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# General methodology for exergy balance in ProSimPlus<sup>®</sup> process simulator

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## A B S T R A C T

This paper presents a general methodology for exergy balance in chemical and thermal processes integrated in ProSimPlus<sup>®</sup> as a well-adapted process simulator for energy efficiency analysis. In this work, as well as using the general expressions for heat and work streams, the whole exergy balance is presented within only one software in order to fully automate exergy analysis. In addition, after exergy balance, the essential elements such as source of irreversibility for exergy analysis are presented to help the user for modifications on either process or utility system. The applicability of the proposed methodology in ProSimPlus<sup>®</sup> is shown through a simple scheme of Natural Gas Liquids (NGL) recovery process and its steam utility system. The methodology does not only provide the user with necessary exergetic criteria to pinpoint the source of exergy losses, it also helps the user to find the way to reduce the exergy losses. These features of the proposed exergy calculator make it preferable for its implementation in ProSimPlus<sup>®</sup> to define the most realistic and profitable retrofit projects on the existing chemical and thermal plants.

### Keywords:

Exergy analysis  
Process design  
Process integration  
Process simulator

## 1. Introduction

Industrial sector accounts for one third of global energy consumption. A common feature of industrial processes is reliance on fossil fuels as the primary source of energy and a large part of the energy consumption is spent on production of utilities (electricity, steam at various pressure levels, hot/cold water, hot flue gas, ...). As this reliance on fossil fuels has huge negative impact on the environment, the scientific world makes a significant effort to find alternative sources of energy. However, even by the most optimistic assessments, all these alternatives are long-term solutions and many projections show that in near future fossil fuels will remain as primary sources of energy.

The mode of production and management of utilities provide a great potential source for energy savings in the industrial sector as a whole but most particularly in the process industry. In this regard, recently in France, the working group, "*Lutter contre les changements climatiques et maîtriser l'énergie*" ("Fight against climate change and control of energy"), gathered at the recent "*Grenelle de l'environnement*" concluded that "approximately one third of the

energy consumption of industrial (or final energy 11 Mtep) comes from processes called "utility" (steam, hot air, heaters, electricity, etc.). The margins for improving the effectiveness of these processes exist. The dissemination and implementation of best practices can save up to 2 Mtep without requiring technological breakthroughs." One of the mechanisms identified by the working group to reduce energy consumption and greenhouse gas emissions is "the establishment of more efficient means of using process utilities" within production units. Then, efforts must be made to seek best practice that will minimize the damage caused by the fossil fuels. A short term and sustainable solution consists in improving energy efficiency of industrial processes [1].

Among the approaches existing to tackle this challenge, exergy analysis has been shown by Kotas [2] to be a useful tool as it exploits the concept of energy quality to quantify the portion of energy that can be practically recovered. Unfortunately, contrary to enthalpy, this concept is rather difficult to handle and this physical quantity is rarely implemented in process simulators. In order to make exergy analysis more understandable and to demonstrate its value for the analysis of the energy efficiency of the process and its utilities, this paper presents a fully-automated exergy analysis tool integrated in a process simulator. This paper starts with some basic exergy concepts and then presents the exergy calculation methodologies for material, heat and work streams as well as their implementation aspects in ProSimPlus<sup>®</sup>. To provide the essential elements for

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## Nomenclature

### General symbols

$B$	exergy flow, W
$b$	molar exergy, J/mol
$G$	Gibbs free energy flow, W
$g$	molar Gibbs free energy, J/mol
$H$	enthalpy flow, W
$h$	molar enthalpy, J/mol
$n$	molar flowrate, mol/s
$N$	number of species, –
$NS$	number of streams, –
$P$	pressure, bar
$Q$	heat flow, W
$q$	heat per mole, J/mol
$R$	universal gas constant, J/(mol.K)
$S$	entropy flow, W/K
$s$	molar entropy, J/(mol.K)
$T$	absolute temperature, K
$W$	power, W
$w$	work per mole, J/mol
$x$	liquid fraction, –
$y$	vapour fraction, –
$z$	global composition of material stream, –

### Greek symbols

$\omega$	vapour ratio
$\Delta G_{y \rightarrow L}^\circ$	standard Gibbs energy of condensation (J/mol)
$\Delta G_f^\circ$	standard Gibbs energy of formation (J/mol)
$\eta$	simple exergy efficiency
$\Psi$	rational exergy efficiency

### Subscripts

$c$	components in the given material stream
$el$	reference element
$f$	formation
$gen$	generated entropy
$j$	reference substance
$j, i$	reference substance $j$ from process substance $i$
$M$	related to material stream
$Q$	related to heat stream
$ref$	reference substance
$rev$	reversible
useful	useful stream
$W$	related to work stream
waste	waste stream

### Superscripts

*	perfect gas
$ch$	chemical
$E$	excess enthalpy or entropy
$l$	liquid phase
$ph$	physical
$v$	vapour phase
$W$	work
$\Delta P$	mechanical component of physical exergy
$\Delta T$	thermal component of physical exergy
$in$	input streams
$out$	output streams
$0$	standard state (pure-component, perfect gas, $T^0 = 298.15$ K, $P^0 = 1$ atm)
$00$	standard dead state

exergy analysis, exergy balance and the most commonly used exergy efficiencies are also presented. Finally, the applicability of our methodology developed in ProSimPlus<sup>®</sup> is shown through a simple scheme of Natural Gas Liquids (NGL) recovery process.

