#### Introduction

The Waste Reduction Algorithm Graphical User Interface (WAR GUI) was developed to compare the environmental friendliness of chemical process designs ( <u>Hilaly and Sikdar, 1994</u>). The WAR GUI does not contain a process simulator. However, the interface allows the user to enter process design information for several different designs in order to compare them on an environmental basis. The pertinent process design information includes the chemicals used, the flow rates of the streams entering and leaving the process, and the energy usage of the process.

The WAR algorithm involves the concept of a <u>Potential Environmental Impact</u> (PEI) balance (analogous to a mass or energy balance) (<u>Cabezas et al., 1999</u>). The balance involves the flow of environmental impact across system boundaries (as opposed to mass or energy). The flow of impact can be due to mass or energy crossing the system boundaries (<u>Young and Cabezas, 1999</u>). From the PEI balance, PEI indexes are calculated which provide a relative indication of the environmental friendliness or unfriendliness of the chemical process.

### Theory

The overall impact balance for a general chemical process is illustrated in Figure 1:



Figure 1. The overall impact balance around a chemical process facility including the energy generation facility. The system boundary is designated with a dashed line.

The potential environmental impact balance is as follows:

$$\frac{\partial [I_t]}{\partial t} = \dot{I}_{in}^{(cp)} + \dot{I}_{in}^{(ep)} - \dot{I}_{out}^{(cp)} - \dot{I}_{out}^{(ep)} - \dot{I}_{we}^{(cp)} - \dot{I}_{we}^{(ep)} + \dot{I}_{gen}^{(t)}$$
(1)

For steady state processes, Equation (1) reduces to

$$0 = \dot{I}_{in}^{(cp)} + \dot{I}_{in}^{(ep)} - \dot{I}_{out}^{(cp)} - \dot{I}_{out}^{(ep)} - \dot{I}_{we}^{(cp)} - \dot{I}_{we}^{(ep)} + \dot{I}_{gen}^{(t)}$$
(2)

The waste energy emissions of both the chemical process and the energy generation process will be neglected since these will have minor impacts when compared to the amount of energy and materials that are consumed and produced through non-fugitive streams. Also, the impact of the input streams to the energy process will be neglected (Young and Cabezas, 1999). This reduces Equation (2) to

$$0 = \dot{I}_{in}^{(cp)} - \dot{I}_{out}^{(cp)} - \dot{I}_{out}^{(ep)} + \dot{I}_{gen}^{(t)}$$
(3)

The environmental impact of the energy usage of a chemical process is accounted for in the impact of the streams leaving the energy generation process (expressed in the third term in Equation 3). Click <u>here</u> for more information on the calculation of the impact of energy generation.

This can be re-written yet again as

$$0 = \dot{I}_{in}^{(t)} - \dot{I}_{out}^{(t)} + \dot{I}_{gen}^{(t)}$$
(4)

The **total input rate of PEI** can be approximated by known and measurable quantities by

$$\dot{I}_{in}^{(t)} = \sum_{i}^{EnvCat} \left[ \alpha_i \middle| \dot{I}_{i,in}^{(t)} \right] = \sum_{i}^{EnvCat} \alpha_i \sum_{j}^{Streams} \sum_{k}^{Comps} \left[ x_{kj} \middle| \psi_{ki}^s \right] + \dots$$
(5)

In the current version of WAR, the combinatorial effects resulting from chemical mixtures (the additional terms given in equation 5) are neglected.

The **normalized impact score** for chemical *k* for category *i* is calculated using the following normalization scheme:

$$\psi_{ki}^{s} = \frac{\left[ (Score)_{ki} \right]}{\left[ \left\langle (Score)_{k} \right\rangle_{i} \right]}$$
(6)

Potential Environmental Impact Indexes

Equations 4-6 can be used to generate indexes that characterize the relative environmental efficiency of a process. There are two different classes of indexes: those associated with PEI output and those associated with PEI generation.

