A CAPE OPEN Unit Operation for the Evaluation of Environmental Impact of a Chemical Process

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Maurizio Fermeglia
mauf@dicamp.units.it
Gennaro Longo
longo@ics.trieste.it
Letitia Toma
toma@ics.trieste.it

Agenda

- Goal and importance of the project
- The Waste Reduction Algorithm (WAR)
- The implementation of WAR in a CAPE OPEN Unit Operation
- Case study
- Conclusions

Sustainability

"Sustainability in Chemical Engineering means continuous effort to protect and improve ecosystems, social balance and economic prosperity by a systematic and integral improvement of

- Environmental protection
- Raw material exploitation
- Energy efficiency
- Safety and health protection

in all kinds of material conversion processes and material production"

(*EFCE definition*)

Goal of the project

- To introduce the concept of sustainability in the process design

Importance of the project

- Industry is an important factor for the economical growth
- Many factors go into investment decisions
- To evaluate the environmental impact of the chemical plants, situated in the developing countries, is essential because:

1. The old polluting industries are situated in the developing countries
2. The decision to invest and build a factory into a virgin area is very tempting because the developing countries offer facilities at a very low cost

The role of ICS-UNIDO

Promotion of and assistance in the development, selection, transfer and use of technology in favor of developing countries.

General Conference Vienna 3/7 December 2001-GC. 9/12/Add.1

Photo by: Luca D'Agostino

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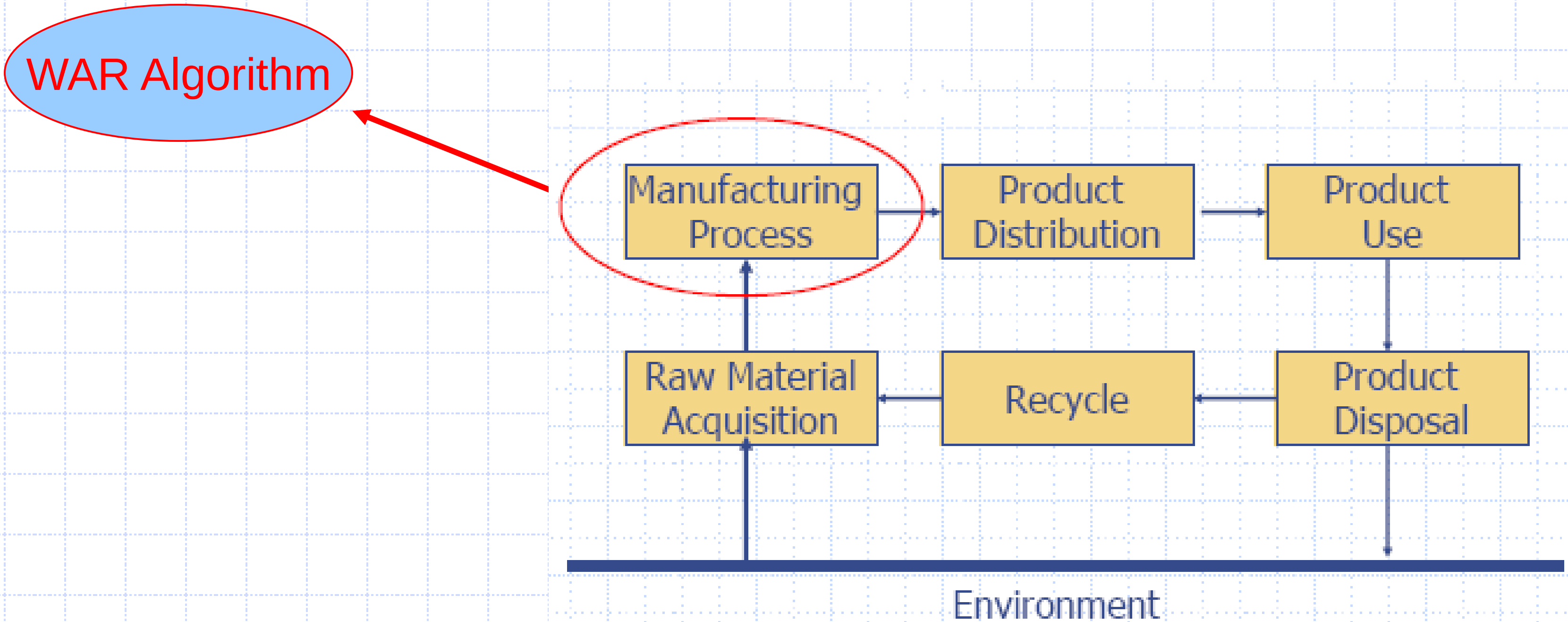
What is Waste Reduction Algorithm (WAR)?

