



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

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# 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.**

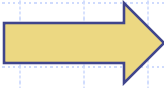
General Conference Vienna 3/7 December 2001-GC. 9/12/Add.1



Photo by: Luca D'Agostino

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# What is Waste Reduction Algorithm (WAR)?

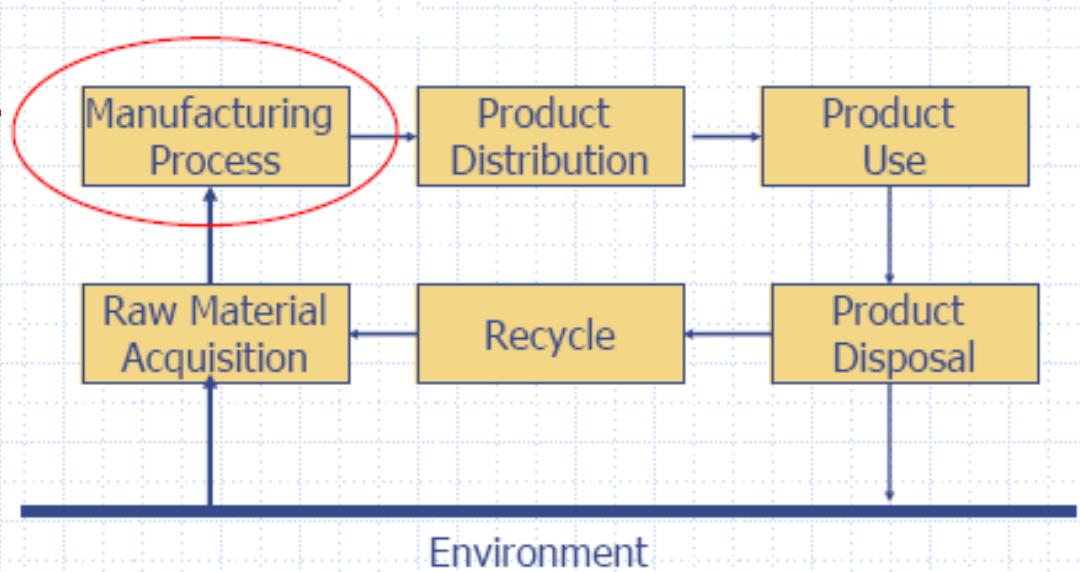
- ◆ Is a tool used to evaluate the environmental friendliness of a chemical process
- ◆ The evaluation is made through environmental impact indexes

