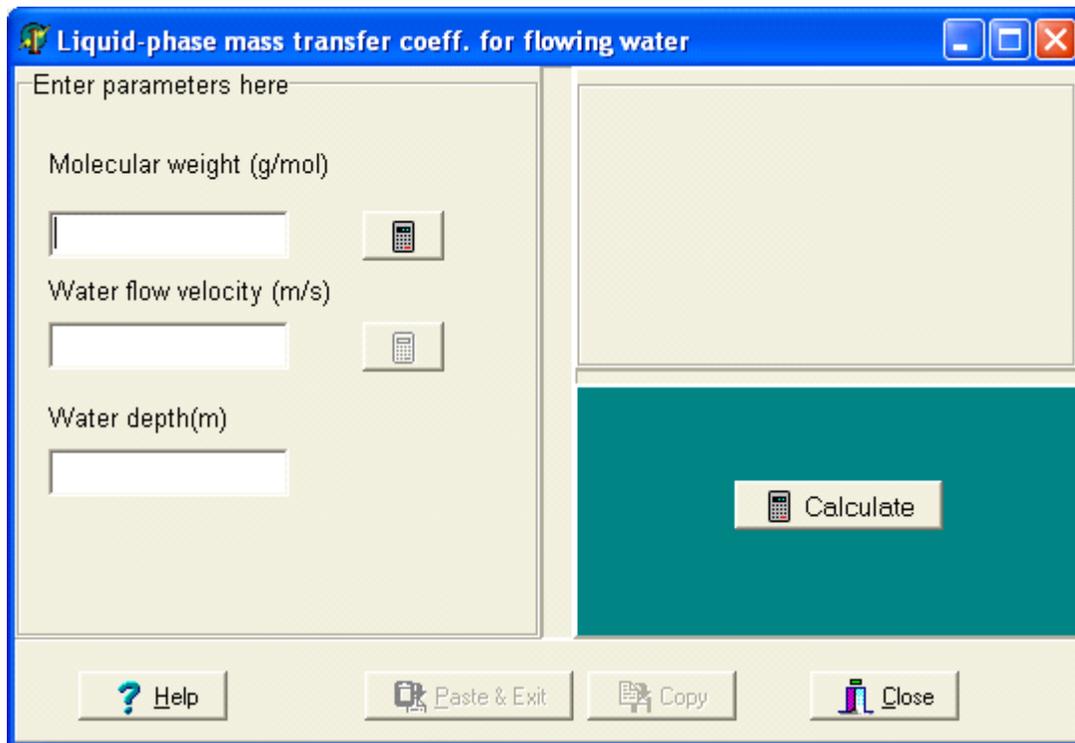

Figure 16. Calculation Screen for Liquid-Phase Mass Transfer Coefficient for Moving Water.

4.3.3 Overall Mass Transfer Coefficient

Generic
Overall mass transfer coefficients are often used to estimate pollutant emissions from tap water and water-based consumer products. This generic method (Equations 28 and 29) is not a parameter estimation method per se. Rather, it gives the definition of overall mass transfer coefficient (Lyman, et al., 1990; ch 15, p11) and is used to calculate the overall mass

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transfer coefficient from the gas- and liquid-phase mass transfer coefficients and Henry's constant. Figure 17 shows the calculation screen.

$$\frac{1}{K_{OL}} = \frac{1}{k_L} + \frac{1}{k_g\,H} \tag{28}$$

$$\frac{1}{K_{OG}} = \frac{H}{k_L} + \frac{1}{k_g} \tag{29}$$

where K_{OL} = overall liquid-phase mass transfer coefficient in meters per hour,

k_L = liquid-phase mass transfer coefficient in meters per hour,

k_g = gas-phase mass transfer coefficient in meters per hour,

H = dimensionless Henry's constant (i.e., air/water partition coefficient).

Since the two overall mass transfer coefficients (K_{OL} and K_{OG}) are linked by Equation 30, one can be calculated from the other.

$$K_{OL} = H\,K_{OG} \tag{30}$$

Still Water Pools and Films

For still water pools and films, Guo and Roache (2003) proposed a three-step calculation method.

Step 1. Use Equation 20 to estimate the gas-phase mass transfer coefficient (k_g);

Step 2. Use Equation 27 to estimate the liquid-phase mass transfer coefficient (k_L); and

Step 3. Use Equation 28 to calculate the liquid-phase overall mass transfer coefficient.

Once the overall liquid-phase mass transfer coefficient (K_{OL}) is known, the overall gas-phase mass transfer coefficient (K_{OG}) can be easily obtained from Equation 30. Calculators for k_g and k_L are provided in the calculation screen (Figure 18).

4.4 Molar Volume

Molar volume (often in cubic centimeters per mole) is a measure of molecular size and is used to estimate