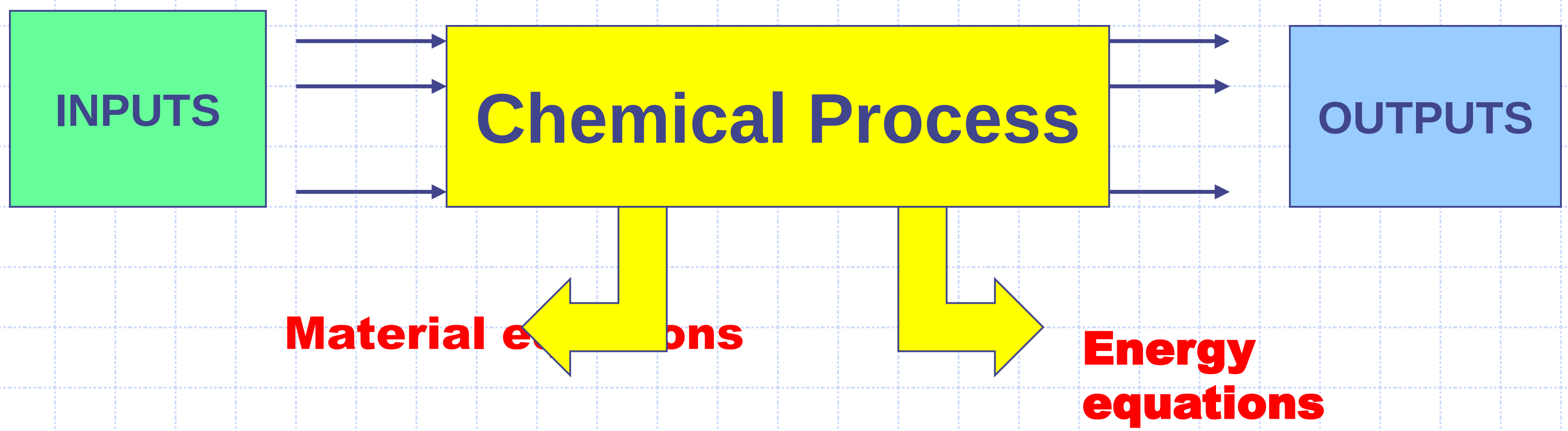
- Is a tool used to evaluate the environmental friendliness of a chemical process
- The evaluation is made through environmental impact indexes