In process simulators, implementation of exergy analysis as a useful tool in evaluating processes along with the traditional energy- and mass- balances needs at first exergy calculation. For a given unit operation, the exergy inputs and outputs have different forms corresponding to work, heat, and material streams. For the purpose of exergy balance, one needs to deal with all of these types of exergy and calculate the exergy of all material, heat and work streams in a process and utilities. To facilitate this step of exergy analysis, there are some exergy methodologies integrated with process simulator [3–6].

Hinderink et al. [3] developed ExerCom as an exergy calculator of material streams for Aspen Plus<sup>®</sup>. Exergy is considered to be composed of three components of physical, chemical and mixing exergy. The value of mixing exergy is dependent on the thermodynamic model chosen in the process simulator. The most commonly used standard chemical exergy table defined by Szargut et al. [7] is used. To implement this exergy calculation methodology, two different tools integrated with Aspen Plus<sup>®</sup> have to be used. As a first tool, ExerCom uses the output of the Aspen Plus<sup>®</sup> simulation, along with internal databases of standard chemical exergies and enthalpies to calculate exergy of material streams. An additional tool like Psage-developed program [8] which interfaces with both Aspen Plus<sup>®</sup> and ExerCom must be used to calculate the exergies of heat and work. Dealing with more than one interface makes exergy analysis inconvenient for the user. ExerCom was used for exergy analysis of advanced separation enhanced water-gas-shift

membrane reactors [9] and an oxy-combustion process for a supercritical pulverized coal power plant with CO<sub>2</sub> capture [10].

Later, based on the method described by Hinderink et al. [3], Montelongo-Luna et al. [4] developed an open-source exergy calculator of material streams for the open-source chemical process simulator Sim42 [11]. As Sim42 is an open source program, this permitted the seamless inclusion of the exergy calculations into the source code of the simulator without linking any external computer routines to the simulator. Unlike most chemical exergy calculators, its chemical exergy is calculated based on the reference environment defined by van Gool [12]. This exergy calculator does not carry out the full exergy balance including heat and work streams. This open-source exergy calculator was recently used for development of the relative exergy array [13] which is a tool to measure the relative exergetic efficiency and the controllability of a process when a proposed process and control structure is postulated.

Zargarzadeh et al. [5] developed Olexan as a tool for online exergy analysis which interfaces with the plant online data system to gather the required stream data and also with a process simulator to compute the missing data. It also provides various thermodynamic measures of effectiveness of the process such as second law efficiency, exergy effectiveness, exergy improvement potentials and irreversibilities. However, Olexan cannot deal with unit operations such as reactors and distillation columns where chemical exergy changes.

Recently, Querol et al. [14] has developed a Microsoft Excel-based exergy calculator for Aspen Plus<sup>®</sup> which facilitates the thermoeconomic analysis. It calculates exergy of heat, work and material streams where the mixing exergy is being considered to be a part of physical exergy. The reference environment is based on Szargut et al. [7].

More recently, Abdollahi-Demneh et al. [6] has developed a VB-based exergy calculator of material streams for Aspen HYSYS® where the chemical exergy is itself being considered to be composed of different components. The reference environment is based on Szargut et al. [7] and can be adapted to the case under study by modifying the reference temperature, pressure and composition but its database covers a limited number of chemical elements.

Although such computer-aided exergy calculations (see Table 1) make exergy analysis more accessible, exergy analysis within process simulators is not still straightforward. This paper presents a general methodology for exergy balance in chemical and thermal processes integrated in ProSimPlus® as a well-adapted process simulator for energy efficiency analysis. In this work, as well as using the general expressions for heat and work streams, all of exergy balance is presented within only one software in order to fully automate exergy analysis. In other words, unlike the most of existing methodology which use the some VB-based subroutines in integration of process simulators, this papers presents a calculator which becomes a part of ProSimPlus® process simulator without further need to any other external programs to perform exergy balance like the traditional enthalpy balance. In addition, after exergy balance, the essential elements (e.g. sources of irreversibility) for exergy analysis are presented to help the user for modifications on either process or utility system. These features of our methodology make it preferable for its implementation in process simulators to analyze the process and its utilities, to define the most profitable retrofit projects. In addition, the exergy efficiency can be chosen as a variable in exergetic optimizations.

## 2. Calculation of exergy of streams

For the purpose of exergy balance, all types of exergy associated with material, heat and work streams in a process and its related utilities, has to be calculated. In this section, after reviewing basic exergy concepts, formulations for exergy calculations and their implementation aspects in ProSimPlus® are presented.

### 2.1. Basic exergy concepts and definitions

According to Szargut et al. [7] and as illustrated on Fig. 1, exergy is defined as “the maximum work which can be extracted when a material stream is brought to a state of thermodynamic equilibrium with the common components of the natural surroundings by means of reversible processes, involving interaction only with the above mentioned components of nature”.

To complete the definition of exergy, we have to define the *Exergy Reference Environment (RE)* such as the one defined by Szargut et al. [7] which is partially shown in Table 2. Moreover, to easily define the different components of exergy, it is necessary to define the concepts of *process state*, *environmental state* and *standard dead state*.