Figure 17. Calculation Screen for Overall Gas- and Liquid-Phase Mass Transfer Coefficients.
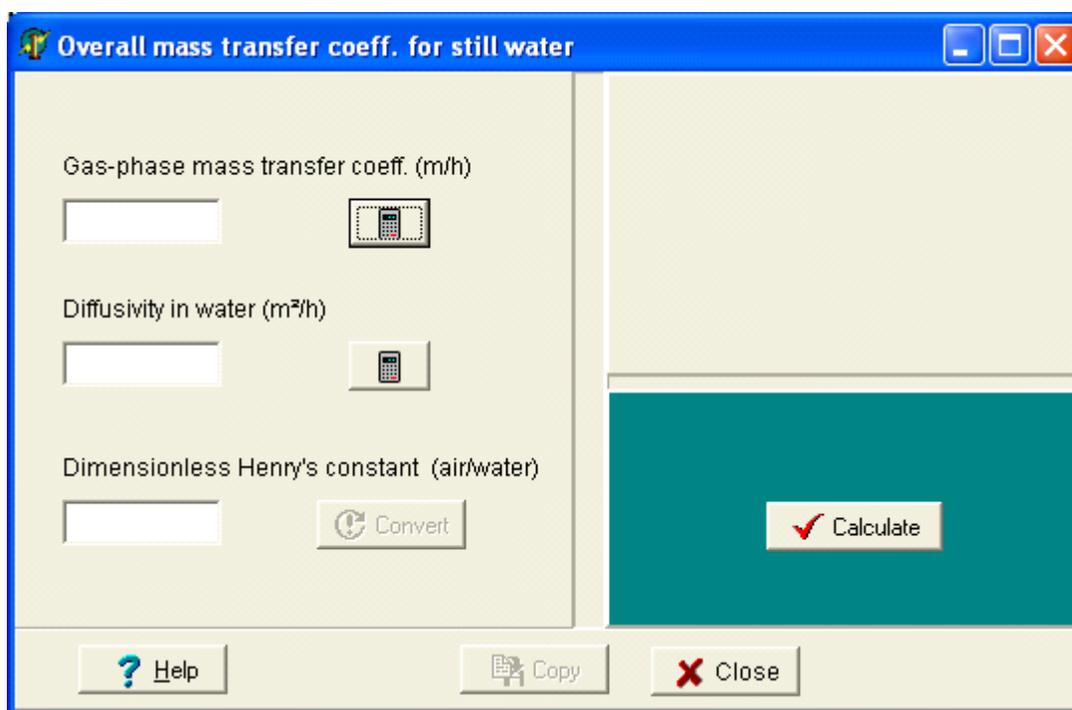
Figure 18. Calculation Screen for Overall Gas- and Liquid-Phase Mass Transfer Coefficients for Still Water Pools and Films.

the diffusion coefficient in air, water, and solids. Two methods are commonly used. One is based on atomic and structural diffusion volume increments and the other is known as the Le Bas molar volume, which is determined at the normal boiling point of the substance. The relationship between these two parameters is shown in Equation 31.

$$V_{mol} = (0.85 \, to \, 0.9) V_{LB} \qquad (31)$$

where V_{mol} = molar volume of gas at normal temperature in cubic centimeters per mole, and
V_{LB} = Le Bas molar volume in cubic centimeters per mole.

4.4.1 Atomic and Structural Diffusion Volume Increments
In this method, the molar volume is the sum of the volume for each atom and structure (Fuller, et al., 1966). The data table used in this program is from Lyman, et al.(1990, ch 17, p 11). For instance, the diffusion volume increments for carbon, hydrogen,

and the aromatic ring are, respectively, 16.5, 1.98, and -20.2 cm³/mol. Thus, the molar volume for benzene ($C_6 H_6$) is

$$V_{mol} = 6 \times 16.5 + 6 \times 1.98 - 20.2 = 110.9 \, (cm^3/mol)$$

The drawback of this method is that the incremental molar volumes are only available for six atoms: C, H, O, N, Cl, and S. Furthermore, the values for N, Cl, and S are based on limited experimental data. The calculation screen for this method is shown in Figure 19.

4.4.2 Le Bas Molar Volume
The Le Bas method estimates the molar volumes of liquids at their respective normal boiling points. Like the method described above, the Le Bas volume is also additive. The original data table is used in this program (Reid, et al., 1977 p 58; Lyman, et al., 1990, ch 17, p 11). This method pays more attention to the molecular structure than the previous method (Section 4.4.2). For instance, oxygen has five incremental
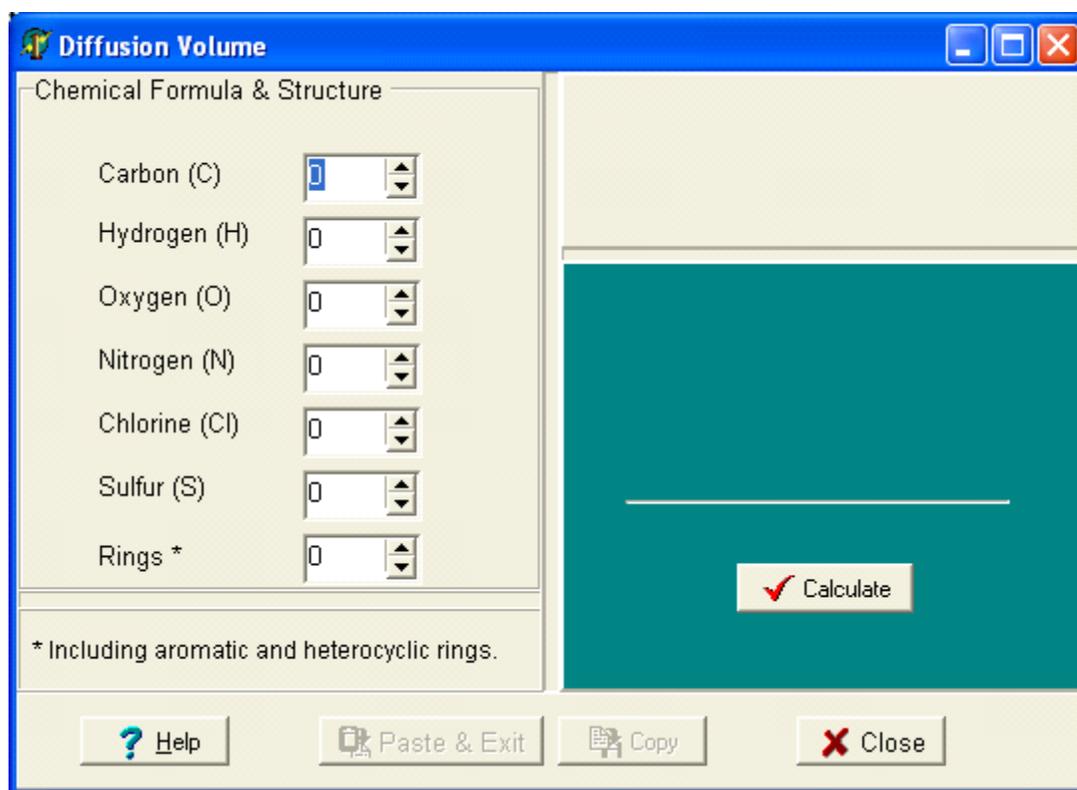
20

Figure 19. Calculation Screen for Molar Volume Based on Atomic and Structural Diffusion Volume Increments.

volumes depending on its bonding with other atoms (e.g., esters and acids). Incremental volumes are available for nine atoms: C, H, O, N, Br, Cl, F, I, and S . The calculation screen is shown in Figure 20.