From D.M.Young and H.Cabezas, 1999

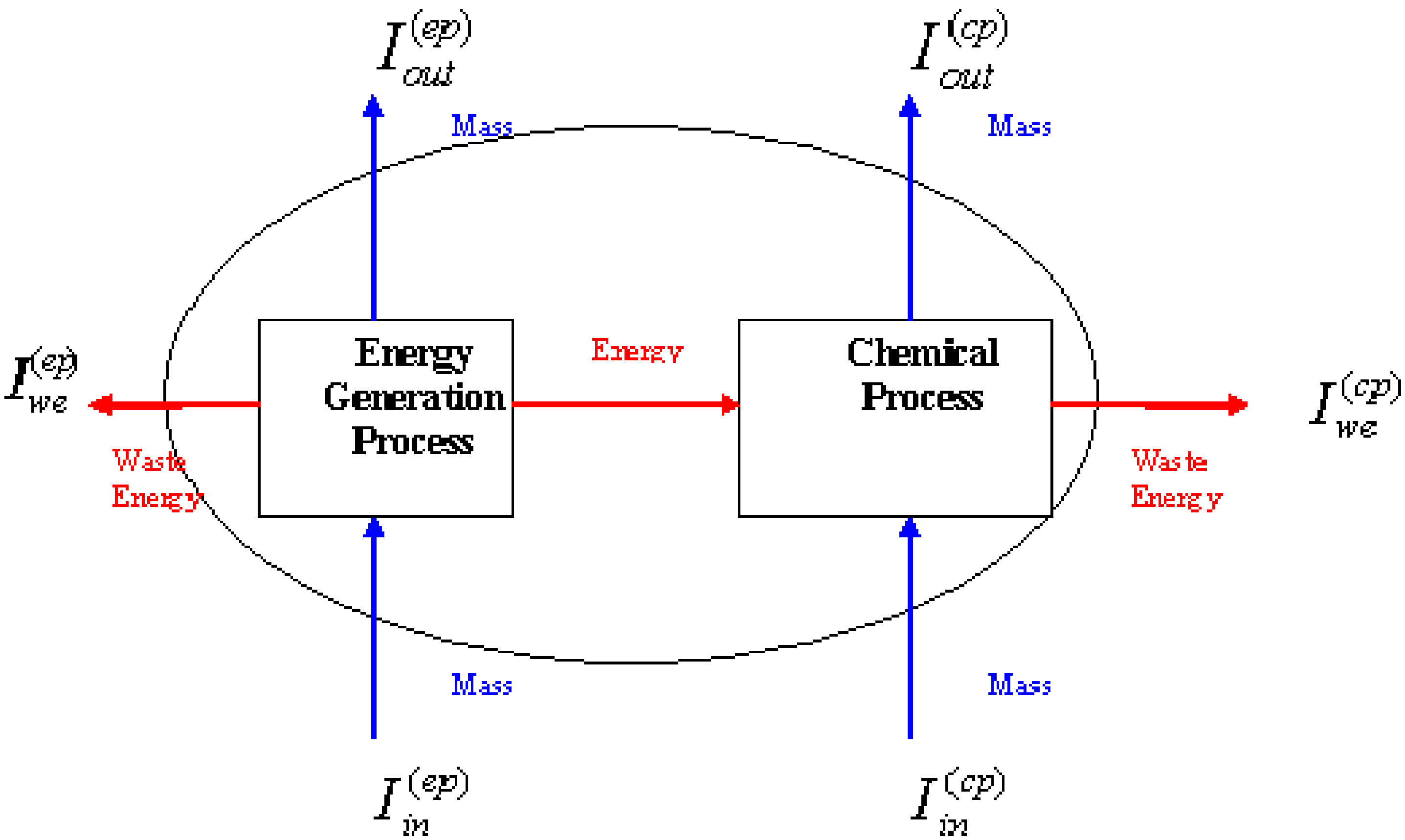
Today's approach of Process Simulation



From D.M.Young and H.Cabezas, 1999


INPUTS
Chemical Process
OUTPUTS
Material e
ons
Energy
equations

The environmental balance



From D.M.Young and H.Cabezas, 1999

PEI Balance

- General form of the equation

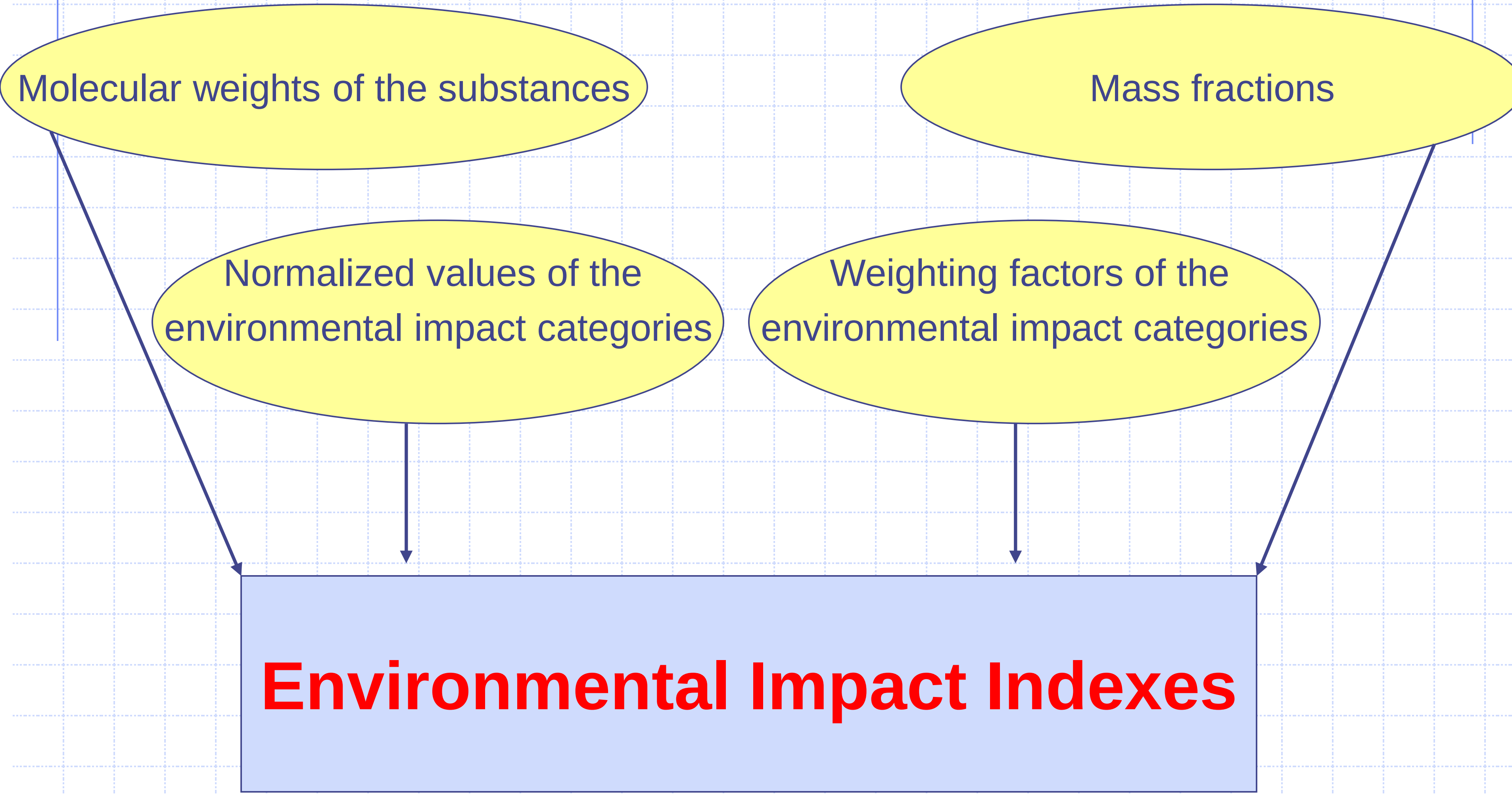
$$\frac{\partial I_{syst}}{\partial t} = I_{in}^{(cp)} + I_{in}^{(ep)} - I_{out}^{(cp)} - I_{out}^{(ep)} - I_{we}^{(cp)} - I_{we}^{(ep)} + I_{gen}^{syst}$$

