THE POLLUTION INDEX PROGRAM

USER'S MANUAL

AND

TUTORIAL

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TABLE OF CONTENTS

LIST OF FIGURES

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INSTALLATION

The Pollution Index Program must be installed under Windows 95 or Windows NT. The procedure to install the program is described as following:

1) Insert CD-ROM in CD-ROM Drive and run the “pollinstall.exe” program.
2) The default destination directory is “C:\Program Files\pollution” into which the program will be copied when the setup program is run.
3) The short cut will be created Under start Programs Advanced Process Analysis.
4) Run the program “pollution.exe” in the installation directory.

Introduction

Cost minimization has traditionally been the objective of chemical process design. However, growing environmental awareness now demands process technologies that minimize or prevent production of wastes. The development of such environmentally benign processes requires a tool which can perform a quantitative measurement of the pollution impact of a process**.**

The pollution index program is a pollution prevention and measurement module, which can be used to assess the environmental impact of chemical and refinery processes. It is based on the pollution index methodology of EPA (Hilaly and Sikdar, 1995). This approach defines pollution indices which can be used to compare the performance of different chemical processes.

Methodology

There is a wealth of information on methods for pollution prevention for chemical and refinery processes. Some methods currently being developed are the Waste Reduction Algorithm (WAR) by Hilaly and Sikdar, (1995), the Environmental Impact Theory by Cabezas et al., (1997), the Clean Process Advisory System (CPAS) by Baker et.al.(1995) and the Mass Exchange Network Methodology by Papalexandri et al.(1994).

The Pollution Index Program uses the Waste Reduction Algorithm (WAR). The WAR algorithm can be used to minimize waste in the design of new processes as well as in the modification of existing processes. It is based on the generic pollution balance of a process flow diagram as given below.

Pollution Accumulation = Pollution Inputs + Pollution Generation - Pollution Output. (1)

In the WAR algorithm, a quantity called as the 'Pollution Index' is defined to measure the waste generation in a process. This index also allows comparison of pollution production of different processes.

The Environmental Impact Theory (Cabezas et. al., 1997)

This theory is a generalization of the WAR algorithm which discusses the methodology for evaluating potential environmental impacts and illustrating its use in the design and modification of chemical processes. The environmental impacts of a chemical process are generally caused by the energy and material that the process takes from and emits to the environment. The potential environmental impact is a conceptual quantity that can not be measured. However, it can be calculated from related measurable quantities.

The generic pollution balance equation of the WAR algorithm (Eqn. 1) is now applied to the conservation of potential environmental impact in a process. The flow of impact in and out of the process is related to mass and energy flows but is not equivalent to them. The conservation equation can be written as

$$\frac{dI_{sys}}{dt} = \dot{I}_{in} - \dot{I}_{out} + \dot{I}_{gen} \tag{2}$$

In the conservation equation, I_{sys} is the potential environmental impact content inside the process, I_{in} is the input rate of impact, I_{out} is the output rate of impact and I_{gen} is the rate of impact generation inside the process by chemical reactions or other means.

Application of this equation to chemical processes requires an expression that relates the conceptual impact quantity to measurable quantities. This can be written as

$$\dot{I}_i = \sum_j \dot{I}_j^{(i)} = \sum_j \dot{M}_j^{(i)} \sum_k x_{kj} \Psi_k \tag{3}$$

where I_i is the total impact flow in the input or the output. The sum over j is taken over all the process streams. For each stream, a sum is taken over all the chemicals where M_j is the mass flow rate of the stream j and x_{kj} is the mass fraction of chemical k in that stream. Ψ_k is the characteristic potential impact of chemical k.

The process streams are divided into three types: Input, Product and Non-product. All non-product streams are considered as containing pollutants, and all product streams are considered to have zero potential impact. This assumption is made because the objective of the methodology is to reduce the impact and amount of waste materials released into the environment. Since the product streams are not released into the environment, they are considered to have zero potential impact.

$$\dot{I}_{gen}^{NP} = \dot{I}_{out}^{NP} - \dot{I}_{in}^{NP}$$

The potential environmental impact of a chemical species is calculated using the following expression.

$$\Psi_k = \sum_l \ {}_l\Psi^s_{k,l} \qquad (4)$$

where the sum is taken over the categories of environmental impact. " $_{l}$ is the relative weighting factor for impact of type l independent of chemical k. Q $_{k,l}^{s}$ is the potential environmental impact of chemical k for impact of type l.

