USER'S GUIDE FOR THE NAPL-SCREEN AND NAPL-ADV MODELS FOR SUBSURFACE VAPOR INTRUSION INTO BUILDINGS

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Purpose

The NAPL-SCREEN and NAPL-ADV models are designed to forward calculate incremental cancer risks or noncarcinogenic hazard quotients due to subsurface soil vapor intrusion into buildings. The models are specifically designed to handle nonaqueous phase liquids or solids in soils. The user may specify up to 10 soil contaminants, the concentrations of which form a residual phase mixture. A residual phase mixture occurs when the sorbed phase, aqueous phase, and vapor phase of each chemical have reached saturation in soil. Concentrations above this saturation limit for all of the specified chemicals of a mixture will result in a fourth or residual phase (i.e., nonaqueous phase liquid or solid).

Previous vapor intrusion models (SL-SCREEN and SL-ADV) handled only a single contaminant and only when the soil concentration was at or below the soil saturation limit (i.e., a three-phase system). Use of these models when a residual phase is present, results in an overprediction of the soil vapor concentration and subsequently the building vapor concentration.

Residual Phase Theory

The three-phase system models discussed above (SL-SCREEN and SL-ADV) estimate the equilibrium soil vapor concentration at the emission source (C_{source}) using the procedures from Johnson et al. (1990):

$$C_{source} = \frac{H'_{TS} C_R r_b}{q_w + K_d r_b + H'_{TS} q_a} \qquad (1)$$

where:

C_{source}	=	Vapor concentration at the source of contamination, g/cm^3
H'_{TS}	=	Henry's law constant at the soil temperature, dimensionless
C_R	=	Initial soil concentration, g/g
r_b	=	Soil dry bulk density, g/cm^3
q_w	=	Soil water-filled porosity, cm^3/cm^3
K_d	=	Soil-water partition coefficient, cm^3/g (= $K_{oc} \times f_{oc}$)
q_a	=	Soil air-filled porosity, cm^3/cm^3
K_{oc}	=	Soil organic carbon partition coefficient, cm^3/g
f_{oc}	=	Soil organic carbon weight fraction.

In Equation 1, the equilibrium vapor concentration is proportional to the soil concentration up to the soil saturation limit. When a residual phase is present, however, the vapor concentration is independent of the soil concentration but proportional to the mole fraction of the individual component of the residual phase mixture. In this case, the equilibrium vapor concentration must be calculated numerically for a series of time-steps. For each time-step, the mass of each constituent that is volatilized is calculated using Raoult's law and the appropriate mole fraction. At the end of each time-step, the total mass lost is subtracted from the initial mass and the mole fractions are recomputed for the next time-step.

The NAPL-SCREEN and NAPL-ADV models use the procedures of Johnson et al. (1988) to calculate the equilibrium vapor concentration at the source of emissions for each time-step. Within each model, the user-defined initial soil concentration of each component in the mixture is checked to see if a residual phase is present. This is done by calculating the product of the activity coefficient of component *i* in water (a_i) and the mole fraction of *i* dissolved in soil moisture (y_i) such that:

$$a_i y_i = \frac{M_i}{\left[\left(P_i^v(T_S) q_a V / RT_S\right) + \left(M^{H2O} / a_i\right) + \left(K_{d,i} M_{soil} / a_i MW_{H2O}\right) d\left(M^{H2O}\right)\right]} \qquad (2)$$

where:

M_i	=	Initial moles of component *i* in soil, moles
$P_i^v(T_S)$	=	Vapor pressure of *i* at the average soil temperature, atm
q_a	=	Soil air-filled porosity, cm^3/cm^3
V	=	Volume of contaminated soil, cm^3
R	=	Ideal gas constant, 82.05 atm-cm^3/mol-^oK
T_S	=	Average soil temperature, ^oK
M^{H2O}	=	Total moles in soil moisture dissolved phase, moles
a_i	=	Activity coefficient of *i* in water, unitless
$K_{d,i}$	=	Soil-water partition coefficient of *i*, cm^3/g
M_{soil}	=	Total mass of contaminated soil, g
MW_{H2O}	=	Molecular weight of water, 18 g/mol
$d(M^{H2O})$	=	1 if $M^{H2O} > 0$, and
$d(M^{H2O})$	=	0 if $M^{H2O} = 0$.

