# Development of a
# Process Sustainable Prediction (PSP) framework

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This work describes a general framework for the prediction of industrial sustainability integrated with process simulators. Even if sustainability is a complex concept, it can be estimated using some indicators or metrics.

Two kinds of sustainability indicators are used in the present work: (i) three-dimensional indicators (3D-indicators) and (ii) one-dimensional indicators (1D-indicators). The methodology proposed by Martins, containing 3D-indicators, is used in this framework as a first evaluation of the global sustainability of the process under study. The methodology takes into account the material intensity, the energy intensity, the potential chemical risk and the potential chemical impact. The 3D-indicators are calculated using the results obtained from process simulation coupled with the database included in the framework.

Sometimes, this information is not sufficient for deciding the best solution, in terms of sustainability, from different alternative design. In this case one may resort to the evaluation of 2D-indicators and 1D-indicators. One relevant 1D indicator is the Waste Reduction Algorithm (WAR). In PSP the algorithm is implemented in a CAPE OPEN standard methodology which is able to interact with most process simulators software available on the market.

The paper describes the development of the Weighting Factors Interface, the development of CAPE OPEN Modules and the development of the Potential Environmental Indexes Interface, which are the most important elements of the implementation of the WAR.

PSP is made up by the CO interfaced to process simulators, a relational database containing toxicological and risk information and a set of software modules. The framework was tested using two process simulators: PROII and Aspen Plus. Representative examples of applicability of PSP are presented in order to validate the framework.

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## 1. Introduction

The concept of sustainable development plays an important role in the 21st century. The three aspects of the sustainable development are: economy, environment and society. The attention of the people who work in the field of sustainable development is focused on the quantification of each aspect as well as on the all possible interactions between the three elements of the sustainable development.

Sikdar(2003) proposed a typology of indicators, considering the three dimensions of sustainable development in three distinct groups:

1. One dimensional (1D) indicators which provide information about one aspect of sustainable development: economical, ecological or societal.
2. Two dimensional (2D) indicators which provide information about two aspects of sustainable development: socio-ecological, socio-economic or economic-ecological.
3. Three dimensional (3D) indicators which provide information about all the three aspects of sustainable development.

The goal of the present work is to introduce the concept of sustainable development during the design step of the process and to offer a valid tool for evaluating the sustainability.

The methodology proposed by Martins(2006), containing 3D-indicators, is used in this framework as a first evaluation of the global sustainability of a chemical process. The methodology takes into account the material intensity, the energy intensity, the potential chemical risk and the potential chemical impact. The material intensity represents the amount of nonrenewable resources required to obtain a unit mass of products. The energy intensity measures the energy demands of the process. The potential chemical risk regards the risk associated with the manipulation, storage and use of hazardous chemical substances in the process. The potential chemical impact is due to emissions and discharges of hazardous chemicals to the environment. The choice of these four metrics was made taking into account the relevant data from a chemical plant and the three aspects of the sustainable development.

One forward step in PSP is represented by the implementation of 2D and 1D indicators. One relevant 2D indicator is the eco-efficiency indicator which takes into account economical and environmental aspects of the process. The environmental impact of the chemical processes is an important issue of our days. In the present work the environmental aspect is taken into account in the design stage of the chemical process. The evaluation of the environmental impact is made through the WAR Algorithm, which represents a 1D indicator.

The elements presented above are discussed in detail in the next section.

## 2. Development

A general schema of the PSP development is presented in Figure1.

The implementation was made according to Martins et al.(2006) and Vincent(2005).The two starting points for calculating the sustainability indicators are the process simulator and the database containing toxicity and risk phrases data. Beside the database two CAPE OPEN (CO) Modules were developed. These modules will be inserted in the process flow-sheet as follows: the first CO Module will be connected to the input and output streams of the process and its goal is to extract data for calculating the material intensity (MI), the energy intensity (EI) and the potential environmental impact indicators (PEI) and the second CO Module will be inserted in one strategic point of the plant in order to extract data for evaluating the potential chemical risk (PCR). The data obtained through the CO Modules are processed in the PSP software. The results are the 3D sustainable indicators.