The **total output rate of PEI** (or total output PEI index) can be approximated using an equation similar to the one used for the total input rate of PEI:

$$\dot{I}_{out}^{(t)} = \sum_{i}^{EnvCat} \alpha_i \left[ \dot{I}_{i,out}^{(t)} \right] = \sum_{i}^{EnvCat} \alpha_i \sum_{j}^{Streams} \sum_{k}^{Comps} x_{kj} \psi_{ki}^{s}$$

$$(7)$$

In the calculation of the output PEI index the user can decide whether or not to include the impact of the product streams. For example if the product is the feedstock for another process one may not want to include its impact in the analysis.

The **total PEI generation rate** (or total PEI generation index) can then be calculated from Equations (4-7).

The output and generation PEI indexes can be evaluated on rate basis (PEI/time) or on a production basis (e.g. PEI/mass of product). The indexes presented so far are in terms of rate evaluations, PEI/time. To evaluate the PEI output index on a production basis, a simple transformation can be made



A similar transformation can be made to convert the PEI generation index into terms of PEI/mass of product

$$\hat{I}_{gen}^{(t)} = \frac{\dot{I}_{gen}^{(t)}}{\frac{\Pr odStreams}{p}} \sum_{p} \dot{P}_{p}$$
(9)

The intended use of the WAR Algorithm is to provide a means for comparing the PEI of alternative designs for a process. In the WAR Algorithm, the four indexes shown in Equations (8-9) are used to compare the environmental friendliness of the possible process designs. Designs with lower PEI index values represent more environmentally desirable designs.

For a more detailed discussion on the interpretation of the results from the WAR GUI, click <u>here</u>.

Click here for Nomenclature

### Specific Chemical Environmental Impacts

To provide an indication of the potential environmental impact of a chemical process, a database of relative environmental impact scores has been created for as many as chemicals as data are available drawing on government and non-government sources.

Eight different categories of impact potential are considered:

<u>Human Toxicity Potential by Ingestion</u> or HTPI, <u>Human Toxicity Potential by Inhalation or Dermal Exposure</u> or HTPE, <u>Ozone Depletion Potential</u> or ODP, <u>Global Warming Potential</u> or GWP, <u>Photochemical Oxidation Potential</u> or PCOP <u>Acidification Potential</u> or AP, <u>Aquatic Toxicity Potential</u> or ATP, and <u>Terrestrial Toxicity Potential</u> or TTP.

### Weighting Factors

Weighting factors are used to combine PEI categories into a single PEI index (see Equations 5 and 7). They represent the relative or site-specific concerns of the user. For instance, if the user was evaluating a process that was located in the Los Angeles area the weighting factor for smog formation (PCOP) would probably receive a high value. Whereas, if the user was evaluating a process in the Northeast the weighting factor for acid rain (AP) would probably receive a high value. The default values used in this program weight all the categories equally.

The user, however, has wide latitude to weight the relative importance of these environmental effects to suit particular applications.

# Nomenclature

In order of appearance:

Symbol	Definition	Units	
$I_t$	Total Amount of potential environmental impact inside the system	PEI/time	
$\dot{I}_{in}^{(cp)}$	Input rate of PEI to the chemical process	PEI/time	
$\dot{I}_{in}^{(ep)}$	Input rate of PEI to the energy generation process	PEI/time	
$\dot{I}_{out}^{(cp)}$	Output rate of PEI to the chemical process	PEI/time	
$\dot{I}_{out}^{(ep)}$	Output rate of PEI to the energy generation process	PEI/time	
$\dot{I}_{we}^{(cp)}$	Output rate of PEI from waste energy lost from the chemical process	PEI/time	
$\dot{I}_{we}^{(ep)}$	Output rate of PEI from with waste energy lost from the energy generation process	PEI/time	
$\dot{I}_{gen}^{(t)}$	Total generation rate of PEI	PEI/time	
$\dot{I}_{in}^{(t)}$	Total input rate of PEI	PEI/time	
$\dot{I}_{out}^{(t)}$	Total output rate of PEI	PEI/time	
$\alpha_i$	Weighting factor associated with impact category <i>i</i>	dimensionless	
$\dot{I}^{(t)}_{ijn}$	Total input rate of PEI for impact category <i>i</i>	PEI/time	
$\dot{M}_{j,m}$	Mass flow rate of input stream <i>j</i>	mass/time	
$x_{kj}$	Mass fraction of component k in stream <i>j</i>	mass of chemical k / mass of stream j	
$\Psi_{ki}^{s}$	Normalized impact score for chemical k for category i	PEI/mass of che mical k	

Continued...