If the sum of all the values of $a_i y_i$ for all of the components of the mixture is less than 1, the mixture does not contain a residual phase and the models are not applicable. In such cases, the SL-SCREEN or SL-ADV model can be used to estimate the building concentration.

Once it has been determined that a residual phase does exists, the mole fraction of each component (x_i) is determined by iteratively solving Equations 3 and 4 subject to the constraint that the sum of all the mole fractions equals unity ($\Sigma x_i = 1$):

$$x_i = \frac{M_i}{\left[\left(P_i^v(T_S) q_a V / RT_S\right) + M^{HC} + \left(M^{H2O} / a_i\right) + \left(K_{d,i} M_{soil} / a_i MW_{H2O}\right) d\left(M^{H2O}\right)\right]} \qquad (3)$$

and,

$$x_i = \frac{M_i^{HC}}{M^{HC}} \qquad (4)$$

where M_i^{HC} is the number of moles of component *i* in residual phase and M^{HC} is the total number of moles of all components in residual phase. The solution is simplified by assuming that M^{H2O} is approximately equal to the number of moles of water in the soil moisture. With the mole

fraction of each component at the initial time-step, the equilibrium vapor concentration at the source of emissions is calculated by Raoult's law:

$$C_{source} = \frac{x_i P_i^v(T_S) MW_i}{RT_S} \qquad (5)$$

where MW_i is the molecular weight of component *i* (g/mol).

At the beginning of each succeeding time-step, the number of moles of each chemical remaining in the soil from the previous time-step are again checked to see if a residual phase is present using Equation 2. When a residual phase is no longer present, the equilibrium vapor concentration at the source of emissions is calculated by:

$$C_{source} = \frac{a_i y_i P_i^v(T_S) MW_i}{RT_S}. \qquad (6)$$

Ancillary Calculations

The activity coefficient of component *i* in water (a_i) is estimated from its solubility. Because hydrocarbons are typically sparingly soluble in water, the following generalization has been applied to compounds that are liquid or solid at the average soil temperature:

$$a_i = (1/y_i) = (55.55 \text{ moles/L}) MW_i / S_i \qquad (7)$$

where S_i is the solubility of component *i* (g/L). For gases at the average soil temperature, the corresponding relationship is:

$$a_i = (1/y_i)\left(1atm / P_i^v(T_S)\right) = (55.55 \text{ moles}/L)\left(MW_i(1\ atm)/S_i P_i^v(T_S)\right). \qquad (8)$$

Assuming that the vapor behaves as an ideal gas with a relatively constant enthalpy of vaporization between 70 ^oF and the average soil temperature, the Claussius-Clapeyron equation can be used to estimate the vapor pressure at the desired temperature:

$$P^v(T_S) = P^v(T_R) \times \exp\left[\left(\frac{T_B \times T_R}{(T_B - T_R)}\right)\left(\frac{1}{T_S} - \frac{1}{T_R}\right)\ln\left(\frac{P^v(T_R)}{P_B}\right)\right] \qquad (9)$$

where:

$P^v(T_S)$	=	Vapor pressure at the desired temperature T_S, atm
$P^v(T_R)$	=	Vapor pressure at the reference temperature T_R, atm
T_B	=	Normal boiling point, ^oK
T_R	=	Vapor pressure reference temperature, ^oK
T_S	=	The desired temperature, ^oK
P_B	=	Normal boiling point pressure = 1 atm.

Building Concentration

The vapor concentration within the building or enclosed space ($C_{building}$) is calculated using the steady-state solution of Johnson and Ettinger (1991) such that:

$$C_{building} = aC_{source}. \qquad (10)$$

The steady-state attenuation coefficient (a) is calculated by:

$$a = \frac{\left[\left(\frac{D_T^{eff} A_B}{Q_{building} L_T}\right) \times \exp\left(\frac{Q_{soil} L_{crack}}{D^{crack} A_{crack}}\right)\right]}{\left[\exp\left(\frac{Q_{soil} L_{crack}}{D^{crack} A_{crack}}\right) + \left(\frac{D_T^{eff} A_B}{Q_{building} L_T}\right) + \left(\frac{D_T^{eff} A_B}{Q_{soil} L_T}\right)\left[\exp\left(\frac{Q_{soil} L_{crack}}{D^{crack} A_{crack}}\right) - 1\right]\right]} \qquad (11)$$

where:

a	=	Steady-state attenuation coefficient, unitless
D_T^{eff}	=	Total overall effective diffusion coefficient, cm^2/s
A_B	=	Area of the enclosed space below grade, cm^2
$Q_{building}$	=	Building ventilation rate, cm^3/s
L_T	=	Source-building separation, cm
Q_{soil}	=	Volumetric flow rate of soil gas into the enclosed space, cm^3/s
L_{crack}	=	Enclosed space foundation or slab thickness, cm
A_{crack}	=	Area of total cracks, cm^2
D^{crack}	=	Effective diffusion coefficient through the cracks, cm^2/s.