- *Process state*: The *process state* refers to the initial state of the system under study ( $T, P, z$ ).
- *Environmental state*: The restricted equilibrium refers to a state where the conditions of mechanical and thermal equilibrium between the system and the environment are satisfied. It requires the pressure and the temperature of the system and environment to be equal. The state that satisfies the condition of restricted equilibrium with the environment will be referred as the *environmental state* ( $T^{00}, P^{00}, z$ ).
- *Standard dead state*: In the unrestricted equilibrium not only the pressure and the temperature but also the chemical potentials of the substances of the system and environment must be equal to satisfy the conditions of full thermodynamic equilibrium

**Table 1**  
A comparison of existing exergy calculators with process simulators.

Reference	Simulator	Exergy components	RE	Possibility to change $T^{00}$ and $P^{00}$	Chemical exergy data base	Heat & work	Implementation	Thermoeconomic	Dependent on the thermodynamic model	Comments	Application
ExerCom Hinderink et al. [3]	Aspen Plus®	Physical, chemical and mixing	Szargut et al. [7]	No	Complete	No	External subroutine	No	Yes	Highly dependent on the thermodynamic model	Water-gas-shift membrane reactors [9], CO2 capture [10]
Montelongo-Luna et al. [4]	Sim42	Physical, chemical and mixing	van Gool [12]	No	Complete	No	Included in simulator	No	Yes	No external subroutines	Development of the relative exergy array [13]
Olexan Zargarzadeh et al. [5]	Online	Physical	–	No	–	Yes	External calculator	No	No	Interface with the online data	Liquefied natural gas (LNG) process [5]
Querol et al. [14]	Aspen Plus®	Physical and chemical	Szargut et al. [7]	No	Complete	Yes	Excel-based	Yes	Yes	Suitable for thermoeconomic analysis	Air separation unit [14]
Abdollahi-Demneh et al. [6]	Aspen HYSYS®	Physical and chemical	Szargut et al. [7]	Yes	Partial	No	VB-based	No	Yes	A limited number of chemical elements	Combustion [6]

**Table 2**

Partial data of the reference environment from Szargut et al. [7] (partial pressure of components is calculated at the mean atmospheric pressure 99.31 kPa).

$T^{00}$	25 °C
$p^{00}$	101.325 kPa
Reference substance	Partial pressure (kPa)
CO <sub>2</sub>	0.0335
H <sub>2</sub> O	2.2
N <sub>2</sub>	75.78
O <sub>2</sub>	20.39
Ar	0.9
D <sub>2</sub>	0.000 342
He	0.000 485
Kr	0.000 485
Ne	0.001 77
Xe	0.000 000 09

between the system and the environment. Under these conditions, the value of exergy of the system is zero because the system cannot undergo any changes of state through any form of interaction with the environment. This state of the system is called the *standard dead state* ( $T^{00}, p^{00}, z^{00}$ ).

## 2.2. Exergy component of a material stream

Like energy, exergy of a material stream can be divided into distinct components: kinetic exergy, potential exergy, physical exergy, chemical exergy (see Fig. 2). Neglecting kinetic and potential exergy, physical exergy and chemical exergy will be the two major contributors. The total exergy of a material stream at given conditions is then expressed as the sum of chemical exergy and physical exergy. Physical exergy as a first component of exergy is defined as: “the maximum amount of work obtainable when it is brought from its *process state* to the *environmental state*, by physical process involving thermal and mechanical interaction only with the environment” whereas chemical exergy is defined as “the maximum work obtainable when a given system is brought from *environmental state* to the *standard dead state*”.

Using these definitions, the following sections will establish general expressions for physical and chemical exergy.

### 2.2.1. Physical exergy

Thermal and mechanical exergy modules shown in Fig. 3 represent ideal devices in which the material stream undergoes some reversible processes. The state of the stream at the entrance of the module is defined by the *process state* and the exit state corresponds to the *environmental state*, i.e. the pressure and temperature of the stream are  $p^{00}$  and  $T^{00}$ . The first law of thermodynamics for the thermal exergy module provides:

$$h(T, P, \mathbf{z}) - h(T^{00}, P, \mathbf{z}) + q_{rev,I} + w_{rev,I} = 0 \quad (1)$$

Then the second law of thermodynamics leads to the following relation:

$$s(T, P, \mathbf{z}) - s(T^{00}, P, \mathbf{z}) + \frac{q_{rev,I}}{T^{00}} = 0 \quad (2)$$

Eliminating the heat transfer rate between the last two equations the specific thermal exergy can be finally defined as follows:

$$b^{\Delta T} = -w_{rev,I} = h(T, P, \mathbf{z}) - T^{00}s(T, P, \mathbf{z}) - \left[ h(T^{00}, P, \mathbf{z}) - T^{00}s(T^{00}, P, \mathbf{z}) \right] \quad (3)$$

Likewise for mechanical exergy module, the definition for the specific mechanical exergy is obtained:

$$b^{\Delta P} = -w_{rev,II} = h(T^{00}, P, \mathbf{z}) - T^{00}s(T^{00}, P, \mathbf{z}) - \left[ h(T^{00}, p^{00}, \mathbf{z}) - T^{00}s(T^{00}, p^{00}, \mathbf{z}) \right] \quad (4)$$

Then, the physical exergy as shown by Kotas [2] is the sum of thermal and mechanical exergies:

$$b^{ph} = b^{\Delta T} + b^{\Delta P} \quad (5)$$

$$b^{ph} = -w_{rev,I} - w_{rev,II} = h(T, P, \mathbf{z}) - T^{00}s(T, P, \mathbf{z}) - \left[ h(T^{00}, p^{00}, \mathbf{z}) - T^{00}s(T^{00}, p^{00}, \mathbf{z}) \right] \quad (6)$$

### 2.2.2. Chemical exergy

In determining physical exergy, the final state of stream is the *environmental state*. Now, this state will be the initial state in the reversible processes which are dedicated to determine the chemical exergy of this material stream. According to the definition of exergy, the final state to which the substance will be reduced is the *standard dead state*. Thus, chemical exergy is defined as “the maximum work obtainable when the substance under consideration is brought from *environmental state* to the *standard dead state* by process involving heat transfer and exchange of substances only with the environment”.