4.5 Molecular Diffusivity
The software contains algorithms for calculating diffusivity in solids as a function of either molecular weight or molar volume, in water, and in air by two methods.

4.5.1 Diffusivity in Air
The method of Fuller-Schettler-Giddings (FSG) and the method of Wilke and Lee (WL) are the two most commonly used methods for estimating molecular diffusivity in air. Overall, the WL method is more accurate, but requires knowledge of the boiling point of the chemical of interest.

FSG method
This method is based on Equation 32 (Fuller, et al., 1966). It is most accurate for non-polar gases at low to moderate temperature and is less accurate for the polar acids and glycols.

$$D_A = \frac{10^{-3}\, T^{1.75}\, \sqrt{M_r}}{P\left(V_A^{1/3} + V_B^{1/3}\right)^2} \tag{32}$$

$$M_r = \frac{M_A + M_B}{M_A\, M_B} \tag{33}$$

where D_A = molecular diffusivity in square centi-
meters per second,
  T = temperature in Kelvin,
  M_A = molecular weight for air = 28.97 g/mole,
  M_B = molecular weight for the chemical of interest in grams per mole,
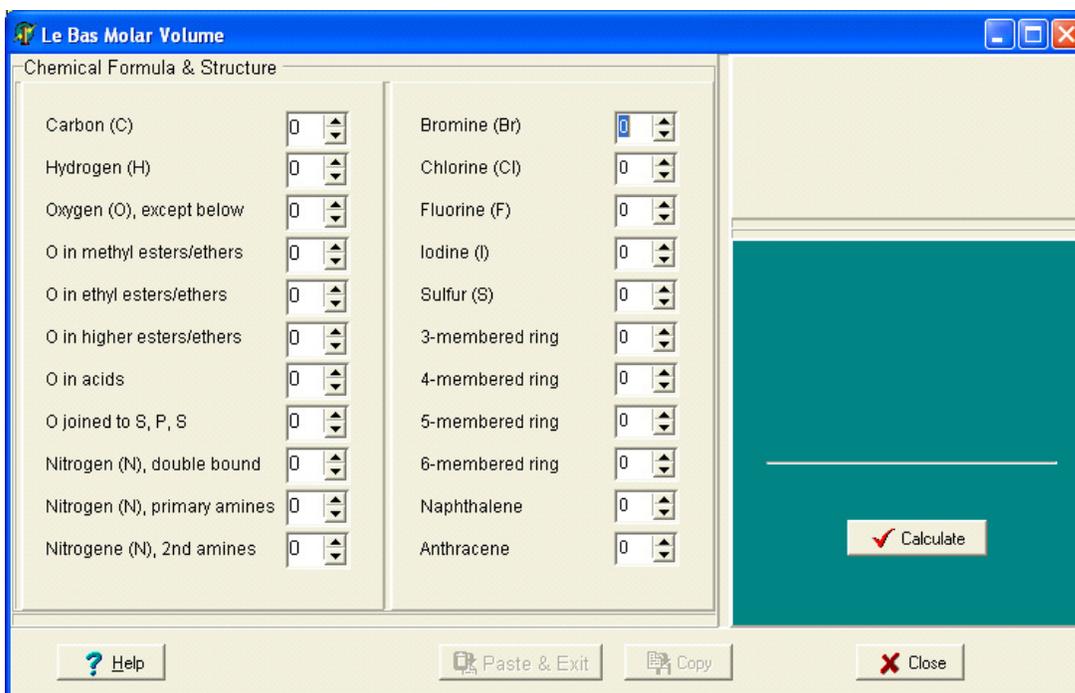 P = atmospheric pressure in atmospheres,

Figure 20. Calculation Screen for Le Bas Volume.

V_A = molar volume for air (20.1 cm³/mol), and

V_B = molar volume for the chemical of interest in cubic centimeters per mole.

There are two methods for estimating V_B: (1) from atomic and structure diffusion volume increments (see Section 4.4.1) and (2) from the Le Bas volume (see Section 4.4.2). This program implements both methods, which are assigned FSG method 1 and FSG method 2, respectively. In FSG method 2, a mean value of 0.875 is used for the constant in Equation 31 (see Lyman, et al., 1990, ch 17, p 13). The calculation screens for FSG methods 1 and 2 are shown in Figures 21 and 22, respectively.

WL method
This method (Equation 34) is usable for a wider range of compounds and temperatures than the FSG method (Wilke & Lee, 1955).

$$D_a = \frac{B' \, T^{2/3} \, \sqrt{M_r}}{P_0 \, \sigma_{AB}^2 \, \Omega} \qquad (34)$$

where B' = a function of molecular weight of air and that of the chemical of interest,

P_0 = atmospheric pressure in atmospheres,

σ_{AB} = characteristic length of the chemical of interest interacting with air, and

Ω = collision integral.

Calculations of B', σ_{AB}, and Ω are by no means difficult, but rather, are tedious. The user is encouraged to read the original paper for more details (Lyman, et al., 1990, ch. 17, pp13-14). The calculation screen for the WL method is shown in Figure 23.

4.5.2 Diffusivity in Water
The Hayduk and Laudie method for estimating the diffusivity in water is based on Equation 35 (Hayduk and Laudie, 1974):

$$D_L = \frac{13.26 \times 10^{-5}}{\eta_w^{1.14} \, V_{LB}^{0.589}} \qquad (35)$$

where D_L = diffusivity in water in square centimeters per second,

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Figure 21. Calculation Screen for Diffusivity in Air with FSG Method 1, in Which the Molar Volume Is Estimated from Atomic and Structure Diffusion Volume Increments.