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

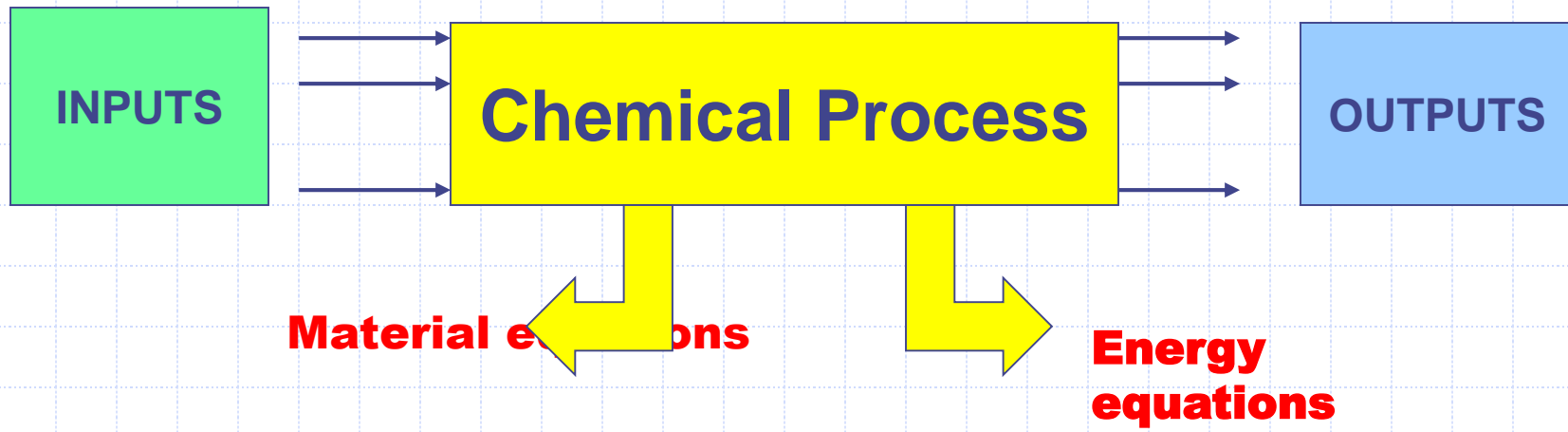


# Today's approach of Process Simulation

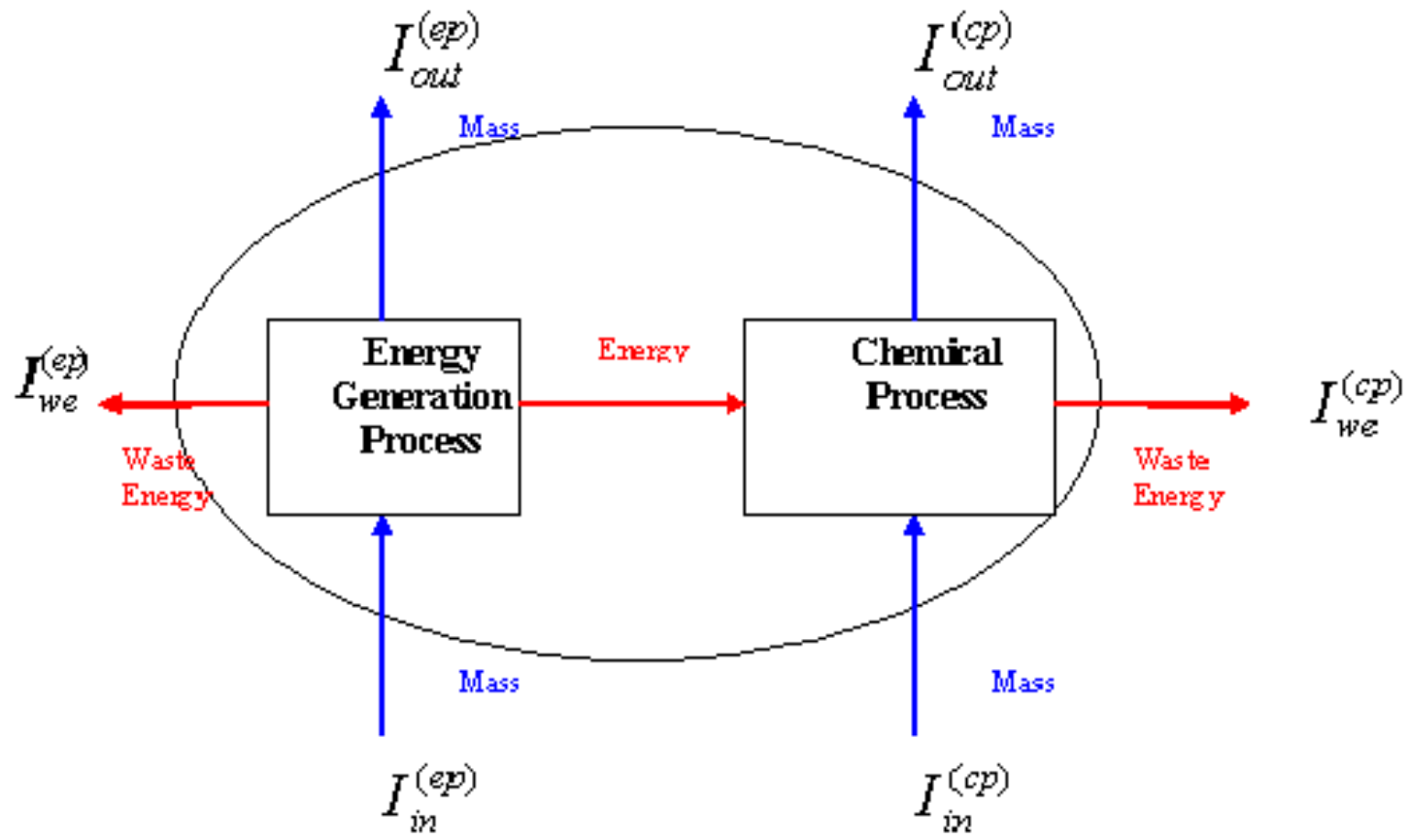
WAR Algorithm



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