- The equation at steady state

$$0 = I_{in}^{(cp)} + I_{in}^{(ep)} - I_{out}^{(cp)} - I_{out}^{(ep)} - I_{we}^{(cp)} - I_{we}^{(ep)} + I_{gen}^{syst}$$

From D.M.Young and H.Cabezas, 1999

Necessary elements to calculate the terms of the equation



Expressions for the chemical process

- The impacts due the emission of waste energy directly into the environment will be neglected
- Chemical process plants do not generally emit large amounts of waste energy into the environment
- For the chemical process plants, the environmental impact associated with the emission of mass is usually much greater than that associated with the emission of energy

$$I_{in}^{(cp)} = \sum_{j}^{cp} I_j^{(in)} = \sum_{j}^{cp} \dot{M}_j^{(in)} \sum_{k} x_{kj} \cdot \Psi_k + \ldots$$

$$I_{out}^{(cp)} = \sum_{j}^{cp} I_j^{(out)} = \sum_{j}^{cp} \dot{M}_j^{(out)} \sum_{k} x_{kj} \cdot \Psi_k + \ldots$$

$$I_{we}^{(cp)} = \sum_{i}^{cp} \dot{E}_j^{(cp)} \cdot \Psi_{we} \approx 0$$

From D.M.Young and H.Cabezas, 1999

Expressions for the energy generation process

- The PEI of the mass inputs is assumed to be zero

$$I_{in}^{(ep)} = \sum_{j}^{ep} I_j^{(in)} = \sum_{j}^{ep} \dot{M}_j^{(in)} \sum_k x_{kj} \cdot \Psi_k + \ldots \approx 0$$

- The PEI of the mass outputs are divide into gaseous and solid streams

$$I_{out}^{(ep)} = \sum_{j}^{cp} I_j^{(out)} = \sum_{j}^{ep-g} \dot{M}_j^{(out)} \sum_k x_{kj} \cdot \Psi_k + \sum_{j}^{ep-s} \dot{M}_j^{(out)} \sum_k x_{kj} \psi_k + \ldots$$

$$\approx \sum_{j}^{ep-g} \dot{M}_j^{(out)} \sum_k x_{kj} \cdot \Psi_k + \ldots$$

- The energy generation process is assumed to be a coal-fired electrical power plant and the mass inputs to this process consist mainly of coal and air along with water

$$I_{we}^{(ep)} = \sum_{i}^{ep} \dot{E}_j^{(ep)} \cdot \Psi_{we} \approx 0$$

From D.M.Young and H.Cabezas, 1999

Environmental Impact Categories

Local Toxicological		Global Atmospheric	
Human	Ecological	Global Warming Potential (GWP) 	Acidification Potential (AP) 
Human Toxicity Potential by Ingestion (HTPI) 	Aquatic Toxicity Potential (ATP) 		
Human Toxicity Potential by Inhalation and Dermal Exposure (HTPE)	Terrestrial Toxicity Potential (TTP)	Ozone Depletion Potential (ODP) 	Photochemical Oxidation Potential (PCOP) 

Environmental Impact Indexes

- Associated with PEI output (PEI/h or PEI/kg of product):
  - total rate of impact output $I_{out}^{(t)}$
  - total impact output per mass of products $\hat{I}_{out}^{(t)}$
- Associated with PEI generation (PEI/h or PEI/kg of product):
  - total rate of impact generation $I_{gen}^{(t)}$
  - total impact generated per mass of products $\hat{I}_{gen}^{(t)}$

From D.M.Young and H.Cabezas, 1999

Observations:

- The lower the value of these indexes the higher the environmental efficiency of a process
- The prudent course of action is to generate as little PEI as possible consistent with engineering constrains and societal needs

