

# INCORPORATION OF ENVIRONMENTAL IMPACT CRITERIA IN THE DESIGN AND OPERATION OF CHEMICAL PROCESSES

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**Abstract** - Environmental impact assessment is becoming indispensable for the design and operation of chemical plants. Structured and consistent methods for this purpose have experienced a rapid development. The more rigorous and sophisticated these methods become, the greater is the demand for convenient tools. On the other hand, despite the incredible advances in process simulators, some aspects have still not been sufficiently covered. To date, applications of these programs to quantify environmental impacts have been restricted to straightforward examples of steady-state processes. In this work, a life-cycle assessment implementation with the aim of process design will be described, with a brief discussion of a dynamic simulation for analysis of transient state operations, such as process start-up. A case study shows the importance of this analysis in making possible operation at a high performance level with reduced risks to the environment.

**Keywords:** environmental impact, process design, life-cycle assessment.

## INTRODUCTION

During the past years, chemical process simulation software has become a basic tool in chemical engineering work. Thanks to the vertiginous growth of computer science, a considerable amount of the current knowledge of chemical engineering has been incorporated in these programs. Recently, dynamic simulation was consolidated as an integral part of the available options. However, there are many aspects not yet directly covered by these programs.

Nonetheless, as a consequence of a growing social conscience, ever more restrictive environmental legislature has forced the chemical

engineer to consider environmental impact throughout the life cycle of a chemical process. Currently some methods have been proposed with the goal of quantifying the environmental impact of a chemical process.

In this work, an implementation in a commercial simulator (HYSYS.Plant v. 2.4) of an environmental impact assessment (EIA) for a chemical process will be presented.

## EXISTING METHODS

Environmental impact assessment (EIA) of a chemical process can be defined as the systematic

identification and evaluation of the potential effects that this chemical process can have on the biological, physical, cultural and socio-economic aspects of environment.

Until recently, the existing methods gave only qualitative orientation with respect to waste minimisation and pollution prevention (Douglas, 1992; Freeman et al., 1992). During the past five years, some new proposals with the aim to quantify the environmental impact of a chemical process (Bauer and Maciel Filho, 1999) have been presented. For the sake of brevity, a detailed discussion of these methods is not aim of this work. Hertwich et al. (1997) and Cano Ruiz and McRae (1998) published good reviews of this topic.

One common feature in these proposals was the difficulty of translating process data into environmental information (Jackson and Clift, 1998).

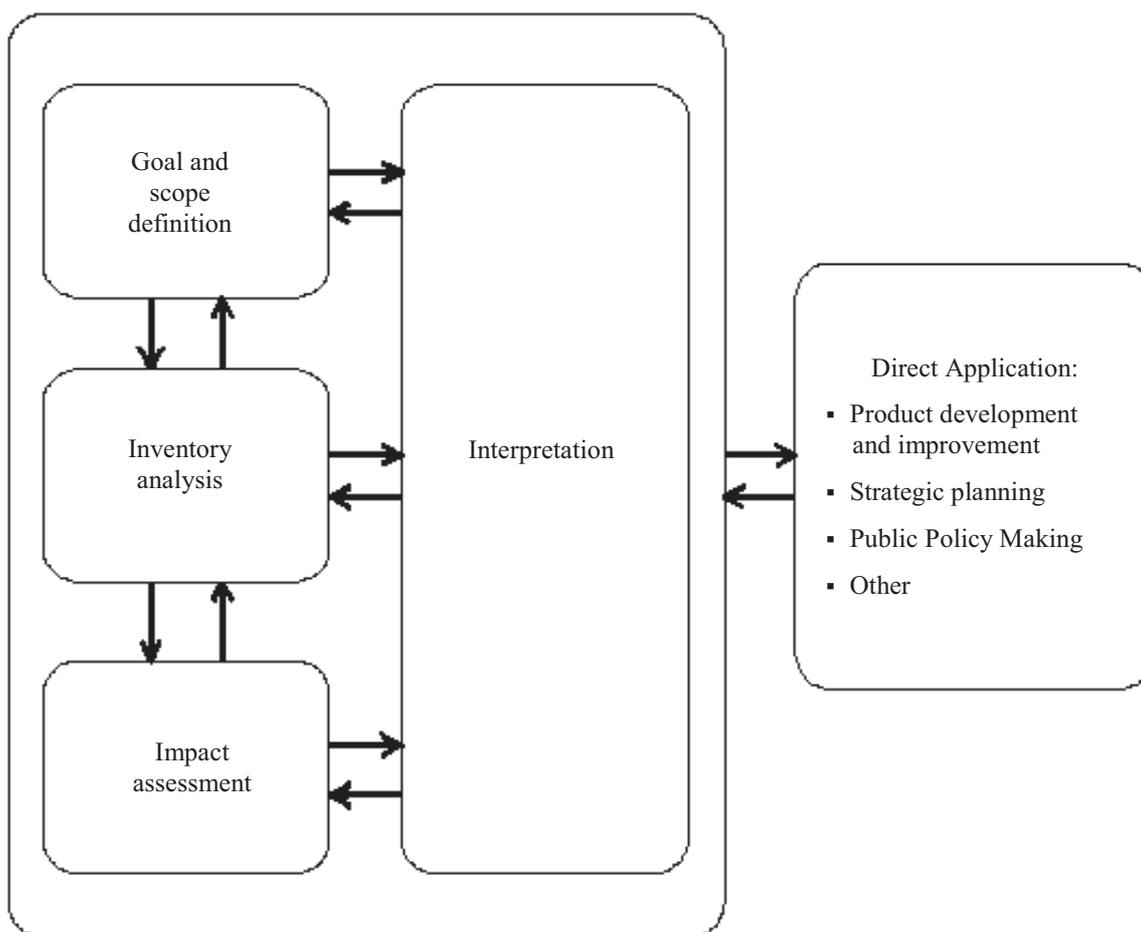
Although it is evident that none of these methods can be applied to all cases or is appropriate for all intended purposes, life-cycle assessment (LCA) has