There are nine different categories of impact. These can be subdivided into four physical potential impacts (acidification, greenhouse enhancement, ozone depletion and photochemical oxidant formation), three human toxicity effects (air, water and soil) and two ecotoxicity effects (aquatic and terrestrial). The relative weighting factor " $_{l}$ allows the above expression for the impact to be customized to specific or local conditions. The suggested procedure is to initially set all the " $_{l}^{s}$ to one and then allow the user to vary them according to local needs.

To quantitatively describe the pollution impact of a process, the conservation equation is used to define two categories of Impact Indices. The first category is based on generation of potential impact within the process. These are useful in addressing the questions related to the internal environmental efficiency of the process plant, i.e., the ability of the process to produce desired products while creating a minimum of environmental impact. The second category measures the potential impact emitted by the process. This is a measure of the external environmental efficiency of the process, i.e., the ability to produce the desired products while inflicting on the environment a minimum of impact.

Within each of these categories, three types of indices are defined. In the first category (generation), the three indices are as follows.

1. $\dot{I}^{NP}_{gen}$ measures the total rate at which the process generates potential environmental impact due to nonproducts. This can be calculated by subtracting the input rate of impact from the output rate of impact as shown in the following equation.

(5)

$\dot{I}^{NP}_{out}$ and $\dot{I}^{NP}_{in}$ can be calculated using equation 3.

2. $\hat{I}^{NP}_{gen}$ measures the potential impact created by all nonproducts in manufacturing a unit mass of all the products. It is calculated by dividing index 1 by the rate at which the process outputs products. This is shown in the following equation.

$$\hat{I}^{NP}_{gen} = \frac{\dot{I}^{NP}_{gen}}{\sum_p \dot{P}_p} = \frac{\dot{I}^{NP}_{out} - \dot{I}^{NP}_{in}}{\sum_p \dot{P}_p} \quad (6)$$

where $\sum_p \dot{P}_p$ is the total rate of output of products.

3. $\hat{M}^{NP}_{gen}$ measures the mass efficiency of the process, i.e., the ratio of mass converted to an undesirable form to mass converted to a desirable form. It is calculated from index 2 by assigning a value of 1 to the potential impacts of all non-products. This is shown in the following equation.

$$\hat{M}^{NP}_{gen} = \frac{\sum_j \dot{M}^{(out)}_j \sum_k x^{NP}_{kj} - \sum_j \dot{M}^{(in)}_j \sum_k x^{NP}_{kj}}{\sum_p \dot{P}_p} \quad (7)$$

The indices in the second category (emission) are as follows.

4. $\dot{I}^{NP}_{out}$ measures the total rate at which the process outputs potential environmental impacts due to non-products. It is calculated using equation 3.

5. $\hat{I}^{NP}_{out}$ measures the potential impact emitted in manufacturing a unit mass of all the products. It is calculated by dividing index 4 by the rate at which the process outputs products This is shown in the following equation.

$$\hat{I}^{NP}_{out} = \frac{\dot{I}^{NP}_{out}}{\sum_p \dot{P}_p} \quad (8)$$

6. $\hat{M}_{out}^{NP}$ measures the amount of pollutant mass emitted in manufacturing a unit mass of product. It is calculated from index 5 by assigning a value of 1 to the potential impacts of all non-products. This is shown in the following equation.

$$\hat{M}_{out}^{NP} = \frac{\sum_j \dot{M}_j^{(out)} \sum_k x_{kj}^{NP}}{\sum_p \dot{P}_p} \quad (9)$$

The first category of indices (indices 1,2 and 3) categorizes generation of potential environmental impact within a process. These indices are most useful in addressing questions related to the internal environmental efficiency of the process plant. Smaller the values of these indices, more environmentally efficient is the process. The second category of indices (indices 4,5 and 6) categorizes emission of potential impact within a process. These are useful in questions related to external environmental efficiency of the process. Indices 1 and 4 can be used for comparison of different designs on an absolute basis whereas the other indices can be used to compare designs independent of the plant size.

In addition to these indices for the process, pollution indices can be defined for the individual streams also. Higher the pollution index of a stream, higher is the pollution impact of that stream on the environment. Since all product streams are considered to have zero potential impact, their pollution index values are zero. The pollution index value for a stream j can be calculated using the following equation.

$$\dot{I}_j = \dot{M}_j \sum_k x_{kj} \Psi_k \quad (10)$$

where M_j is the mass flow rate of the stream j, x_{kj} is the mass fraction of chemical k in that stream and Q_k is the characteristic potential impact of chemical k.

Tutorial Session:

To illustrate the use of WAR Algorithm and the working of the Pollution Index Program, a small tutorial problem (Cabezas et. al., 1997) is given below. The process is of production of methyl ethyl ketone (MEK) from secondary butyl alcohol (SBA). This is a typical chemical engineering process with several unit processes such as reactors, separators, mixers etc. and is thus ideally suited for the purpose of this illustration.