To assess the work potential (i.e. exergy) of a stream of substance by virtue of the difference between its chemical potential and that of the environment, the properties of the chemical elements comprising the stream must be referred to the properties of some corresponding suitably selected substances in the environment (i.e. Reference Substances, RS). Reference Substances can either be gaseous components from the atmosphere, species dissolved in seawater, or solid compounds presents on the earth's surface.

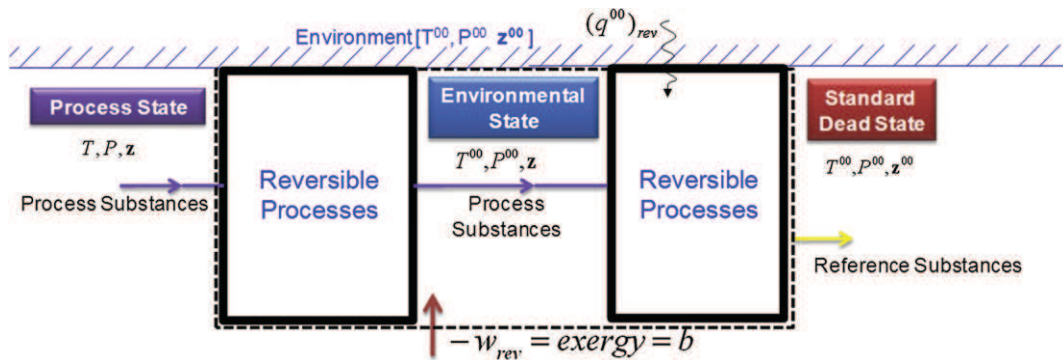


Fig. 1. Definition of exergy of material stream.



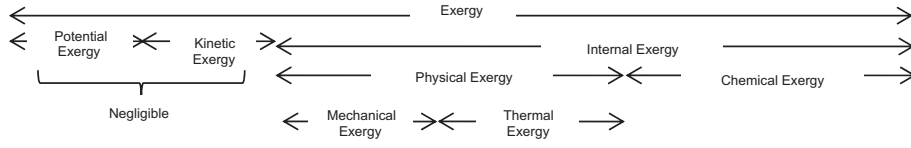


Fig. 2. Exergy components.

To understand the physical meaning of chemical exergy, let us take a general example illustrated in Fig. 4a. Two cases must be examined:

- If the substance under consideration is a RS (for example  $\text{CO}_2$  which is present in the atmosphere as illustrated on Fig. 4b), the evaluation of exergy of material stream only requires a change in the composition of this substance. The partial pressure of gas to a state of chemical equilibrium can be reached by means of *Module CHEM II*.
- On the other hand, if the substance under consideration is a *Non-RS* (for example  $\text{CH}_4$  on Fig. 4c), calculating chemical exergy will involve an additional module (i.e. *CHEM I*) to include a reversible chemical reaction to transform the *Non-RS* under consideration into one or more RS with the aid of RS brought from the environment. This reaction, which is called *Reference Reaction*, occurs in *Module CHEM I*.

From this simple example, the general formulation of the chemical exergy of a given mixture is:

$$b^{ch}(T^{00}, P^{00}, \mathbf{z}) = h(T^{00}, P^{00}, \mathbf{z}) - T^{00} s(T^{00}, P^{00}, \mathbf{z}) - \frac{1}{n} \sum_i^{Nc} \left[ \sum_{j=1}^{N_{ref,i}} n_{j,i} \left[ h_j(T^{00}, P^{00}, \mathbf{z}^{00}) - T^{00} s_j(T^{00}, P^{00}, \mathbf{z}^{00}) \right] \right] \quad (7)$$

where,

- $n_{j,i}$  is the flowrate of the reference substance  $j$  generated by the process substance  $i$
- $N_{ref,i}$  is the number of reference substance  $j$  generated by the process substance  $i$

It results from Eq. (7) that one needs to evaluate the molar enthalpy of each reference substance which is present in the environment. Reference species can be either gaseous component from atmosphere, species dissolved in seawater or solid

compounds from the earth crust. This task requires very precise assumptions concerning the mean concentration of all the *reference substances* in the *reference environment* and complex thermodynamic calculations. To simplify this step, Szargut et al. [7] defined the concept of molar standard chemical exergy as the chemical exergy obtained in the standard state at  $T^0, P^0$ .

$$b_i^0 = h_i^*(T^0, P^0) - T^0 s_i^*(T^0, P^0) - \sum_{j=1}^{N_{ref,i}} \frac{n_{ij}}{n_i} \left[ h_j(T^{00}, P^{00}, \mathbf{z}^{00}) - T^{00} s_j(T^{00}, P^{00}, \mathbf{z}^{00}) \right] \quad (8)$$

The standard chemical exergy can be defined for elements or components. For the given standard chemical exergy value of elements  $b_j^0$ , the standard chemical exergy of component  $i$  can be defined as follows [11]:

$$b_i^0 = \Delta G_f^0 + \sum_{j=1}^{N_{el,i}} n_{i,j} b_j^0 \quad (9)$$

A first table of the chemical exergy of reference substances has been established by Szargut et al. [7] and recently updated by Rivero and Garfias [15].

Assuming that the reference environment is in the standard conditions (i.e.  $T^{00} = T^0$  and  $P^{00} = P^0$ ), it is then possible to extract the standard molar chemical exergy  $b_j^0$  of the component  $i$  from Eq. (9).