been increasingly adopted in chemical process design (Azapagic, 1999; Azapagic and Clift, 1999; Burguess and Brennan, 2001). An extremely detailed and complex methodology, LCA has in most cases been applied in either a streamlined (Curran, 1996) or a limited (Vignes, 2001) form.

## LCA METHODOLOGY

LCA is a tool used to evaluate the environmental effects of a product, process or system from extraction of the raw materials (oil, ores, fresh water, air, and so on) to the final disposal of materials in the environment, commonly known as "cradle to grave" analysis. LCA is normally applied (ISO 14040, 1997), as shown in Figure 1, in four main phases:

- 1) goal and scope definition,
- 2) inventory analysis,
- 3) impact assessment, and
- 4) interpretation.



**Figure 1:** Methodological Framework of an LCA

In the first phase the purpose of the work is defined and the system boundaries (temporal, geographical, and technological) and mainly the environmental impact categories to be used are identified.

The second phase is concerned with data collection and the calculation procedures for preparing the materials and energy inputs and outputs of any unit process producing the LCI. These procedures may be almost completely rigorously implemented using the chemical process simulation software.

The third phase is impact assessment (LCIA), and it is aimed at understanding and evaluating the magnitude and significance of potential environmental impacts of the system under study. It is essentially a quantitative procedure to identify, characterise, and assess the potential impacts of environmental interventions identified in the second phase.

The final phase in an LCA study is interpretation, which may be defined as the systematic procedure to identify, qualify, check, and evaluate the results of the LCI and LCIA. The main aim of interpretation is to analyse the results according to the goals and scope and to formulate the conclusions and the recommendations that can be drawn from the LCA. It can comprise five different kinds of analysis (Heijungs and Kleijn, 2000):

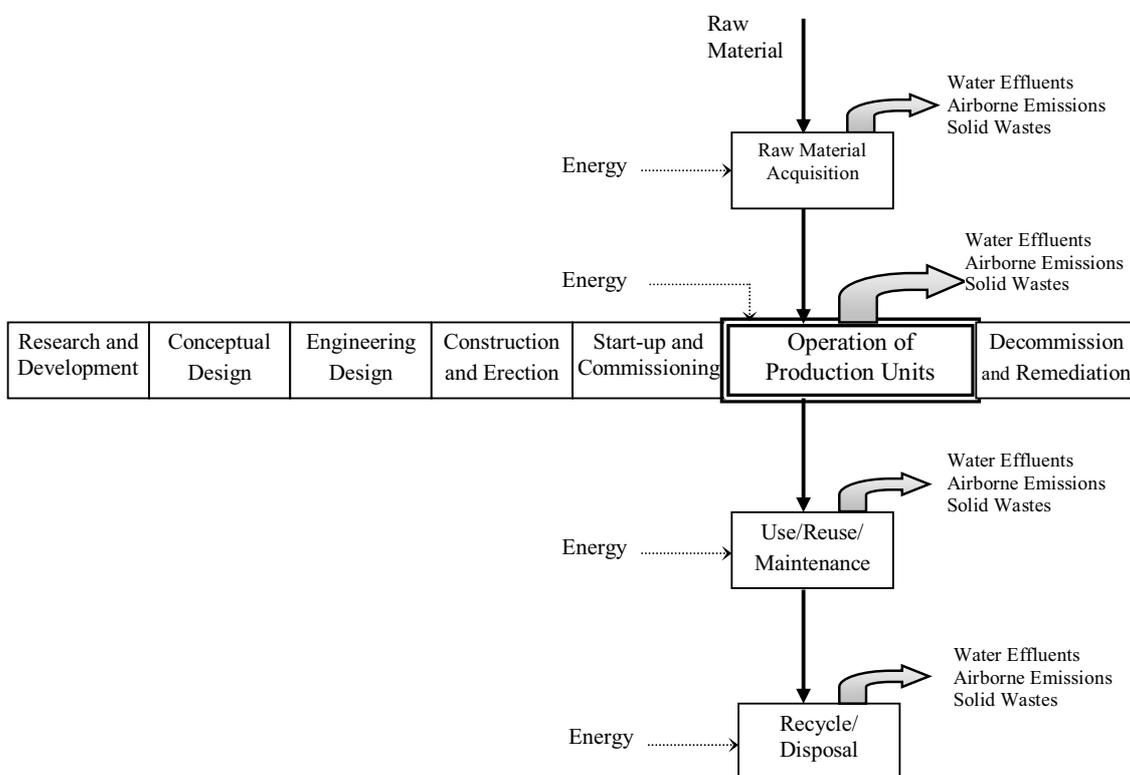
- 1) contribution analysis,
- 2) perturbation analysis,
- 3) uncertainty analysis,
- 4) comparative analysis, and