The process flow diagram for the above process is shown in Figure 1. SBA is fed to a hydrogen scrubber where the feed SBA scrubs residual MEK from the hydrogen stream. The SBA feed is then pumped up to the reaction pressure and heated to the reaction temperature. This feed then enters the reactor. The output of the reactor is then sent to a heat exchanger where it is partially condensed. The mixture of MEK, SBA and hydrogen is cooled further and sent to a separator where the hydrogen is flashed off. The hydrogen is then scrubbed and the liquid phase is then sent to the MEK purification system where it is separated into product MEK and waste SBA.

The mass flow rates (kg/hr) of the input and output streams are given in Table 1, and the potential environmental impact scores for these chemicals are given in Table 2 from Cabezas et al. (1997).

Table 1 Mass Flowrates of Input and Output Streams for the MEK Process

Stream Number	**1**	**2**	**3**	**4**	**5**
SBA	3362	19	3	2670	1
MEK	0	0	567	13	71
H2O	8	0	0	0	8
H2	0	18	0	0	0

Table 2 Potential Environmental Impact Scores for Chemicals in the MEK Process.

	H2	MEK	SBA	H2O
$Q_{j,l}$ (impact / kg)	0	0.42	0.00041	0

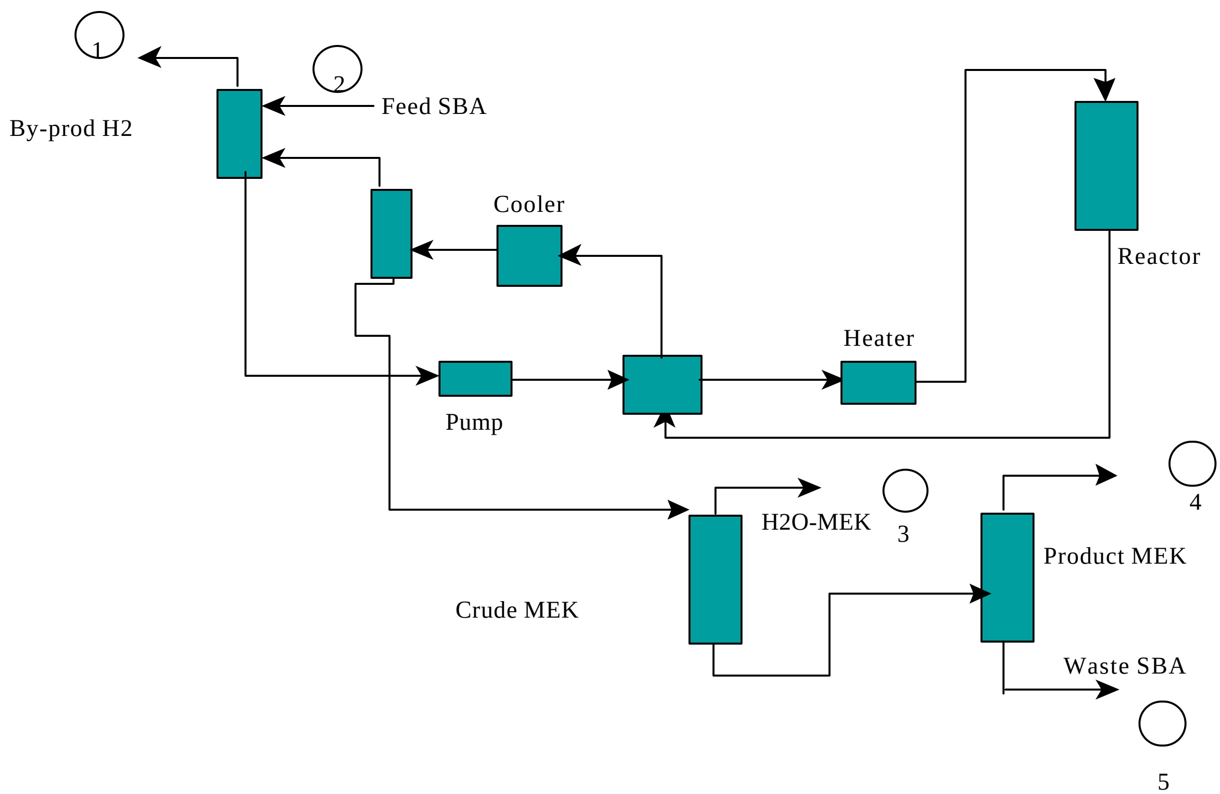


Figure 1: Process Flow Diagram for the MEK Process. (Cabezas et al., 1997)

Now that we have all the necessary data, let us use the Pollution Index Program for this problem. On running the program, the 'Welcome Window' as shown in Figure 2 appears on the screen. It gives a short description of the program's function and the Potential Environmental Impact theory. It asks the user to choose either a new model or an existing model. We will choose the 'New Model' option. (For an existing model, the program shows the 'Open Model' dialog box shown in Figure 3)

Next, the program shows the 'Stream Data' form which is given in Figure 4. Since we have chosen a New model, all the data fields will be initially empty.

