Environmental Life Cycle Assessment in Process Optimisation

Ana María ELICECHE
PLAPIQUI (Universidad Nacional del Sur – CONICET)
Bahía Blanca –ARGENTINA
meliceche@plapiqui.edu.ar

PASI – August 2008 - Mar del Plata

Outline

- Motivation.
- Potential environmental impact evaluation.
- Life cycle environmental impact assessment.
- Minimization of life cycle environmental impact.
- Operation of a steam and power sector.
- Different applications
- Conclusions.

Motivation

- Use environmental objectives to support a decision making process.
- Evaluate potential environmental impact from emissions calculated with process simulation.
- Minimization of life cycle environmental impact in process optimization.
- Contribute to a sustainable development in the environmental and economic aspects.

Challenges

- Selection of an environmental metric.

- Couple environmental objectives
  to rigorous process modelling.
  (From quantified emissions
  evaluate potential environmental impact)

- Environmental impact is directly correlated
  with process emissions so that
  the analysis, operation and design stages
  can be addressed.

- Extend the battery limits to include the main
  environmental impacts in the life cycle.

Environmental impact evaluation

Select a methodology that allows
the quantification of the environmental impacts
from the emissions
evaluated through process simulation.

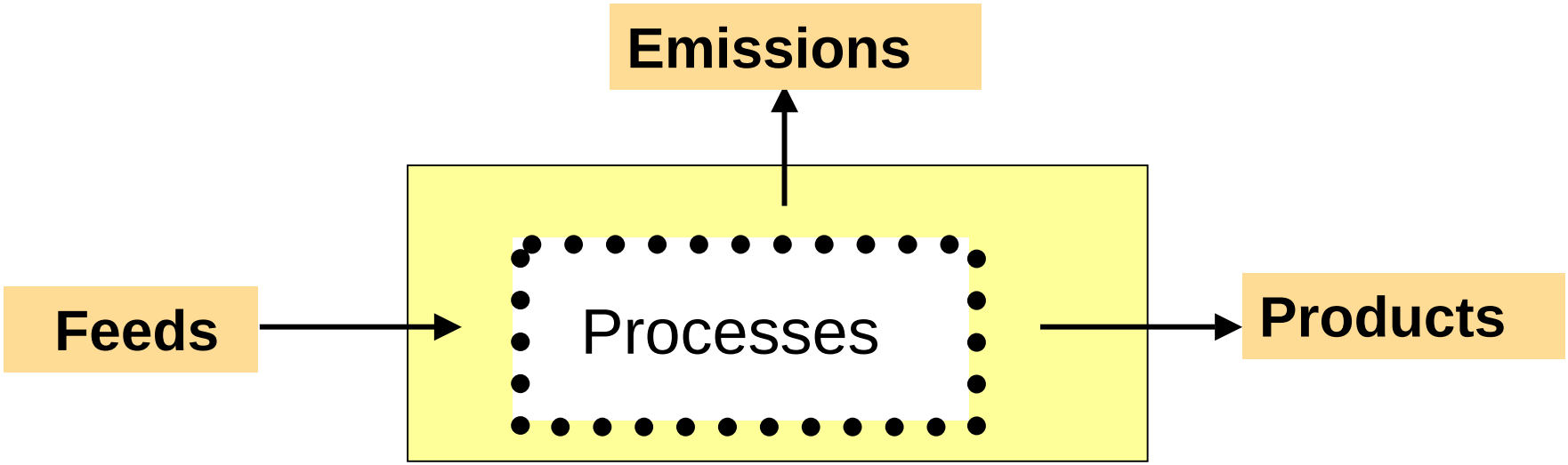
Heijungs et al.(1992)

Emissions quantification

Gaseous, liquids and solids

Process modelling and simulation

Rigorous modelling and simulation to quantify emissions.



Simulation considering small flows and compositions.

Environmental impact evaluation

Potential environmental impact evaluation

from the contribution of different

environmental impact categories.

Evaluate the environmental impact categories that follows

from process plat emissions.

Environmental impact categories

- GLOBAL WARMING
- ACIDIFICATION
- OZONE DEPLETION
- PHOTOCHEMICAL OXIDANTS (SMOG)
- AQUATIC ECOTOXICITY
- HUMAN ECOTOXICITY
- IONIZING RADIATIONS
- RESOURCE CONSUMPTION
  (Non renewable and scarce)