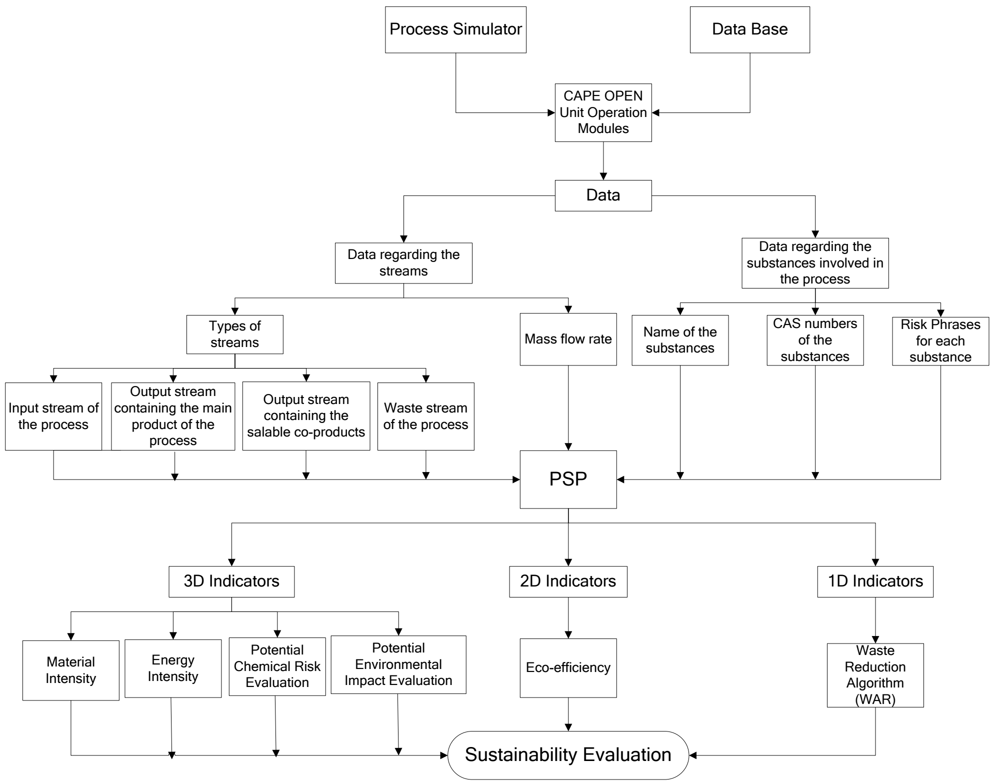


Figure1. General Schema of the PSP development

In order to compare different alternatives design, the methodology described above should be repeated for each particular case. Comparing the indicators obtained for each case the best design, sustainable speaking, could be chosen.

Sometimes, the information of 3D indicators is not sufficient for deciding the best solution from different alternatives design. In this case one may resort to the evaluation of 2D Indicators and 1D Indicators. As mentioned above one relevant 1D indicator is the Waste Reduction Algorithm (WAR) developed by Cabezas et. al(1997). The main elements of the implementation of WAR are: the Weighting Factors Interface, the development of CAPE OPEN Modules and the development of the Potential Environmental Indexes Interface. The weighting factors are essential for the WAR Algorithm because they permit the combination of the impact categories according to local needs and policies. This interface was created with the goal in mind to offer the possibility of modifying the factors. The logical schema of the Weighting Factor Interface is presented in Figure 2.

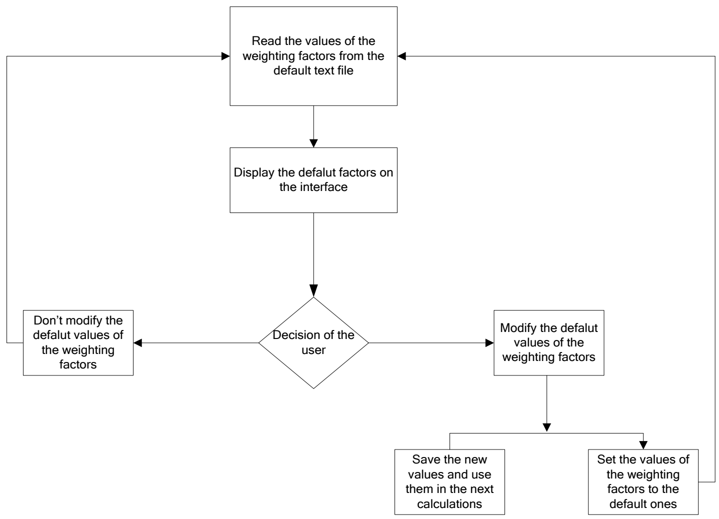


Figure2 Logical Schema of the Weighting Factors Interface development

A forward step was the development of the two CO Modules: one module incorporating the WAR equations and the second CO module incorporating the energy generation process connected to the chemical process. It is important to mention that both modules are linked to the toxicological database containing the impact categories: Global Worming Potential, Acidification Potential, Ozone Depletion Potential, Photochemical Oxidation Potential, Terrestrial Toxicity Potential, Aquatic Toxicity Potential, Human Toxicity Potential by Ingestion, and Human Toxicity Potential by Inhalation. The way the total environmental impact is calculated is summarized in Figure3.