# The environmental balance



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

# PEI Balance

- ◆ General form of the equation

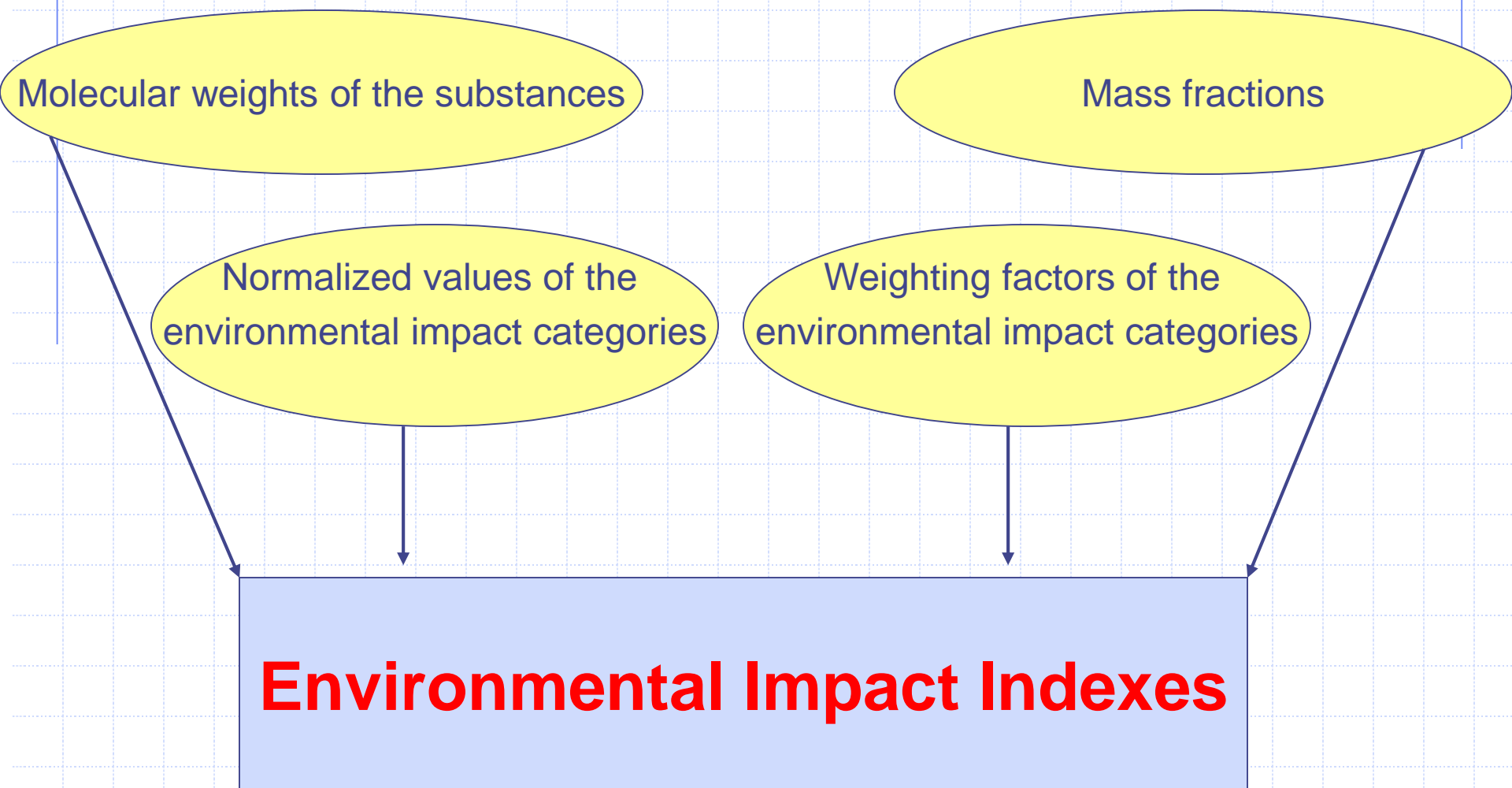
$$\frac{\partial I_{syst}}{\partial t} = I_{in}^{(cp)} + I_{in}^{(ep)} - I_{out}^{(cp)} - I_{out}^{(ep)} - I_{we}^{(cp)} - I_{we}^{(ep)} + I_{gen}^{syst}$$

