Environmental assessment integrated with process simulation for process design

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Abstract: The decisions within design and renovation of processes have traditionally been based only on technical and economic aspects. The impacts that waste emissions have on the environment have been taken in consideration after setting the basic lines of the project and even after having fixed the layout. A new approach, involving all these issues at the same time, has been developed in order to make better use of natural resources. The aim of this work is to integrate both process design and environmental tools in order to develop a methodology that involves, simultaneously, *environmental analysis* and *process modelling*. This methodology integrates both *raw materials* and *energy streams,* and specifies the main elements needed to interconnect the available data and variables. Furthermore, the outputs in the process modelling and environmental analysis are used as feedback in the design process. As an application example of this methodology, the Municipal Solid Waste incineration plant in Tarragona has been studied.

Keywords: Design for Environment; Life Cycle Management, Life Cycle Assessment and Modelling Integration; incineration process

1. INTRODUCTION

The international agreements to decrease the pollutants emitted by industrial processes makes necessary to consider different alternatives of processes and products design. One of these alternatives refers to the identification and quantification *a priori* of the impacts generated in the process. The achievement of this goal requires in most of cases, to a multidisciplinary design team to evaluate simultaneously many different aspects (environment, security, health, operations, control, etc.) [Gradael, 2000]. One of the techniques recently proposed to do it, is the *Design for the Environment* (DfE), which contains systematic considerations regarding environmental health and security objectives, along with the life cycle of the products and processes [Fiksel, 1993]. On the other hand, methodologies to environmental analysis like L*ife Cycle Assessment* (LCA) – that is a chain-oriented methodology applied in evaluations of environmental performance of products, along it all life cycle – are strongly related to process analysis. In this frame, the flow of cross-linked information in a LCA states the importance and novelty of the association between process analysis and the environmental assessment.

The fundamental approaches in process analysis (synthesis, modelling, and design) have particular attributes, require different types of information and provide results applicable in several ways. The strong relationship between them allows their integration with other resources of information transference, cycles revision and retro-feed information. Nowadays there are several software packages available for process analysis. However, great part of them are directly used for life cycle analysis without contemplating environmental impacts, which has to be classified, characterised, and quantified in order to know its magnitude [De Caluwe, (1997].

The environmental and process analysis may be unified under the approach L*ife Cycle Engineering (LCE)*, which permits supporting the decision-making when a product system analysis is performed [Spatari, 2001]. Nevertheless to realise this unification, should be important that LCE would be based on the modelling approach.

In this context, the current work purposes a methodology that permits the introduction of environmental concerns in the process analysis by the on-line prediction of environmental damage for different scenarios of study.

2. METHODOLOGY

2.1 Topics for integration

The integration of information is realised in two stages: *identification of variables*, and *capture-transference of data.* The first stage allows identifying process streams and some basic information regarded to their role in the process (input/output, energy/material and product/by-product). An efficient procedure to perform this task is the process description, which can be easily made by a flowsheet analysis. Nevertheless, the variables in modelling and environmental assessment must have similar characteristics to create a consistent methodology. In the second stage, the process information is transferred and transformed, in order to be used by the subsequent step (Figure 1).

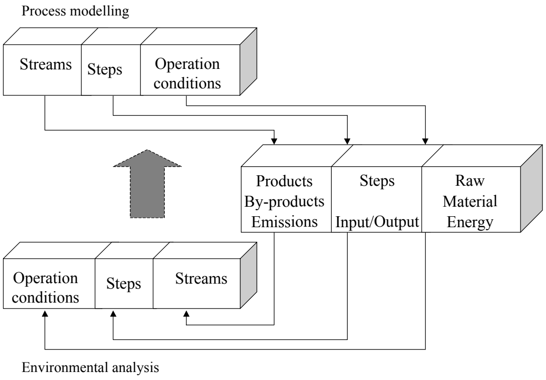

Figure 1. Global integration framework

2.2 Information transfer between tools

To makes the information transfer a connection between the tools must be previously established. An interface - builds up by the application of a computational programming language – permits supply this necessity, as can be seen in Figure 2.

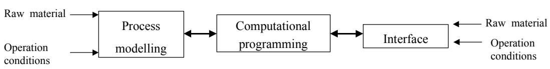

Figure 2. Connection between simulation and spreadsheet

The connection between interface and environmental analysis must consider several aspects. The first of them, is the capability of it in modifying importing and exporting information. The second aspect refers to the evaluation of the relationship between products, by-products and waste. Finally, a third aspect involves the two-way interconnection capabilities. In this case, the main characteristics to be considered are reading, updating and importing/exporting data.