The final step of the implementation of the WAR is represented by the Potential Environmental Indexes Interface. This interface is necessary for the calculation of the environmental indexes: the total rate of PEI leaving the system, the total rate of PEI leaving the system per mass of product, the total rate of PEI generated within a system, the total rate of PEI generated within a system per mass of product of a chemical process. Using these indexes different processes can be compared and the best solution form the environmental point of view can be chosen.

The PSP was implemented in Visual Basic (version 6.0). The DB containing toxicological and risk phrases data was implemented in Microsoft Access and has more then 4500 substances. For the development of the CO Modules the CAPE OPEN Unit Wizard (version 0.9.3) was used.

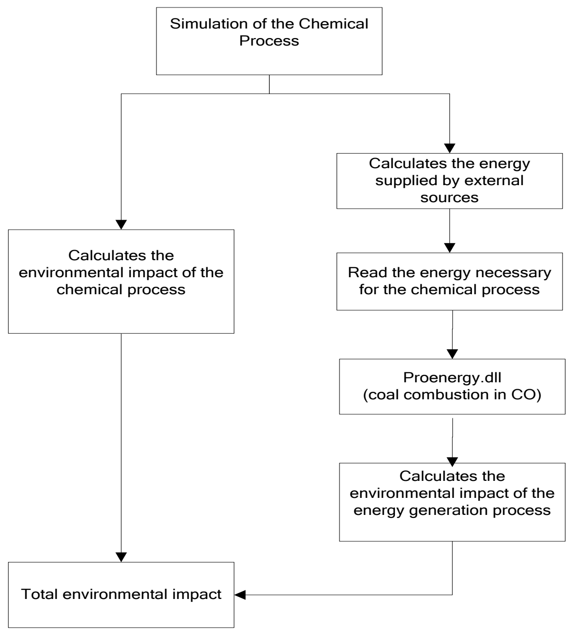


Figure3. Logical Schema for the Calculation of the Environmental Impact using the CO Modules

## 3. Example

A representative example of applicability of PSP is presented in order to validate the framework. The process chosen is the acrylic acid production process presented by Turton(2003). Five alternative designs are proposed for the process. The temperature of the reactor is decreased from 310˚ C up to 210 ˚C. The 3D Indicators obtained in all five cases are presented in Table 1.

| | MI | EI | PCR | PEI |
|---|---|---|---|---|
| Case1 | 2915.066 | 520.461 | 301020 | 8530.52 |
| Case2 | 2877.105 | 494.714 | 301020 | 8530.52 |
| Case3 | 2861.003 | 480.635 | 301020 | 8530.52 |
| Case4 | 2934.939 | 485.545 | 310020 | 8530.52 |
| Case5 | 3134.124 | 1034.755 | 310020 | 8530.52 |

Table1. 3D Indicators obtained in the acrylic acid production

The case with  minors 3D indicators is the case number 3. This represents the most environmental friendly design. For the same cases the WAR was applied. The results are reported in Table2 and these stress one more time the choice of the third alternative design.

| Name of environmental indexes | Name of the cases | | | | |
|---|---|---|---|---|---|
| | Case 1 | Case 2 | Case 3 | Case 4 | Case 5 |
| Iout (PEI/hr) | 17047.553 | 5424.005 | 5074.482 | 5203.7025 | 11665.58 |
| Iout_mp (PEI/kg) | 2.673 | 0.791089 | 0.71691 | 0.74146 | 1.8084 |
| Igen (PEI/hr) | 5668.061 | -5955.487 | -6305.001 | -6175.789 | 286.090 |
| Igen_mp (PEI/kg) | 0.888 | -0.868 | -0.891 | -0.880 | 0.043 |

Table2. Environmental Impact Indexes obtained in the acrylic acid production using WAR Iout- rate of impact leaving the system, Iout_mp- rate of impact leaving the system per mass of product, Igen-rate of impact generatedwithin the system, Igen_mp-rate of impact generated within the system per mass of product

## 4. Conclusions

The present work describes the implementation of a framework used in the evaluation of sustainability. The background of the framework is represenated by the 3D and 1D indicators found in the literature. The software takes into consideration the aspects of sustainability during the design step of a chemical process. The presnt software was tested in several cases and the acrylic acid production process is reported here.

The future work will be focused on the development of the 2D indicator and on the improvement of the database.

## 5. Acknowledgment

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## 6. References

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