Figure 22. Calculation Screen for Diffusivity in Air with the FSG Method, in Which the Molar Volume Is Estimated from the Le Bas Volume.
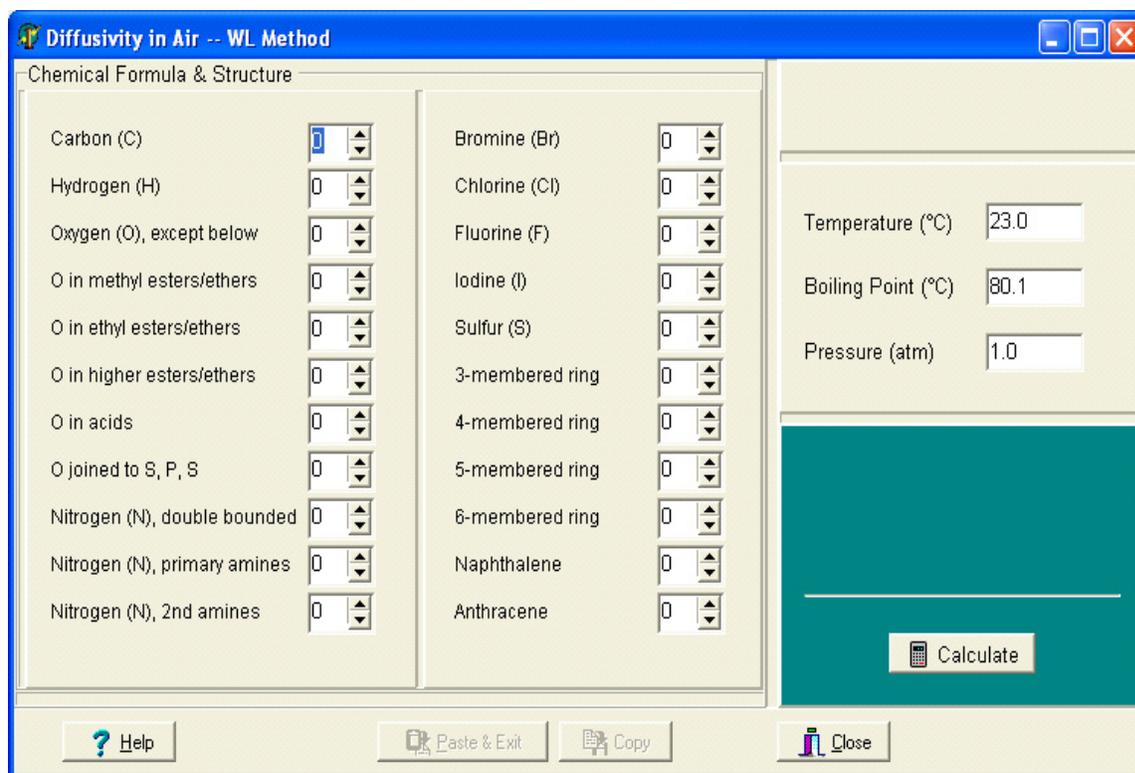
Figure 23. Calculation Screen for Molecular Diffusivity in Air with the WL Method.

η_w = viscosity of water (centiPoise), and
V_{LB} = Le Bas volume in cubic centimeters per mole.

The user needs to enter the molecular formula in the calculation screen (Figure 24), and the two parameters in Equation 35 (η_w and V_{LB}) are calculated internally based on methods described in Sections 4.8.2 and 4.4.3, respectively.

4.5.3 Diffusivity in Solids as a Function of Molecular Weight

For a given solid material and a class of chemicals, correlation exists between the diffusivity of a chemical and its molecular weight (Bodalal, et al., 2001; Cox, et al., 2001). The two constants in Equation 36, A and n, are found from experimental data. Data for nine material/chemical class combinations are available in this program.

$$D_s = \frac{A}{m^n} \tag{36}$$

where D_s = diffusivity in solid in square meters per second,

A = a coefficient specific to a material and a compound class,

m = molecular weight in grams per mole, and

n = an index specific to material and a compound class.

Values of A and n for different materials are provided in the calculation screen (Figure 25). When the user clicks on a material in the table, the selected material/chemicals will be displayed at the upper-right corner. In Figure 25, gypsum board/aromatics are selected and, thus, $A = 44.81$ and $n = 5.99$.