The reader is referred to the *User's Guide for the Johnson and Ettinger (1991) Model for Subsurface Vapor Intrusion Into Buildings (Revised)* (EQ, 2000) for a more detailed discussion of the derivation of Equation 11 and procedures for determining values for model input parameters. Except for the calculation of the equilibrium vapor concentration at the source of emissions, NAPL-SCREEN is identical to the three-phase model SL-SCREEN and NAPL-ADV is identical to the three-phase model SL-ADV.

The NAPL-SCREEN and NAPL-ADV models explicitly solve for the time-averaged building concentration over the exposure duration using a forward finite-difference numerical approach. For each time-step *dt*:

$$M_i(t+dt) = M_i(t) - dt\left(C_{building} \times Q_{building} / MW_i\right) \qquad (12)$$

where $M_i(t)$ is the number of moles of component *i* in soil at the previous time and $M_i(t+dt)$ is the number of moles at the new time. The time-step interval is variable as a function of the percent of mass lost over the time-step. The user may specify a minimum and maximum percent loss allowed; these values are applied to the single component of the residual phase mixture with the highest mass loss rate during each time-step interval. If the user-specified maximum percent

loss is exceeded, the next time-step interval is reduced by half; likewise, if the user-specified minimum percent loss is not achieved, the next time-step interval is increased by a factor of two. The instantaneous building concentration at time = t is calculated using Equation 10 for each time-step. The time-averaged building concentration is estimated using a trapezoidal approximation of the integral.

Model Assumptions and Limitations

The NAPL-SCREEN and NAPL-ADV models operate under the assumption that sufficient time has elapsed since the time of initial soil contamination for steady-state conditions to have been achieved. This means that the subsurface vapor plume has reached the bottom of the enclosed space floor and that the vapor concentration has reached its maximum value. An estimate of the time required to reach near steady-state conditions (t_{ss}) can be made using the following equations from API (1998):

$$t_{ss} \cong \frac{R_v q_a L_T^{\,2}}{D^{eff}} \qquad (13)$$

and,

$$R_v = 1 + \frac{q_w}{q_a H'_{TS}} + \frac{r_b K_d}{q_a H'_{TS}} \qquad (14)$$

and,

$$D^{eff} = D_a \frac{q_a^{10/3}}{n^2} + \left(\frac{D_w}{H'_{TS}} \right) \frac{q_w^{10/3}}{n^2} \qquad (15)$$

where R_v is the unitless vapor phase retardation factor, L_T is the source-building separation (cm), D^{eff} is the effective diffusion coefficient (cm^2/s), D_a is the diffusivity in air (cm^2/s), D_w is the diffusivity in water (cm^2/s), and n is the soil total porosity (cm^3/cm^3). The NAPL-SCREEN and NAPL-ADV models are applicable only when the elapsed time since initial soil contamination meets or exceeds the value of t_{ss} (see **Using the Models**).

Emission source depletion is calculated by estimating the rate of vapor loss as a function of time such that the mass lost at each time-step is subtracted from a finite mass of contamination at the source. This requires the model user to estimate the dimensions of the emission source, e.g., the length, width, and thickness of the contaminated zone. The model should only be used, therefore, when the extent of soil contamination has been sufficiently determined. It should be noted that because the NAPL-SCREEN and NAPL-ADV models are one-dimensional, the areal extent of soil contamination (i.e., length × width) can be less than but not greater than the areal extent of the building floor in contact with the soil.

