

## SECTION 1. A. English Version B. [Version française](#) C. [En Español](#)

This section explains the **general** features of **IH Mod**. Additional help on each specific model is available from each model page via a help button on the model page. Note that this workbook of models is a supplement to the book *“Mathematical Models for Estimating Occupational Exposure to Chemicals”* 2<sup>nd</sup> edition, 2009, and the book provides necessary underpinnings to select the most appropriate model, select appropriate parameters, understand the model limitations, and help understand the meaning of the calculation results. **The book is the main “go to” source for technical questions about the models and their use. Go to that reference for help with issues such as “how do I determine the generation rate?” or “which model should I use first?” or “where can I find values for the turbulent diffusion coefficient?”**

The illustration on the “User Introduction” page has labels that show most of the functions on each model sheet. Note there may be slight differences on the contents for each specific model. The Data Tables (time series of concentrations, or distance series for certain models) are shown below the graphs. Scroll down to see the full data table.

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## General Help

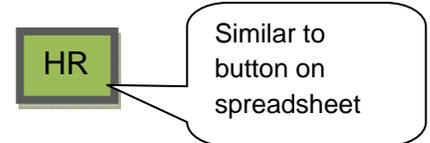
1. The user is expected to know and use Excel to open, and “save as” a working copy of **IH Mod**.
2. The Excel install for Excel 2003 should include the “Analysis Toolpak” in order for certain of the turbulent diffusion models to run correctly. These models need the “error function” (or ERF in Excel). To install, via the Excel menu tree: Tools, Add-Ins, Analysis ToolPak. You may need the install CD for the MS Office 2003 Suite to complete this. Versions of Excel prior to Excel 2003 may need an add-in called “Additional Engineering Functions” installed. The Analysis ToolPak may not need to be installed for Excel 2007.
3. Apple computers running Excel may not handle the Visual Basic coding in **IH Mod**. Thus, **IH Mod** may not run correctly or at all on Apple computers. This is based on limited initial testing on an Apple notebook computer. The testing suggests the Excel version for that system does not support the Visual Basic code used in **IH Mod**. Apple computers emulating MS Windows and using a Windows version of Excel may handle **IH Mod** adequately, but our project team has not verified this.

4. Spreadsheet Protection is enabled to prevent inadvertent changes to the equations and other functions. “**Green**” cells are for user inputs of model parameters, such as the generation rate and room ventilation. Mandatory input parameters are labeled in **red**. The model will not calculate if these **mandatory parameters are not entered**. In certain models and parameters, zero values are not allowed, and will result in the model not running. This will be obvious. As stated in the “disclaimer”, users unlocking and modifying the spreadsheet accept all responsibility for their modifications.
5. Scrolling on each model page is set so that the title and other header information remain visible.
6. More specific help on each model is provided and maybe reached via the help (?) icon on each model page. Each specific model page provides the reference to the relevant chapters of the **text “Mathematical Models for Estimating Occupational Exposure to Chemicals”**, 2<sup>nd</sup> edition, AIHA Press, 2009, C. Keil Editor. Users of **IH Mod** are expected to have the text on hand as a key reference when modeling.
7. Mathematical notation may differ SLIGHTLY for some of the equations when comparing **IH Mod** to that given in the text **“Mathematical Models for Estimating Occupational Exposure to Chemicals”**, 2<sup>nd</sup> edition, AIHA Press, 2009, C. Keil Editor. The most significant difference is in the “well mixed room with back pressure”. **IH Mod** uses an easier to implement in Excel (but equivalent in calculation results) from than in the book.
8. A column to right of the “user input parameter” unprotected cell section gives the user capability to “spin” input parameters to different values to see the effect on the calculation results, in both the graphs and data tables. Note these default to 100% of the user input parameter and can then “spin” to lower values. Modeling larger values for the parameter requires entering larger values in the user input section. There is an exception: in certain models, users may scroll to larger values of distance (using horizontal slider controls) from the generation source origin.
9. **Be careful about your** input units! **IH Mod** specifies the expected units. You may need to do some units conversions outside of **IH Mod** to assure you have the parameters in the expected units. However, **IH Mod** provides a unit conversion utility for commonly encountered units. Look on the right side of the graphs for this utility.
10. A “user calculations” column to the right in the data table segment (below the graph) of each model page is open (not protected) for use in doing any additional calculations on the data the user may wish to perform, such as determining the TWA for intervals rather than the TWA from  $t_0$  to  $t_n$ .
11. Users must set the Maximum time for simulation. The calculations for time intervals in the graphs and data columns are then based on intervals (typically 100) from zero up to this Maximum time. The user may choose and enter shorter or longer times for the simulation in order to better see the early event or late event concentrations. This version of **IH Mod** restricts the Maximum time to values less than 1440 minutes (24 hours).
12. User information will show at the base of graph IF ENTERED in the User Information block. If no user information is entered, the graphs remain unlabeled. The first “user comments” field will show with the graphs, but the second “user comment” field will show only on the “user information” block on this page.
13. Navigation buttons, print icons etc do NOT print with the page print or graph print.
14. Users can navigation from model help to general help, but navigation back from general help to the specific model is via the **IH Mod** Introduction screen.