2.3 Process design involving environmental concerns

The *process design* can be related to the process modelling and the *environmental analysis* by three steps. The first step executes the transference of information from the process simulation to the environmental analysis. In the second one, the environmental analysis computes the main loads and the stages where the pollutants are present. Finally, the results obtained can be used in the decision-making procedure, which completes the integration.

3. CASE STUDY

3.1 Solid Waste Incineration Plant

The Municipal Solid Waste Incinerator (MSWI) plant of Tarragona (SIRUSA) operates since 1991. Located in an industrial area, three kilometers far from Tarragona's town, this is one of the greatest units of solids incineration from all Spain.
In general terms, the incinerator embraces two parallel grate-fired furnaces, each one with primary and secondary chambers. The combustion process is based on Deutsche Babcock Anlagen technology, and was conceived to operate with a capacity of 9.6 tons per hour in each furnance. A general scheme of MSWI is presented in Figure 3.

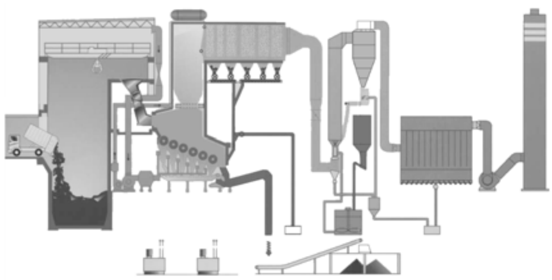

Figure 3. Scheme of the MSWI plant

To develop the simulation, the system was divided into three subsystems: 1) *Combustion,* 2) *Energy generation* and, 3) *Flue gas purification* [Kremer, 1998]. Each of the steps has defined the operation conditions, inlets and outlets. As this process has been object of previous studies, there was enough information available to carry out its simulation [Belevi, 2000].

3.2 Materials and methods

Several tools were used in the study. Initially, to the execution of the modelling process the computational device tool Hysys.Plant® [AEA Technology, 2001] was used to simulate the system. The information related with the resources consume and releases, were withdrawn in the ETH Report [Frischknecht, 1996], and TEAM™ [Ecobilan Group, 1998] databases.

3.3 Results from the simulated process

The MSW incineration process was modelled in the steady state mode of Hysys.Plant®. The main assumptions in the model are related to the inferred of the solids properties and the use of transfer coefficients for the metals [Fernández 1992 and Verhulst, 1996] without what would be really difficult to achieve consistent results. Figure 4 shows the scheme of the final case developed.

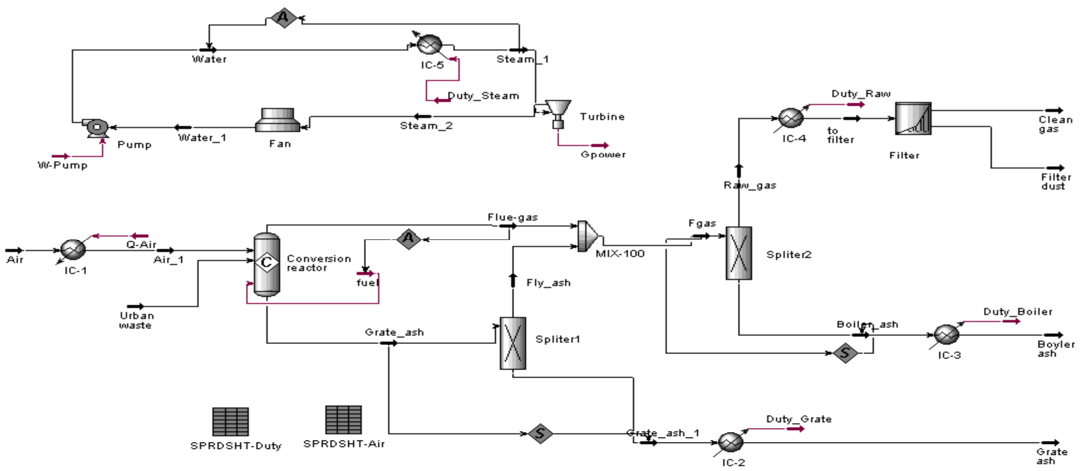

Figure 4. Process Flow Diagram of the Incineration Process

The information related with the properties of the inlet and outlet streams in the model is presented in Table 1. The columns *urban waste* and *clean gas*, contain information that correspond to plant data, provided by SIRUSA S.A. (Tarragona, Spain), which were used to develop the simulation of the process. The columns *grate ash, boiler ash* and *filter dust* by it turns, are results of the modelling.