- ◆ 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

$$I_{in}^{(cp)} = \sum_j^{cp} I_j^{(in)} = \sum_j^{cp} \dot{M}_j^{(in)} \sum_k x_{kj} \cdot \Psi_k + \dots$$

$$I_{out}^{(cp)} = \sum_j^{cp} I_j^{(out)} = \sum_j^{cp} \dot{M}_j^{(out)} \sum_k x_{kj} \cdot \Psi_k + \dots$$

$$I_{we}^{(cp)} = \sum_i^{cp} \dot{E}_i^{(cp)} \cdot \Psi_{we} \approx 0$$

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

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

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

$$\approx \sum_j^{ep-g} \dot{M}_j \sum_k x_{kj} \cdot \Psi_k + \dots$$

$$I_{we}^{(ep)} = \sum_i^{ep} E_j \cdot \Psi_{we} \approx 0$$

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  $I_{out}^{\wedge(t)}$

◆ 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  $I_{gen}^{\wedge(t)}$

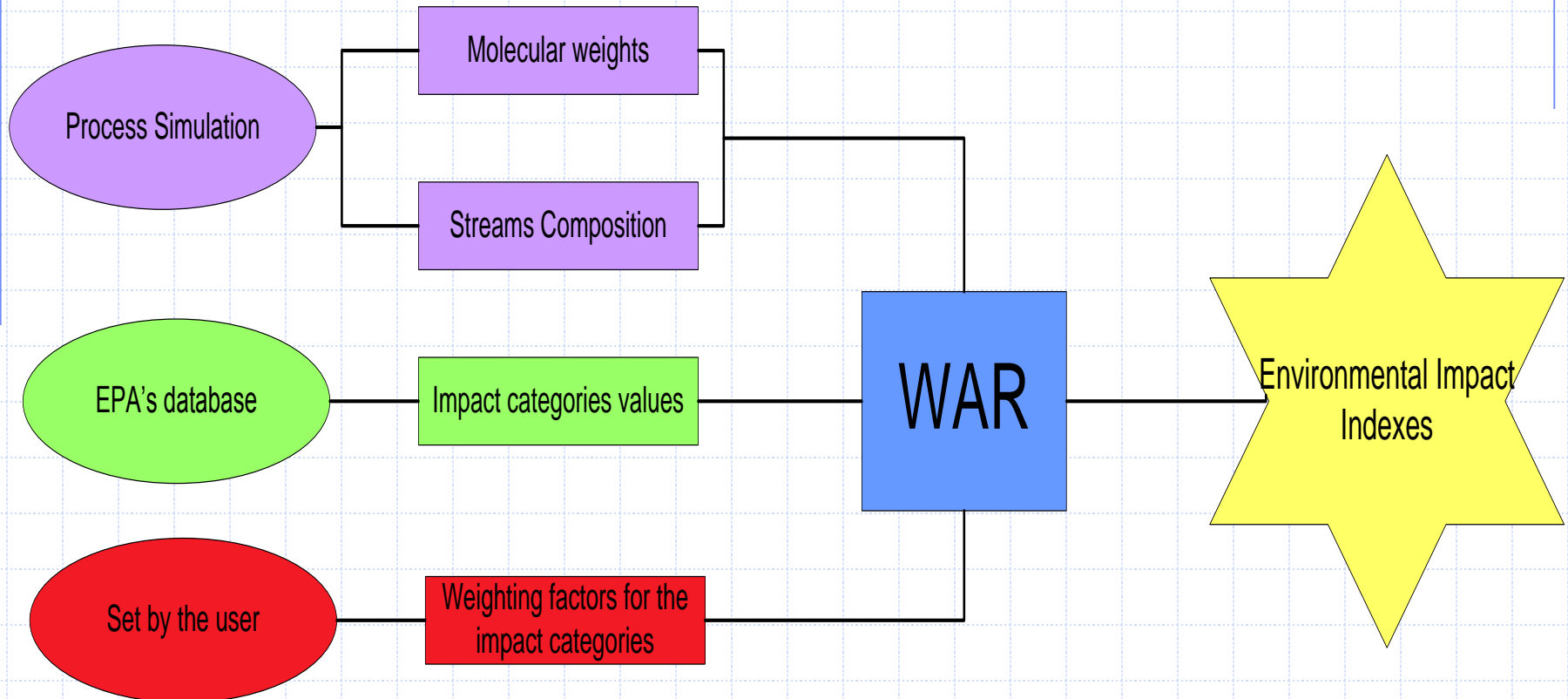
# Observations:

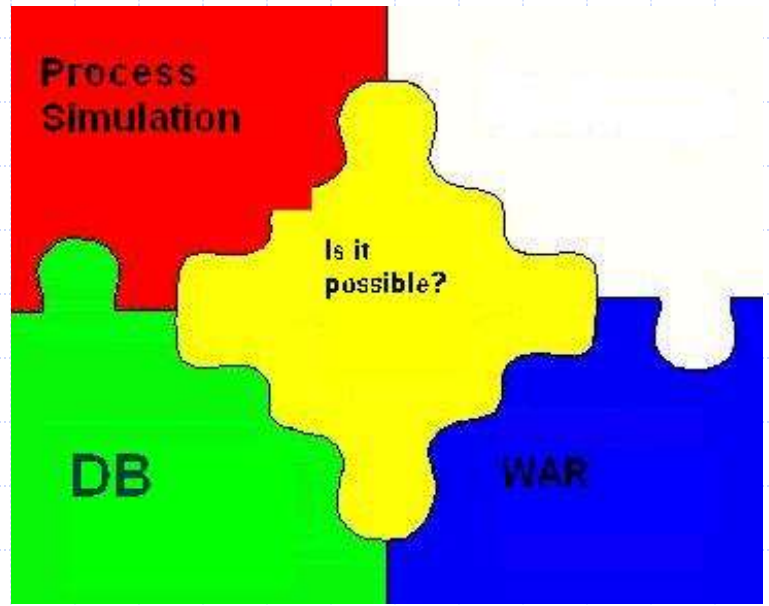
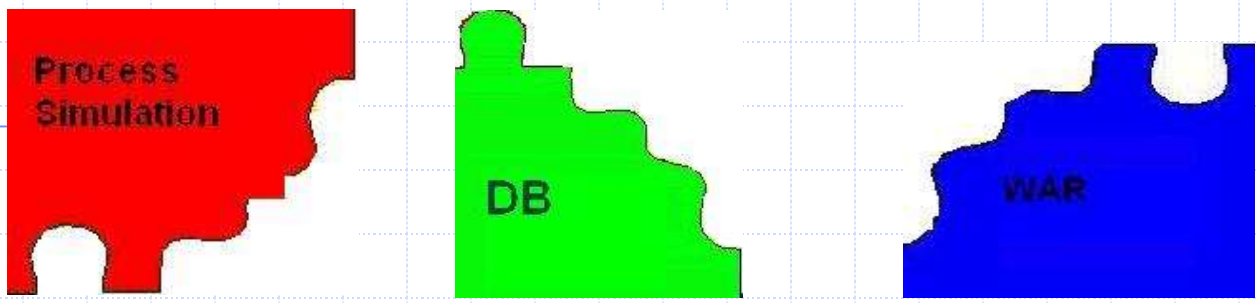
- ◆ The lower the value of these indexes the higher the environmental efficiency of a process
- ◆ The prudent course of action is to generate as little PEI as possible consistent with engineering constraints and societal needs