The table at the top left corner shows the list of streams in the model. New streams can be added by first entering the necessary stream data and then clicking the 'Add Stream to list' button. The necessary stream data includes the stream name, the component data and the stream type. The component data includes the component name and its flowrate. The component flowrates can also be specified in terms of the mass fractions along with the total mass flowrate of the stream.

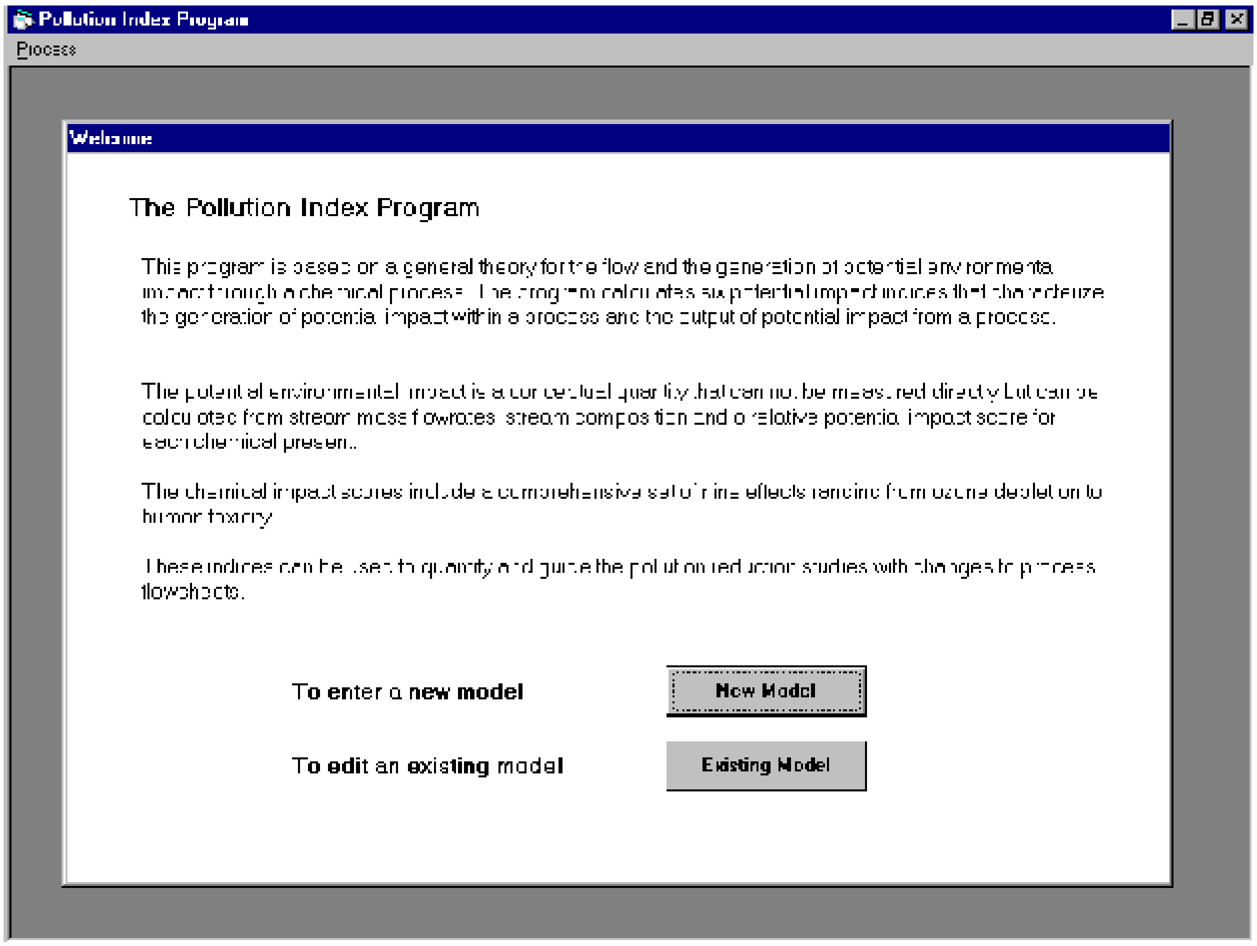
Since we have the data in terms of mass flowrates, we do not need to specify the total flowrate of any stream. So, let us enter the data for the stream number 1. In the box for the stream name, let us enter str1. (We will name all of our streams for this problem as str1, sr2 and so on). We will click the 'Mass flowrates of components' option in the 'Specify' box. In the Components Data table, we will enter the two components: H2O and SBA and their corresponding flowrates. Other components of the system which are not present in this stream need not be entered.