Table 1. Properties of the main streams

Properties	Urban waste	Grate ash	Boiler ash	Filter dust	Clean gas
Temperature (ºC)	25	175	175	265	265
Pressure (kPa)	101.3	101.3	101.3	99[a]	99[a]
Mass flow (kg/h)	9.6E3	1,7E3	38.41	156.1	4.4E4
Heat Flow (kJ/h)	-4.2E+07	1.5E+6	3.4E+4	2.37E+5	- 1.6E+8

Due to natural difficulty of modelling an inorganic system like this, and the lack of information about their transfer coefficients, components as NOx and dioxins, that are really important from the environmental point of view, were not taken into account. In addition, the error made is not calculated due to the assumptions of the model.

Table 2,present the composition of the main streams.

Table 2. Composition for the streams

	Urban waste	Grate ash	Boiler ash	Filter dust	Clean Gas
Elements	(Kg/h)	(Kg/h)	(Kg/h)	(Kg/h)	(Kg/h)
Br	2.76	-	-	-	2.76
H_2O	2.65E+03	-	-	-	6.78E+03
C	2.49E+03	-	-	-	-
H_2	465.9	-	-	-	-
Cl_2	126.2	-	-	-	1.01
S	18.5	-	-	-	-
HF	-	-	-	-	2.47
CO_2	-	-	-	-	9.11E+03
HCl	-	-	-	-	128.8
SO_2	-	-	-	-	37
Ash	1.87E+03	1.69E+03	37.45	149.8	-
Hg	1E-03	-	4.E-06	-	9.E-04
Pb	2.03	1.32	0.01	0.7	-
Zn	5.47	3.49	0.08	1.91	-
Cd	0.05	0.01	-	0.04	-
Cu	6.43	6.24	0.02	0.18	-
Cr	1.11	1.07	0.02	0.02	-

3.4 Interface for information flow

In order to use the results from the process modelling in the environmental analysis, these were automatically sent to the interface by *MicroSoft© Visual Basic*, the computational resource to programming macros. The interface permits the control of the changes made in the operating conditions. These changes can be made with the linking and update features of *Hysys.Plant®* and *Microsoft© Excel*. The interconnection between the modelling process and the interface allows taking information from the simulation and send it to the interface. (Figure 5).

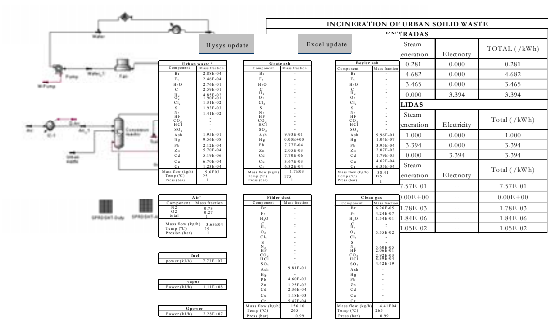

Figure 5. Interface to information transfer

3.4 Environmental analysis

The goal of an environmental analysis is to calculate the environmental impacts in an activity or process. However, in the life cycle assessment method, it is not usually known where and when all the emissions take place [Finnveden G 1999]. Due to this fact, the present study has been limited to three steps in the incineration process and only were defined the environmental loads without calculating the impacts.

In the case in study, the environmental analysis was carried out by means of modules and systems developed in TEAM™ tool. The modules levels represent the defined stages for the process and allow building the systems in study (*combustion, flue gas purification and energy generation*). The modules levels information was obtained by two ways, on one hand, information from process modelling (combustor, energy production and filter modules), and on the other hand, from the TEAM™ database (fuel and electricity modules). The ecological balance makes possible accounting the generated loads and their allocation. In addition, that analysis can be used during the inventory step of the LCA to determine the components of the system that must be evaluated. The loads were defined in terms of the principal emissions (Table 3).

The load balance shows an abridged inventory of the used resources and also, emissions to air, soil and water. Besides, this balance presents both the specific loads in each step, as well as the total load in the studied process. According to the balance, the major loads in the process are related on one hand with emissions of CO_2 and ash (present not only in the combustion process, but in the energy generation as well). And on the other hand, solid ash (generates in both stages: combustion and flue gas purification). Other emissions as SO_2 also were quite important, especially in the combustion process. However and due to the limitations in the model to simulate the real behaviour of the solids, the emissions of heavy metal could not present relevant values.