5) discernibility analysis.

The chemical process design follows a series of stages, beginning with a preliminary structuring of the process, based on an input-output description (Turton et al., 1998) and concluding with a flowsheet of the final process. LCA can assist in the environmental performance analysis during the whole sequence of stages.

## CHEMICAL PROCESS DESIGN

The concept of chemical process life-cycle is well-known to the chemical engineer. Generally speaking, a chemical process life-cycle begins with a research and development stage, followed by a conceptual process design (process synthesis) and then an engineering design (detailed design and layout). After these stages, the plant construction and erection stage begins. The next stage is the start-up and commissioning of the plant. Then the plant has an operational stage during its active lifetime with insets of relatively short maintenance/retrofitting/debottlenecking steps. Finally, the plant is decommissioned and remediation may be conducted, when necessary. These process life-cycle stages are illustrated, although not in scale, in Figure 2, on the horizontal axis.



**Figure 2:** Illustration of Process Life-Cycle and Product Life-Cycle

For products, the life cycle begins when raw materials are extracted or harvested. These materials pass through a series of processing units until the final product is delivered to the customer. After use, the product is disposed of or recycled. The main steps of this product life cycle are shown on the vertical axis in Figure 2.

The economic evaluation and optimisation of a chemical process has been studied for a long time (Bauer, 1978). However, environmental considerations in chemical process optimisation is almost unknown in Brazil and represents a very recent worldwide concern.

A major problem in environmental evaluation is how many and which indicators to use for environmental performance evaluation. The two intermediate phases of LCA, mainly the third, can provide a good framework to realise this work.

## ENVIRONMENTAL CRITERIA

Although complete agreement on the utilisation of environmental metrics in chemical processes does not exist, some indicators have been used frequently. In Table 1 a comprehensive, but not exhaustive, list of the available indicators is presented. In addition to these, when necessary, more specific indicators (lost

heat, odour, noise, ionising radiation, etc.) can be used.

In the LCA framework environmental quantification is known as characterisation step and consists in the calculation of a common base for any impact category, allowing aggregation into a single value: the environmental indicator for the category being addressed.

The environmental impact of a chemical process is assessed using characterisation models that establish relationship between the composition of a specific input or output stream in the process and each environmental impact category.

The category impact indicator related to impact category  $i$  for specific stream  $k$  of the process is calculated by the general equation:

$$CII(i, k) = \sum_j CF(i, j) * m(j, k) \quad (1)$$

where  $CF(i, j)$  is the characterisation factor for impact category  $i$  for chemical  $j$  and  $m(j, k)$  is the mass emission rate for chemical  $j$  in stream  $k$  ( $\text{kg}\cdot\text{h}^{-1}$ ).

Most of the commercial simulators have no feature for evaluation of direct environment impact. However, through the use of generic features available in these programs it is possible perform a satisfactory impact quantification.

**Table 1: Potential Indicators of Environmental Impact**

Indicator	Environmental Effect	Source Examples
DAR	Depletion of Abiotic Resources	Depletion of minerals, fossil fuels, and metal ores.
DBR	Depletion of Biotic Resources	Depletion of forests and vegetable fuels.
LUT	Land Use and Transformation	Land occupation and transformation, loss of biodiversity.
DWR	Depletion of Water Resources	Groundwater extraction for industrial supply.
GW	Global Warming	Greenhouse effect gases ( $\text{CO}_2$ , $\text{CH}_4$ , $\text{CO}$ , and $\text{NO}_x$ )
OD	Ozone Depletion	Chlorofluorocarbons, volatile organic compounds.
HAT	Human Air Toxicity	Compounds toxic to human health released into air.
HWT	Human Water Toxicity	Compounds toxic to human health released into water.
HST	Human Soil Toxicity	Compounds toxic to human health released into soil.
AET	Aquatic Ecotoxicity	Toxic compounds released into aquatic ecosystem.
TET	Terrestrial Ecotoxicity	Toxic compounds released into terrestrial ecosystem.
POF	Photochemical Oxidant Formation	Volatile organic compounds.
ARC	Acid Rain Compounds	$\text{SO}_x$ , $\text{NO}_x$ , and $\text{NH}_x$ .
EMN	Eutrophication by Macronutrients	Nitrogen (N) and phosphorus (P).