15. The models given in **IH Mod** were all independently verified for calculation integrity. We thank AIHA members Renee Anthony, Fred Boelter, Michael Jayjock, Perry Logan, James Stewart, ,Monika Vadali, Steven Jahn in particular for their help in the calculation checks and other review procedures completed.

## High Time Resolution Option

Several of the models have an option to increase the number of time increments used in the calculation. This option is shown as a green button underneath the graph, on the left under the version number. This button looks similar to the one shown below. This button triggers a macro that inserts 5000 time-intervals over the “maximum time for simulation”. This is not the default because this can significantly slow the calculations, particularly in older computers, and the increased time-resolution is often not needed. It MAY be of use in a situation where there is a short initial release and the users wants to track the decay over a time interval significantly longer than the duration of the release.



## TWA Concentration – Alternate Estimation

An alternative to calculate the applicable TWA over a “long” period from a “short” exposure follows. This example is specifically for the NF-FF model (Two-zone model) but the principle applies to other models too. The 8 hour (480 minute) or other time period (e.g., 24 hours or 1440 minutes) time-weighted average (mg/m<sup>3</sup>) in the near field and far field equation (two zone model) can be calculated using the following relationship which is simply the average generation rate (G) in mg/min for the 8 hrs (480 minutes) or other time in minutes divided by the ventilation rate (m<sup>3</sup>/min) in the volume of interest (either NF or FF):

Thus, the-time weighted concentration for any solvent that is totally evaporated into and subsequently purged from a volume during that time is directly proportional to the mass spilled (M0) and inversely proportional to the constant ventilation rate within that volume.

$$\text{Time Weighted Average in Zone} = \left[ \frac{\left[ \frac{\text{MassEmitted}}{\text{TWATime}} \right]}{\text{Ventilationrate}} \right]$$

For example, for a mass of 5000 mg and 480 minute TWA time with a ventilation rate, far field of 50 m<sup>3</sup>/min,

$$\text{TWA 480 minute} = \frac{5000\text{mg} / 480 \text{ min}}{50\text{m}^3 / \text{min}} = 2.1 \text{ mg/m}^3$$

Ventilation rate in the far field = Q.

$$\text{Ventilation rate in the near-field} = \left[ \frac{\beta}{\beta + Q} \right] \cdot Q$$

Thus, the-time weighted concentration for any solvent that is totally evaporated into and subsequently purged from a volume during that time is directly proportional to the mass spilled (M0) and inversely proportional to the constant ventilation rate within that volume.

Note that several of the models in the current version of IH Mod give the option to estimate the mass emitted to time t based on the Generation Rate (G). This Mass Emitted estimate can be used with the formulae as shown above.

## Specific Model Comments

1. Constant Generation rates. Several of the models include Generation Rates as constant values. These models do not consider a limitation on the quantity of the material leading to the generation rate. In some circumstances, when the material is not refreshed/replaced, the concentration predictions cannot extend indefinitely. In such cases, users should determine the appropriate time course.

2. In several of the models, we have implemented a calculation to show the quantity of contaminant emitted to the time t specified by the user. This will be the time set in the scrolling Time box at the top right of the model, which can be scrolled to the “time generation cease”, or to any other time between zero “Maximum time for the simulation.” This can be used as a mass balance check if the user can estimate the initial mass of contaminant available for release.

