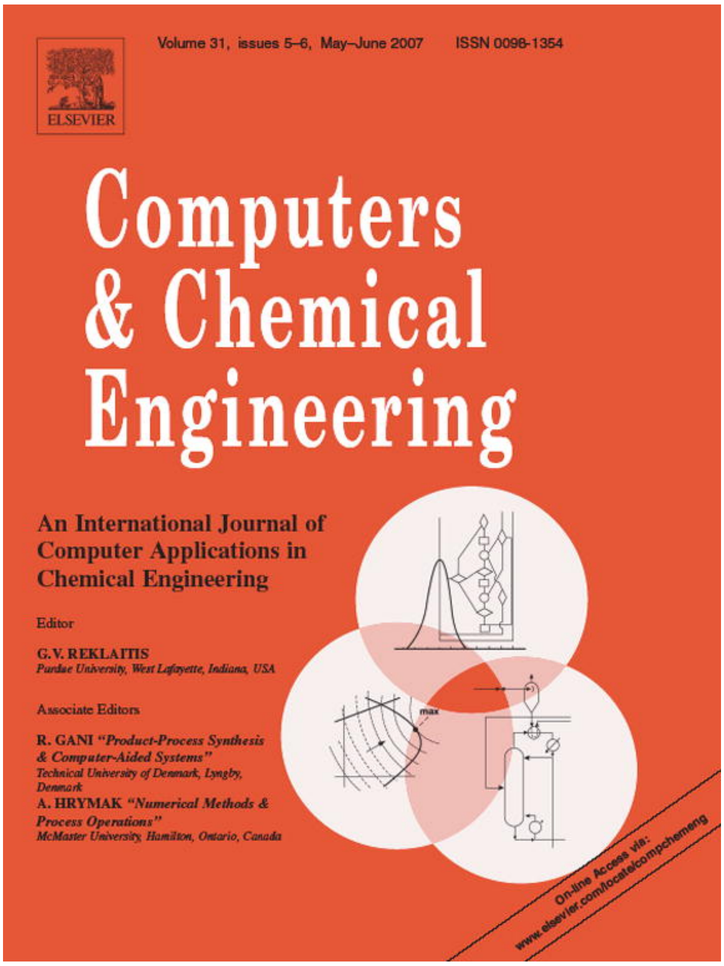
Volume 31, issues 5–6, May–June 2007 ISSN 0098-1354
ELSEVIER
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An International Journal of Computer Applications in Chemical Engineering
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Computers and Chemical Engineering 31 (2007) 648–656
Computers & Chemical Engineering
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Environmental life cycle impact as a tool for process optimisation of a utility plant

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Received 4 December 2005; received in revised form 7 September 2006; accepted 11 September 2006
Available online 4 December 2006

Abstract

The purpose of this paper is to minimize environmental life cycle impact when a detail process modelling is available. A methodology is presented to calculate the optimum operating conditions of an ethylene process utility plant. The overall environmental impact is calculated as a weighted sum of global warming, acidification, eutrophication, photochemical oxidation, ozone depletion, human toxicity and ecotoxicity. The battery limits of the plant are extended to include the relevant environmental impacts corresponding to the imported electricity generated in thermoelectric, hydroelectric and nuclear plants. A mixed integer non-linear programming problem is formulated and solved in GAMS. Significant reductions in environmental impact particularly in global warming, the most relevant category, are obtained choosing the pressure and temperature of high, medium and low pressure steam headers together with the selection of optional drivers and boilers. Improvements achieved simultaneously in natural gas and electricity consumption and operating cost are also reported.

Keywords: Environmental life cycle impact; Utility; Optimisation

1. Introduction

The purpose of this paper is to show that environmental life cycle impact assessment can be used as a quantitative objective function for process optimisation when utility plant process model is available. Environmental life cycle impact assessment is therefore associated to process optimisation rather than to a product as it has been extensively used in the literature. This is a new approach that leads to important improvements. The utility plant has been chosen as the case study due to its significant contribution to energy consumption in process plants and consequently to the operating cost in a scenario of increasing fuel costs. Furthermore, in the steam and power generation plant analysed, when the battery limits are extended to include the environmental impact of the imported energy, the optimal operating conditions calculated minimizing the operating costs and the environmental impact are similar. Significant reductions in the consumption of fossil fuels are achieved reducing simultaneously the combustion emissions in the boilers, mainly carbon dioxide helping to comply with Kyoto Protocol. Thus, a new methodology and a useful computational tool are developed to promote sustainable development. In the utility plant, improvements in environmental impact and operating cost are achieved simultaneously, because both functions are directly related to the amount of fuel burned in the boilers. A detailed modelling of the utility plant is carried out using a property prediction of steam and water enthalpy and entropy.

The need to incorporate environmental objectives in process optimisation has been recognised in the last decade by authors like Stefanis, Livingston, and Pistikopoulos (1995), Dantus and High (1999), Cabezas, Bare, and Mallick (1999) and Young, Scharp, and Cabezas (2000). Environmental life cycle impact has been traditionally used to quantify and assess the environmental performance of a product. Azapagic and Clift (1999) have proposed the application of life cycle assessment to aid the decision making process for environmental improvement, with multiple objectives for the mineral boron production. Fu and Diwekar (2003) have proposed the minimisation of cost and greenhouse emissions with a multiobjective framework. Hashim, Douglas, Elkamel, and Croiset (2005) studied the Ontario energy system to minimise CO_2 emissions using linear programming. Initiatives have also been taken to develop best

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doi:10.1016/j.compchemeng.2006.09.005