Symbol	Definition	Units	
$(Score)_{ki}$	Impact value of chemical k on some arbitrary scale for category <i>i</i>	varies for each category	
$\langle (Score)_k \rangle_i$	Average impact value for all chemicals in category <i>i</i>	varies for each category	
$\dot{I}_{i,out}^{(t)}$	Total output rate of PEI for impact category i	PEI/time	
$\dot{M}_{j,out}$	Mass flow rate of output stream <i>j</i>	mass/time	
$\hat{I}_{out}^{(t)}$	Total PEI leaving the system per mass of products leaving the system	PEI/mass of product streams	
$\dot{P_p}$	Mass flowrate of the product stream $p$	mass/time	
$\hat{I}_{gen}^{(t)}$	Total PEI generated within a system per mass of products leaving the system	PEI/mass of product streams	

### Interpretation of the results of the WAR GUI

The WAR GUI allows the user to calculate several <u>potential environmental impact</u> <u>indexes</u>. In general processes with lower PEI indexes will be more environmentally friendly. From the PEI indexes one can identify the most environmentally friendly process design from several alternatives. However, the need to design processes with lower PEI must be constrained by the considerations of engineering economics and the human need for the products that the process manufactures.

The **total output rate of PEI** allows one to compare alternative processes in terms of the potential effect on the environment external to the process. The total output rate of PEI is most useful in assessing whether a particular site is able to accommodate a given process plant. For example a process with a low output rate of PEI could be located in a more ecologically sensitive area than would be the case for a process with a high rate of impact output.

The **total generation rate of PEI** allows one to compare different processes in terms of their generation of new PEI within the process. The generation rate of PEI is important because once it is created, it will likely take resources to keep the PEI from becoming actual impacts on the environment. The total generation rate of PEI allows one to determine if the chemical reactions occurring within the process produce products that are less environmentally friendly than the feed stock chemicals.

The total PEI leaving the system per mass of products and the total PEI generated within a system per mass of products allow one to compare alternative processes regardless of the manufacturing plant size. For example, one can compare the environmental consequences of having one large plant versus several small ones. The amount of PEI per mass of products decreases if the amount of PEI emitted has decreased or because the mass flow rates of the product streams have increased or both. This illustrates that by lowering the amount of PEI per mass of products one also improves the material utilization efficiency of the process.

### Product vs. Nonproduct analysis

The default setting for the program is **not** to include the environmental impact of the product streams in the analysis. In general one should not be penalized for manufacturing a product that has market value. Thus one should focus on minimizing the environmental impact of the waste streams, the by-product streams, and the energy produced by the process. One should include the impact of the product streams if a stream is likely to be emitted into the environment (e. g. consumer products) or if one is evaluating several different product alternatives. One should not include a product if the product is simply an intermediate product that will be directly used as a feed elsewhere in the manufacturing facility.

## Impact of energy consumption

The energy consumption of a process has an effect on the total potential environmental impact of a process (click <u>here</u> for further information). In general a reduction in the energy consumption of a process will also reduce the potential environmental impact of a process. However in some cases decreasing the energy usage may increase the PEI of a process. For example if one decreases the reflux ratio of a product distillation column the energy usage will decrease but the separation efficiency will also decrease. This causes a larger amount of the product to be present in the waste stream, which then may increase the PEI of the process. One may choose not to include the impact of energy generation if the energy generation is unknown or is assumed to have a negligible impact.