Environmental impact evaluation

$$\Psi = \sum_j \omega_j \times \psi_j$$

Total potential environmental impact: sum of the contributions of categories

$$\psi_j = \sum_k \psi_{kj}$$

Environmental impact category *j*

ω_j waiting factor for each category *j*

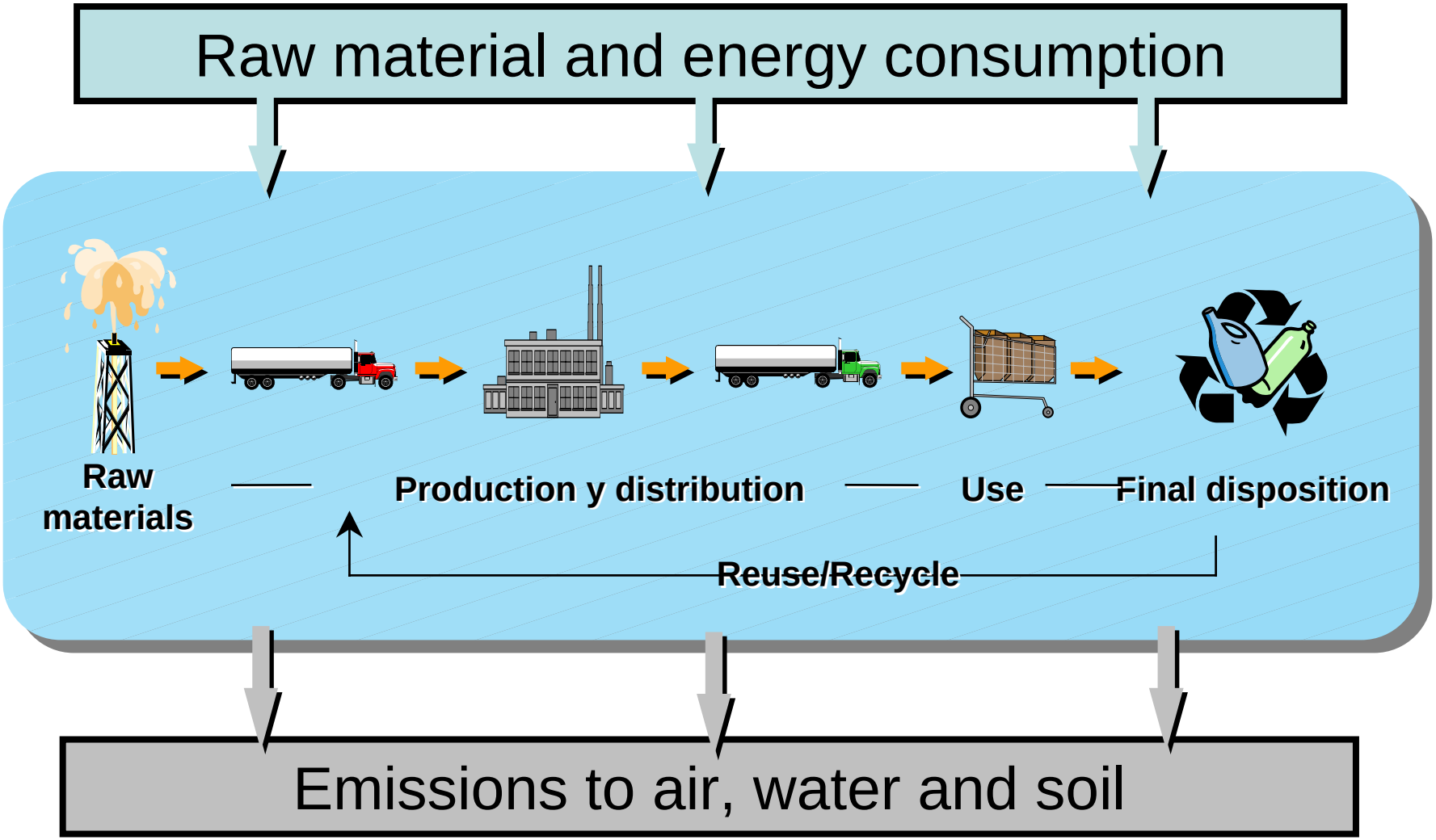
$$\psi_{kj} = F_k \ \gamma_{kj}$$

F_K flow rate of component *k*

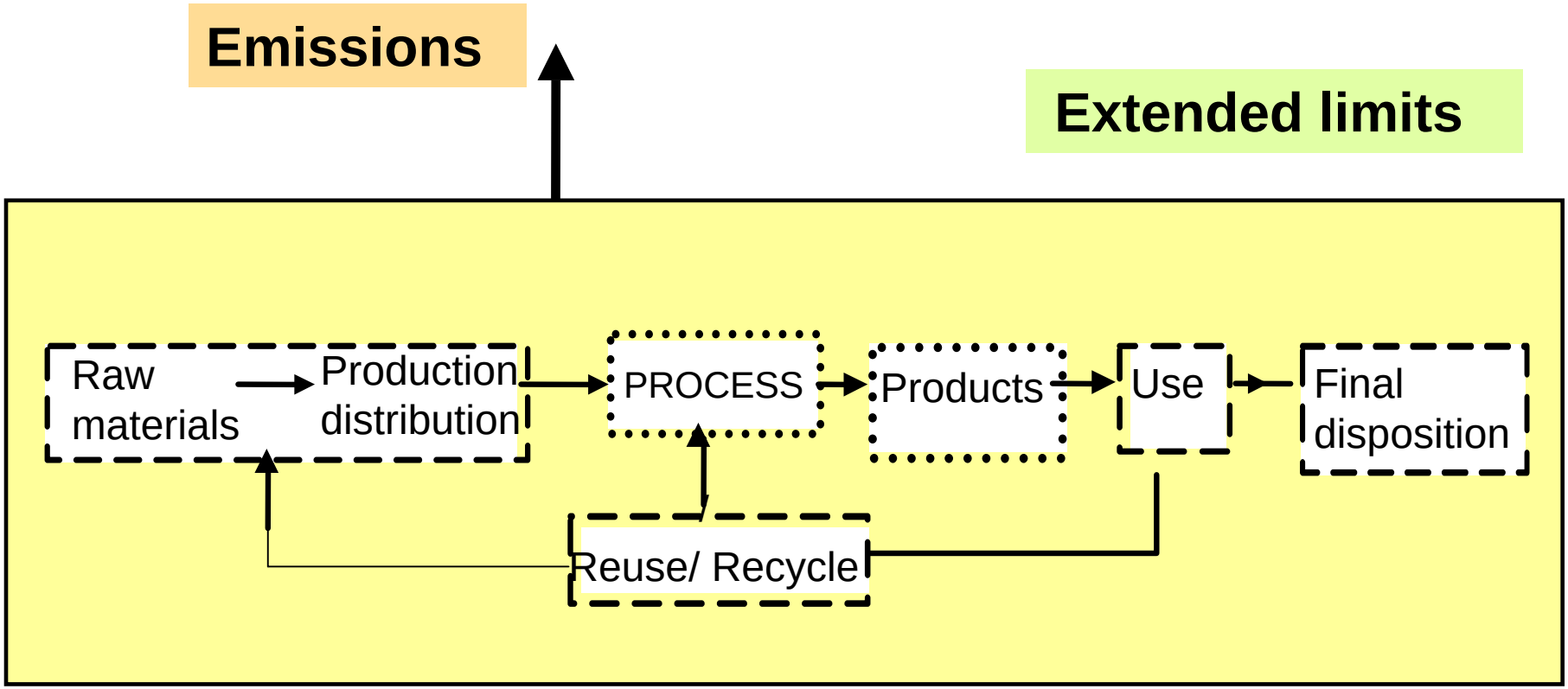
γ_{kj} characterization factor
contribution of component *k*
in category *j*

Heijungs et al, 1992

Environmental life cycle assessment



Life cycle limits



Estimate emissions in the life cycle extended limits.

Environmental life cycle

Environmental life cycle has been associated to
products and technologies.

Environmental life cycle will be associated
to process optimization.

Minimize environmental life cycle:

to select

operating conditions and analysis or design

with rigorous modelling and simulation.