4.5.4 Diffusivity in Solids as a Function of Molar Volume

Correlations described in Section 4.5.3 are specific to
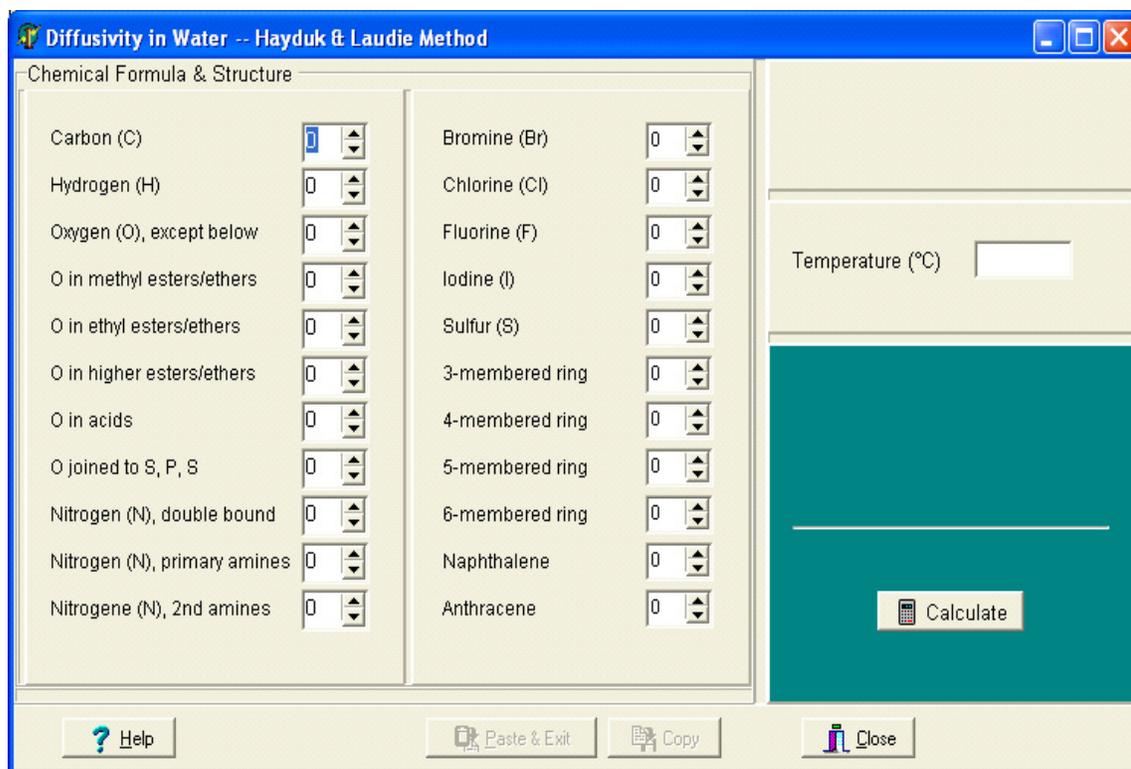
24

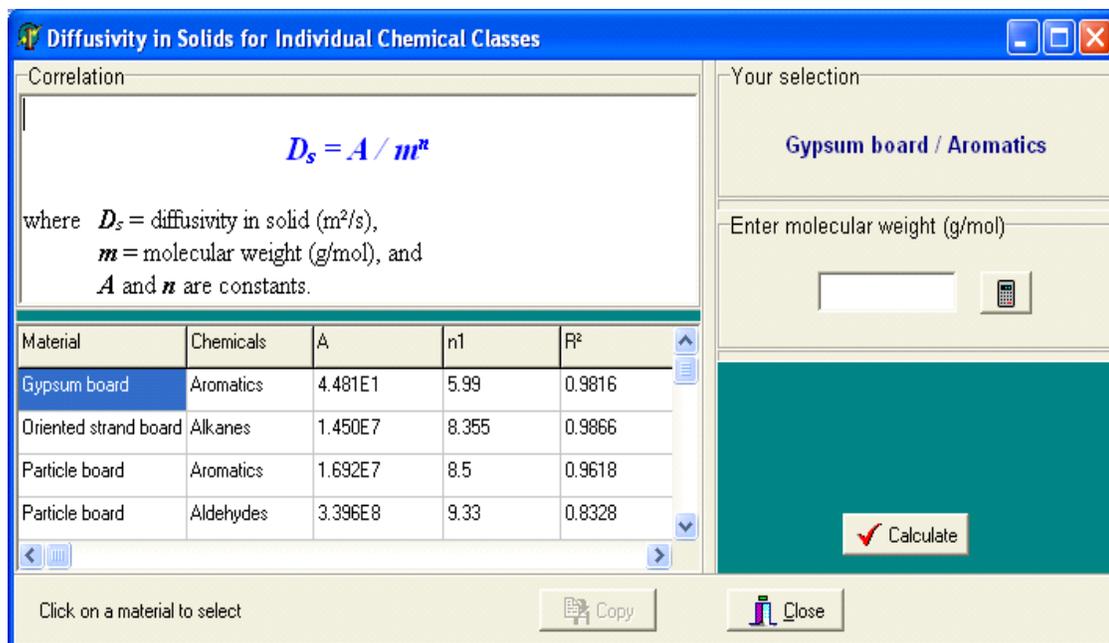**Figure 24. Calculation Screen for Molecular Diffusivity in Water.**

Figure 25. Calculation Screen for Diffusivity in Solid Material. This Method Is Specific to Given Material/Chemical Class Combinations.

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certain material/chemical class combinations. To loosen such restrictions, Guo (2002b) suggested that D_s be correlated to the molar volume. Equation 37 can be applied to mixed chemical classes.

$$\ln(D_s) = A + B \ln(V_m) \qquad (37)$$

where V_m = molar volume in cubic centimeters per mole.

Coefficients A and B for different materials are provided in the calculation screen (Figure 26). The user is expected to select a material, enter the molar volume and then click the <Calculate> button. A calculator is available for computing the molar volume.

4.6 Solid-Air Partition Coefficient

Solid-air partition coefficient is a key parameter in models for pollutant emissions from building materials and is defined by Equation 38.

$$K_P = \frac{C_s}{C_a} \qquad (38)$$

where K_P = solid-air partition coefficient (dimensionless),

C_s = concentration in solid material in mass/volume, and

C_a = concentration in air at equilibrium with solid phase in mass/volume.

Thus, if a chemical has a large K, it tends to stay in the solid phase. The reciprocal of K is known as the air/solid partition coefficient.

4.6.1 Material and Chemical Specific Methods
For a given solid material and a chemical class, correlations exist between solid-air partition coefficient and vapor pressure (Equation 39).

$$K_P = \frac{B}{P^n} \qquad (39)$$

where P = vapor pressure in millimeters Hg).

Constants B and n have been reported for ten material/chemical class combinations (Zhao, et al, 1999; Bodalal, et al, 2001). All are implemented in this program, and the data are shown in the calculation

Figure 26. Calculation Screen for Molecular Diffusivity in Solid Materials. This Method Is Not Specific to a Particular Compound Class.

screen (Figure 27). The square of correlation coefficient (r^2) ranged from 0.689 to 0.997.