## Tutorial

In this tutorial we will evaluate the environmental friendliness of two process designs used to produce phthalic anhydride. The first design produces phthalic anhydride from o-xylene and the second design produces it from naphthalene. The process flow diagram for the process that uses o-xylene is as follows:



Phthalic anhydride

The first step is to create a new case history file. Do this by clicking on the **New** case history file button (located next to Step 1). This creates a blank case history file ("Untitled.war").

The second step is to add the first case study. Open the Add case screen by clicking on the **New case study** button (located next to Step 2). Case studies that will be compared are stored in the same case history file.

Name the first case study "Unit 700" (in the text box next to Step 2a).

For the description of Unit 700 type "o-xylene feed stock" (Step 2b).

Once the case study is added to the case history file, the next step is to add chemicals to the case study.

## Adding chemicals to the Unit 700 case study

Open the add chemicals screen by clicking on the **Edit/Add Chemicals** button (Step 2c). Chemicals can be added to the case study by a number of ways. This tutorial will discuss them all.

First, we'll add chemicals by using the Chemical Abstract Service (CAS) registry number. Click on the **Search by CAS Number** option button. This loads a list of CAS numbers. The first chemical we want to add is phthalic anhydride. Type "85-44-9" in the search text box. When the CAS number for phthalic anhydride appears, single click on it. This will display "phthalic anhydride" in the name box below the list of CAS numbers. The chemical can be added to the case study by double clicking on its CAS number in the list or by clicking on the **Add from list** button.

Next, we'll add chemicals by their name. Click on the **Search by Name** option button. This loads a list of chemical names. The next chemical we want to add is "maleic anhydride". Type "maleic anhydride" in the search text box. When "maleic anhydride" is highlighted in the list box add it to the case study.

Next, we'll add chemicals by their chemical formula. Click on the **Search by formula** option button. This loads a list of chemical formulas. The next chemical we want to add is o-xylene. Type its formula (C8H10) in the search text box. Double click on the formula when it appears. This brings up a list of all chemicals in the database with this formula. If one clicked on the wrong formula one can reload the list of formulas by clicking on the **Up** button located next to the list box. Add o-xylene to the case study.

Next, we'll add chemicals by the substring of their name. Click on the **Search by Substring** option button. The next chemical we want to add is oxygen. Type "oxyg" in the search text box. The list box below should then display oxygen since it is the only chemical in the database with the substring "oxyg". Add oxygen to the case study.

Add water, carbon dioxide and nitrogen (in that order) by using the any of the options just discussed.

View the data for phthalic anhydride by double clicking on it in the list chemicals in the case study (or single click on its name in the list and click on the **View/edit chemical** button). Change the impact value for Fathead minnow LC50 to 9.4 mg/L. Click on the **Calculate scores** button to update the normalized score in the text box on the right. Restore the literature value by clicking on **Restore Default Values**. Click **OK** to return to the Add chemicals screen.

For practice, let's add the wrong chemical to chemical list and then delete it. Click on the **Search by CAS Number** option button. Add p-chloronitrobenzene (CAS

number: 100-00-5) to the case study. Delete this p-chloronitrobenzene by clicking on its name in the list of chemicals in the case study and clicking the **Delete Chemical** button.

Click here for screen shot of what Add chemicals screen should look like.

Click **OK** to close the Add chemicals screen.

#### Adding streams to the Unit 700 case study

The next step is to add input and output streams to our case study. Click on **Edit/Add Streams** to open the Add streams screen (Step 2d).

The units for our flowrate data is in kg/hr. To display the proper units first click on the **Options** button. Make sure that "kg" is selected on the **Mass units** combo box and "hr" is selected on the **Time units** combo box. We are going to add stream data using the mass fractions of the components so make sure that the **mass fractions** option is selected in the component data frame. Click on the **OK** button to return to the Add streams screen.

Click on the **Add stream** button (it should be flashing). Enter "Air feed" as the name for the first stream (in the text box below the **Delete** button).

Click on the box below the stream name in the grid to choose a stream type. Choose "Inlet" from the drop down list. The column width can be resized if necessary.

Click on the box below the stream type and enter a flow rate of 63967 kg/hr.