Nomenclature

a^{na}	constant coefficient in the linear correlation for an air fan power
a^{np}	constant coefficient in the linear correlation for a water pump power
b^{na}	constant coefficient in the linear correlation for an air fan power
b^{np}	constant coefficient in the linear correlation for a water pump power
c_{CW}	cooling water treatment cost
c_E	electrical power cost
c_{FW}	fresh water cost
c_{NG}	natural gas cost
C	utility plant operating cost
d	constant coefficient in purge enthalpy linear correlation
e	constant coefficient in purge enthalpy linear correlation
ef_{ks}	emission factor for chemical k from power source s
$[\mathrm{EC}]_s$	electricity imported from power source s
F_n^m	mass flowrate from unit n to unit m
$F_n^{m,LB}$	lower bound on flowrate F_n^m
$F_n^{m,UB}$	upper bound on flowrate F_n^m
h_{kj}	Heijung's factor for chemical k in environmental category j
h_{nb}	specific enthalpy in boiler nb
h_{nh}	specific enthalpy in header nh
h_{np}	specific enthalpy associated to stream F_{np}
$h_{nt,ISO}$	isoentropic steam enthalpy in an ideal isoentropic expansion in the nt turbine
h_p	specific enthalpy associated to purge stream
h_{nh}^{il}	constant coefficient in the bivariate polynomial for the steam enthalpy prediction
I_n	set defining input streams to unit n
K_j	number of chemical compounds contributing to environmental impact category j
LHV	lower heating value of natural gas
$n\mathrm{a} = 1, \ldots, N_a$	subset of air fans
$n\mathrm{b} = 1, \ldots, N_b$	subset of boilers
$n\mathrm{e} = 1, \ldots, N_e$	subset of electrical motors
$n\mathrm{h} = 1, \ldots, N_h$	subset of steam headers
$n\mathrm{p} = 1, \ldots, N_p$	subset of pumps
$n\mathrm{t} = 1, \ldots, N_t$	subset of steam turbines
N	set of units present in the superstructure
O_n	set defining output streams from unit n
P_{nh}	pressure of steam header nh
q_k	chemical k mass flowrate
q_{ks}	mass flowrate of chemical k from the power source s
QI_n	set defining the heat inputs to unit n
QO_n	set defining the heat outputs from unit n
$\dot{Q}_n^m$	heat rate transferred from unit n to unit m
s_{nh}^{il}	constant coefficient in the bivariate polynomial for the steam enthalpy prediction
S_{nh}	specific entropy of header nh
T_{nh}	temperature of header nh
$\dot{W}_n^m$	shaft work rate transferred form unit n to unit m
$\dot{W}_{ne}^{UB}$	upper bound on power provided by an electrical motor
$\dot{W}_{nt}^{UB}$	upper bound on power provided by a steam turbine
WI_n	set defining shaft work inputs to unit n
WO_n	set defining shaft work outputs from unit n

Greek symbols

α_j	normalizing factor for environmental impact category j
η_{nt}	efficiency of turbine nt
η_{nb}	global efficiency of boiler nb
ω_j	relative weighting factor of the environmental impact category j
Ψ	overall environmental impact
Ψ_j	contribution of each environmental impact category j
Ψ_{kj}	contribution of component k emission to a given environmental impact category j
ω_j	relative weighting factor of the environmental impact category j

available practice to integrate life cycle assessment, risk assessment and ecological considerations by Finnveden et al. (2003).

In this work, the aim is to select the operating conditions of the utility plant minimizing the life cycle environmental impact. In the utility plant there are continuous and binary optimisation variables. The operating conditions selected are the temperature and pressure of high, medium and low-pressure steam headers, deaerator tank pressure, and letdowns flow rates. Binary variables are introduced to select alternative driver configurations, steam turbines or electrical motors and also to select if some equipment such as boilers, air fans, steam turbines or electrical motors are on or off. A mixed integer non linear programming problem is formulated and solved in GAMS, Brooke, Kendrick, Meeraus, and Raman (2003), to minimize environmental life cycle impact. A rigorous simulation of the utility plant is implemented and posed as constraints in the optimisation problem.

The potential environmental impact is modelled according to the methodology presented by Heijungs et al. (1992). Several potential environmental impacts categories associated to global warming, acidification, eutrophication, photochemical oxidation, ozone depletion, human toxicity and ecotoxicity are added to obtain an overall environmental impact as suggested by Cabezas et al. (1999) in the waste reduction algorithm.

The numerical results of Table 1 show that significant reductions of more that 15% in the environmental life cycle impact, operating cost, natural gas consumption and electricity imported can be achieved in the utility plant with the method-

Table 1
Minimising the environmental life cycle impact

Optimisation variables	Bounds		Initial point	Optimal solution
	Lower	Upper		
HPSH pressure (bar)	48.00	52.00	49.00	52.00
MPSH pressure (bar)	18.00	26.00	18.00	23.90
LPSH pressure (bar)	3.00	5.00	4.50	3.00
HPSH temperature (°C)	400.00	450.00	410.00	450.00
MPSH temperature (°C)	310.00	370.00	330.00	310.00
LPSH temperature (°C)	150.00	250.00	230.00	150.00
Deaerator Pressure (bar)	1.20	3.00	1.50	2.715

	Initial Point	Optimal Solution	% Reduction
Environmental LC impact (PEI/h)	633.098	528.298s	16.554
Operating cost, ($/h)	1256.132	1022.666	18.586
Natural gas (tonnes/h)	8.664	7.191	16.994
Electrical power (kWh)	2315.763	925.604	60.030

ology presented indicating the significance of the approach proposed.