The results here obtained can give support in the decision-making procedure. Furthermore, this information is helpful in the projection of environmental loads.

Table 3. Main loads in the Ecobalance**.**

Article	Units	Total load	Loads per step		
		Incineration	Combustion	F, G, purification	Energy generation
(r) Barium Sulphate	kg	5,29E-02	5,23E-02	-	6,20E-04
(r) N Gas (in ground)	kg	5,21E+05	5,15E+01	-	5,93E-01
(r) Sand (in ground)	kg	4,39E-02	4,30E-02	-	9,46E-04
(r) Sodium Chloride	kg	2,55E-01	2,46E-01	-	9,53E-03
(r) Zinc	kg	3,76E-07	3,72E-07	-	4,41E-09
Electricity	MJ	241	241	-	-
Land Use	m^2	2,87E-06	2,87E-06	-	-
Waste	kg	9,60E+00	9,60E+00	-	-
Water Used (total)	L	5791,91	5,72E+03	-	7,17E+01
Grid power	MJ	1,00E+03	-	-	1,00E+03
(a) Acetaldehyde	kg	9,31E-06	1,12E-06	--	8,19E-06
(a) Arsenic	kg	3,84E-05	3,33E-05	--	5,13E-06
(a) Ash	kg	1,08E+02	1,04E-02	--	3,96E-04
(a) Benzene	kg	1,08E+02	1,04E-02	--	3,96E-04
(a) Cadmium	kg	7,85E-04	7,83E-04	--	2,23E-06
(a) Calcium	kg	2,56E-03	2,99E-04	--	2,26E-03
(a) Carbon Dioxide	kg	4,31E+02	4,03E+02	--	2,80E+01
(a) Carbon Monoxide	kg	4,53E-01	2,25E-01	--	2,28E-01
(a) Carbon Tetrafluoride	kg	1,25E-08	1,24E-08	--	1,47E-10
(a) Chromium	kg	2,00E-02	2,00E-02	-	-
(a) Cobalt	kg	8,86E-05	8,31E-05	--	5,48E-06
(a) Copper	kg	1,82E-02	1,82E-02	--	7,92E-06
(a) Hydrogen Sulphide	kg	7,35E-04	4,96E-04	--	2,39E-04
(a) Mercury	kg	9,13E-06	8,54E-06	--	5,93E-07
(a) Nitrogen Oxides	kg	1,16E-04	1,11E-04	--	5,71E-06
(a) Sulphur Oxides	kg	2,93E+00	2,77E+00	--	1,60E-01
(s) Ash	kg	1,90E+03	1,76E+03	1,41E+02	--
(s) Cadmium	kg	4,76E-02	1,36E-02	3,39E-02	1,43E-12
(s) Calcium	kg	2,70E-03	2,67E-03	--	3,16E-05
(s) Copper	kg	6,67E+00	6,50E+00	1,69E-01	7,26E-12
(s) Lead	kg	2,03E+00	1,37E+00	6,60E-01	3,32E-11
(w) Arsenic	kg	5,79E-05	5,76E-05	--	3,05E-07
(w) BOD5	kg	3,14E-03	3,14E-03	--	5,25E-06
(w) Cadmium	kg	4,74E-05	4,73E-05	--	9,64E-08
(w) COD	kg	6,00E-02	5,99E-02	--	8,44E-05

r = resources; a = air; s= soil; w = water

4. CONCLUSIONS AND OUTLOOKS

The present study allows observing that the integration of the tools of modelling process and environmental analysis lets using the results of each one of them recurrently. After establishing the design and operating conditions with the process modelling, the results are used to carry out the application of the environmental analysis.
With this methodology, the results obtained in an environmental analysis can be used (after their evaluation) as input information in a new modelling. Consequently, it will be possible to make decisions about improvements in the process,

such as a new unit, changes in the composition, and/or new operation conditions.
In the studied process and according to the balance, the major emissions were present in the combustion process and the flue gas purification.
The evaluation through the tools should help to the identification of the process stages that present the most significant environmental damages.
The chosen process is very uncomplicated, and the work not intend to be a rigorous study, nevertheless, the results may be used like

departure point for the knowledge of the main releases (and therefore of the impacts or risks) of this industrial activity.

Finally, from the process analysis approach, it is possible to define –at early stages of design-, the environmental implications of a process, and to determine their environmental impacts through a load balance. In the future, this should permit describing which is their real effect in specific geographical areas.

5. ACKNOWLEDGEMENTS

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