4.6.2 Method for All Materials and Compound Classes

By combining all experimental data (see Section 4.6.1), Guo (2002b) found a correlation for all materials and compound classes. Equation 40 (n=56; r^2= 0.734) is useful for roughly estimating the solid-air partition coefficient without any experimental data. Figure 28 shows the calculation screen.

$$\ln(K_P) = 8.86 - 0.785\ln(P) \tag{40}$$

4.7 Volatility of Organic Compounds

The software has algorithms for computing the vapor pressure of individual organic compounds and the total vapor pressure of petroleum-based solvents.
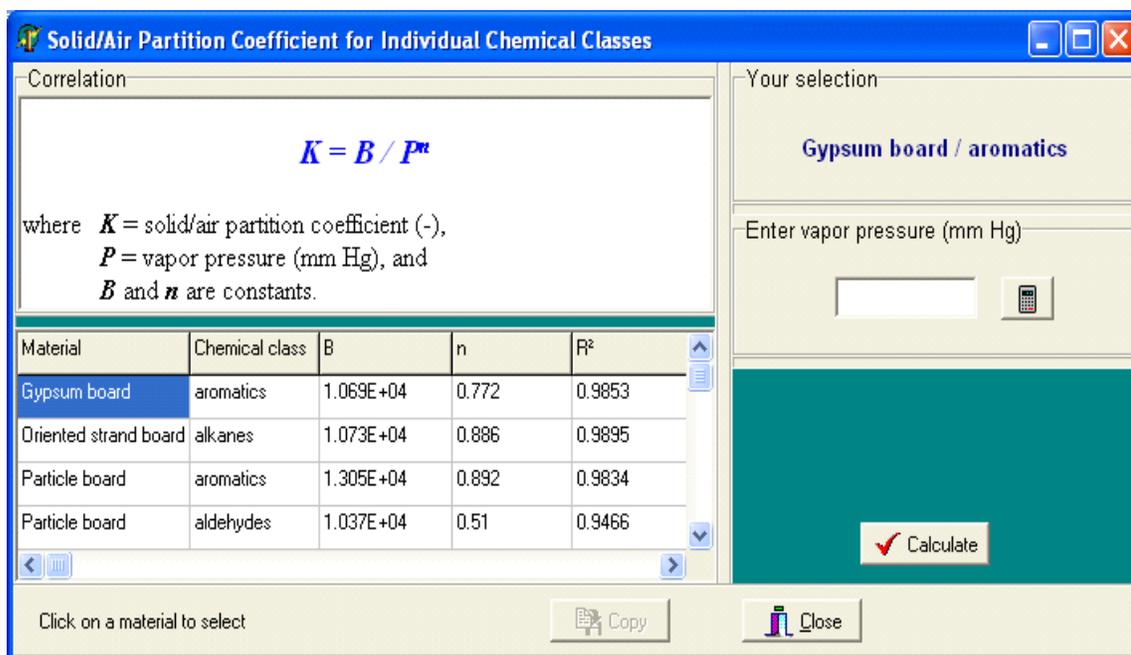

Figure 27. Calculation Screen for Solid-Air Partition Coefficient. This Method Is Material and Chemical Specific.
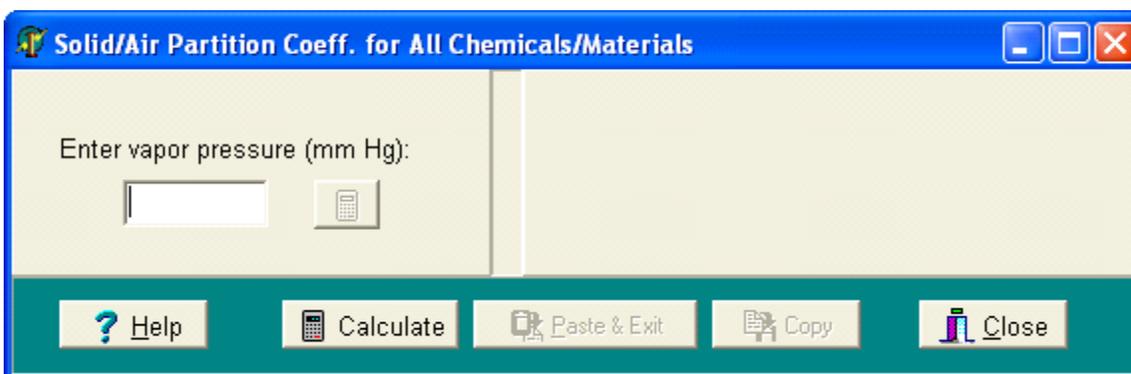

Figure 28. Calculation Screen for Solid-air Partition Coefficient. This Method Is Not Specific to Compound Classes.

4.7.1 Makar Method for Pure Organic Compounds

A method developed by Makar (2000) allows the user to estimate the vapor pressure for an organic compound by knowing (1) its compound class, (2) the carbon number in the molecule, and (3) the temperature of interest. In doing so, Makar divided organic compounds into 39 classes (e.g., n-alcohols, n-alkanes, and polyaromatics). For each compound class, the 12 coefficients in Equation 41 were found based on available experimental data and are given in a table.

$$\log_{10} P = a_0 + a_1 T + a_2 T^2 + a_3 T^3$$
$$+ n(b_0 + b_1 T + b_2 T^2 + b_3 T^3) \qquad (41)$$
$$+ n^2(c_0 + c_1 T + c_2 T^2 + c_3 T^3)$$

where P is in millimeters Hg and T is in Kelvins.

In general, the correlations are good. This method is very useful in the absence of experimental data at room temperature. It is the user's responsibility, however, to determine the class to which a given compound belongs. In other words, the user must know the molecular structure of the compound.