2. Modelling of the steam and power generation plant

The utility plant provides mainly steam and power to the chemical plant. It consumes fossil fuels, a non-renewable resource burnt in the boilers and also a scarce resource as water. The pollution comes mainly from the combustion emissions and purged water. A schematic flow sheet of an ethylene process utility plant is presented in Fig. 1. Boilers produce superheated steam at high pressure. The main equipment in utility plants are: boilers, high, medium and low pressure steam headers, steam turbines, pumps, deaerator tank, vents, let-down streams, water treatment plant, heat exchangers, air fans and electrical motors. A rigorous modelling of the main equipment involved and the property prediction to evaluate the steam and water enthalpy and entropy is used. The modelling equations are posed as equality constraints in the optimisation problem. The plant has alternative drivers such as electrical motors and steam turbines for the

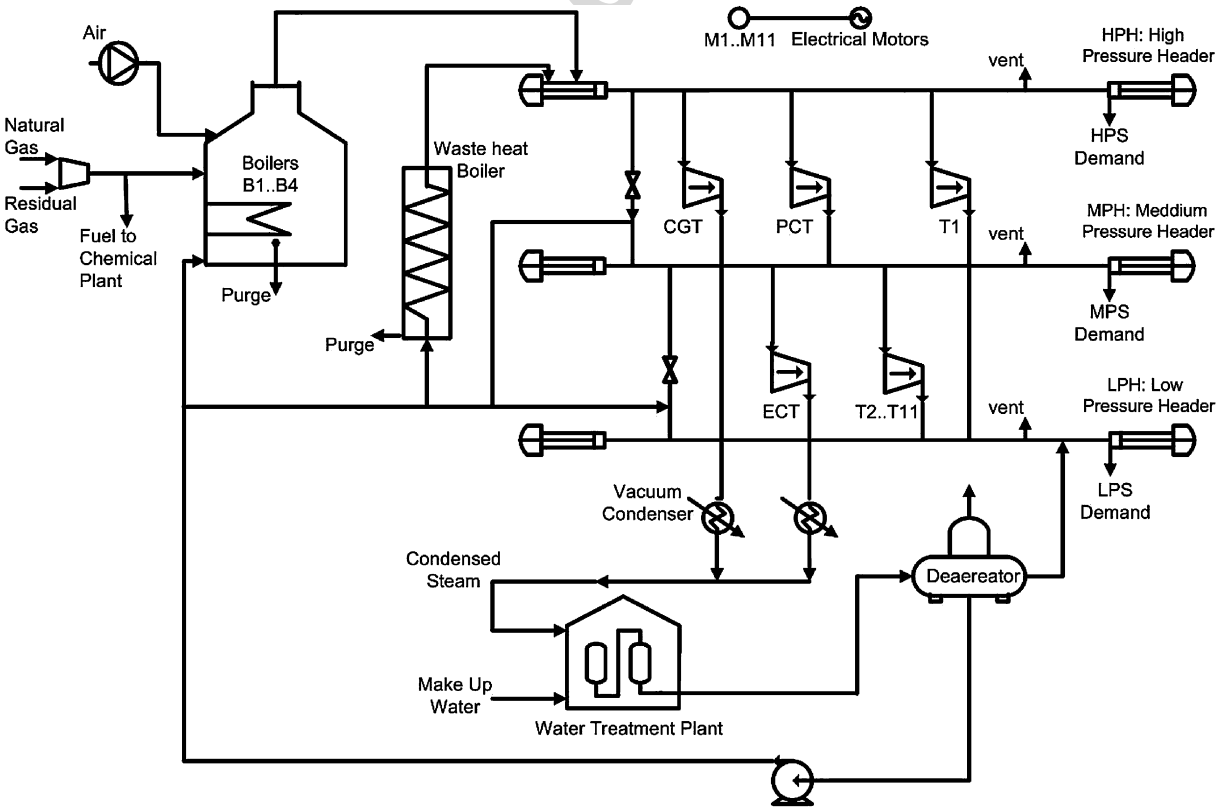

Fig. 1. Steam and power generation plant.

pumps. Binary variables are used for the selection of alternative drivers and other equipment that can be on or off, such as boilers and their auxiliary equipment.

Condensing and backpressure turbines are the most common types of steam turbines, with the latter having the widest application. Both can be multistage machines, with more than one steam input or output. The output of condensing turbines commonly goes to a vacuum condenser to increase the power. More power can also be obtained increasing the difference between inlet and outlet pressures, although the cost of steam production or vacuum generation grows. Turbines take their steam from a header and release the steam to a lower pressure header. In the headers, the steam temperature and pressure is controlled by desuperheating water and by high-pressure steam letdowns. The condensed steam returning from the heat exchangers is re-used to generate steam. The recycled condensate cannot be re-used without previous water treatment to prevent corrosion in boilers and turbines.