- *First case:* The process mixture is in the vapour phase. In that case, Eq. (7) can be rewritten as follows:

$$b^{ch,V}(T^{00}, P^{00}, \mathbf{y}) = h^V(T^{00}, P^{00}, \mathbf{y}) - T^{00} s^V(T^{00}, P^{00}, \mathbf{y}) - \frac{1}{n} \sum_i^{Nc} \left[ \sum_{j=1}^{N_{ref,i}} n_{j,i} \left[ h_j(T^{00}, P^{00}, \mathbf{z}^{00}) - T^{00} s_j(T^{00}, P^{00}, \mathbf{z}^{00}) \right] \right] \quad (10)$$

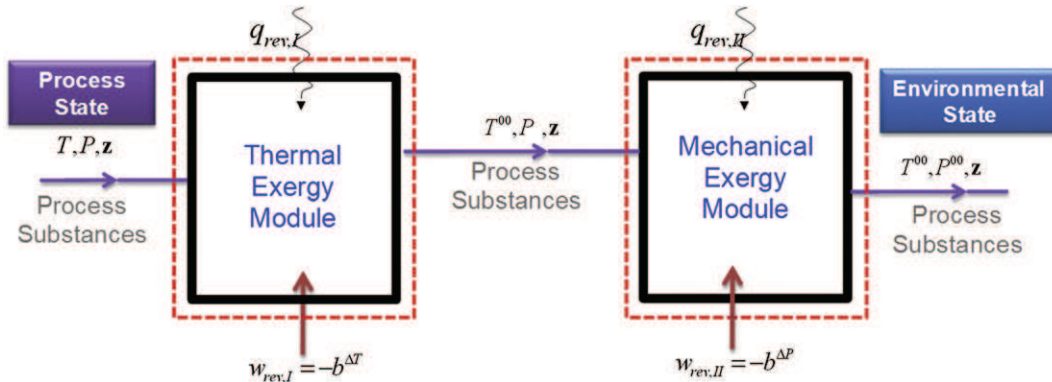


Fig. 3. Definition of physical exergy (thermal and mechanical modules).

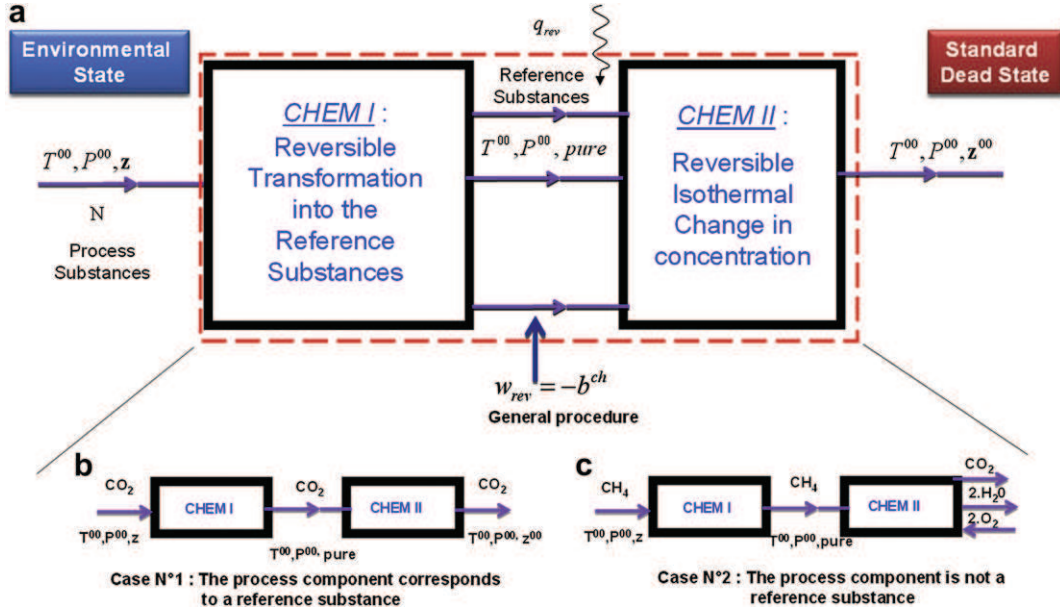


Fig. 4. Definition of chemical exergy.

Assuming that the vapour phase at  $T^{00}$  and  $P^{00}$  behaves as a perfect gas, we can write:

$$b^{ch,V}(T^{00}, P^{00}, \mathbf{y}) = \sum_i^{Nc} y_i \left[ h_i^*(T^{00}, P^{00}) - T^{00} s_i^*(T^{00}, P^{00}) + RT^{00} \ln(y_i) - \sum_{j=1}^{N_{ref,i}} \frac{n_{ij}}{y_i n} \left[ h_j(T^{00}, P^{00}, \mathbf{z}^{00}) - T^{00} s_j(T^{00}, P^{00}, \mathbf{z}^{00}) \right] \right] \quad (11)$$

Eq. (11) can be expressed as a function of the standard molar chemical exergy, we finally obtain:

$$b^{ch} = \sum_i^{Nc} y_i (b_i^\circ + RT^{00} \ln(y_i)) \quad (12)$$

- *Second case:* The process mixture is in the liquid phase. In the case of non-ideal mixture, chemical potential is:

$$\mu_i(T, P) = \mu_i^0(T, P) + RT \ln(\gamma_i x_i) \quad (13)$$

Therefore, the term  $\gamma_i$  has to be introduced as follows:

$$b^{ch}(T^{00}, P^{00}, \mathbf{z}) = b^{ch,L}(T^{00}, P^{00}, \mathbf{x}) = \sum_i^{Nc} x_i \left[ h_i^{0,L}(T^{00}, P^{00}) - T^{00} s_i^{0,L}(T^{00}, P^{00}) + RT^{00} \ln(\gamma_i x_i) - \sum_{j=1}^{N_{ref,i}} \frac{n_{ij}}{x_i \cdot n} \left( h_j(T^{00}, P^{00}, \mathbf{z}^{00}) - T^{00} s_j(T^{00}, P^{00}, \mathbf{z}^{00}) \right) \right] \quad (14)$$