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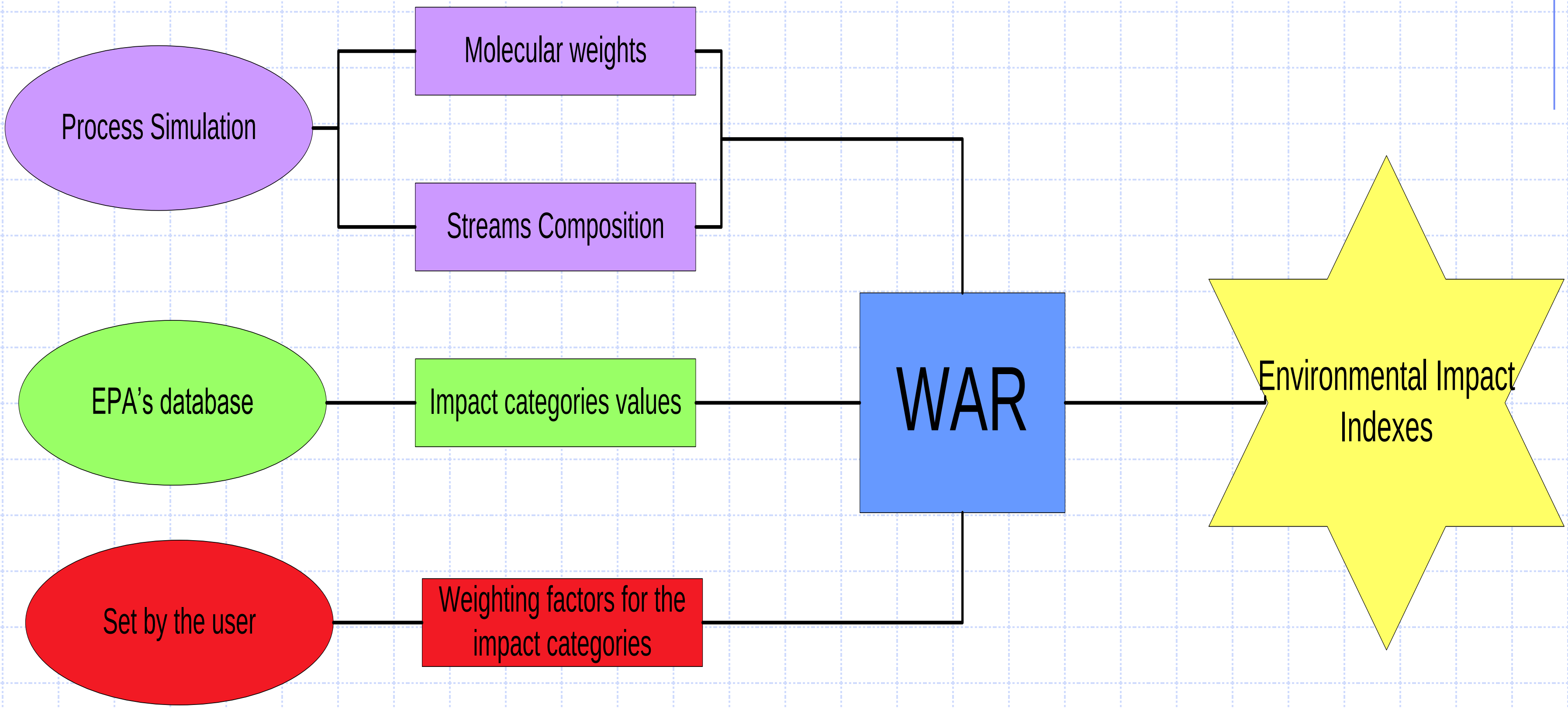
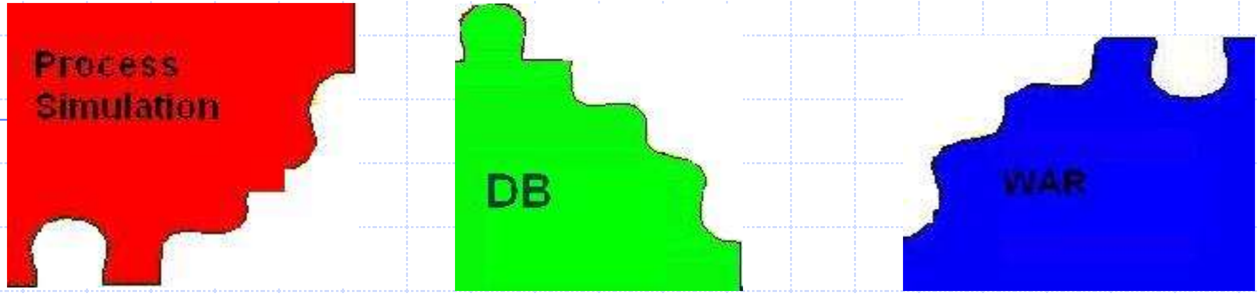
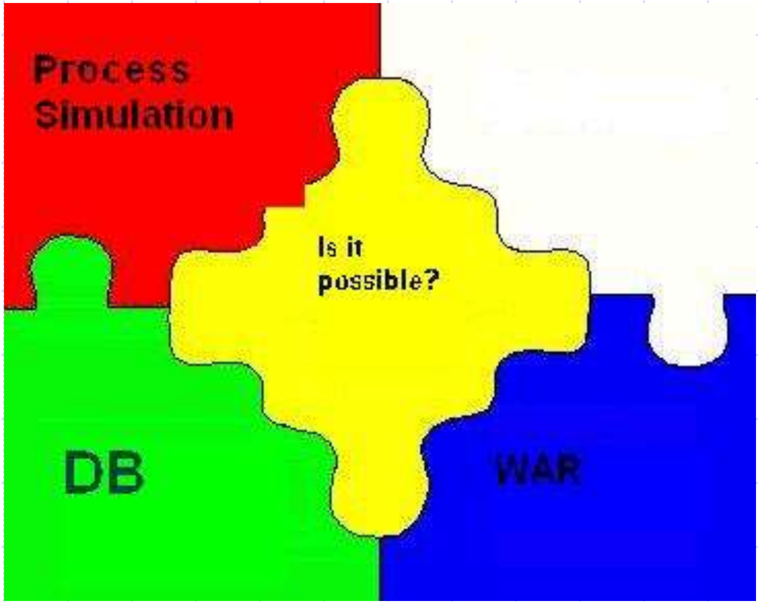
Necessary data for WAR