Minimize environmental life cycle

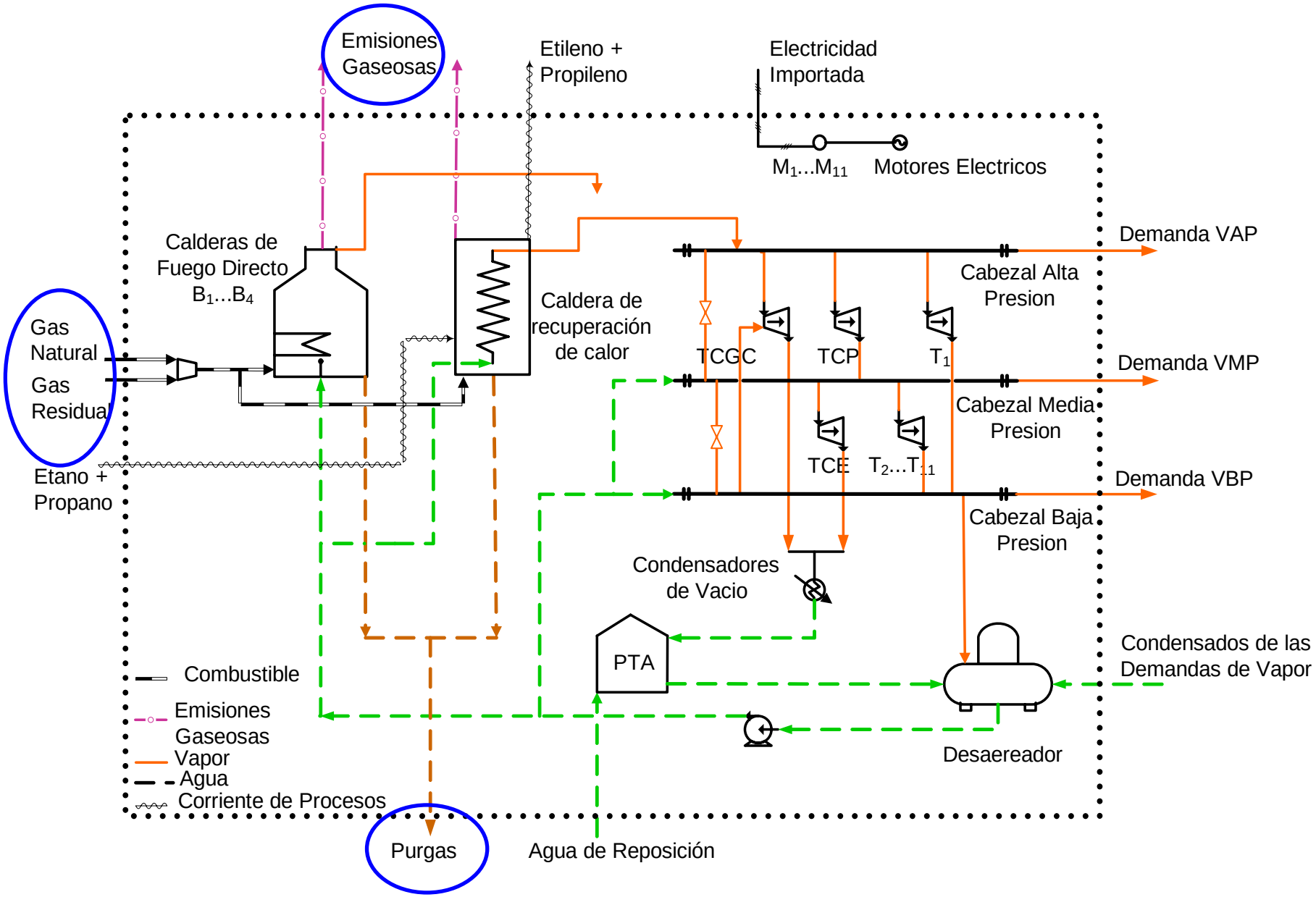
SELECTION OF THE OPERATING CONDITIONS

WITH RIGOROUS MODELLING AND SIMULATION.

CASE STUDY:

STEAM AND POWER SECTOR OF AN ETHYLENE PLANT

Steam and power sector



Selection of the operating conditions

Minimize environmental impact

$$\underset{x,y}{Min} \quad \Psi^{UP}(x, y)$$

$$s.t.: \quad h(x) = 0$$

$$g(x) + A(y) \leq 0$$

$$x^{LB} \leq x \leq x^{UB}$$

$$x \in R^{n}$$

$$y \in \{0,1\}^{m}$$

MINLP problem formulated in GAMS

Operating conditions of steam and power plant

CONTINUOUS OPERATING CONDITIONS :

Temperature and pressure of high, medium and low pressure steam headers.
Deareator pressure.

BINARY OPERATING CONDITIONS :

Drivers selection between steam turbines and electrical motors for pumps.

Selection of equipment that is *ON* or *OFF* related to
heaters and their auxiliary air fans and pumps.

Environmental impact evaluation

Emissions evaluation: combustion of natural and residual gases and purges.

$$F_k^{UP} = F_{gn} \times e_{k,gn} + F_{gr} \times e_{k,gr} + e_{k,Aq} \times \sum_p F_p$$

Contribution of component k to category j

$$\psi_{kj} = F_k^{UP} \gamma_{kj}$$

Environmental category j

$$\psi_j = \sum_k \psi_{kj}$$

Total potential environmental impact

$$\Psi^{UP} = \sum_j \omega_j \times \psi_j$$

Minimize environmental impact

Operating conditions selection

$$\underset{x,y}{Min} \quad \Psi^{UP}(x, y)$$

$$s.t.: \quad h(x) = 0$$

$$g(x) + A(y) \leq 0$$

$$x^{LB} \leq x \leq x^{UB}$$

$$x \in R^n$$

$$y \in \{0,1\}^m$$

Equality constraints include modelling and property predictions.

Inequality constraints include operating conditions and logic constraints.

Improvements achieved

Objectives and operating conditions		Initial point	Min Environ. Impact	% change
Environmental impact	**PEI/h**	33188.070	**28591.310**	**13.85**
Operating cost	**$/h**	1938.341	1777.522	**8.30**
Natural Gas	**tn/h**	8.546	6.995	**18.15**
Imported electricity	**Kwh**	1074.806	3806.508	**- 254.18**
Make up water	**tn/h**	32.000	22.000	**31.25**
High vapour pressure	**tn/h**	193.457	169.568	**12.35**
Heaters purges	**tn/h**	5.327	4.122	**22.62**
HPS Temperature	**°C**	420.000	445.055	-----
HPS Pressure	**bar**	50.500	52.000	-----
MPS Temperature	**°C**	320.000	310.00	-----
MPS Pressure	**bar**	23.000	23.465	-----
LPS Temperature	**°C**	210.000	150.00	-----
LPS Pressure	**bar**	3.000	5.000	-----
Deareator pressure	**bar**	2.500	3.000	-----

CPU time: 11.82 sec, 13 major iterations

Main numerical results

Simultaneous reductions in environmental impact, cost, natural gas, make up water, high pressure steam generated are observed.

Increasing the efficiency of the process both environmental impact and cost are reduced simultaneously indicating that they are not conflictive objectives.

Electricity imported has increased.