The utility plant superstructure is described by the set of units $N=\{n\}$ and by the following sets defining interconnections:

$$I_n = \{m|\text{unit}\, n \text{ has input flowrate from unit}\, m\} \tag{1}$$

$$O_n = \{m|\text{unit}\, n \text{ has output flowrate to unit}\, m\} \tag{2}$$

$$WI_n = \{m|\text{unit}\, n \text{ has shaft work input from unit}\, m\} \tag{3}$$

$$WO_n = \{m|\text{unit}\, n \text{ has shaft work output to unit}\, m\} \tag{4}$$

$$QI_n = \{m|\text{unit}\, n \text{ has input heat from unit}\, m\} \tag{5}$$

$$QO_n = \{m|\text{unit}\, n \text{ has output heat to unit}\, m\} \tag{6}$$

The set $\{n\}$ is composed by the following subsets:

$$\{n\} = \{n\text{a}, n\text{b}, n\text{e}, n\text{h}, n\text{p}, n\text{t}\} \tag{7}$$

where: $n\text{a}=1, \ldots, N_\text{a}$ air fans; $n\text{b}=1, \ldots, N_\text{b}$ boilers; $n\text{e}=1, \ldots, N_\text{e}$ electrical motors; $n\text{h}=1, \ldots, N_\text{h}$ steam headers; $n\text{p}=1, \ldots, N_\text{p}$ pumps; $n\text{t}=1, \ldots, N_\text{t}$ turbines.

The mass (8) and energy balances (9) for each equipment n can be stated as follows:

$$\sum_{m\,\in\, I_n} F_m^n - \sum_{m\,\in\, O_n} F_n^m = 0 \tag{8}$$

$$\sum_{m\,\in\, I_n} F_m^n h_m - \sum_{m\,\in\, O_n} F_n^m h_n + \sum_{m\,\in\, QI_n} |\dot{Q}_m^n| - \sum_{m\,\in\, QO_n} |\dot{Q}_n^m| + \sum_{m\,\in\, WI_n} \dot{W}_m - \sum_{m\,\in\, WO_n} |\dot{W}_n| = 0 \tag{9}$$

F_n^m represents the flowrate from unit n to unit m, h_n is the specific enthalpy associated to F_n^m, $\dot{Q}_m^n$ is the heat rate transferred from unit m to unit n and $\dot{W}_m$ is the power released or consumed by a unit n. The summations are made over the sets defined in Eqs. (1)–(6). Absolute values of work and heat transfer rate are used to become independent of the sign convention for both terms.

The enthalpy $h_{n\text{h}}$ and entropy $S_{n\text{h}}$ of steam header nh are predicted using a bivariate-polynomial as a function of the pressure $P_{n\text{h}}$, and temperature $T_{n\text{h}}$.

$$S_{n\text{h}}(T_{n\text{h}}, P_{n\text{h}}) = \sum_{i=0}^{3}\sum_{l=0}^{3} s_{n\text{h}}^{il}(T_{n\text{h}})^i (P_{nh})^l, \quad i+l \le 3 \tag{10}$$

$$h_{n\text{h}}(T_{n\text{h}}, P_{n\text{h}}) = \sum_{i=0}^{3}\sum_{l=0}^{3} h_{n\text{h}}^{il}(T_{n\text{h}})^i (P_{nh})^l, \quad i+l \le 3 \tag{11}$$

The coefficients $s_{n\text{h}}^{il}$ and $h_{n\text{h}}^{il}$ were obtained correlating steam data in the temperature and pressure operating range of header nh.

In particular the energy balance of steam turbine nt is formulated using the turbine efficiency η_{nt} and an isoentropic expansion as follows:

$$\eta_{nt} F_{n\text{h}}^{n\text{t}}(h_{n\text{h}} - h_{n\text{t,Iso}}) = \dot{W}_{nt}^{lt} \tag{12}$$

Where nh indicates the header that provides steam to the turbine nt and $h_{n\text{h}}$ is the enthalpy of header nh and stream $F_{n\text{h}}^{n\text{t}}$. The power $\dot{W}_{nt}^{lt}$ is provided by turbine nt to unit lt, where $h_{n\text{t,Iso}}$ is the isoentropic steam enthalpy of the ideal isoentropic expansion.

Binary variables are introduced in order to model the on/off options. Then, a binary variable y^n is equal to zero if unit n is off or equal to one if that unit is on. The related flowrates F_n^m that enters the unit m, are constrained by the following inequalities:

$$y^n F_n^{m,\text{LB}} \le F_n^m \le y^n F_n^{m,\text{UB}} \tag{13}$$

Where $F_n^{m,\text{LB}}$ and $F_n^{m,\text{UB}}$ are the lower and upper bounds of flowrate F_n^m. Then, if unit is off ($y^n=0$) the related flowrates are zero. If unit n is on, all the inlet flowrates are nonnegative and operate in their specified range.

In some cases, a certain priority is assigned and it is modelled as follows:

$$y^n \le y^m \tag{14}$$

Thus unit n can be on, only if unit m is also on. In other words, unit m must be switched on before unit n. This order of priority applies for example to boilers and its auxiliary equipment such as feed water pumps and air fans. The power of boilers pumps and air fans are calculated using a linear function of the water and air flowrates:

$$\dot{W}_m^{n\text{p}} = a^{n\text{p}} y^{n\text{p}} + b^{n\text{p}} F_{n\text{p}}^{n\text{b}} \tag{15}$$

$$\dot{W}_m^{n\text{a}} = a^{n\text{a}} y^{n\text{a}} + b^{n\text{a}} F_{n\text{a}}^{n\text{b}} \tag{16}$$

Where $a^{n\text{p}}$, $b^{n\text{p}}$, $a^{n\text{a}}$ and $b^{n\text{a}}$ are constant coefficients. For each boiler, an air-fan is used to provide the air needed for the natural gas combustion. As the fan na is on, if and only if boiler nb is on, then the same binary variable is assigned to model the on/off states for both units. However, as a given air fan can receive its power either by an electrical motor ne or a steam turbine nt, a binary variable is introduced to represent this option. Then,

$$\dot{W}_m^n = \dot{W}_{n\text{e}}^n + \dot{W}_{n\text{t}}^n \tag{17}$$

$$0 \le \dot{W}_{n\text{e}}^n \le \dot{W}_{n\text{e}}^{\text{UB}}(1 - y^{n\text{b}}) \tag{18}$$

$$0 \leq \dot{W}_{nt}^{n} \leq \dot{W}_{nt}^{\mathrm{UB}} y^{n\mathrm{b}} \quad (19)$$

The power is provided by an electrical motor ne if $y^{n\mathrm{b}} = 0$ or by a steam turbine nt if $y^{n\mathrm{b}} = 1$. The power provided by a motor or a turbine has a range of variation between 0 and an upper bound. The driver that has been switched on provides a power equal to its upper bound while the driver that has been switched off provides no power, as indicated by the inequalities of Eqs. (18) and (19).