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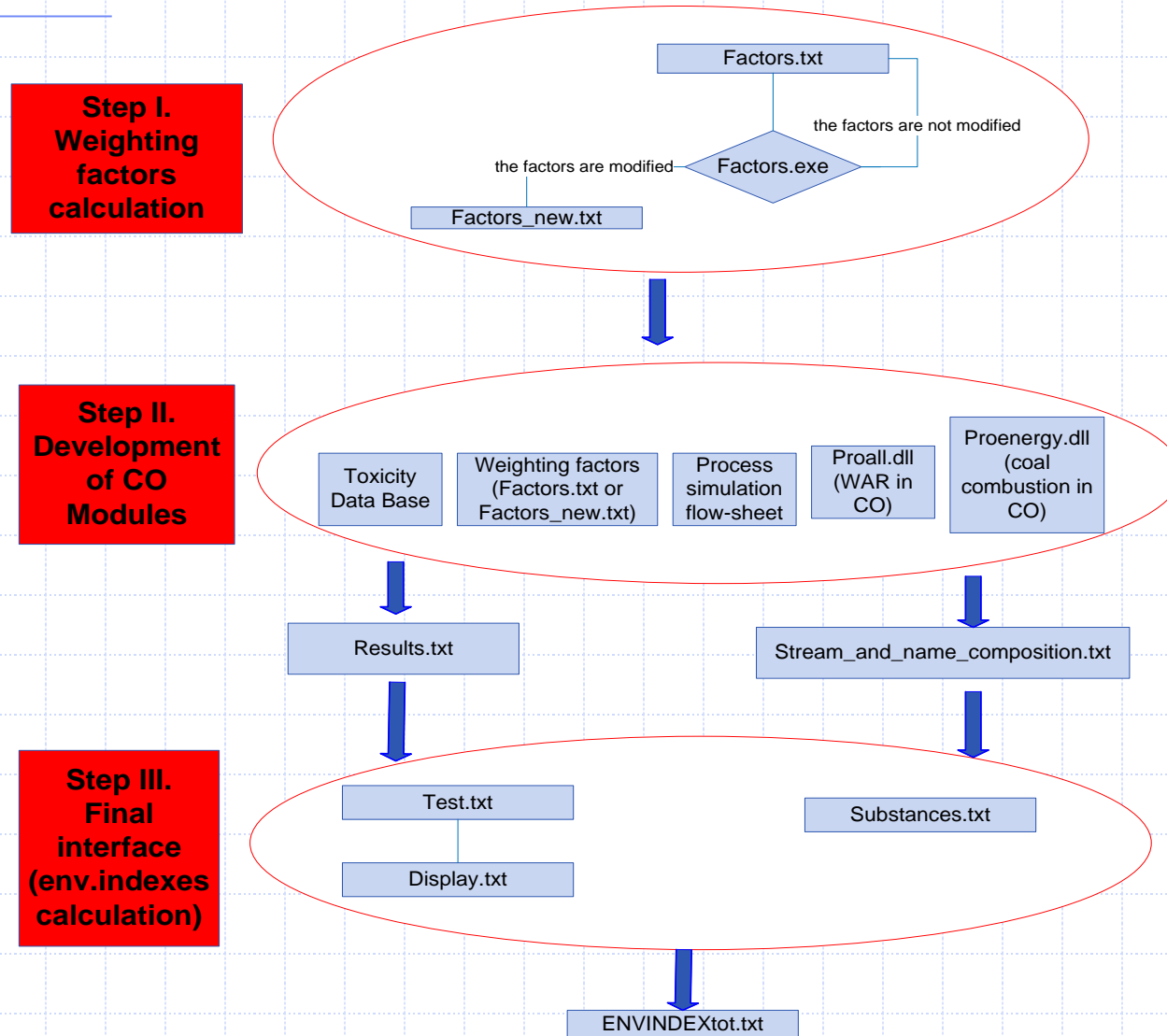
# Necessary data for WAR





# CAPE OPEN

# Main framework of the implementation



# Step1, Weighting Factors Interface...

Form1

## Weighting Factors

**GWP\_factor**

**ODP\_factor**

**PCOP\_factor**

**AP\_factor**

**HTPE\_factor**

**HTPI\_factor**

**TTP\_factor**

**ATP\_factor**

**Save the new values of the weighting factors**

**Set the weighting factors to the default values**

**STOP**

- What are the weighting factors?  
The weighting factors are numbers.
- Why are they used?  
The weighting factors are used to emphasize or de-emphasize specific concerns that are relevant or irrelevant to their process conditions and locality.
- Which are the default values?  
The WAR assigns a default value of unity (1) for all weighting factors. This implies that all the impact categories are equally important.
- Which are the values they can assume?  
Typically the weighting factors should range between 0 and 10 (according to local needs and policies).
- Some examples of the weighting factors
  - PCOP would be weighted more heavily than others impacts in an area that suffers from smog.
  - ATP would be weighted more heavily than others impacts if the process plant is discharging in a water body.
  - AP would have small values if the chemical plant is situated in the desert.