Each model treats the contaminated zone directly below the building as a box containing a finite mass of each specified compound. The initial contamination contained within the box is assumed to be homogeneously distributed. After each time-step, the remaining contamination is assumed to be instantaneously redistributed within the box to homogeneous conditions. The diffusion path length from the top of contamination to the bottom of the enclosed space floor therefore remains constant with time. Use of this simplifying assumption means that the degree of NAPL soil saturation is not required in the calculation of the total overall effective diffusion coefficient (D_T^{eff}).

As time proceeds, the concentration of the mixture of compounds within the soil column may reach the soil saturation limit. Below this point, a residual phase will cease to exist and the vapor concentration of each chemical will decrease proportional to its total volume soil concentration. Theoretically, the vapor concentration will decrease asymptotically, approaching but never reaching zero. Because of the nature of the numerical solution to equilibrium vapor concentration, however, compounds with high effective diffusion coefficients (e.g., vinyl chloride) may reach zero soil concentrations while other less volatile contaminants will not. If the initial soil concentrations are significantly higher than their respective values of the soil saturation concentration, a residual phase may persist up to the user-defined exposure duration.

Model assumptions and limitations concerning vapor transport and vapor intrusion into buildings are those specified for the SL-SCREEN and SL-ADV three-phase models. The user is referred to EQ (2000) for a discussion of these assumptions and limitations.

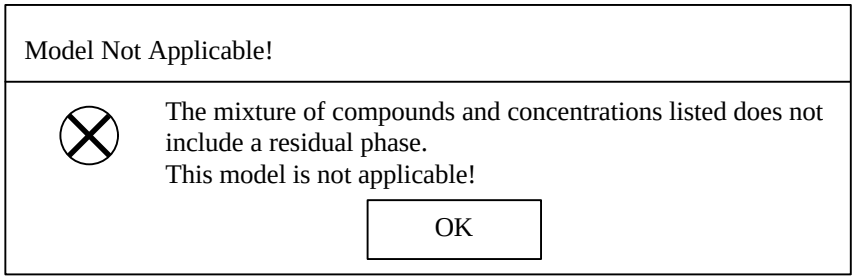
Using the Models

Each model is constructed as a Microsoft® Excel workbook containing five worksheets. The DATENTER worksheet is the data entry worksheet and also provides model results. The VLOOKUP worksheet contains the "Chemical Properties Lookup Table" with 93 listed chemicals and associated chemical and toxicological properties. It should be noted that the toxicological properties for many of these chemicals were derived by route-to-route extrapolation (see Appendix C of EQ, 2000). In addition, the VLOOKUP worksheet includes the "Soil Properties Lookup Table" containing values for model intermediate variables used in estimating the soil vapor permeability. The CHEMPROPS worksheet provides a summary of the chemical and toxicological properties of the soil contaminants selected by the user. In addition, the CHEMPROPS worksheet provides calculated values for the soil saturation concentration (C_{sat}) and the time to reach steady-state conditions (t_{ss}) once all required data are entered into the DATENTER worksheet. The INTERCALCS worksheet contains calculated values of intermediate model variables. Finally, the COMPUTE worksheet contains the numerical solutions for equilibrium vapor concentration and building vapor concentration as a function of time.

Both models use the Microsoft® SOLVER add-in algorithms to simultaneously solve Equations 3 and 4 for each of up to 10 chemicals specified by the user. In order to run NAPL-SCREEN or NAPL-ADV, the SOLVER add-in must be loaded into EXCEL. The user is referred to the EXCEL instructions for loading the SOLVER add-in.

On the DATENTER worksheet, the user may specify up to 10 soil contaminants by CAS number along with associated soil concentrations in units of mg/kg. The CAS number entered must match exactly one of the 93 chemicals listed in the VLOOKUP worksheet or the error message "CAS No. not found" will appear in the "Chemical" box. If the list of chemicals and concentrations entered does not constitute a residual phase, the error message in Figure 1 will appear after starting the model.

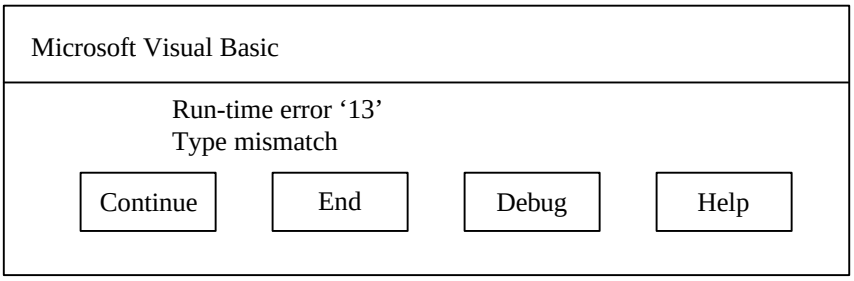
Figure 1. Residual Phase Error Message



If this error message box appears, use either the SL-SCREEN or SL-ADV model to estimate subsurface vapor intrusion into the building.