## A Few Words about Monte Carlo Simulation with IH Mod

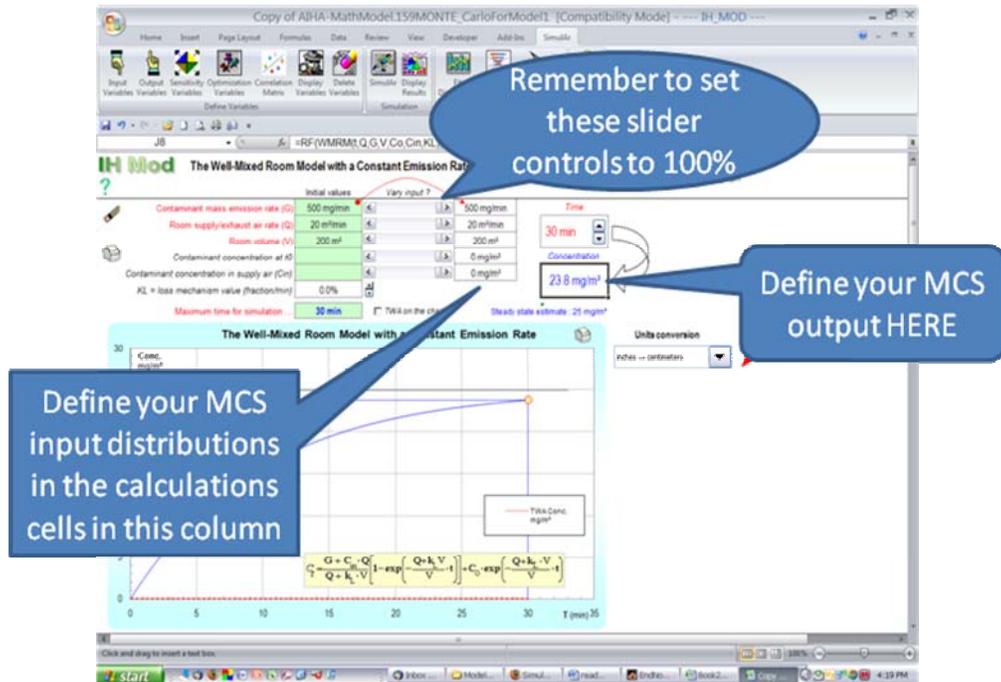
IH Mod was not intended as a tool for those with extensive need for Monte Carlo simulation (MCS) work. For extensive MCS work, a custom-built (by the user) sheet may be faster and more satisfactory. That said, one CAN do MCS work in IH Mod, with certain add-in packages. As of the time we developed this note, Crystal Ball (one of the commercial, powerful and fast MCS software packages) was not compatible with IH Mod. We have not tried other commercial MCS software, such as @Risk. However, we have tried two “FREEWARE” packages that are “add-ins” to Microsoft Excel. These work with IH Mod, albeit somewhat slowly. The faster of the two (for Excel 2007) is SimuLAR, [available at: <http://www.simularsoft.com.ar>]. SimuLAR is licensed as “emailware” meaning the developer requests users to send and share models developed using SimuLAR. The other freeware package is Simulacion [available at: [http://www.cema.edu.ar/~jvarela/index\\_eng.htm](http://www.cema.edu.ar/~jvarela/index_eng.htm)]. Note you are on your own obtaining, setting up and running these packages.

Setting up either requires un-protecting the specific model sheet used in Excel. That is (in Excel 2007) under the menu “Home, Format, Protection. Then, set up the VARY INPUT cells (to the right of the green parameter input cells in IH Mod) as the INPUT VARIABLES. Define the OUTPUT as the concentration cell on the right, below the “time” scroll controls. Note to set a relevant “max time for simulation”, make sure all parameters are set to their 100% value (via vary input? sliders). See Figure 1 (following, last page) for a screen capture illustrating these points.

## Frequently Asked Questions

(to be developed)

Fig. 1. Screen Capture Illustrating Set Up of IH Mod for Monte Carlo Simulations



Also remember to "unprotect" the worksheet!

*En Francais*

**Translation Here**

## Espanol

Translation here