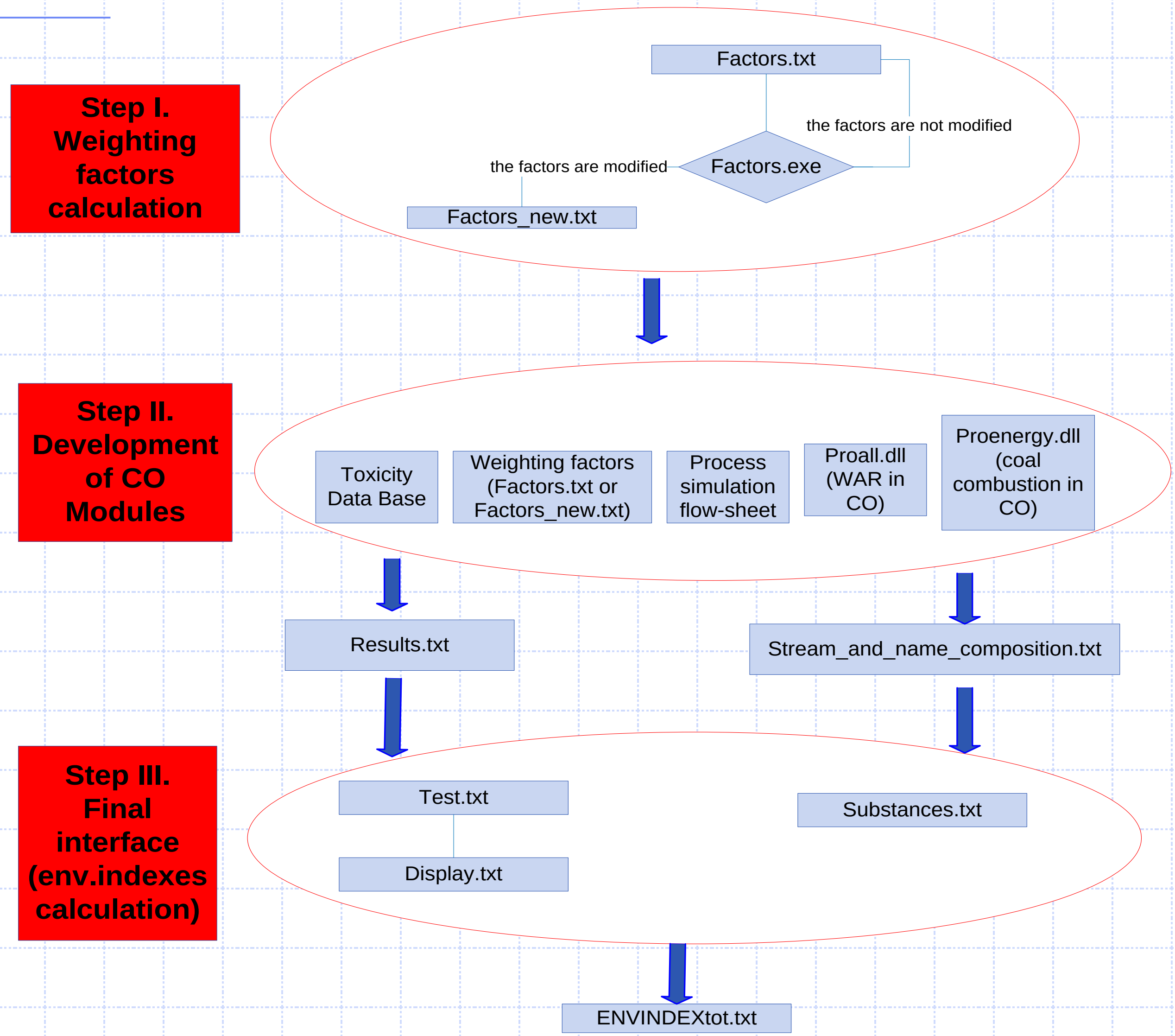



Process
Simulation
DB
WAR


Process
Simulation
Is it
possible?
DB
WAR

CAPE OPEN

Main framework of the implementation



Step1, Weighting Factors Interface…

Step2, Development of the CO Modules WAR implemented in a CO Module

The CO containing the WAR has:

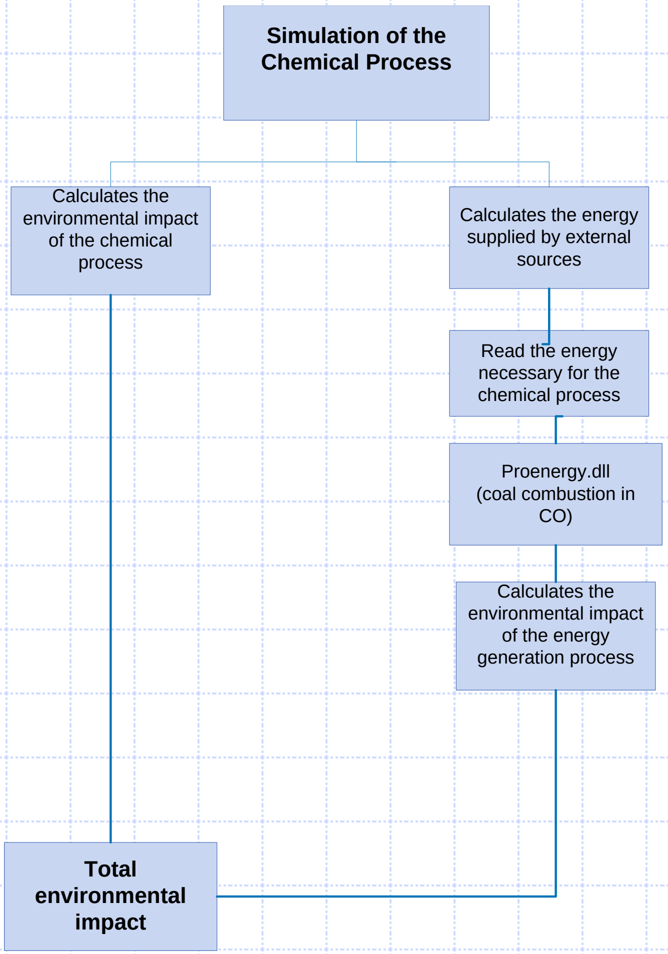
- One input port
- One output port
- Three parameters