Driver/Equipment	Initial point	MINLP Solution
Impulsor Bomba agua torre quenching Nº 1	Turbine	Motor
Impulsor Bomba agua torre quenching Nº 2	Turbine	Motor
Impulsor Bomba lubricación Nº 1	Turbine	Motor
Impulsor Bomba lubricación Nº 2	Turbine	Motor
Impulsor Bomba lubricación Nº 3	Turbine	Motor
Impulsor Bomba condensado Nº 1	Turbine	Motor
Impulsor Bomba condensado Nº 2	Turbine	Motor
Impulsor Compresor aire	Turbine	Motor
Bomba agua caldera Nº 1, (turbina)	OFF	OFF
Bomba agua caldera Nº 2, (turbina)	OFF	OFF
Bomba agua caldera Nº 3, (motor elec.)	ON	Motor
Bomba agua enfriam. Nº 1,(turbina)	ON	OFF
Bomba agua enfriam. Nº 2 (turbina)	ON	OFF
Bomba agua enfriam. Nº 3, (motor elec.)	ON	Motor
Bomba agua enfriam. Nº 4, (motor elec.)	OFF	Motor
Bomba agua enfriam. Nº 5, (motor elec.)	OFF	OFF
Impulsor Ventilador caldera Nº 1	OFF	OFF
Impulsor Ventilador caldera Nº 2	Turbine	Motor
Impulsor Ventilador caldera Nº 3	Turbine	Motor
Impulsor Ventilador caldera Nº 4	Turbine	OFF
Caldera Nº 1	OFF	OFF
Caldera Nº 2	ON	ON
Caldera Nº 3	ON	ON
Caldera Nº 4	ON	OFF