HYSYS is a well-known static/dynamic simulator (Hyprotech Ltd., 2001). One of its features is the user property utility, where any impact category indicator for any process stream can be calculated. The value of any indicator is a function of its composition, normally calculated by the simulator. The values of the characterisation factors for each chemical species are available elsewhere (Guinée et al., 2002) and should be supplied to the simulator.

The user property option in the simulation basis manager allows definition of the mass flow rate as mixing basis. Equation (2) is used as the mixing rule:

$$(P_{mix})^{f1} = f2 * \sum_{i=1}^N (x(i) * P(i)^{f1}) \quad (2)$$

where  $f1$  and  $f2$  are parameters utilised with the default value of 1;  $x(i)$  and  $P(i)$  are, respectively, the mass flow rate and the characterisation factor for a specific environmental impact category for the chemical species  $i$ ; and  $P_{mix}$  is the value of the category impact indicator for the environmental category considered for a specific process stream.

Thus, each (material or energy) stream will have a vector that represents its environmental impact potential (or its environmental load). The dimension of this "environmental vector" will be equal to the number of indicators (impact categories) utilised.

For each input stream the related "environmental vector" includes the accumulated environmental impact load ("environmental history") from the acquisition of natural resources ("cradle") to the process considered ("gate").

Although their "environmental vector" can be easily determined, the internal streams will not be used in the environmental balance, as they are confined within the boundaries defined.

Each waste stream of the process will have its own "environmental vector" where each category indicator will be calculated by Equation (2).

In each process unit, the environmental load of a product stream, represented by its "environmental vector," is the sum of environmental loads of the (materials and energy) streams that enter the process with the environmental loads of the (materials and energy) waste streams. As is true for the whole process, the environmental impact of the product is the sum of all input streams and all waste streams.

An optional but recommended step in impact assessment is normalisation, which is defined as the calculation of the magnitude value of each indicator relative to reference information to better understand the relative importance of the results in the system.

Over a defined period of time, this reference may be related to a given community (the population of a city, a country, or even the world) or an "average" person.

The next step (also optional) is grouping, in which the impact categories are aggregated into one or more sets.

The final step is weighting, in which the (normalised) indicators for each category assessed are multiplied by numerical factors (weights) according to their relative importance and possibly aggregated. One of the most controversial questions regards the aggregation of indicators. On one hand, using a large number of indicators becomes very difficult the study of waste minimisation. On the other hand, the aggregation of several indicators into a single indicator requires the definition of a weight set for different categories. This weight set, though very useful in a particular system under study, may be influenced by the subjectivity inherent in any process involving the choice of values.

For instance, the aggregation of the desired indicators permits calculation of the environmental impact index, where the weight factors will all be considered equal to one. This corresponds to considering all the impacts as being of the same environmental importance. Equation (3) gives this calculation for process stream  $k$ :

$$EII_k = \sum_{j=1}^M (\alpha(j) * P_{mix}(j)) \quad (3)$$

where  $\alpha(j)$  and  $P_{mix}(j)$  are, respectively, the weight factor and the value of the category indicator  $j$ , calculated by Equation (2), and  $EII_k$  is the environmental impact index for the  $M$  category indicators utilised.

The final calculations are made on the spreadsheet, a logic operation of HYSYS that is similar to the Excel spreadsheet. The values determined in the user property utility are first transferred to the spreadsheet. It is then possible to compute the environmental impact index for the process, considering only the input streams and the waste streams of the whole process.

## CASE STUDY

As an example of utilisation of the methodology, the production of propylene glycol by propylene oxide hydration will be considered. This is a well-known process, described in detail by Fogler (1999). The flowsheet considered is presented in Figure 3.

The whole plant involves other stages that are not shown, where the principal is the reactor for partial oxidation of propylene with air or oxygen.

In a first stage water is mixed with propylene oxide at a molar ratio ranging from 10 to 20. The reactor effluent is separated in a dehydration column. Then vacuum distillation columns separate the glycols (mono, di and tripropylene glycol). Due to an

exothermic reaction, the temperature of the reactor effluent reaches 130°C.

Table 2 gives the environmental data needed to compute the desired indicators. As no data were found in the literature on the heavier propylene glycols (di and tri), for both, data on monopropylene glycol were used (they were considered one single compound).