After starting the model calculations, other error message boxes may appear if data entry values are missing on the DATENTER worksheet or if entered values do not conform to model assumptions. If such an error message box appears, fill-in missing data or re-enter data as appropriate. If entered data values are outside the expected range or if text values are entered where numeric values are expected, the model calculation macro will be suspended and the run-time error message in Figure 2 will appear.

Figure 2. Run-Time Error Message



Should this error message appear, click on the "End" button to terminate the macro and return to the DATENTER worksheet. At this point, the user should review all of the entered values and make the appropriate corrections.

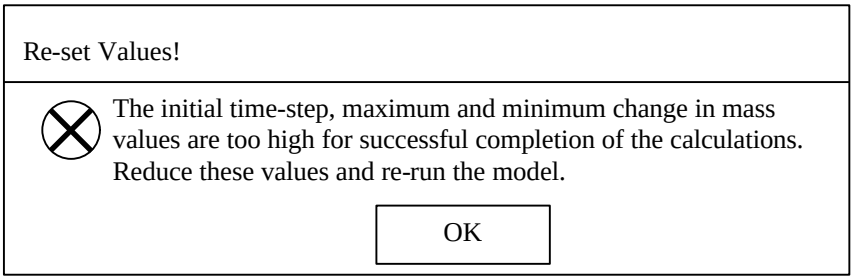
In addition to contaminant data, soil properties data, zone of contamination data, and exposure assumptions must also be specified in the DATENTER worksheet. Similar to the SL-SCREEN three-phase model, the NAPL-SCREEN model allows for only one soil stratum between the top of contamination and the bottom of the building floor in contact with the soil. In addition, the NAPL-SCREEN model uses built-in default values for all building variables (e.g., building dimensions, air exchange rate, total crack area, etc.). These default values are for

single-family detached residences; therefore, the NAPL-SCREEN model should only be used for the residential exposure scenario.

The NAPL-ADV model, like the SL-ADV model, allows for up to three different soil strata between the top of contamination and the bottom of the building floor. In addition, the NAPL-ADV model allows the user to enter values for all model variables. This allows for the estimation of soil vapor intrusion into buildings other than single-family residences. The user is referred to EQ (2000) for a discussion of model input variables.

For each model, the user must also enter the duration of the first (initial) time-step interval. The maximum and minimum change in mass for each time-step must also be specified. The values of the initial time-step interval, and the maximum and minimum change in mass are important. If these values are too low, the model will calculate very small increments in the mass lost over time which will greatly extend the run-time of the model. In general, if the concentrations of the least volatile chemicals in the mixture are well above their respective values of the soil saturation concentration, a relatively large initial time-step interval, and maximum and minimum change in mass should be specified (e.g., 4 days, 10%, and 5%, respectively). For comparison, the value of the soil saturation concentration (C_{sat}) for each chemical specified by the user may be found in the CHEMPROPS worksheet after all data have been entered on the DATENTER worksheet. If, however, the soil concentrations of the most volatile constituents are very close to their respective saturation limits, large values of the initial time-step interval, and the maximum and minimum change in mass will result in the error message in Figure 3 after starting the model.

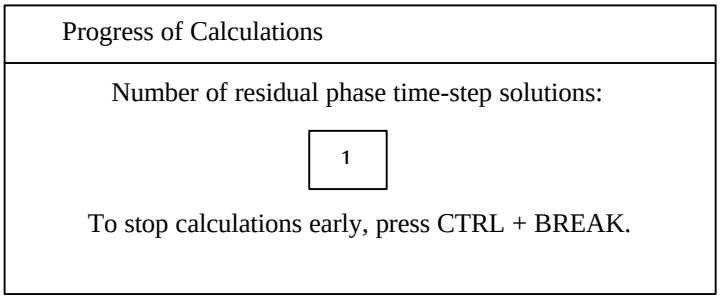
Figure 3. Time-Step and Change in Mass Error Message



Should this error message occur, reduce the value of the initial time-step interval and the values of the maximum and minimum change in mass to smaller values and re-run the model. The error message will be repeated until the values of these variables are sufficiently small.