Binary variables

Initial point

Motors: 2

Turbines: 13

Solution point

Motors: 13

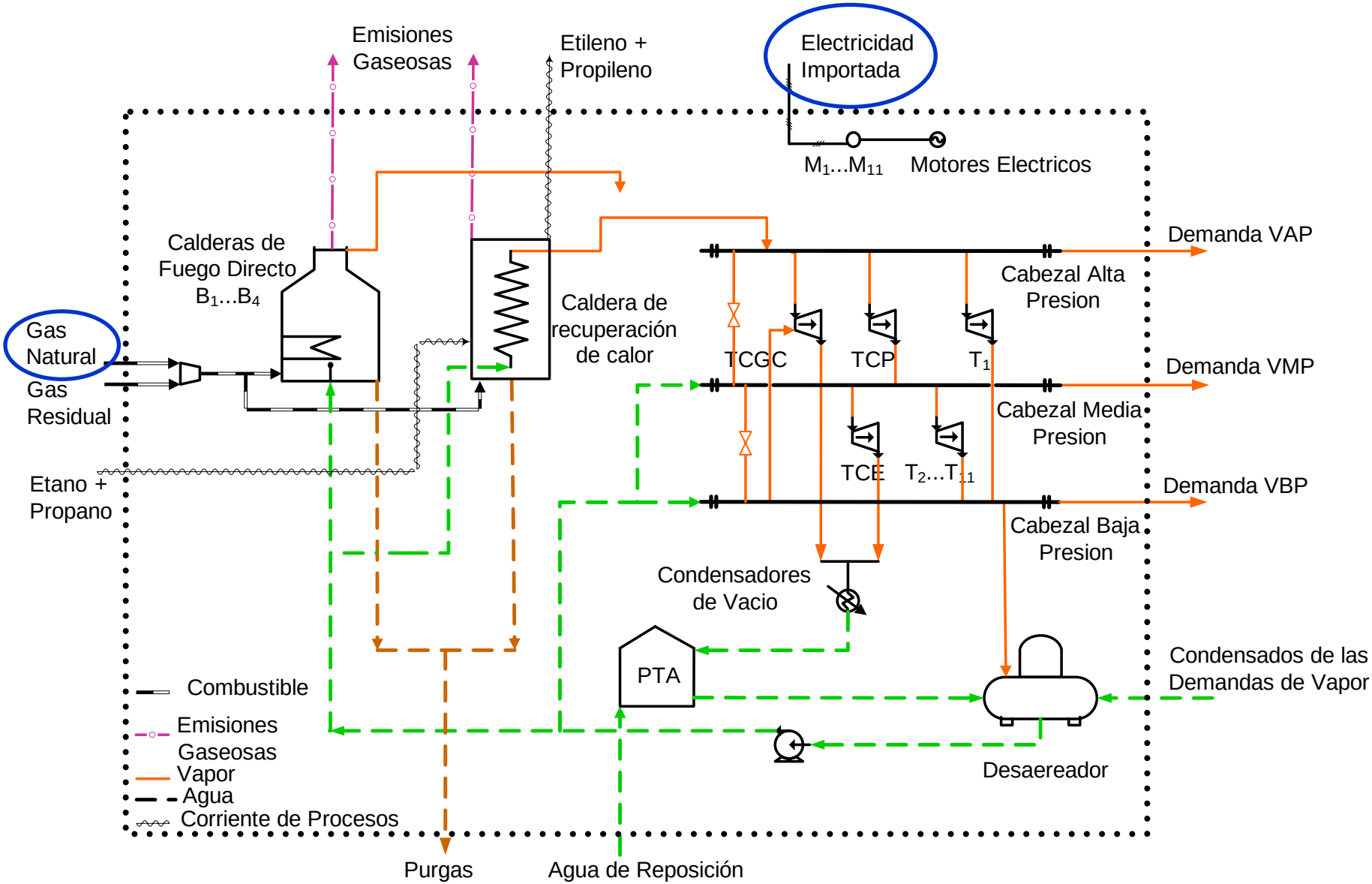
Turbines: 0

Environmental impact categories contribution

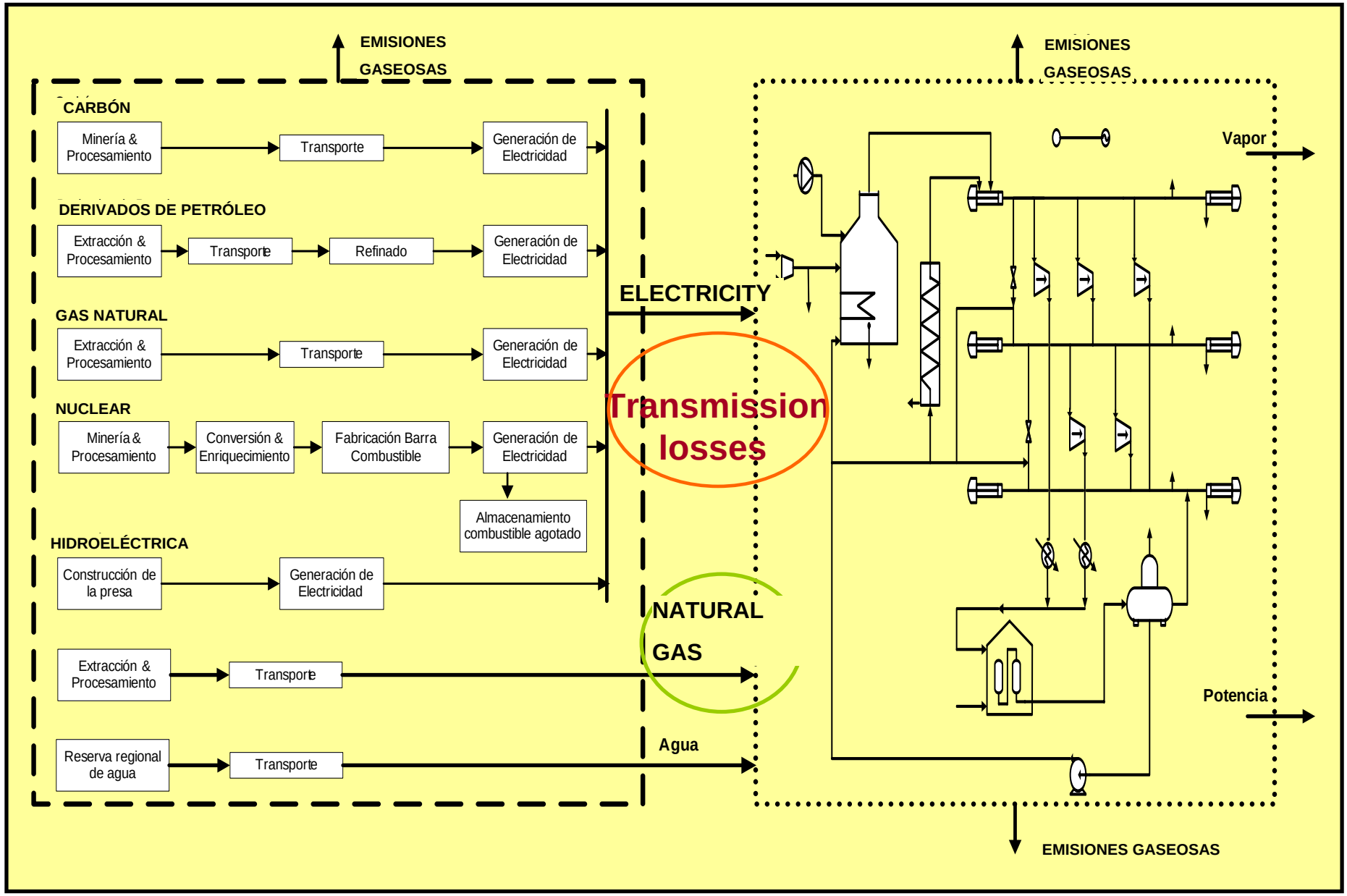
Environmental Impact Category		Environmental impact	Contribution %
Global Warming	**CO_2 kg eq**	**28483.380**	**99.623**
Acidification,	**SO_2 kg eq**	51.575	0.180
Human toxicity	**1- 4, DCB kg eq**	51.527	0.180
Aquatic eco toxicity	**1- 4, DGB kg eq**	2.804	0.010
Photochemical oxidation	**ethylene kg eq**	2.017	0.007
Eutrofization	**PO^{-3}_4 kg eq**	0.004	1.559 E-05
Stratospheric O_3 depletion	**CFC-11 kg eq**	---	---
Ionizing Radiations	**yr**	---	---
Non renewable Resource		6.0 E-08	2.099 E-10
Scarce renewable Resource		2.216 E-11	7.752 E-14
Total	**PEI/h**	**28591.310**	100

Global worming is the main contribution, due to combustion emissions.

Life cycle environmental emissions



Life cycle environmental emissions and impacts



Minimization of life cycle environmental impact

$$\underset{x,y}{Min} \quad \Psi^{CVUP}(x, y)$$

$$s.t.: \quad h(x) = 0$$

$$g(x) + A(y) \leq 0$$

$$x^{LB} \leq x \leq x^{UB}$$

$$x \in R^n$$

$$y \in \{0,1\}^m$$

MINLP problem size

13563 constraints, 13570 variables, 24 binary variables.