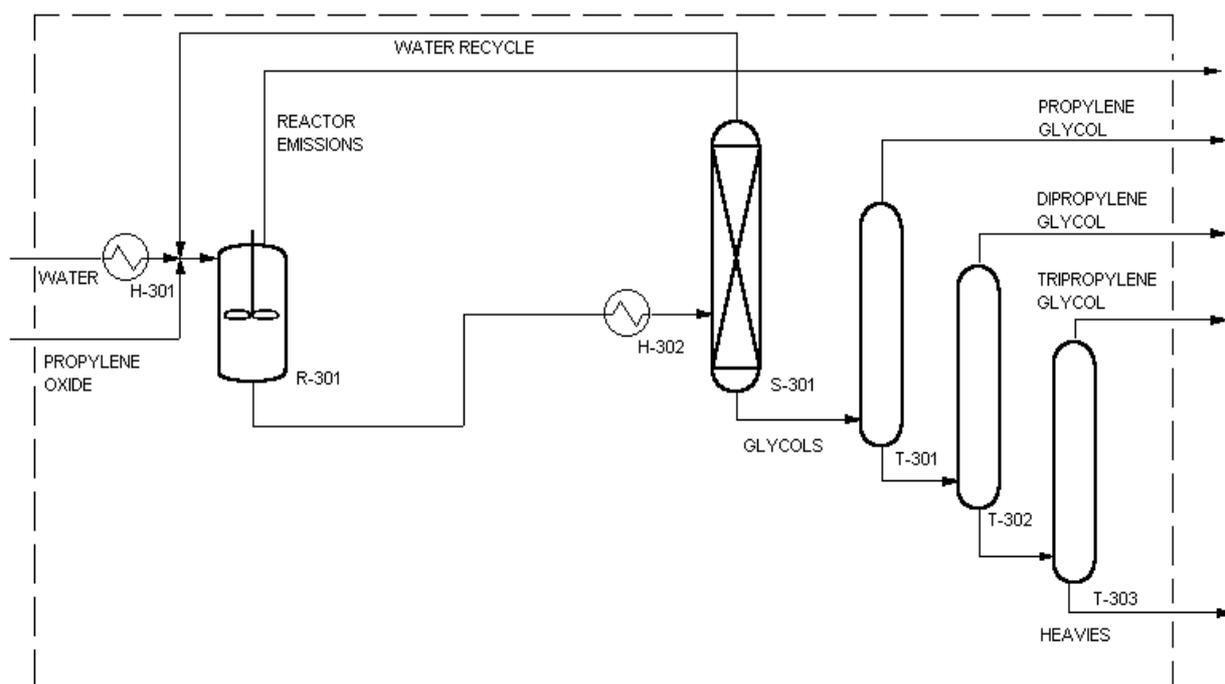


Figure 3: Process Flowsheet

Table 2: Characterisation Factors for Impact Categories

Characterisation Factors	Propylene Oxide	Propylene Glycol
Factor for DAR (kJ.mol <sup>-1</sup> )	1914	1803
Factor for HAT (kg 1, 4 DCB eq.kg <sup>-1</sup> )	1.3 E3	—
Factor for HWT (kg 1, 4 DCB eq.kg <sup>-1</sup> )	2.6 E3	—
Factor for HST (kg 1, 4 DCB eq.kg <sup>-1</sup> )	5.9 E2	—
Factor for AET (kg 1, 4 DCB eq.kg <sup>-1</sup> )		
Air	3.7 E-2	—
Water	4.0 E0	—
Industrial soil	4.8 E-1	—
Factor for TET (kg 1,4 DCB eq.kg <sup>-1</sup> )		
Air	1.5 E-3	—
Water	6.5 E-4	—
Industrial soil	1.2 E-1	—
Factor for POF (kg ethylene eq.kg <sup>-1</sup> )	—	0.457

In this case study indicators of the following categories of environmental impact will be considered: depletion of abiotic resources (DAR), human air toxicity (HAT), human water toxicity (HWT), human soil toxicity (HST), aquatic ecotoxicity (AET), terrestrial ecotoxicity (TET), photochemical oxidant formation (POF).

The DAR indicator for each process stream is given by Equation (2) where  $x(i)$  and  $P(i)$  are, respectively, the molar flow rate and the characterisation factor for DAR (exergy) for the chemical species  $i$  and  $P_{mix}$  is the value of the DAR indicator for a specific process stream.

The human toxicity indicator depends on which environmental compartment the stream is released (air, water or soil) and is given by Equation (2) where  $x(i)$  and  $P(i)$  are, respectively, the mass flow rate and the characterisation factor for the compartment considered for the chemical species  $i$  and  $P_{mix}$  is the value of the air, water or soil human toxicity indicator (HAT, HWT or HST) for a specific process stream.

The aquatic ecotoxicity and terrestrial ecotoxicity indicators for each process stream are given by Equation (2) where  $x(i)$  and  $P(i)$  are, respectively, the mass flow rate and the characterisation factor (aquatic or terrestrial) for the chemical species  $i$  in the compartment into which the stream is released and  $P_{mix}$  is the value of the aquatic ecotoxicity indicator or terrestrial ecotoxicity indicator) for a specific process stream.

The POF indicator for each process stream is given by Equation (2) where  $x(i)$  and  $P(i)$  are,

respectively, the mass flow rate and the characterisation factor for POF for the chemical species  $i$  and  $P_{mix}$  is the value for the POF indicator for a specific process stream.