The Air feed stream contains only oxygen and nitrogen so enter a mass fraction of 0.2330 for oxygen and 0.7670 for nitrogen. All other components have a mass fraction of zero for the Air feed stream.

Enter data for the remaining streams as follows:

Name	o-Xylene feed	Waste gas	Maleic anhydride	Phthalic anhydride
Туре	Inlet	Outlet Waste	Outlet Waste	Product
Flow rate	10469	62634	1750	10044
X(PHTHALIC ANHYDRIDE)	0.0000	0.0016	0.0412	0.9993
X(MALEIC ANHYDRIDE)	0.0000	0.0014	0.9588	0.0007
X(o-XYLENE)	1.0000	0.0025	0.0000	0.0000
X(OXYGEN)	0.0000	0.0089	0.0000	0.0000
X(WATER)	0.0000	0.0947	0.0000	0.0000
X(CARBON DIOXIDE)	0.0000	0.1075	0.0000	0.0000
X(NITROGEN)	0.0000	0.7833	0.0000	0.0000

Click on the **Check mass balance** button. A message box should indicate that the total inlet flow rate is nearly equal to the outlet flow rate (within 1%).

Click here for screen shot of what Add streams screen should look like.

Click **OK** to close the Add streams screen.

### Completing the Unit 700 case study

The user has the option of including the energy consumed by the process into the calculation of its environmental friendliness. It is up to the user to determine this amount.

For this case study, enter an energy usage of 62,035 MJ/hr (in the text box next to Step 2e).

Select "Coal" for the fuel type.

Click **OK** to complete the addition of the case.

Click on the **Edit Cases** button (next to Step 3). Click on the **View/Edit Chemicals** button and verify that the list of chemicals in the case study is correct. Click on the **View/Edit Streams** button and verify that the stream data is correct.

Click **OK** to return to the main screen.

Click the **View/Edit Weights** button (next to Step 4) to open the Impact weights screen.

The weights for all the impact categories are set to unity by default. The weights can be adjusted by typing in the text boxes provided or by dragging the slider bars. For example the acidification potential can be more heavily weighted by moving its slider bar to 3. For this tutorial we want to keep all the weights equal to unity. Click on the **Default** button to set all the weights equal to unity.

Click **OK** to return to main screen.

Save the case history file by selecting **Save case history file as ...** from the **File** menu. Save the file as "tutorial.war".

Note: A complete case history file for the tutorial ("unit 700 (for tutorial).war") is included in the MyFiles directory.

## Adding the Unit 701 Case Study

In the next case study (Unit 701), phthalic anhydride is produced from naphthalene. The process flow diagram for this process is as follows:



Instead of inputting all of the data manually as we did for the previous case study, we will import the data for this case study directly from an ASPEN Plus report file.

## Importing unit 701 case study information from ASPEN

The program will read in chemical and stream information that is found in an ASPEN PLUS report file (.rep). For chemical information, the program will focus on the formula for the chemicals. If there is only one match in the WAR database for a particular formula, the program will automatically assign the chemical name and CAS number associated with that formula. The user should verify that the program has assigned the correct chemical to the case study.

If more than one match is found in the WAR database for a particular formula, the user will have to select the proper chemical by double clicking on that chemical in the grid.

Begin importing the file by clicking on the **Import case study from ASPEN** button.

Select "napthalene.rep" from the list of files in the MyFiles directory and click on **Open**.

## Completing the Unit 701 case study

Click the **Finish** button to finish importing the ASPEN file.

The program informs us that it had to convert from molar flowrates to mass flow rates and reminds us to check the stream types for each stream. Finally it signals the completion of file import.

Clicking on the finish button opens the Edit case screen automatically.

Change the name of the case to "Unit 701" (in the case name field).

Enter "naphthalene feed stock" in the case description text box.

Click on the **View/Edit Chemicals** button and verify that the list of chemicals in Unit 701 is correct. Click **OK** button to return to the Edit case screen.