# 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

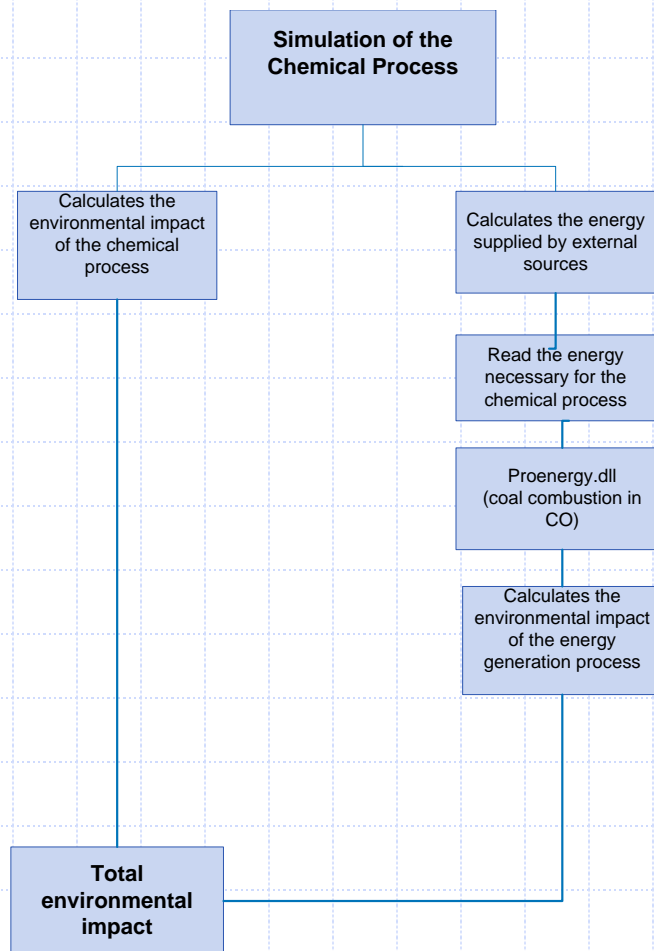
Chemical Process			Energy Generation Process		
Name of the parameter	Value	Results obtained after the simulation	Name of the parameter	Value	Results obtained after the simulation
<b>Process_Type (type)</b>	0		<b>Process_Type (type)</b>	1	
<b>CAPE_position (Ind)</b>	0 (for the input stream)	Value for In CP	<b>CAPE_position (Ind)</b>	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"			
<b>CAPE_ID (name)</b>	0		<b>CAPE_ID (name)</b>	0	
	1 . N-number of CAPE OPEN modules inserted in the process			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

### Available streams

input stream of the chemical process  
 stream name: S10  
 mass flow rate: 2540.11491394043

input stream of the chemical process  
 stream name: S3  
 mass flow rate: 5344.29334320769

input stream of the chemical process  
 stream name: S2  
 mass flow rate: 17876.2939417655

input stream of the chemical process  
 stream name: S1  
 mass flow rate: 38045.634773648

output stream of the chemical process  
 stream name: S30

### Selected streams for chemical process input

add clear

Selected stream for chemical process output

add clear

Selected streams for chemical process waste:

add clear

Selected streams for energy process input

add clear

Selected streams for energy process waste:

add clear

### Available compounds

PROPENE  
 WATER  
 OXYGEN  
 NITROGEN  
 ACETIC  
 ACRYLIC  
 CO2  
 DIFE

Choose the main product of the process

Main product

Remove the product

Run

STOP

tout  PEI/hr

tout\_mp0  PEI/kg

tout\_mp1  PEI/kg

tout\_mp2  PEI/kg

igen  PEI/hr

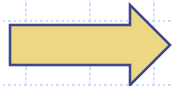
igen\_mp0  PEI/kg

igen\_mp1  PEI/kg

igen\_mp2  PEI/kg

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# Processes developed

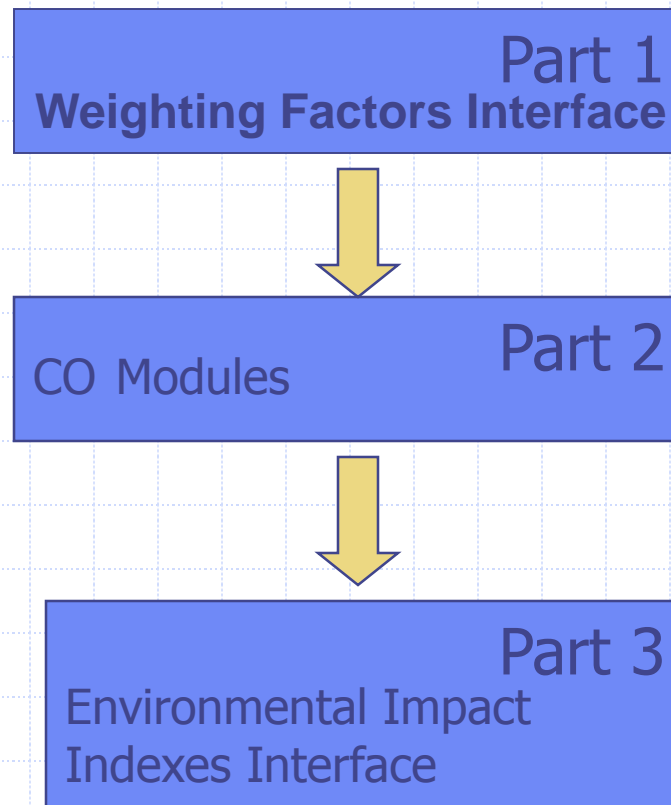
- ◆ Acrylic Acid production
- ◆ Phthalic Anhydride production
- ◆ Formaldehyde production
- ◆ Mobile incineration of heavy oil laden soil
- ◆ Sweetening natural gas by means of diglycolamine absorption
- ◆ Dimethyl ether production