After all required data are entered into the DATENTER worksheet, the model is run by clicking on the “Execute Model” button which will change from reading “Execute” to “Stand by...”. In addition, the message box in Figure 4 will appear keeping a running count of the number of residual phase time-step solutions achieved by the model.

Figure 4. Progress of Calculations Message Box

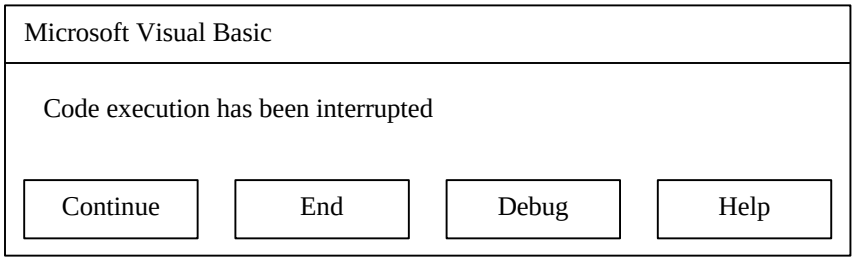


Each SOLVER trial solution can also be seen running in the status bar at the bottom of the screen. When the model is finished calculating, the "Execute Model" button will read "Done" and the Progress of Calculations message box in Figure 4 will disappear. The time-averaged building concentrations, incremental cancer risks, and/or hazard quotients will then be displayed under the "RESULTS" section of the DATENTER worksheet. In addition, an "X" will appear beside the calculated risk or hazard quotient of each contaminant for which a route-to-route extrapolation was employed. It should be noted that a route-to-route extrapolation was used for any chemical without a unit risk factor (URF) or a reference concentration (RfC) as specified in the EPA 1996 Soil Screening Guidance. Therefore, the user should evaluate the resulting cancer risks and/or hazard quotients of such chemicals. Once a solution has been achieved and the user wishes to save the results, the file should be saved under a new file name. If the user wishes to delete all of the data previously entered on the DATENTER worksheet, this may be accomplished by clicking on the "Clear Data Entry Sheet" button.

Stopping Calculations Early

As mentioned previously, the user-defined values of the initial time-step interval, and the maximum and minimum change in mass should be chosen carefully. If the model run-time is excessive or if the user simply wishes to terminate the calculations, the model may be stopped by pressing CTRL + BREAK. If termination occurs in-between SOLVER solutions, the message box in Figure 5 will appear.

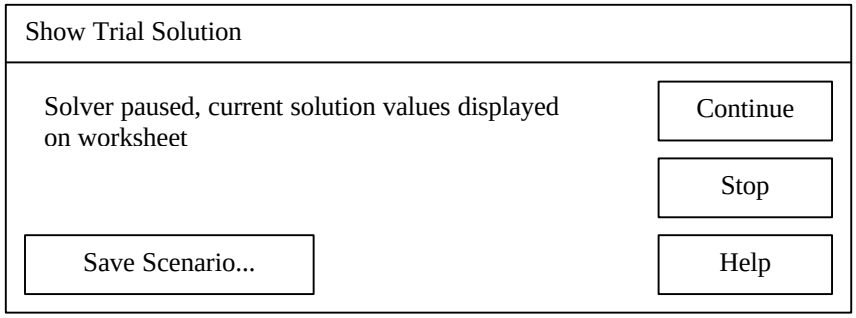
Figure 5. Code Interruption Message Box



If this message box appears, click on the "End" button to terminate the macro.

If the termination occurs during a SOLVER solution, the message box in Figure 6 will appear. If this message box appears, click on the "Stop" button. This will stop the SOLVER solution but not the program macro. Depending on where in the macro code the interruption occurs, the model may continue to operate after clicking on the "Stop" button in Figure 6. If this happens, press CTRL + BREAK again. At this point, the message box in Figure 5 will appear; click on the "End" button to terminate the macro.

Figure 6. Solver Interruption Message Box



At this point, the user may examine the model results up to the point of termination on the COMPUTE worksheet. The values of the "Change in mass", the "Time-step interval", and the "Cumulative time" should be examined to determine if changes are necessary in the values of the initial time-step interval, and the maximum and minimum change in mass. After these or any other values are changed on the DATENTER worksheet, the model may be re-run by clicking on the "Execute Model" button.