Note also that standard molar chemical exergy was defined for vapour species. As a consequence, if the chemical exergy concerns a liquid mixture, it is necessary to add a term corresponding to Gibbs free energy of condensation. Finally, Eq. (7) becomes:

$$b^{ch} = \sum_i^{Nc} x_i (b_i^\circ + \Delta G_{v \rightarrow L}^\circ + RT^{00} \ln(\gamma_i x_i)) \quad (15)$$

- *Third case:* The process mixture is in the vapour–liquid phase. In that case, the chemical exergy is expressed as a function of the vapour ratio:

$$b^{ch} = (1 - \omega) \left[ \sum_i^{Nc} x_i (b_i^\circ + \Delta G_{v \rightarrow L}^\circ + RT^{00} \ln(\gamma_i x_i)) \right] + \omega \left[ \sum_i^{Nc} y_i (b_i^\circ + RT^{00} \ln(y_i)) \right] \quad (16)$$

- *Fourth case:* The process stream is a mixture of liquid–liquid. In that case, the chemical exergy is expressed as a function of fractions of liquid I and II:

$$b^{ch} = \omega^I \left[ \sum_i^{Nc} x_i^I (b_i^\circ + \Delta G_{v \rightarrow L}^\circ + RT^{00} \ln(\gamma_i x_i^I)) \right] + (1 - \omega^I) \times \left[ \sum_i^{Nc} x_i^{II} (b_i^\circ + \Delta G_{v \rightarrow L}^\circ + RT^{00} \ln(\gamma_i x_i^{II})) \right] \quad (17)$$

- *Fifth case:* The process stream is a mixture of liquid/liquid/vapour. In this case, the chemical exergy is expressed as a function of fraction of liquid and vaporisation ratio:

$$b^{ch}(T, P, \mathbf{z}) = (1 - \omega) \left( \omega^I \left[ \sum_i^{Nc} x_i^I (b_i^\circ + \Delta G_{v \rightarrow L}^\circ + RT^{00} \ln(\gamma_i x_i^I)) \right] + (1 - \omega^I) \left[ \sum_i^{Nc} x_i^{II} (b_i^\circ + \Delta G_{v \rightarrow L}^\circ + RT^{00} \ln(\gamma_i x_i^{II})) \right] \right) + \omega \left( \sum_i^{Nc} y_i (b_i^\circ + RT^{00} \ln(y_i)) \right)$$



Calculation of the molar chemical exergy of a mixture by the equations given above, results in 1.5% and 5.8% deviation from the examples given in Kotas [2] and Hinderink et al. [3].

### 2.2.3. Exergy of work stream

Exergy is defined as the equivalent work of a given energy form. Consequently, shaft-work (either mechanical or electrical work) is equivalent to exergy [16].

### 2.2.4. Exergy of heat stream

The exergy of a heat stream is determined from the maximum work that could be obtained from it using the environment as a reservoir of zero-grade thermal energy. For the specified control surface of the Carnot cycle shown in Fig. 5, first and second laws of thermodynamics result in Eqs. (18) and (19).

$$|Q_H| - |W_{MAX}| - |Q_C| = 0 \quad (18)$$

$$\frac{|Q_H|}{T_H} - \frac{|Q_C|}{T_C} = 0 \quad (19)$$

$$|W_{MAX}| = |Q_C| \left( 1 - \frac{T_C}{T_H} \right) \quad (20)$$

Considering a heat stream provided by a given utility (e.g. heat source) to a process unit operation, the temperature of the cold source ( $T_C$ ) becomes equal to the ambient temperature ( $T^0$ ). Temperature of heat source ( $T_H$ ) is regarded as the temperature at the system boundary at which the heat transfer occurs. When the heat transfer occurs at a varying temperature such as the case of heat exchanger, the thermodynamic average temperature ( $\bar{T}$ ) [17] can be defined. It can be determined by combining first and second laws around the heat source. Heat transfer shown in Fig. 6 is assumed to be reversible, therefore in accordance with second law of thermodynamic we have:

$$s_{out} - s_{in} = \int \frac{dq}{T} \quad (21)$$

According to the first law of thermodynamics we also have:

$$h_{out} - h_{in} = \int dq \quad (22)$$

By definition, the thermodynamic average temperature ( $\bar{T}$ ) is equal to:

$$\bar{T} = \frac{\int dq}{\int \frac{dq}{T}} \quad (23)$$

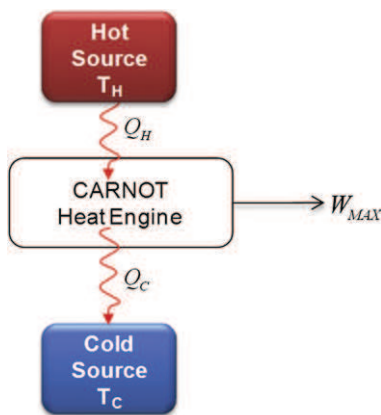


Fig. 5. Carnot cycle.

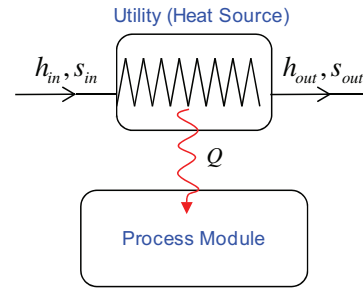


Fig. 6. Exergy of heat stream.