Formulated and solved in GAMS. MINLP Solver : DICOPT,

MIP sub problem: CPLEX, NLP sub problem: CONOPT2

Eliceche, Corvalán and Martinez (2007)

Improvement minimizing life cycle environmental impact

Objectives and operating conditions		Initial point	Min LCEI	% change
Environmental impact	**PEI/h**	33627.33	**29544.101**	**12.14**
Operating cost	**$/h**	1938.341	1638.355	**15.48**
Natural Gas	**tn/h**	8.546	7.167	**16.13**
Imported electricity	**Kwh**	1074.806	1138.947	**- 5.97**
Make up water	**tn/h**	32.000	22.000	**31.25**
High vapour pressure	**tn/h**	5.327	4.205	**21.06**
Heaters purges	**tn/h**	193.457	170.90	**12.03**
HPS Temperature	**°C**	420.000	450.000	-----
HPS Pressure	**bar**	50.500	52.000	-----
MPS Temperature	**°C**	320.000	310.000	-----
MPS Pressure	**bar**	23.000	23.816	-----
LPS Temperature	**°C**	210.000	150.00	-----
LPS Pressure	**bar**	3.000	4.015	-----
Deareator pressure	**bar**	2.500	2.683	-----

CPU time: 3.10 sec, 3 major iterations

Driver / Equipment	Initial point	MINLP Solution
Impulsor Bomba agua torre quenchinq Nº 1	Turbine	Turbine
Impulsor Bomba agua torre quenchinq Nº 2	Turbine	Turbine
Impulsor Bomba lubricación Nº 1	Turbine	Turbine
Impulsor Bomba lubricación Nº 2	Turbine	Turbine
Impulsor Bomba lubricación Nº 3	Turbine	Turbine
Impulsor Bomba condensado Nº 1	Turbine	Turbine
Impulsor Bomba condensado Nº 2	Turbine	Turbine
Impulsor Compresor aire	Turbine	Turbine
Bomba agua caldera Nº 1, (turbina)	OFF	OFF
Bomba agua caldera Nº 2, (turbina)	OFF	OFF
Bomba agua caldera Nº 3, (motor elec.)	ON	ON
Bomba agua enfriam. Nº 1,(turbina)	ON	ON
Bomba agua enfriam. Nº 2 (turbina)	ON	OFF
Bomba agua enfriam. Nº 3, (motor elec.)	ON	ON
Bomba agua enfriam. Nº 4, (motor elec.)	OFF	OFF
Bomba agua enfriam. Nº 5, (motor elec.)	OFF	OFF
Impulsor Ventilador caldera Nº 1	OFF	OFF
Impulsor Ventilador caldera Nº 2	Turbine	Turbine
Impulsor Ventilador caldera Nº 3	Turbine	Turbine
Impulsor Ventilador caldera Nº 4	Turbine	OFF
Caldera Nº 1	OFF	OFF
Caldera Nº 2	ON	ON
Caldera Nº 3	ON	ON
Caldera Nº 4	ON	OFF

BINARY VARIABLES

Initial point

Motors: 2

Turbines: 13

Solution point

Motors: 2

Turbines:11

PEI / Kwh

PS = 0.276

EI = 0.387

Ratio of environmental impact to power generated

Life cycle potential environmental impact
for each type of electricity generation.

Generators	**Environmental Impact PEI / h**	**Electricity Imported Kwh**	**PEI / Kw**
Hydro electric	90.092	442.601	0.204
Thermo Natural Gas -Gas turbine	158.159	325.368	0.486
Thermo Natural Gas - Vap turbine	58.795	104.716	0.561
Thermo Fuel Oil - Vap turbine	57.413	63.580	0.903
Thermo Gas Oil - Vapour turbine	57.038	89.750	0.636
Thermo Carbon - Vapour turbine	11.767	11.221	1.049
Nuclear	7.707	101.709	0.076
Total – Medium value	440.972	1138.947	**0.387**

Environmental impact categories contribution

Categorías de Impacto Ambiental		Impacto Ambiental	Contribución %
Global Warming	**Kg. CO_2 eq**	**29431.249**	**99.618**
Human Toxicity	1- 4, DCB kg eq	53.879	0.182
Acidification	SO_2 kg eq	52.646	0.178
Aquatic toxicity	1- 4, DCB kg eq	4.232	0.014
Photochemical oxidants	ethylene kg eq	2.075	0.007
Eutrofization	PO^{-3}_4 kg eq	0.021	7.126 E-05
O_3 stratospheric reduction	CFC-11 kg eq	3.430 E-06	1.161 E-08
Ionizing radiations	yr	2.000 E-08	6.770 E-11
Non Renewable resources		6.000 E-08	2.030 E-10
Scarce renewable resources		2.420 E-11	8.191 E-14
Total, PEI/h		**29544.101**	100

Global worming is the main contribution, due to combustion emissions.