In accord with the Environmental Impact Theory, the process streams are divided into three categories: Input, Product and Non-Product. Str1 is an input stream. So, in the Stream Type list, we will choose 'Input'. Having entered all the information for this stream, we can now click the 'Add stream to list' button. The stream now gets added to the Stream List table at the top. In this manner, we can add all the five streams to our model.

The list at the right hand top of the form shows the list of all the components in the process. Whenever, a new component is added to the model, it is automatically added to this list. Each of these components has Specific Environmental Impact Potentials, $Q^s_{j,l}$ for each of the nine different categories of impacts. The user has to click on the component name in the list and then enter the $Q^s_{j,l}$ values in the table. All the impact potentials have a default value of zero.

So, let us click on SBA in the 'Choose component' list and enter the value of 0.00041 in the first impact type. Also, click on MEK and enter 0.42.

Figure 2: Welcome Window



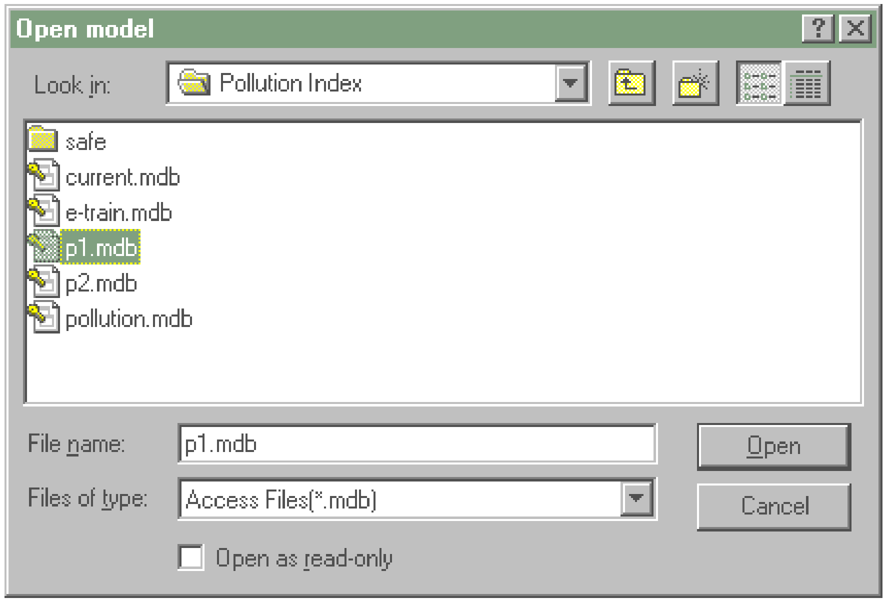


Figure 3: Open Model Dialog Box

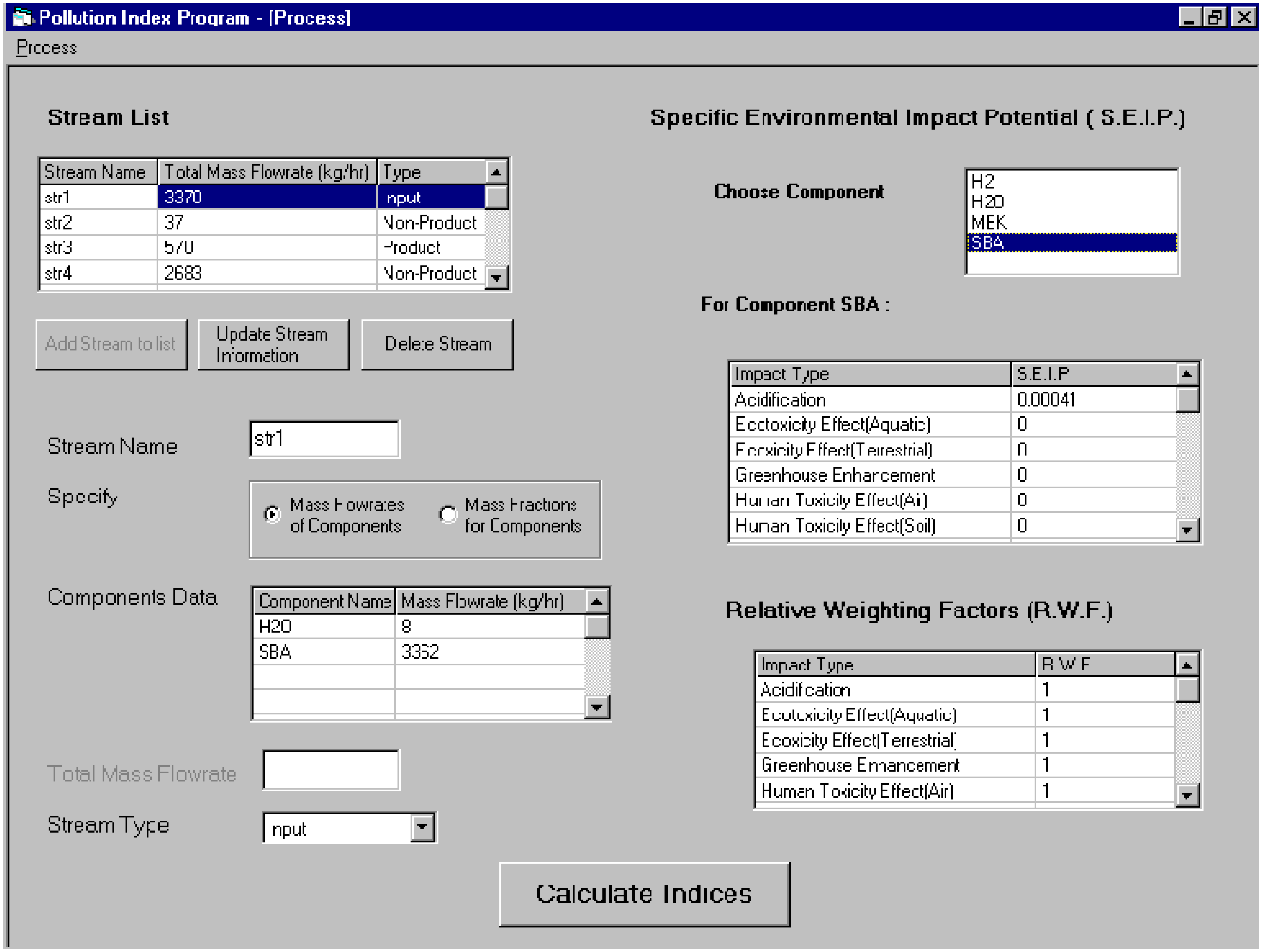


Figure 4: Stream Data

Also, the user has to enter the Relative Weighting Factors ($"_1$) for the process. In accordance with the theory, all the $"_1$ s are initialized to one. For this problem, we will retain these default values.

To modify the information for any stream, the user simply has to click on that stream in the list, and the data for that stream appears in the boxes. The user can make the required changes and click the 'Update Stream Information' button. Similarly, to delete a stream, the user has to select the stream first and press the 'Delete Stream' button.

All of this model information is written to a temporary buffer. At any time, the user can save the model by choosing the 'Save' option in the menu. Let us save our model in a file called 'example.mdb'. (The model is stored as a Microsoft Access database file. So, it must have the '.mdb' extension.)

Now that we have entered and saved the model, the 'Calculate Indices' button can be clicked to view the values of the six pollution indices defined earlier. On clicking this button, the program uses the data entered by the user to evaluate these indices using equations 5-9. It then displays on the screen the 'Pollution Indices' form which shows the results of these evaluations. This form is shown in Figure 5. The column on the left-hand side shows the indices based on the generation of potential environmental impact and the right-hand side column shows the indices based on the emission of environmental impact. Each index is accompanied by a Help button. Clicking the 'Help' displays more information about that particular index at the bottom of the screen. The results for this problem are given in Table 3.

Table 3 Results for the MEK process.