# Phthalic Anhydride Production

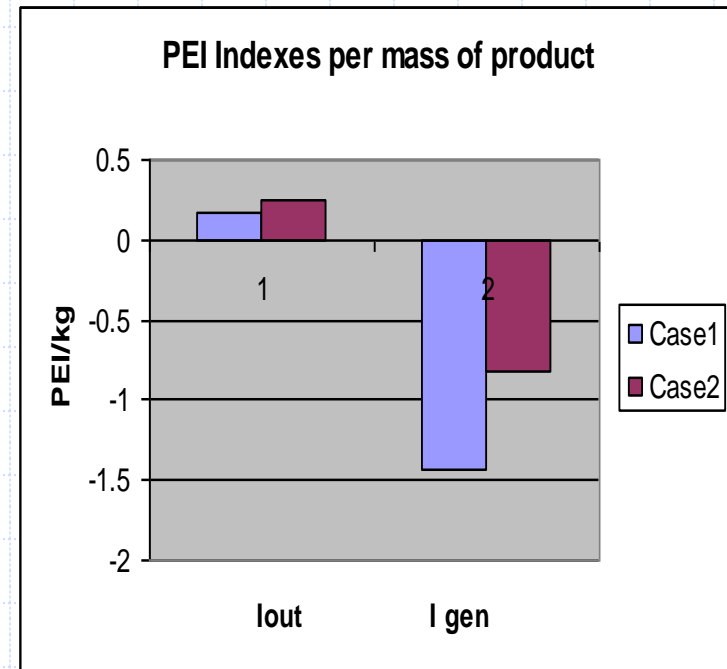
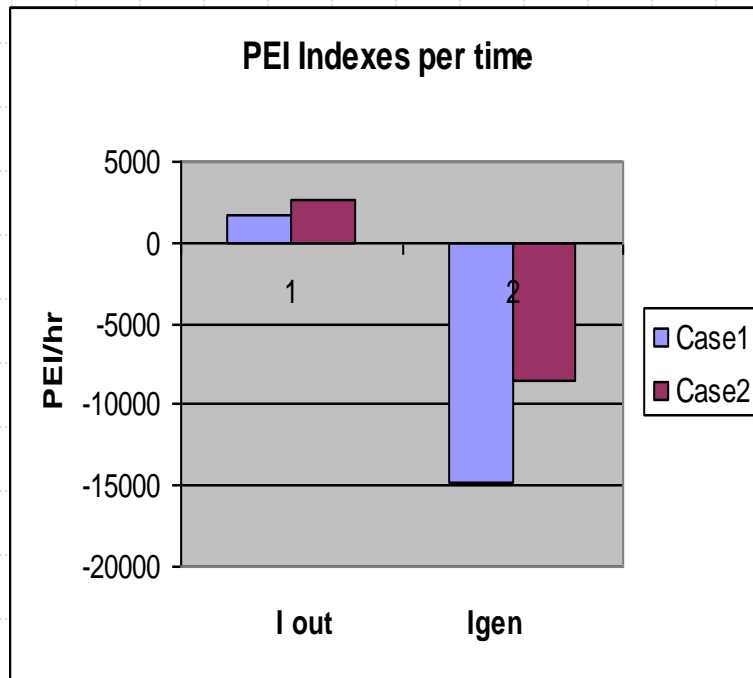
- ◆ From o-xylene
- ◆ From naphthalene

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

# Practical demonstration...



# 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
- ◆ Michel Pons, CO-LaN
- ◆ ICS-UNIDO
- ◆ University of Trieste