The boilers are modelled using a global efficiency $\eta_{n\mathrm{b}}$. The energy balance for boiler $n\mathrm{b}$, where inlet water is transformed into superheated steam by the combustion of natural gas $F_{\mathrm{NG}}^{n\mathrm{b}}$ that has a lower heating value of LHV, it is represented by:

$$\sum_{np} F_{np}^{n\mathrm{b}} h_{np} - F_{n\mathrm{b}}^{n\mathrm{h}} h_{n\mathrm{b}} - F_{n\mathrm{b}}^{\mathrm{p}} h_{\mathrm{p}} = \eta_{n\mathrm{b}} \times F_{\mathrm{NG}}^{n\mathrm{b}} \times \mathrm{LHV} \quad (20)$$

Condensed water and make up water $F_{np}^{n\mathrm{b}}$ are fed to the boiler, and the output flowrates are the high pressure steam produced $F_{n\mathrm{b}}^{n\mathrm{h}}$ and a purge $F_{n\mathrm{b}}^{\mathrm{p}}$. The purge is assumed to be saturated water at the boiler's operating pressure $P_{n\mathrm{b}}$ and its enthalpy h_{p} is calculated with the linear correlation (21) in the operating range of boiler pressures:

$$h_{\mathrm{p}} = d + eP_{n\mathrm{b}} \quad (21)$$

Where d and e are constant coefficients.

Finally, the operating cost of the plant is proportional to the flows of natural gas $F_{\mathrm{NG}}^{n\mathrm{b}}$, electrical power imported $\dot{W}_{\mathrm{imp}}^{\mathrm{E}}$, fresh water F_{FW}^{np} and cooling water treatment $F_{\mathrm{CW}}^{n\mathrm{b}}$.

$$C = c_{\mathrm{NG}} F_{\mathrm{NG}}^{n\mathrm{b}} + c_{\mathrm{E}} \dot{W}_{\mathrm{imp}}^{\mathrm{E}} + c_{\mathrm{FW}} F_{\mathrm{FW}}^{np} + c_{\mathrm{CW}} F_{\mathrm{CW}}^{np} \quad (22)$$

Where c_{NG} is the natural gas cost, c_{E} is the electrical power cost, c_{FW} the fresh water cost, c_{CW} is the cooling water treatment cost.

3. Environmental life cycle impact assessment

Life cycle is a holistic accounting of the environmental impact of all relevant sectors of the supply chain related with the product or service analysed. It is also called "a cradle to grave" study of a given product or service. The ISO14042 (1999) standard has been developed for environmental life cycle assessment providing a framework, terminology and some methodological choices. The environmental life cycle assessment methodology, as indicated in the ISO14042, comprises four main phases:

(i) *Goal and scope definition,* where the boundaries of the system are established in order to include all relevant processes contributing to the global environmental impact;
(ii) Inventory analysis, where the mass and energy flow rates are quantified;
(iii) *Impact assessment,* where the environmental and human health effects of the mass and energy flows are estimated;
(iv) *Interpretation,* where the results are analysed in order to achieve further improvement on the environmental performance.

In practice the process is iterative, as the results from subsequent stages will often require previous assumptions about system boundaries, required data, data quality, etc., to be modified. In this work the four stages have been considered simultaneously to improve the operating conditions of the utility plant.

The limits of the production plant are extended to contemplate raw material extraction, transport, production, use and waste disposal. The system boundary definition is extended compared with the conventional analysis in which the systems boundary is drawn around the process plant. Environmental life cycle impact assessment considers the whole material and energy supply chains. The material and energy flows that enter or leave the system include material and energy resources and emission to air, water and soil. These are referred to as environmental burdens and they arise from activities encompassing extraction and refining of raw material, transportation, production, use and waste disposal. Although environmental life cycle impact assessment has been associated with a product, in this work it will be applied to analyse and select optimally the process operation. It will be incorporated as a tool in process optimisation, rather than in products or technology selection at a decision making level.

While process engineering is normally concerned with the operations within the plant boundaries (battery limits) (1) in Fig. 2, environmental life cycle impact assessment considers the material and energy balances in the extended boundary (2) in Fig. 2, so that the limits between the system and the environment need to be defined including the main processes whose environmental impacts should be considered from raw material extraction to final disposal. Then, the limits of the system are extended to include the generation of the electricity imported, as shown in Fig. 2. The main environmental impacts of imported electricity generated by thermoelectric, hydroelectric and nuclear plants are evaluated. The electrical interconnected network in Argentina has approximately the following distribution: 53% of thermo electrical, 35% of hydro electrical and 12% of nuclear generation. The distribution of thermoelectric energy is: 30% gas turbine, 59% steam turbine burning natural gas, and 11% steam turbine burning fuel oil or gas oil. The combustion of oil, coal and natural gas releases pollutants, such as nitrogen oxide, carbon monoxide, particulate matter, sulphur dioxide, volatile organic compounds, organic hydrocarbons and trace metals into the air. The emissions associated with exploration, extraction, transport and refining were taken into account for oil, coal and natural gas consumed in the electric power generation.