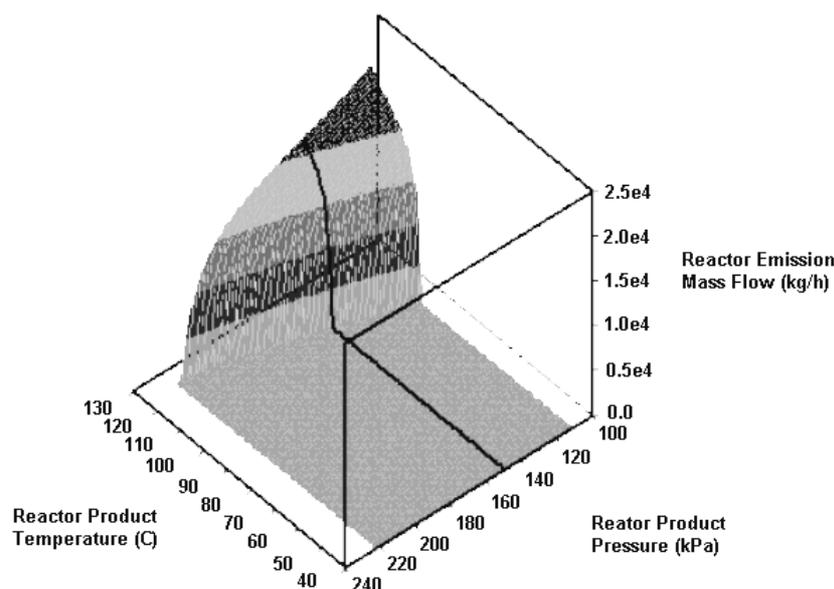
Initially, a study of only the reactor, without the recycle, was conducted. Figures 4, 5, and 6 show the dependence on temperature and pressure, of the reactor emission stream, conversion, and EII, respectively. The dependence of water/propylene oxide molar ratio on the dependent variables described was also analysed, as shown in Figure 7. This ratio doesn't show a major influence and is important only when considering di and tripropylene glycol formation.

This study allows analysis of dependence not only for the conversion and mass flow rate of the reactor emission stream but also of the environmental impact index.

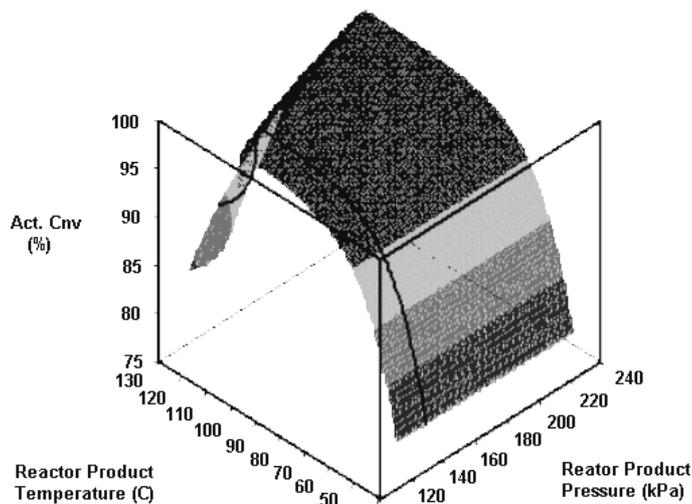
Figure 8 shows a PFD for the process under study and the spreadsheet with the values of indicators for the categories utilised for the process streams and the EII for the reactor emission stream and for the whole process.

To simplify, a "gate-to-gate" case was analysed, i. e., preprocess steps were not considered.

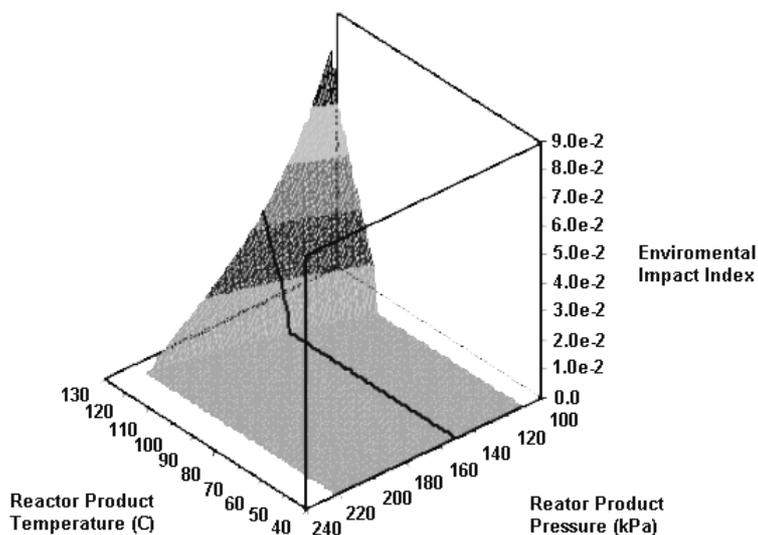
In Figure 8 the flowsheet for the process in steady state is presented. The transition to dynamic situation is made with some care in creation of the model. With the model run in the dynamic mode, it is possible to analyse the behaviour of environmental impact in situations of operation in transient regime, such as in plant start-up and shutdown or evaluations of disturbances in the process variables.