Index Type	**Value**	**Units**
Based on Generation of Potential Environmental Impact		
Total rate of Impact Generation	35.00448	Impact / hr
Specific Impact Generation	0.061411	Impact / kg product
Rate of Generation of pollutants / product	-1	kg pollutants / kg products
Based on Emission of Potential Environmental Impact		
Total rate of Impact Emission	36.3829	Impact / hr
Specific Impact Emission	0.063827	Impact / kg product
Rate of Emission of pollutants / product	4.91228	kg pollutants / kg products

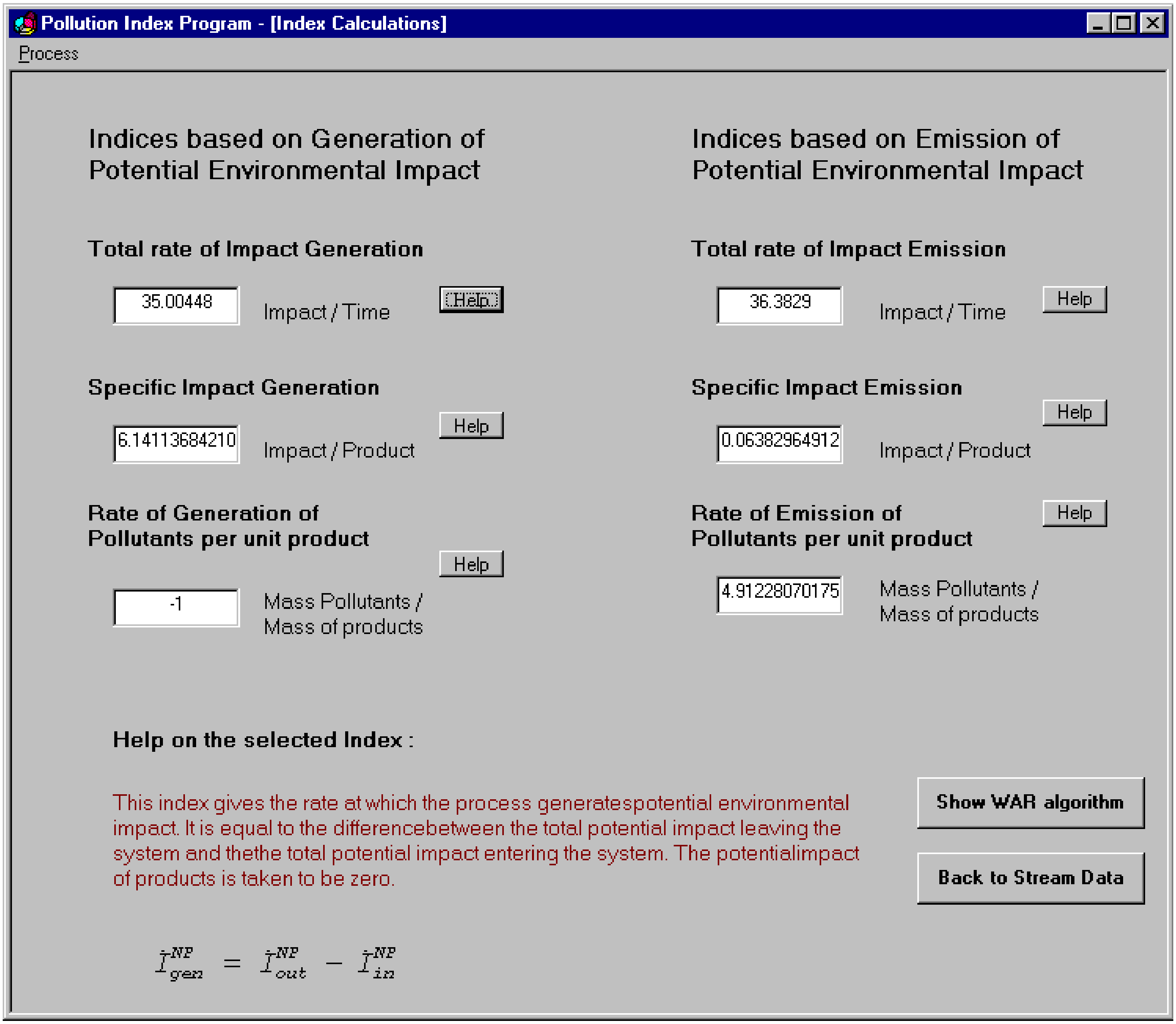


Figure 5: Pollution Indices

Let us click the 'Show the WAR algorithm' button which will display the 'WAR Algorithm' window shown in Figure 6. In this figure, the table on the left side shows the pollution index values for the individual streams. These values are obtained by applying equation 10 to all the process streams. A comparison of these values can help in identifying streams with high pollutant content.

The pollution index values for the individual streams in the MEK process are given in Table 4. We can see that stream 5 has a very high pollutant content followed by stream 4. Stream 3 has no pollutants because it is a product stream. The form also shows the important steps of WAR Algorithm which gives a systematic way of approaching the waste minimization problem. Process modifications should be made to reduce the pollutant contents of streams 4 and 5. Clicking the 'Back' button will bring us back to the 'Indices' form.