Step-By-Step Procedures for Running the Models

The following gives the step-by-step procedures for running either the NAPL-SCREEN or the NAPL-ADV model.

1. On the DATENTER worksheet, enter the CAS number of each soil contaminant in the residual phase mixture (do not include dashes in the CAS numbers). After the CAS numbers have been entered, the respective chemical names will appear in the "Chemical" box.

2. On the DATENTER worksheet, enter the soil concentration of each contaminant in units of mg/kg as well as values for all remaining variables except the "Initial time-step", the "Maximum change in mass", and the "Minimum change in mass".

3. On the CHEMPROPS worksheet, note the calculated values of the "Time to steady state" (t_{ss}) for each contaminant. Calculated values of the time-averaged building concentration and associated risks for contaminants with values of t_{ss} greater than the actual elapsed time since initial soil contamination will be artificially high.

4. On the CHEMPROPS worksheet, note the calculated values of the "Soil saturation concentration" (C_{sat}) for each contaminant. Use these data to help determine appropriate user-defined values for the initial time-step, and the maximum and minimum change in mass.

Typical values for these variables might be 2 days, 7%, and 4%, respectively, but may be considerably higher or lower depending on the number of chemicals in the analysis and the starting soil concentrations (see the discussion on page 8).

5. Click on the "Execute Model" button to begin the model calculations. If data are missing on the DATENTER worksheet, or entered values do not conform to model assumptions, an error message box will appear after the model is started informing the user of the type of error encountered. Enter the appropriate values on the DATENTER worksheet and re-run the model. Once the model has successfully started, note the number of residual phase time-step solutions achieved by the model in the Progress of Calculations message box (Figure 4). Use this information to help establish new values for the initial time-step interval and the maximum and minimum change in mass if the number of time-steps needs to be increased or decreased.

6. When the NAPL-SCREEN model has finished calculating, check column "O" on the COMPUTE worksheet to determine how many time-steps were calculated while a residual phase was present; one time-step is equal to one row (when using the NAPL-ADV model check column "P"). A residual phase is present when the value in column "O" or "P", as appropriate, is equal to 1.000. In general, a greater number of time-steps means a more accurate estimate of the time-averaged building concentration. If the starting soil concentrations of the most volatile contaminants are very close to their respective values of C_{sat}, a minimum of 5 to 10 time-steps should be calculated by the model. For all other cases, a reasonable number of time-steps is between 40 and 70. To increase the number of time-steps calculated by the model, decrease the values of the initial time-step interval and the maximum and minimum change in mass. The opposite is true when the number of time-steps is to be decreased.

7. If the message box in Figure 1 appears after starting the model, the mixture of compounds and concentrations specified does not include a residual phase. Use the SL-SCREEN or SL-ADV model to calculate indoor air concentrations and risks for each contaminant separately.

8. If the message box in Figure 3 appears after starting the model, reduce the input values of the initial time-step, and maximum and minimum change in mass and re-run the model.

9. If the run-time of the model is excessive, terminate the model macro by pressing CTRL + BREAK (see the discussion under **Stopping Calculations Early** on pages 9 and 10). Examine the calculated values of the "Change in mass", the "Time-step interval", and the "Cumulative time" on the COMPUTE worksheet. Re-enter new lower values for the initial time-step interval, and the maximum and minimum change in mass and re-run the model.

10. After successful completion of a model run, note the calculated values of the "Time-averaged building concentration", "Incremental cancer risk", and/or "Hazard quotient" in the "RESULTS" section of the DATENTER worksheet. Also note for which contaminants a route-to-route extrapolation was employed. <u>If the model results are to be retained, save the file under a new file name</u>.

Adding, Deleting or Revising Chemical Data

Up to 150 chemicals can be listed in the "Chemical Properties Lookup Table" within the VLOOKUP worksheet. To add, delete or revise chemicals, the VLOOKUP worksheet must be unprotected using the password "ABC" in capital letters. Row number 171 is the last row that may be used to add new chemicals. If new chemicals are added or chemicals deleted, the user must sort all the data in the "Chemical Properties Lookup Table" (except the column headers) in ascending order by CAS number. After sorting is complete, the worksheet should again be protected.

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