Substituting Eqs. (21) and (22) in Eq. (23),  $\bar{T}$  can be evaluated:

$$\bar{T} = \left( \frac{h_{out} - h_{in}}{s_{out} - s_{in}} \right) \quad (24)$$

### 2.3. ProSimPlus® implementation

To implement exergy balance in ProSimPlus® [18], a set of subroutines are integrated in the flowsheet as a programming module. The exergy calculator in ProSimPlus® allows the user to call the available functions from Simulis® thermodynamics.

Fig. 7 shows the flowchart of the exergy calculator dedicated to the calculation of physical and chemical exergy of a material stream. Three main procedures to calculate exergy of a material stream are explained as follows:

- *Definition Reference Environment*: This procedure is used to define the conditions for the reference environment. The database of standard chemical exergy proposed by Rivero and Garfias [15] is used at the fixed temperature, pressure and composition.
- *PhysExergy Material Stream*: This procedure calculates the physical exergy of the material stream. It uses procedure of CalcH&S to call enthalpy and entropy functions from Simulis® thermodynamics.
- *ChemExergy Material Stream*: This procedure calculates the chemical exergy of the material stream starting with calling *StdChemExergy DataBank* as a procedure to calculate the standard chemical exergy of the component found in the flowsheet based on the calculation methodology of Rivero and Garfias [15]. *ElementStdChemEx* as a database containing the chemical exergy of all elements including the standard database available with Simulis® thermodynamics with a subroutine of *DecompFormula* which break down each chemical compound into its constituent chemical elements, are matched together to calculate the chemical exergy.

### 3. Exergy balance and exergy analysis

Given the procedure dedicated to the calculation of exergy of individual streams, it is now possible to carry out exergy balance. Contrary to energy balance directly deduced from the first law of thermodynamics, exergy balance is deduced from the first and second laws of thermodynamics and requires a contribution of the engineer. Indeed, to enable the evaluation of internal and external losses thanks to exergy balances, first waste streams have to be distinguished from useful ones.

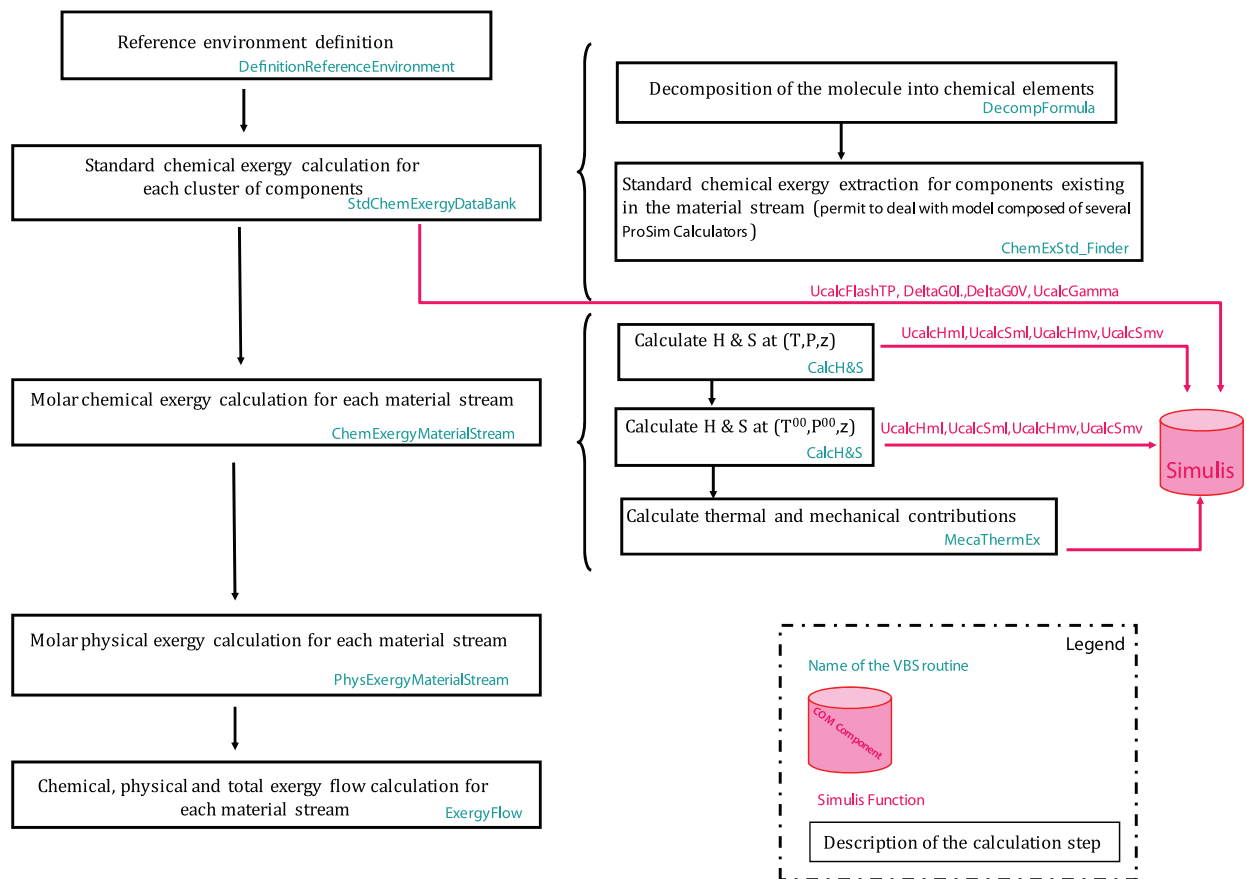


Fig. 7. Calculation of exergy of material streams in ProSimPlus®

### 3.1. Waste stream vs. useful streams

The generic system illustrated in Fig. 8. can either represent a single unit operation, a global flowsheet or a part of a flowsheet. In this system, inputs material, heat and work are transformed into output ones by thermal and chemical operations. In such a system, some material and heat output streams are not useful ones and can be considered as waste streams (it can be waste materials that need to be recycled). Energy and exergy balances do not consider these waste streams in the same way.