Table 4 Pollution Index Values for Streams in the MEK Process

str1	str2	str3	str4	str5
1.37	0.00779	0	6.55	29.8

To make modifications in our model, we can click the 'Back to Stream Data' button which will again display the 'Stream Data' window. We can now add and delete streams, change data for existing streams, change the Impact Potentials for the components etc. and again click the 'Calculate Indices' button to see the results for the modified model. In order to save the changes to the model, the 'Save' option on the menu must be used.

Thus, we can make changes in the model and see the effect on the pollution indices by going back and forth in these windows. The 'Exit' button in the menu will quit the application.

General Information:

The pollution index program is written using Visual Basic 5.0. It uses Microsoft Access 97 as the database.

Acknowledgments:

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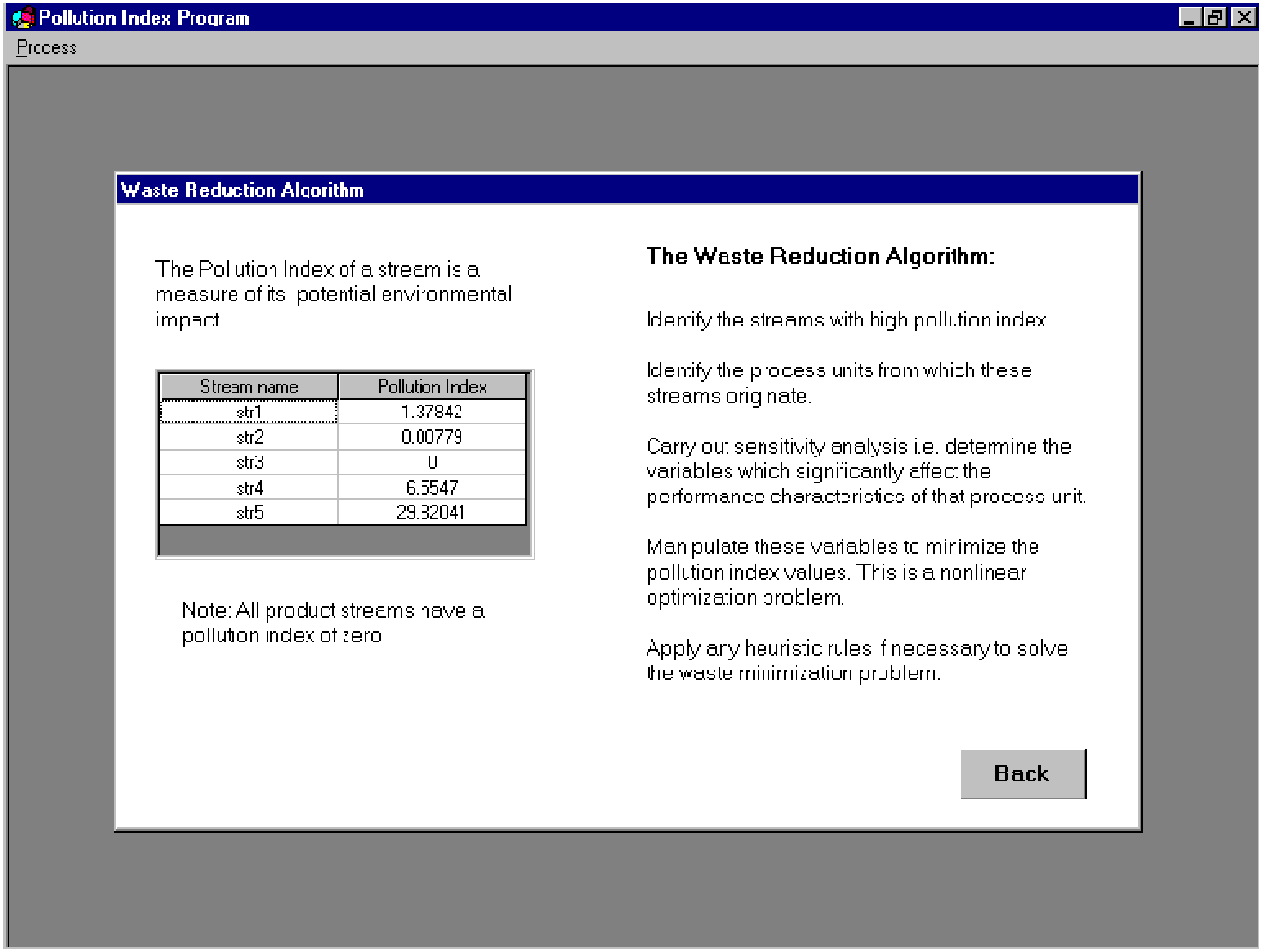

Figure 6: WAR Algorithm

References:

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