Environmental impact of each stage of the life cycle

	Electricity generators							Utility plant	
Life cycle stage	**Hidro Elec.**	**Natural gas Vapour Turbine**	**Fuel Oil Vapour Turbine**	**Gas Oil Vapour Turbine**	**Carbon Vapour Turbine**	**Gas Natural Gas Turbine**	**Nuclear**	**Natural Gas**	**Resd Gas**
CONSTRUCTION	5.214	-----	-----	-----	-----	-----	16.766	-----	-----
EXTRACTION	-----	1.354	0.111	0.022	0.720	1.461	6.587	1.461	
CONVERSION	-----	-----	-----	-----	-----	-----	1.198	-----	-----
ENRICHMENT	-----	-----	-----	-----	-----	-----	44.910	-----	-----
FUEL FABRICATION	-----	-----	-----	-----	-----	-----	4.192	-----	-----
TRANSPORT	-----	6.801 E-03	0.037	0.011	0.026	7.337 E-03	-----	7.368 E-04	-----
REFINING	-----	-----	0.031	0.06	-----	-----	-----	-----	-----
REPROCESSING	-----	-----	-----	-----	-----	-----	7.185	-----	-----
OPERATION	**94.786**	**98.639**	**99.821**	**99.960**	**99.254**	**98.531**	**19.162**	**98.538**	**100**

Minimizing operating cost

$$C = c_{NG} F_{NG} + c_E \dot{W}_{imp}^E + c_{FW} F_{FW} + c_{CW} F_{CW}$$

Cost of : natural gas + electricity + make up water + water treatment

Formulation of the MINLP Problem

$$\begin{aligned} &\underset{x,y}{Min} \quad C\ (x, y) \\ &s.t. : \quad h(x) = 0 \\ &\qquad g(x) + A(y) \le 0 \\ &\qquad x^{LB} \le x \le x^{UB} \\ &\qquad x \in R^n \\ &\qquad y \in \{0,1\}^m \end{aligned}$$

Solutions minimizing environmental impact and operating cost

Objective Function		Min Cost	% Dev	Min LCEI	% Dev	Min IA Utility	% Dev
Cost	$ / h	1624.133	0	1638.355	**0.868**	1777.522	**8.629**
Life Cycle EI	PEI / h	29595.394	**0.173**	29544.101	0	30065.070	**1.733**
Utility EI	PEI / h	29335.360	**2.536**	29103.130	**1.759**	28591.310	0

Similar solutions are found when minimizing operating cost and life cycle environmental impact, with variations between 0.1 to 1 %.

While comparing results with between cost and environmental impact of the utility plant ,
differences of 8.6 % in cost and 2.5 % in environmental impact are observed .

In this case study, environmental impact and cost are not conflictive objectives if bounds are properly defined.

IT IS VERY IMPORTANT TO EXTEND THE LIMITS TO INCLUDE THE MAIN ENVIRONMENTAL IMPACTS FROM ESTIMATED EMISSIONS.

APPLICATIONS

SELECTION OF THE ELECTRICITY GENERATORS IN THE ARGENTINIAN INTERCONECTED NETWORK.

DESIGN OF THE PERVAPORATION MEMBRANE MODULES IN A HYBRID SEPARATION SYSTEM WITH AN AZEOTROPIC DESTILLATION COLUMN.

CONCLUTIONS

DEVELOPMENT OF METHODOLOGIES TO:

- **Quantify potential environmental impact of industrial process and plants.**
- **Estimate the main environmental impacts associated to process life cycle.**
- **Minimize life cycle environmental impact in process optimization.**

APPLICATION TO:

- **Operation of a steam and power generation plant.**

REFERENCES

Azapagic A., 1999, Life Cycle Assessment and its applications on process selection design and optimization. *Chemical Engineering Journal*, 73, 1-21.

Azapagic A. and Clift R., 1999, The application of life cycle assessment to process optimization. *Computers and Chemical Engineering*, 23 (10), 1509-1526.

Cabezas H., Bare J. and Mallick S. 1999. Pollution prevention with chemical process simulator the generalized waste reduction algorithm. *Computers and Chemical Engineering,* 23, 623-634.

Dantus M. and K. High , 1999, Evaluation of waste minimization alternatives under uncertainty: a multiobjective optimization approach, *Computers and Chemical Engineering*, 23, 1493-1508.

Eliceche, A., Corvalán, S. and Martinez, P. 2007. Environmental life cycle impact as a tool for process optimization of a utility plant, *Computers and Chemical Engineering*, 31, 648-656.

Eliceche, A.M. and Martinez, P.E. 2007. Minimization of life cycle CO2 emissions in a petrochemical utility plant. Chemical Engineering Transaction, Vol.XII, 2007 - PRES'07 Proceedings.

Heijungs, R., Guinée, J., Huppes G., Lankreijer, R.M., Ansems, A.A.M., Eggels, P.G., van Duin, R. de Goede, H.P. 1992. Environmental Life Cycle Assessment of Products-Guide and Backgrounds. Centre of Environmental Science (CML).Leiden.

Martinez P., and Eliceche A. 2007. Minimization of life Cycle CO2 emissions in the operation of a steam and power plant. 17th European Symposium on Computer Aided Process Engineesing – ESCAPE17. V. Plesu and P.S. Agachi (Editors).

Young D., Scharp R. and Cabezas H. 2000. The waste reduction (WAR) algorithm: environmental impacts, energy consumption, and engineering economics. *Waste Management* 20 (8), 605-615.