Click on the **View/Edit Streams** button. Phthalic anhydride is the product for our process so change the stream type for the PHTHANHY stream to "Product". Click **OK** button to return to the Edit case screen.

Enter an energy usage of "59592" MJ/hr in the text box next to Step 1e.

Select "Coal" for the fuel type.

Click **OK** to complete the addition of the case.

Click the **Save** toolbar button.

#### Viewing the results graph (tutorial)

Click on the **View Results Graph** button (Step 5). The calculation results using the default options are now displayed.

For help in interpreting the results of the WAR GUI, click here.

According to the graph the total output rate of potential environmental impact (PEI) is higher for Unit 701 than it is for Unit 700. The main reason is that the naphthalene fed process produces a byproduct stream containing naphthoquinone that is a relatively toxic chemical.

In terms of the generation rate of PEI, the impacts of the processes are roughly equivalent. The PEI generation rate is calculated by subtracting the environmental impact of the input streams from that of the output streams. Thus as the inherent toxicity of the input streams increases, the PEI generation rate decreases. The naphthalene input stream is inherently more toxic than the o-xylene stream, which explains why here the cases yield approximately equivalent results.

Also shown on the Results graph are the output and generation rates of PEI per mass of product. These are useful indicators for cases in which the product flow rates are significantly different. In this example the product flow rates in both cases are nearly equivalent so that the results are the same as those given by the indexes in units of PEI/time.

To edit the display options select **Options** from the **Graph** menu. Check the **Include product stream in analysis** box and click **OK**. The difference in the PEI between the cases does not change since both processes had the same product flow rate. Return to the Options screen and uncheck the **Include product stream in analysis** box.

Now uncheck the **Include energy in analysis** box and click **OK**. The total output rate of PEI for each unit should have decreased slightly. Return to the Options screen and recheck the **Include energy in analysis** box.

Now we would like to compare the processes in terms of the individual impact categories. Return to the Options screen and check the **Individual impact categories** box. Checking this box enables one to choose a PEI index to display. For this example choose the generation index (in units of PEI/time). Click **OK** to return to the Results graph. From this graph it is apparent that Unit 700 has a large negative contribution to the PEI generation rate from the PCOP (smog formation) category. Suppose for example that the plant was located in a remote area so that this category is not relevant. To remove the influence of the PCOP category on the total impact, return to the main screen by clicking on the **Back to main** button, then click on **View/Edit Weights**, change the weight for photochemical oxidation to zero, click **OK**, and return to the graph by clicking **View Results Graph**. Now the results

indicate that Unit 701 has a significantly lower impact generation rate. Return to the Impact weights screen and reset the weights to the default values. Click **OK** to return to the Main screen.

Return to the Results graph options screen and uncheck the **Total impact** box, and click **OK**. Now only the individual categories are displayed. Displaying only the individual categories is useful to more easily see the differences in the individual categories.

It is up to the user to decide on to evaluate all of the options discussed here. The user should apply a weighting profile that is appropriate for their specific location and concerns. The user must also decide on how to evaluate the results presented by the program, i.e. is it more important to look at output or generation, and is it more important to look at PEI/time or PEI/production rate. Most likely, the user will find useful information from combinations of those discussed above.

Return to the Results graph options screen, select **Black and white** (in the patterns box), and click **OK**. Now the impact data bars are shaded instead of colored. This is a useful option for printing the graph on black and white printers.

To print the graph, select **Print...** from the **Graph** menu.

Suppose for example that we would only like to change the plot order on the graph. Choose **Select cases to plot** from the **Graph** menu. Add both cases by clicking on **Add all cases**. Click on Unit 700 in the selected cases list and click on the **Move down** button. Click **OK** to confirm the changes to the plotted cases.

Click on **Back to Main** button to return to the main screen.

#### Viewing the results table (tutorial)

Click on the **View Results Table** button (Step 5). The calculation results are now displayed in tabular format.

The displayed results can be changed by selecting **Options** from the **Table** menu. The available options are similar to the graph options in the <u>previous section</u> of the tutorial. However, if one selects the **Total PEI indexes** option from the Displayed data set of radial buttons, the results table also displays the contribution of the energy generation process to the PEI indexes.