Liquid effluents like cooling water purge, boiler blow down, demineralised water, etc. that are discharged from the utility plants and fossil fuel electric power generation release pollutants (chlorine, heavy metals, phosphorus, etc.) into surface waters as reported by Elliot (1989) and the Electric Power Research Institute report (1985). Creation of a hydroelectric reservoir can contribute to greenhouse gas emissions when a large biomass is flooded during impounding as reported by International Energy Agency (2000). Gases generated by aerobic and anaerobic decomposition are mainly carbon dioxide, methane, and to a lesser extent nitrous oxide.

The environmental impacts corresponding to the utility plant and the generation of the electricity imported have

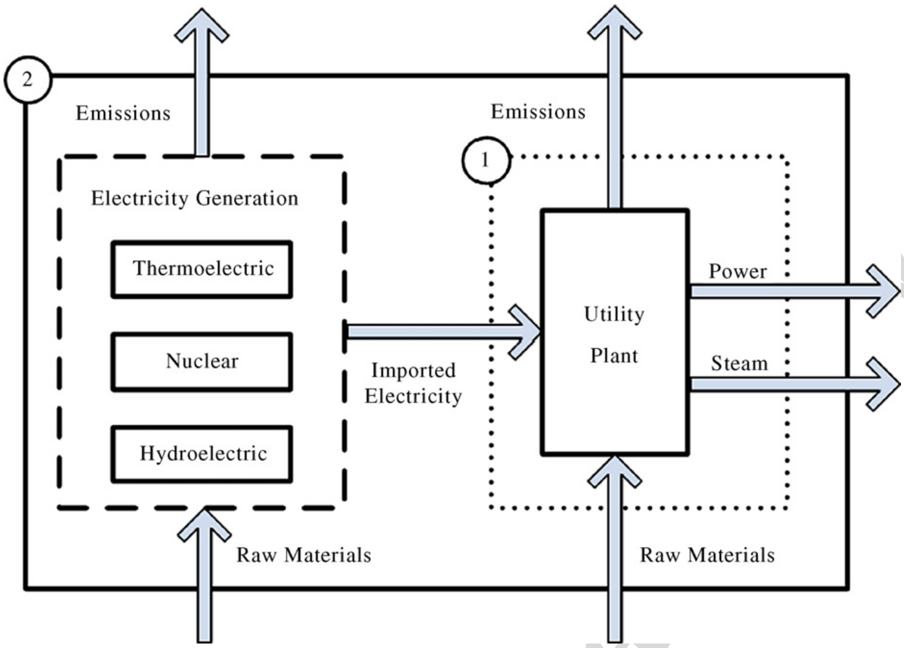

Fig. 2. Steam and power plant battery limits (1) and extended limits to include the generation of imported electricity (2).

been calculated and incorporated in the objective function for the selection of the operating conditions, following the methodology presented in the next section.

4. Environmental impact evaluation

The overall environmental impact is evaluated considering the contribution of the following environmental categories as described by Heijungs et al. (1992): global warming potential, acidification, photochemical oxidation, ozone depletion, human toxicity in air and water, ecotoxicity and eutrophication. These environmental categories are described briefly in the following section. Gagnon, Belanger, and Uchiyama (2002) considered global warming potential and acidification for the Canadian energy generation sector.

4.1. Impact categories

Global warming is caused by emissions of the greenhouse gases (GHG): CO_2, N_2O, CH_4, SF_6 (sulphur hexafluoride), hydrofluorcarbons (CFCs) and perfluorcarbons. The absorption and loss of radiant energy by the earth and the atmosphere are almost totally responsible for earth's weather. The heat that the earth absorbs reradiates energy back into space in the form of long wave radiation (infrared radiation). In the atmosphere, however, the GHG can absorb this reradiated energy, converting it to heat. Being heated, the molecules can now also reradiate the heat they absorb back to the earth (Seinfeld, 1998).

Depletion of stratospheric ozone quantifies stratospheric ozone breakdown as a result of human activities. Because of the dilution of the ozone layer, a large fraction of the sun's UV-B radiation reaches the surface of the earth. Ozone depletion indicates the potential of chlorofluorocarbons (CFCs) and chlorinated hydrocarbons for depleting the ozone layer.

Acidification is based on the contributions of SO_2, NO_x, HC1 and NH_3 to the potential acid deposition, i.e. on their potential to form H^+ ions. For example, sulphuric acid result when SO_2 discharged from combustion processes reacts with the moisture in the air.

Photo oxidant formation is the formation of reactive substances, which are injurious to human and ecosystem health (e.g. smog formation). Photo oxidant can be formed in the troposphere via photochemical oxidation of volatile organic compounds or carbon monoxide in the presence of NO_x and under the influence of UV light. Photochemical oxidants are caused primarily by volatile organic compounds, including: alkanes, halogenated hydrocarbons, alcohols, ketones, esters, ethers, olefins, aromatic, etc.

Nitrification/eutrophication is defined as the potential to cause over-fertilisation of water and soil. This enrichment may cause an undesirable shift in the composition of species and an increased production within aquatic and terrestrial ecosystems. Emissions of NO_x, $NH_4{}^+$ and $PO_4{}^{-3}$ are considered to be the main contributions to eutrophication.

Human toxicity is estimated here as the possible effect of chemicals releases to air and/or water that are toxic to humans either by inhalation or ingestion. They are calculated using acceptable human daily intake of the toxic substances.