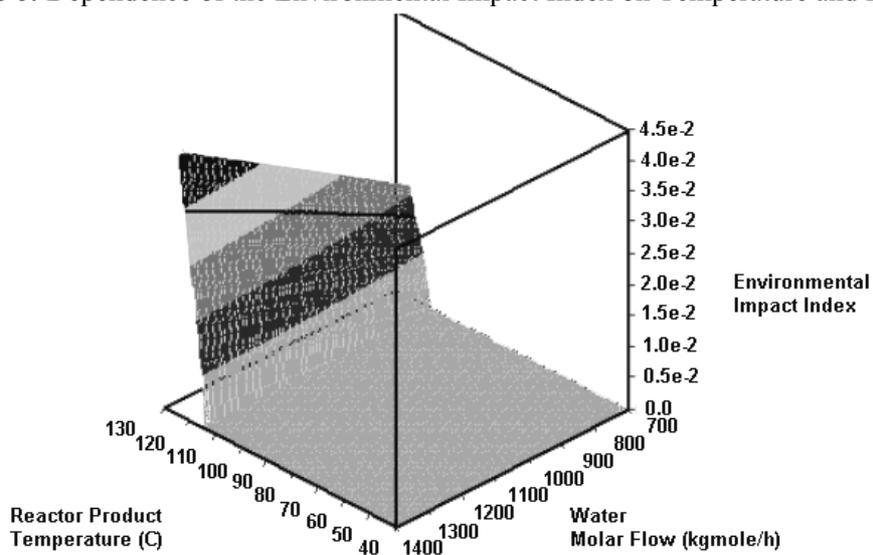
**Figure 4:** Dependence of the Reactor Emission Stream on Temperature and Pressure