Coefficients for different compound classes are stored in a database table, invisible to the user. The user is expected to select a compound class from the list, select the carbon number, and enter the temperature (Figure 29). Note that the range of allowable carbon numbers for each compound class is defined by the method developer.
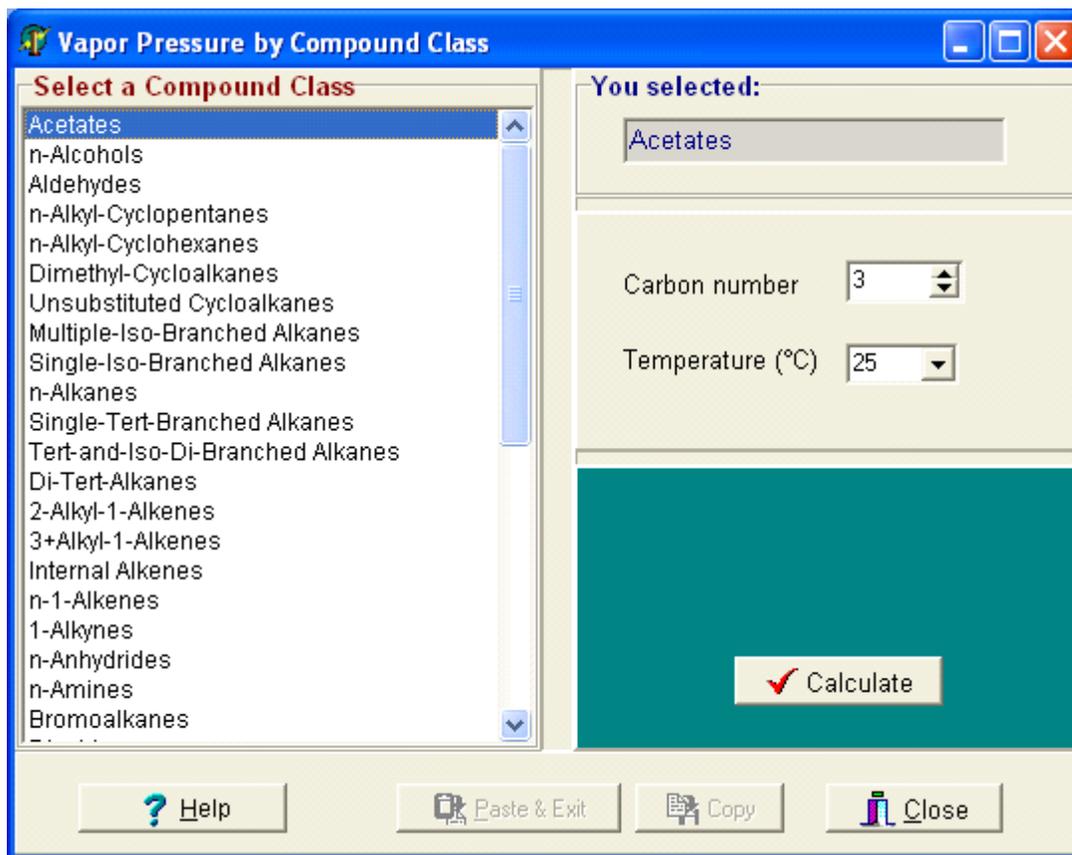

Figure 29. Calculation Screen for Estimating the Vapor Pressure Based on Compound Class.

4.7.2 Total Vapor Pressure of Petroleum-Based Solvents

Predicting the emissions of TVOCs from petroleum-based paint or solvents requires knowledge of the total vapor pressure for TVOC. Assuming ideal solution, the total vapor pressure is the sum of the partial pressures for all compounds in the solvent mixture, but it is difficult to quantify all the components of a petroleum-based solvent, which contains hundreds of compounds. Guo, et al. (1999) suggested that total vapor pressure be approximated by that of an imaginary solvent consisting of the known major components in the mixture (Equation 42). Knowledge of the contents of about a dozen major components in the solvent—normally achieved by GC analysis—is sufficient for a reasonable estimate of the total vapor pressure.

$$P_T = \sum_{i=1}^{q} \frac{P_i\, y_i}{m_i} \bigg/ \sum_{i=1}^{q} \frac{y_i}{m_i} \qquad (42)$$

To simplify the calculations, this program contains a mini-database for the properties of common VOCs in petroleum solvents (Figure 30). The user is expected to enter the contents of individual VOCs in the coating materials in the last column. The user can, of course, add new VOCs to the table. This method also calculates the average molecular weight based on Equation 43.

$$\overline{m} = \sum_{i=1}^{n} y_i \bigg/ \sum_{i=1}^{n} (y_i / m_i) \qquad (43)$$

4.8 Properties of Water

The software has algorithms for calculating the vapor pressure and viscosity of water.

4.8.1 Vapor Pressure of Water

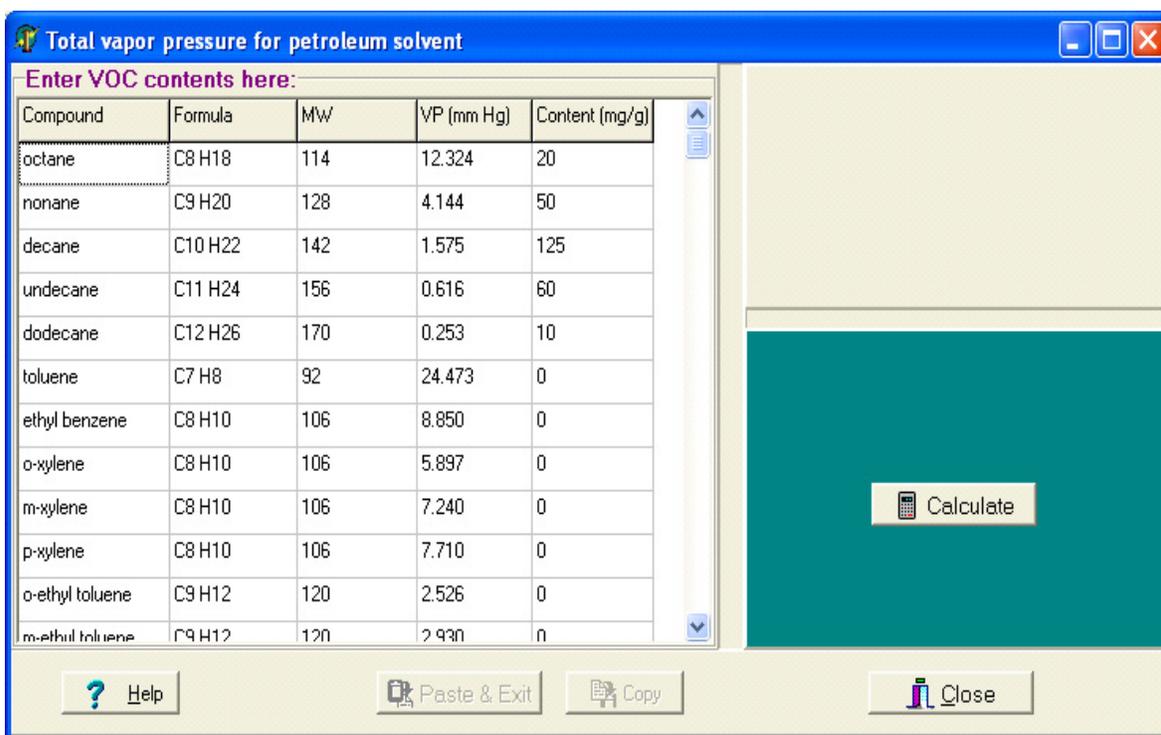The vapor pressure for water is calculated from Equation 44 (Yaws, 1994a, page 345)