Eco-toxicological impacts are the effects of toxic substances on aquatic and terrestrial ecosystems. This impact depends on the maximum tolerable concentrations on water and soil, that represent the concentration considered to protect 95% of the species in a certain ecosystem.

4.2. Overall environmental impact assessment

The contribution of a given component emission to the environmental categories is evaluated by multiplying its flow rate with the corresponding Heijungs factor. The contribution of component k emission to a given environmental impact category j, Ψ_{kj} is evaluated by multiplying the flow rate q_k emitted into the environment by the factor h_{kj} published by Heijungs et al. (1992). The Heijungs factor, h_{kj}, represents the potential effect that chemical k has on the environmental impact category j.

$$\psi_{kj} = q_k h_{kj} \tag{23}$$

q_k represents either the emission flowrate of the utility plant or the emission flowrate in the generation of the imported electricity.

The environmental impact of each category Ψ_j is calculated adding the contribution of all the components k as follows:

$$\psi_j = \alpha_j \sum_k \psi_{kj} \tag{24}$$

The normalizing factor α_j has been suggested by Cabezas et al. (1999) in the waste reduction algorithm and has been used by his co-workers Smith, Mata, Young, Cabezas, and Costa (2004) for designing an environmentally friendly hydrodealkylation of toluene plant considering fugitive and open emissions. This normalizing factor is calculated as the inverse of the average value of the Heijungs factors of the components contributing to category j, where K_j is the number of chemical compounds k that contribute (total number of compounds with non-zero scores in the database) to the environmental impact category j as stated by Heijungs et al. (1992):

$$\alpha_j = \frac{K_j}{\sum_k (h_{kj})} \tag{25}$$

The overall environmental impact Ψ is calculated as the sum of the contribution of each environmental impact (EI) category Ψj, as shown in Eq. (24), with ω_j representing the relative weighting factor of the EI category j.

$$\psi = \sum_j \omega_j \psi_j \tag{26}$$

Thus, the simulation of the utility plant and the main processes in the extended limits should provide the emission flow rates q_k to end up calculating the overall environmental impact Ψ. Considerable uncertainty and lack of information can be found along the extended limits of the environmental life cycle assessment. So the environmental impact quantification relies on the data available outside the battery limits of the plant being analysed.

4.3. Environmental impact assessment of the electricity generation

The burden of a given component k emitted into the environment q_k from a specific power source s is calculated using the following general equation:

$$[\mathrm{EC}]_\mathrm{s} \times \mathrm{ef}_{k\mathrm{s}} = q_{k\mathrm{s}} \tag{27}$$

Where $[\mathrm{EC}]_\mathrm{s}$ is the electricity consumed from power source s in $\mathrm{kW\,h^{-1}}$, ef_{ks} is the emission factor of chemical k from the power source s, in $[\mathrm{kg\,kW\,h^{-1}}]$.

4.4. Hydro electrical and nuclear generation

In hydro electrical power generation the emissions of CO_2, NO_x and SO_2 are considered. The emission factors take into account the dam building, mainly the material transport in trucks with internal combustion engines which emit greenhouse gases (CO_2, SO_2 and NO_x) and submerged biomass decay, which mainly emit CH_4 and CO_2. Therefore, the CO_2 emission factor has contributions from gaseous emissions of transport and from submerged biomass decay, (for further discussion on this point, see Gagnon & van de Vate, 1997).

For nuclear power generation the source emissions factors take into account the power plant emissions during the energy production, which are mainly aqueous ones and also consider the gaseous emissions during the power plant construction stage: CO_2, NO_x and SO_2. These factors include the life cycle assessment of fuel fabrication: uranium mining, milling, conversion, enrichment, and fuel fabrication (AEA, 1998). The following chemical compounds are present in liquid effluents of nuclear plants and are calculated as reported by AEA (1998): chlorides, thiosulphate, ammonia, antimonium, arsenics, berylium, cadmium, chromium(III), copper, iron, lead, manganese, mercury, nickel, phosphorous, sulphur and zinc. These chemicals contribute to the following environmental impact categories: water human toxicity, ecotoxicity and nitrification.

4.5. Thermo electrical power generation: natural gas, gas oil, fuel oil and coal

In the case of thermo electrical power sources, the electricity consumed from each source (natural gas, gas oil, fuel oil and coal) is multiplied by a factor that includes the lower heating value of the fuel and the efficiency of the power source. It is converted to fuel mass and multiplied by the emission factors reported by U.S. Environmental Protection Agency (1998) to give the emissions flow rates. These factors include the following LCIA stages: exploration, extraction, transport, refining and power generation itself (for petroleum derived fuels), electricity transport and waste disposal. In the case of natural gas the refining and waste disposal stages are not considered.

Once the chemical emissions corresponding to the different electricity generation sources are calculated, they are multiplied by the corresponding Heijungs's factor to predict their contribution to the potential environmental impact (PEI/h) using the Eqs. (23), (24) and (26).