Chemical Process			Energy Generation Process		
Name of the parameter	**Value**	**Results obtained after the simulation**	**Name of the parameter**	**Value**	**Results obtained after the simulation**
Process_Type (type)	0		Process_Type (type)	1	
Cape_position (Ind)	0 (for the input stream)	Value for In CP	Cape_position (Ind)	0 (for the input stream)	Value for In EP
	1 (for the waste stream)	Value for Out CP		1 (for the waste stream)	Value for Out EP
	2 (for the output-product-stream)	Value for Output stream of the chemical process			
	3 (for the internal stream of chemical process)	Message "Internal stream of the chemical process"			
cape_ID (name)	0 1 . N-number of CAPE OPEN modules inserted in the process		cape_ID (name)	0 1 . N-number of CAPE OPEN modules inserted in the process	

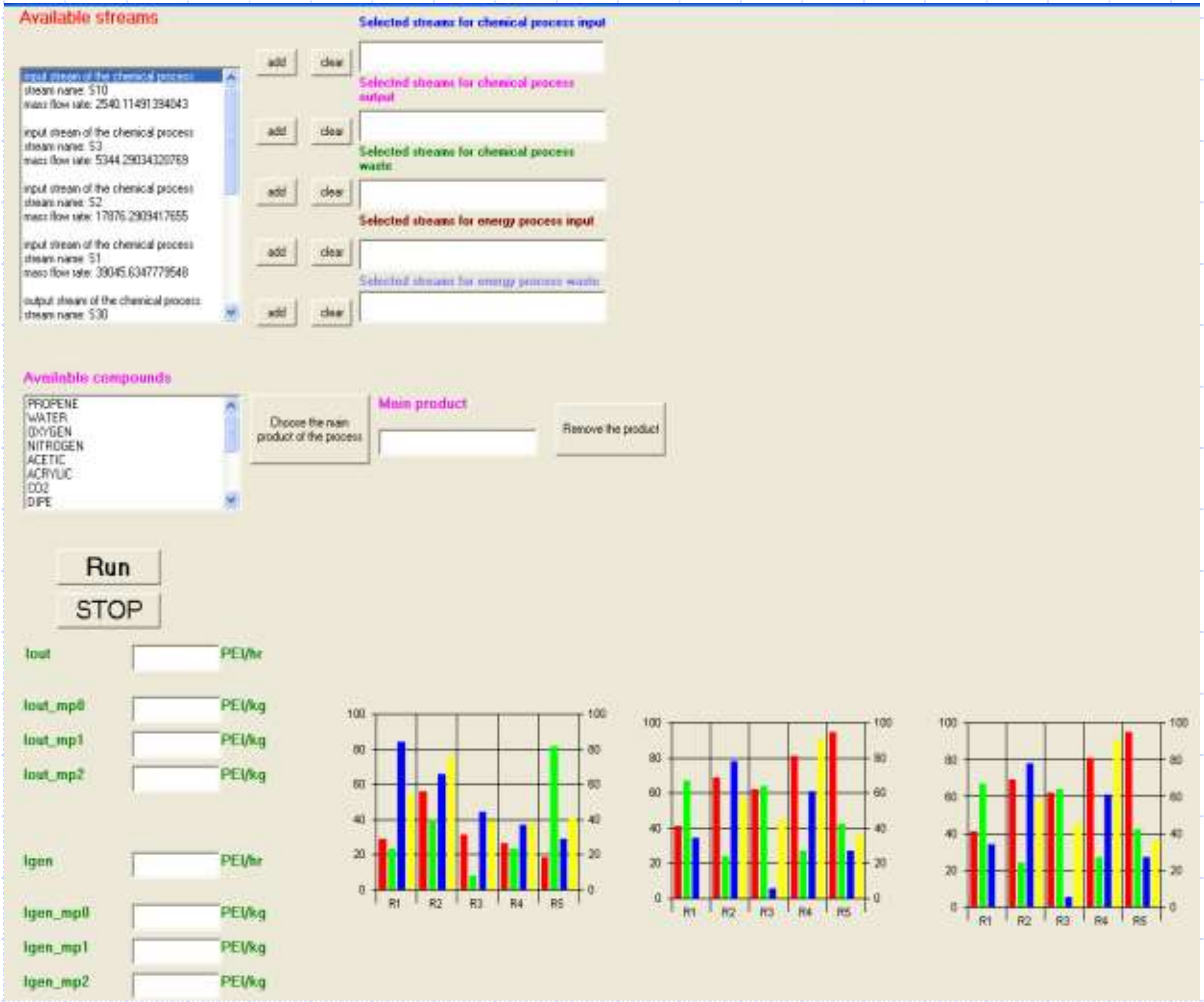
The energy generation process

- The energy is obtained from the combustion of the coal
- Only the gaseous streams are considered in the calculation of the environmental impact
- The material and the energy balance equations for the combustion of the coal were implemented in a CO Unit Operation