Compound	Formula	MW	VP (mm Hg)	Content (mg/g)
octane	C8 H18	114	12.324	20
nonane	C9 H20	128	4.144	50
decane	C10 H22	142	1.575	125
undecane	C11 H24	156	0.616	60
dodecane	C12 H26	170	0.253	10
toluene	C7 H8	92	24.473	0
ethyl benzene	C8 H10	106	8.850	0
o-xylene	C8 H10	106	5.897	0
m-xylene	C8 H10	106	7.240	0
p-xylene	C8 H10	106	7.710	0
o-ethyl toluene	C9 H12	120	2.526	0
m-ethyl toluene	C9 H12	120	2.930	0

Figure 30. Calculation Screen for Total Vapor Pressure of Petroleum-Based Solvents.

$$\log_{10} P_{w0} = A + B\,/\,T + C\log_{10} T$$
$$+ D\,T + E\,T^2 \tag{44}$$

where P_{w0} = water vapor pressure in millimeters Hg,
T = temperature in Kelvins,
A = 29.8605,
B = -3.1522×10³,
C = -7.3037,
D = 2.4247×10⁻⁹, and
E = 1.8090×10⁻⁶.

Temperature is the only user input (Figure 31).

4.8.2 Viscosity of Liquid Water
The absolute viscosity of liquid water is calculated

from Equation 45 (Yaws, 1994b).

$$\log_{10} \eta = A + B\,/\,T + C\,T + D\,T^2 \tag{45}$$

where η = liquid viscosity (centiPoise),
T = temperature in Kelvins and 273 K < T < 642 K,
A = -10.2158,
B = 1.7925×10⁻³,
C = 1.7730×10⁻², and
D = -1.2631×10⁻⁵.

Temperature is the only user input in the calculation screen (Figure 32). Note that 1 centiPoise = 0.01 Poise = 0.01 (g/s/cm).

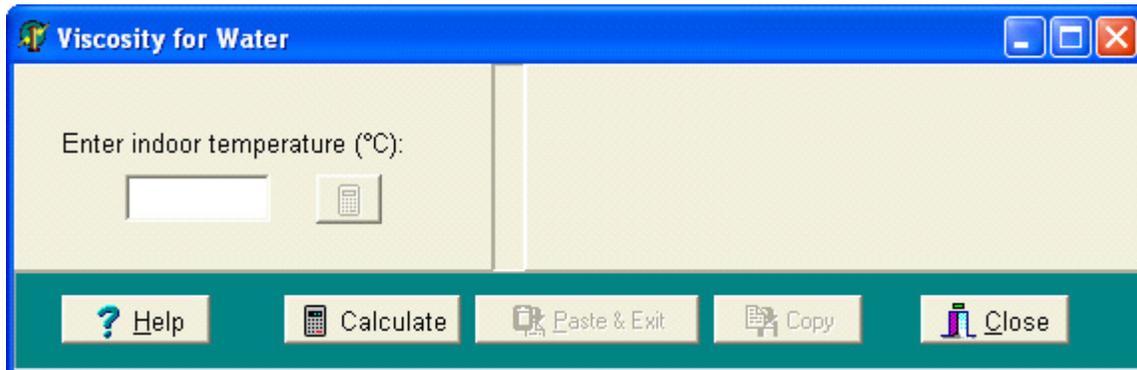**Figure 31. Calculation Screen for Water Vapor Pressure.**

Figure 32. Calculation Screen for Water Viscosity.

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16. ABSTRACT

The report describes a Microsoft Windows-based computer program that implements 30 methods for estimating the parameters in indoor emissions source models, which are an essential component of indoor air quality (IAQ) and exposure models. These methods fall into eight categories: (1) the properties of indoor air, (2) the first-order decay rate constants for solvent emissions from indoor coating materials, (3) gas-phase, liquid-phase, and overall mass transfer coefficients, (4) molar volume, (5) molecular diffusivity in air, liquid, and solid materials, (6) solid-air partition coefficient, (7) vapor pressure and volatility for pure organic compounds and petroleum-based solvents, and (8) the properties of water. Potential users include those who develop or use IAQ and exposure models and those who develop or use quantitative structure-activity relationship (QSAR) models. In addition, many calculations are useful to researchers in areas other than indoor air quality. Users can benefit from this program in two ways: first, it serves as a handy tool by putting commonly used parameter estimation methods in one place; second, it saves users time by taking over tedious calculations. It should be pointed out, however, that the methods implemented in this program cover only a fraction of the parameters that appear in the more than 50 indoor emission source models. Furthermore, the methods in the current version are mostly for gaseous pollutants; those for particulate matter are not included.