**Figure 5:** Dependence of the Reactor Conversion on Temperature and Pressure



**Figure 6:** Dependence of the Environmental Impact Index on Temperature and Pressure



**Figure 7:** Dependence of the Environmental Impact Index on Temperature and Water Flow Rate

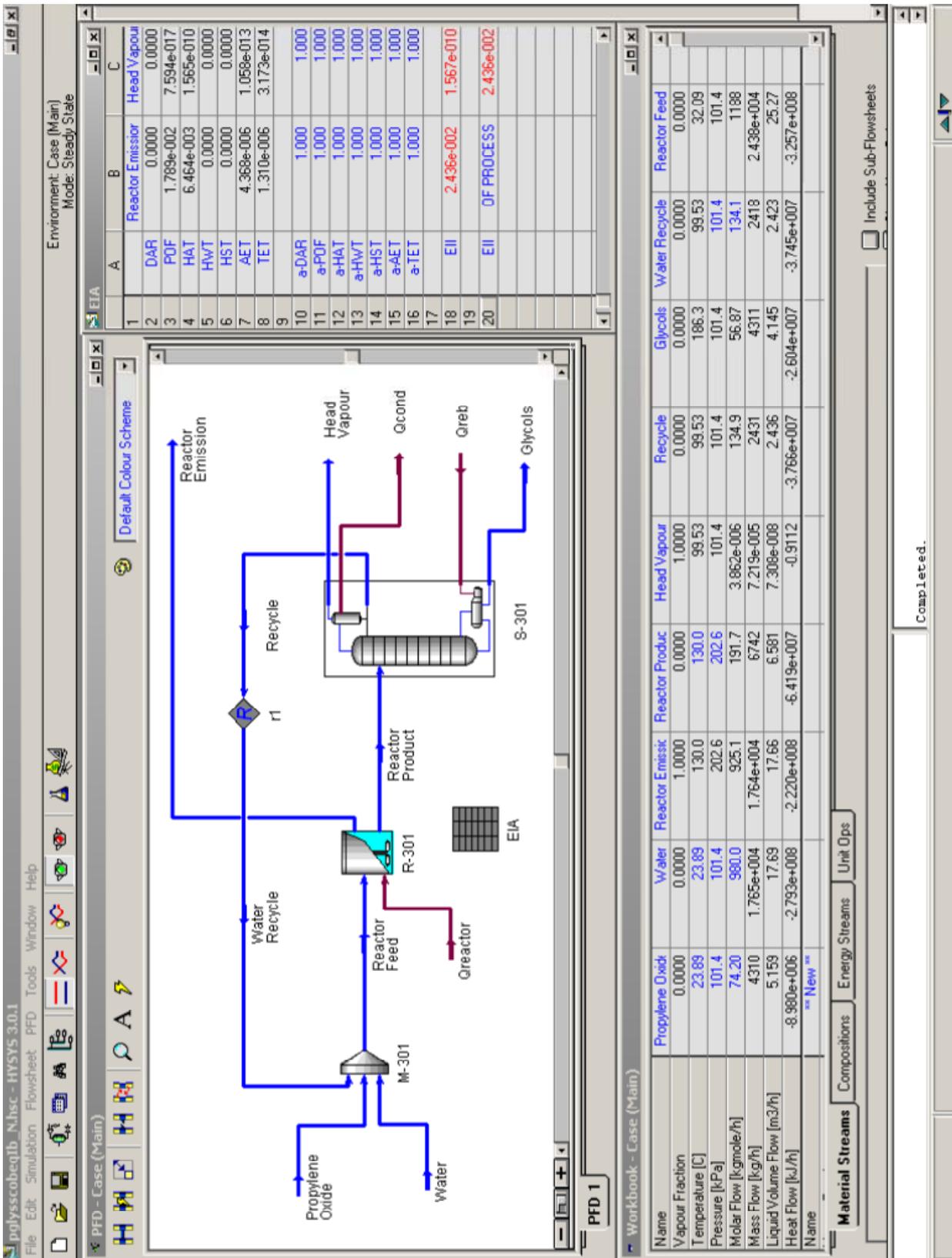


Figure 8: PFD, Workbook, and Spreadsheet for the Process considered

## FINAL REMARKS

The design of new chemical process units requires an environmental impact assessment together with the traditional economic evaluation. This activity must also be considered in development of operating policies in order to guarantee that unit operation will achieve the environmental performance desired.

In both cases, commercial simulators can be used with only minor adjustments. In this work, a practical case of application of HYSYS was presented to quantify the environmental impact of a chemical process.

The results obtained allow the user to quantify the major indicators in order to make decisions during design to minimise the generation of toxic waste as well as to take action during plant monitoring aiming to maintain its operation according to legal environmental standards. In addition to the environmental analysis, it allows for the establishment of heuristics previously based only on economic concerns.

## REFERENCES

- Azapagic, A. and Clift, R., The Application of Life-Cycle Assessment to Process Optimisation, *Comp. & Chem. Eng.*, 23, 1509-1526 (1999).
- Azapagic, A., Life-cycle Assessment and Its Application to Process Selection, Design and Optimisation, *Chem. Eng. J.*, 73, 1-26 (1999).
- Bauer, P.E., Technical-Economic Study of Industrial Use Alternatives for Coal gas (in Portuguese). M.Sc. thesis, Universidade Federal do Rio de Janeiro, Rio de Janeiro (1978).
- Bauer, P.E. and Maciel Filho, R., Methods for Environmental Impact Evaluation in the Chemical Process Design and Operation (in Portuguese), II Congresso de Engenharia de Processos do MERCOSUL, Florianópolis, Brazil (1999).
- Burguess, A.A. and Brennan, D.J., Application of Life-Cycle Assessment to Chemical Processes, *Chem. Eng. Sci.*, 56, 2589-2604 (2001).
- Cano Ruiz, J.A. and McRae, G.J., Environmentally Conscious Chemical Process Design, *Ann. Rev. Energy Environ.*, 23, 499-523 (1998).
- Curran, M.A., *Environmental Life-Cycle Assessment*, McGraw-Hill, New York (1996).
- Douglas, J.M., Process Synthesis for Waste Minimization, *Ind. Eng. Chem. Res.*, 31(43), 238-243 (1992).
- Fogler, H.S., *Elements of Chemical Reaction Engineering*, Upper Saddle River, NJ: Prentice-Hall Inc (1999).
- Freeman, H., Haryen, T., Springer, J., Randall, P., Curran, M.A., and Stone, K., Industrial Pollution Prevention: A Critical Review. *J. Air Waste Manage. Assoc.*, 42, 618-656 (1992).
- Guinée, J.B., Gorrae, M., Heijungs, R., Huppes, G., Kleijn, R., de Koning, L., Wegener Sleswijk, A., Suh, S., Udo de Haes, H.A., de Bruijn, H., Van Duin, R., and Huijbregts, M.A.J., *Handbook on Life-Cycle Assessment Operational Guide to the ISO Standards*, Dordrecht: Kluwer Academic Publishers (2002).
- Heijungs, R. and Kleijn, R., Numerical Approaches towards Life-Cycle Interpretation: Five Examples, WP-SSP Working Paper 2000.001, Centre of Environmental Science (CML), Leiden University, The Netherlands (2000).
- Hertwich, E.G., Pease, W.S., and Koshland, C.P., Evaluating the Environmental Impact of Products and Production Processes: A Comparison of Six Methods, *Sci. Total Environ.*, 196, 13-29 (1997).
- Hyprotech Ltd., *HYSYS.Plant Release 2.4 User Guide*. Calgary: Canada (2001).
- ISO International Standard 14040, *Environmental Management – Life-Cycle Assessment – Principles and Framework*, International Organisation for Standardisation (ISO), Geneve (1997).
- Jackson, T. and Clift, R., Where's the Profit in Industrial Ecology, *J. Ind. Ecol.*, 2, 3-5 (1998).
- Turton, R., Bailie, R.C., Whiting, W.B., and Shaiwitz, J.A., *Analysis, Synthesis, and Design of Chemical Processes*, Upper Saddle River, NJ: Prentice-Hall Inc (1998).
- Vignes, R.P., Use Limited Life-Cycle Analysis for Environmental Decision-Making, *Chem. Eng. Prog.*, 40-54, Feb 2001.