General Schema of the Total Environmental Impact



Step3, Final Interface



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Processes developed

- Acrylic Acid production
- Phthalic Anhydride production
- Formaldehyde production
- Mobile incineration of heavy oil laden soil
- Sweetening natural gas by means of dyglicolamine absorption
- Dimethyl ethere production

Phthalic Anhydride Production

- From o-xylene
- From naphtalene

The environmental impact of both processes was calculated with the described methodology

Practical demonstration…

Part 1
Weighting Factors Interface

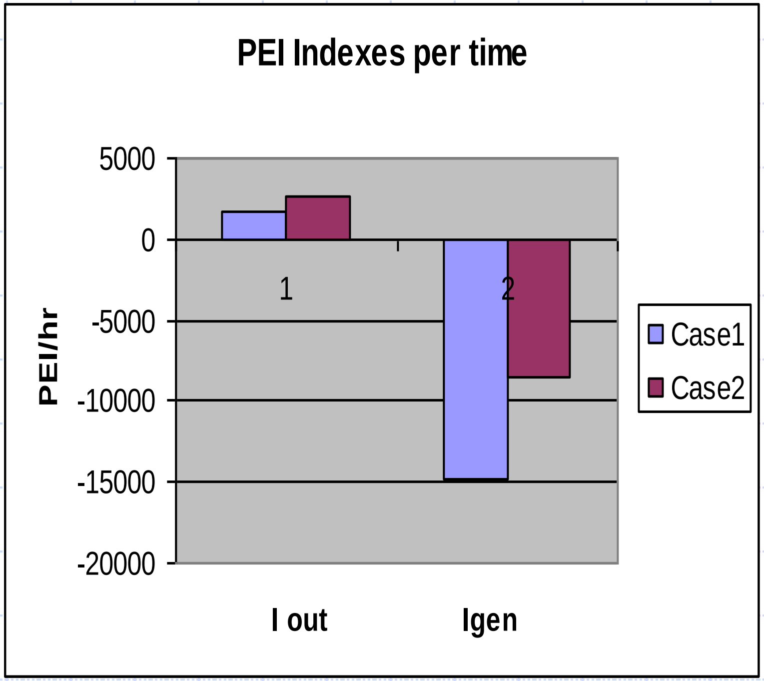
↓

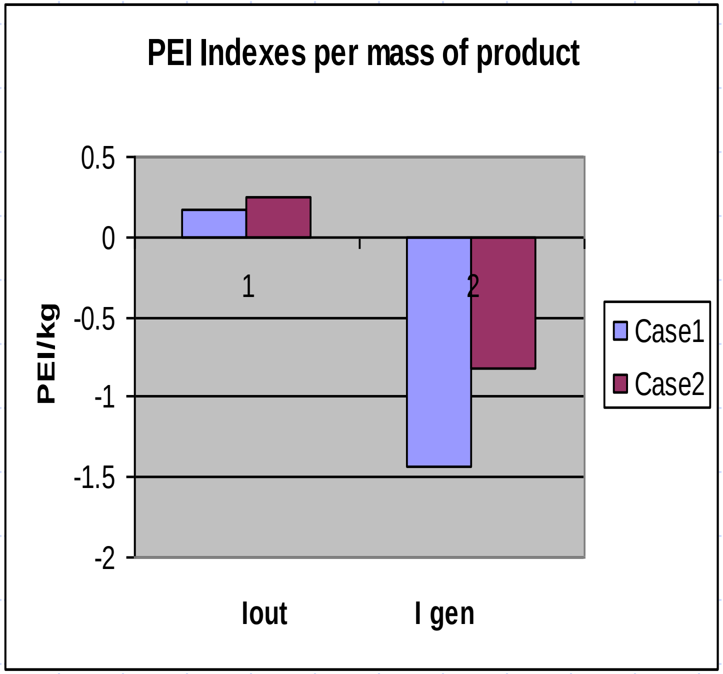
Part 2
CO Modules

↓

Part 3
Environmental Impact Indexes Interface

Environmental Impact Indexes





Conclusions

- It is possible to reduce the generation of the wastes and their environmental impact by modifying the design of the process
- The WAR is a useful tool for the design of new processes as well as modification of the old ones
- WAR was implemented in a CO Unit Operation
- The energy generation process connected to the chemical process is considered too, for a complete evaluation of the environmental impact
- The procedure was tested with success using two process simulators: PROII and Aspen Plus

Acknowledgments

- PROII and Aspen Plus support teams
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- University of Trieste