If one desires to print the table as it appears on the screen, select **Print...** from the **Table** menu.

To display a text version of the table, click on **View as text** on the **Table** menu. The table can be printed by selecting **Print...** from the **Results File** menu.

Return to the main menu.

## Viewing the energy comparison graph(tutorial)

Open the Energy comparison graph by clicking the **View Energy Comparison Graph** button.

This graph allows one to compare the contributions of the chemical process and the energy generation process to the PEI indexes.

Edit the display options by selecting **Options** from the **Energy Graph** menu. Click on the **Default** button to restore the default options. Click **OK** to return to the Energy comparison graph screen.

The graph should now illustrate that the contribution of the energy generation process to the output PEI Index is significantly less than that of the chemical process (for this example).

Now we would like to compare the relative effects of the energy generation process to the chemical process for a given case study for all the individual categories. Return to the Options screen. Select the **Display results for all the impact categories for the following case study:** option. Once this option is chosen one has to pick a case study to evaluate. Choose "Unit 700" from the list box below this option. Click **OK** to return to the graph.

The graph now illustrates that the only significant contribution from the energy generation process to the Total PEI comes from the acidification potential.

As a final example we will now compare the contributions of the energy generation processes to that of the chemical processes for the acidification potential for the different case studies. Return to the options screen. Select the **Compare case studies for the following impact category:** button and select AP from the category drop down list. Return to the graph. The graph now illustrates that the energy generation process is the sole contributor to the energy generation process for both case studies and that Unit 701 contributes less to the acidification potential (since it has a lower energy consumption rate).

Return to the main screen.

## Creating a results file (tutorial)

Previously we created a table that displayed impact results for one set of options at a time. Now we will create a text file that displays the impact calculation results several different ways. The text file will also give a stream report, a chemical report, and list the weighting profile.

To create a results file, first click on the **Create results File** button (Step 6).

Uncheck the box for Include product stream in analysis.

The default text file name is the same as the case history file name with a "txt" extension instead of a "war" extension. If desired, change the file name by editing the path in the text box or by selecting the **Browse...** button.

To create a space delimited text file, make sure **Space delimited** is selected in the text file options box.

To create (and consequently view the file) click the **OK** button.

Once the text file is displayed it can be edited (i.e. to add additional notes).

If desired save the file by selecting **Save as...** from the **Results File** menu.

If desired print the text file by selecting **Print...** from the **Results File** menu.

Click on the **Close** button to return to the main menu.

## Using additional features in the options menu

In this portion of the tutorial we will add a fictitious chemical to the database, view its affect on the average impact scores, and remove it from the database.

Select **View average impact scores** from the **Options** menu. These scores are the average scores used in the denominator of <u>equation 6</u>.

Record the first 4 scores on a piece of paper for reference later.

Return to the main screen (click on **Back to main**).

Now we will add the fictitious chemical "methyl ethyl death" to the database.

Select Add chemical to database from the Options menu.

Type "methyl ethyl death" for the chemical name.

Type "999-99-99" for the CAS number.

Type "C6H12O2" for the chemical formula.

Type "116.0" for the molecular weight.

Input the following impact values:

Rat oral LD50: "1000"

OSHA TWA PEL: "100"

Fathead minnow LC50: "100"

Global Warming potential: "5"

Click on the **Calculate scores** button to calculate the normalized scores for the new compound.

Click **Add** to add the chemical to the database.

Now view the average impact scores again- the values should have changed slightly.

Now we will view the chemical we just added to the database.

Select Edit chemical in database from the Options menu.

Select Search by CAS Number option.

Enter the CAS number for methyl ethyl death (999-99-9) in the search text box.

When the correct CAS number is highlighted in the list box click **View/Edit Chemical**.

Verify that the impact data for the chemical is the same as that which you entered.

Click on **Delete from database** to delete the chemical from the database.

Click **OK** to return to the main screen.

This concludes our tutorial.