5. Optimisation problem formulation

The objective function is the overall environmental impact of the utility plant Ψ as defined in Eq. (26), including the environmental impacts due to the generation of the imported electricity. The continuous operating conditions selected are the temperature and pressure of the high, medium and low pressure steam headers, the deaerator tank pressure and letdown flow rates. The following optimisation problem is formulated:

$$\begin{aligned} \min_{x,y} \quad & \psi(x, y) \\ \text{st.}: \quad & h(x) = 0 \\ & g(x) + Ay \le 0 \\ & x^{\mathrm{L}} \le x \le x^{\mathrm{U}} \\ & x \in R^n \\ & y \in \{0, 1\}^m \end{aligned} \tag{P1}$$

Where x and y are the continuous and binary variables, respectively. Superscripts U and L, indicates upper and lower bounds on vector x, respectively. The equality constraints $h(x)=0$ are the system of non-linear algebraic equations that represent the steady state modelling of the process plant (Eqs. (1)–(21)), including mass and energy balances and property predictions; the inequality constraints $g(x)+Ay \le 0$ represent minimum and maximum equipment capacities and operating constraints. The A matrix includes linear relations between binary variables such as logical constraints.

Pressures and temperatures of high, medium and low pressure steam headers, deaerator pressure and letdowns flow rates are the continuous optimisation variables. The vector y represents integer variables to select alternative drivers and equipment in operation such as boilers and their auxiliary pumps and air fans.

The power and steam demands of the ethylene plant are posed as equality constraints. The main power demands correspond to the cracked gas, ethylene and propylene refrigeration compressors. Other demands posed as equality constraints are the energy recovered from and consumed by the cracking furnace of the ethylene plant. Equality constraints also include the power demands for the condensate pump impellers, air fan impellers, boiler water pumps and cooling water pumps.

In the utility plant there are alternative drivers such as steam turbines and electrical motors for some pumps like condensate and lubricating ones, requiring binary variables to select the driver. There are also binary variables to select whether the equipment is on or off, like cooling tower pumps and boilers and their corresponding air fans and pumps.

6. Environmental life cycle impact minimisation

Mixed integer non linear programming problem (P1) is formulated and solved in GAMS. The modelling equations and water property prediction are posed as equality constraints in GAMS. The number of equations of problem (P1) included in GAMS is in the order of 10,500. The codes used to solve the non linear programming and mixed integer linear programming sub problems in GAMS were CONOPT ++ and OSL. The solution was found in 20 s and four major iterations. In this work, the weighting factors ω_j of Eq. (26) are equal to one, therefore the use of value judgments in weighting various environmental impacts has been equally considered. Different solutions can be obtained changing the values of the weighting factors that should be defined at the decision making level.

Table 2
Environmental impact category contributions

Impact category	PEI/h	% Contribution
Global warming	440.308	83.345
Acidification	86.298	16.335
Photo oxidant formation	1.313	0.249
Human toxicity air	0.359	0.068
Nitrification	0.019	0.004
Human toxicity water	0.001	0.0001
Ecotoxicity	0.00018	0.000034
Ozone depletion	0.0000068	0.000001
Total	528.298	100.00

In the utility plant of an ethylene process, 100 chemical compounds ($k=100$) are considered related mainly to the emissions. The steam and power demands of the chemical plant are formulated as equality constraints. There are 24 binary variables corresponding to: (i) four optional boilers and their corresponding air fans (four) and feeding water pumps (four), (ii) eight optional pump drivers (steam turbines or electrical motors) and (iii) four optional cooling tower pumps.

The initial and solution values of the operating conditions are reported in Table 1, including the temperature and pressure of high (HPSH), medium (MPSH) and low (LPSH) pressure steam headers. The main results minimizing the overall environmental impact Ψ as defined in Eq. (26), including the environmental impacts of the utility plant and the generation of the imported electricity are shown in Table 1. Significant reductions in the environmental life cycle (LC) impact (16%), operating costs (18%), natural gas (17%) and electricity (60%) consumption are obtained simultaneously as can be observed in Table 1. The improvements obtained are highly dependant on the initial point chosen.

Global warming has the highest potential environmental impact contribution representing 83% followed by Acidification with 16%, as shown in Table 2. Both contributions represent approximately 99.68% of the overall potential environmental impact. Therefore, for utility plants, the evaluation of these two environmental categories, global warming and acidification would be sufficient to represent the overall environmental impact.

The optimum operating values for temperature and pressure of high pressure steam header are equal to their upper bounds. Temperature and pressure of low pressure steam header are equal to their lower bounds. The maximum temperature and pressure of the HPSH and minimum temperature and pressure of the LPSH provide the maximum enthalpy gradient between high and low pressure steam headers and therefore the maximum power from the steam, increasing the efficiency or the ratio between power provided versus natural gas burned in the boilers. In this way the natural gas burned is minimised and also the combustion emissions and the corresponding potential environmental impact. Eight binary variables change their values between the initial and optimal points. In the initial point, three boilers out of four are on, while in the solution point two boilers are on, thus the air fan and feed water pump corresponding to boiler 3 and 4 are off.

If only the environmental impact inside the battery limits is considered there is an incentive to choose electrical motors as drivers instead of the steam turbines, because there is not an environmental impact associated with the electricity imported. For that reason an increment in the electricity imported of 46% is observed in this case.

It has been shown that the environmental life cycle impact can be used as the objective function to be minimized in the selection of the operating conditions of processes. It is very important to extend the boundaries of the process plant in the life cycle context, as shown in the case studied of the utility plant, a key part in many chemical and petrochemical plants. Future work will look at multiple objectives such as environmental life cycle impact and economical objectives considering not only cost but also income achieved throughout CO_2 emissions trading.

7. Conclusions

Environmental Life Cycle Impact has been minimized in the selection of the operating conditions of a utility plant. Significant reductions in the environmental impact, operating cost, natural gas and electricity consumption have been achieved simultaneously, increasing the efficiency of the plant. The methodology presented can be extended to the selection of the operating conditions of different processes and plants and to the synthesis and design stages. The evaluation of the main emissions in the life cycle boundaries is required to quantify their potential environmental impact.

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