As illustrated in Eq. (25), for energy balances deduced from the first law of thermodynamics, waste and useful streams do not need to be distinguished:

$$H_M^{\text{in}} + Q^{\text{in}} + W^{\text{in}} = H_M^{\text{out}} + Q^{\text{out}} + W^{\text{out}} \quad (25)$$

Likewise, to write exergy balance, total exergy input and total exergy output are given by the sum of input and output exergy associated with material, work and heat:

$$B^{\text{in}} = \sum_{i=1}^{NS_M^{\text{in}}} B_{M,i}^{\text{in}} + \sum_{i=1}^{NS_Q^{\text{in}}} B_{Q,i}^{\text{in}} + \sum_{i=1}^{NS_W^{\text{in}}} B_{W,i}^{\text{in}} \quad (26)$$

$$B^{\text{out}} = \sum_{i=1}^{NS_M^{\text{out}}} B_{M,i}^{\text{out}} + \sum_{i=1}^{NS_Q^{\text{out}}} B_{Q,i}^{\text{out}} + \sum_{i=1}^{NS_W^{\text{out}}} B_{W,i}^{\text{out}} \quad (27)$$

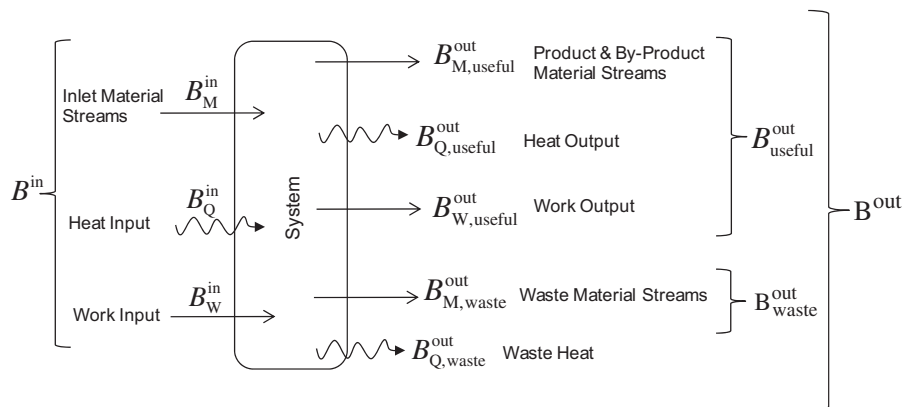


Fig. 8. A general presentation of a process or system.

Contrary to energy balance, the strength of exergy balance relies on the capacity to estimate the exergetic efficiency of the process by classifying the output stream into “useful” or “waste” streams. As a consequence, the exergy of heat and material streams must be expressed as follows:

$$B_M^{\text{out}} = B_{M,\text{useful}}^{\text{out}} + B_{M,\text{waste}}^{\text{out}} \quad (28)$$

$$B_Q^{\text{out}} = B_{Q,\text{useful}}^{\text{out}} + B_{Q,\text{waste}}^{\text{out}} \quad (29)$$

Furthermore, as all work output is assumed to be as “useful”, one can write:

$$B_{W,\text{waste}}^{\text{out}} = 0 \quad (30)$$

$$B_{\text{waste}}^{\text{out}} = \sum_{i=1}^{NS_{M,\text{waste}}^{\text{out}}} B_{M,\text{waste},i}^{\text{out}} \quad (31)$$

As a consequence, the total output exergy flow can be expressed as follows:

$$B_{\text{useful}}^{\text{out}} = \sum_{i=1}^{NS_{M,\text{useful}}^{\text{out}}} B_{M,\text{useful},i}^{\text{out}} + \sum_{i=1}^{NS_{Q,\text{useful}}^{\text{out}}} B_{Q,\text{useful},i}^{\text{out}} + \sum_{i=1}^{NS_{W,\text{useful}}^{\text{out}}} B_{W,i}^{\text{out}} \quad (32)$$

Using the “useful” and “waste” streams concept, the exergy balance can now be written. However, contrary to energy balance, another term corresponding to the exergy destroyed in the system (due to irreversibility of the process) must be introduced in the output terms. Then we have:

$$B^{\text{in}} = B_{\text{useful}}^{\text{out}} + \underline{B_{\text{waste}}^{\text{out}}} + I \quad (33)$$

where underlined term is “external exergy loss” and “I” represents the “internal exergy loss”. These two terms will be discussed in detail in the next section.

Finally, the resulting exergy balance can be written as follows:

$$\sum_{i=1}^{NS_M^{\text{in}}} B_{M,i}^{\text{in}} + \sum_{i=1}^{NS_Q^{\text{in}}} B_{Q,i}^{\text{in}} + \sum_{i=1}^{NS_W^{\text{in}}} B_{W,i}^{\text{in}} = \sum_{i=1}^{NS_{M,\text{useful}}^{\text{out}}} B_{M,\text{useful},i}^{\text{out}} + \sum_{i=1}^{NS_{Q,\text{useful}}^{\text{out}}} B_{Q,\text{useful},i}^{\text{out}} + \sum_{i=1}^{NS_{W,\text{useful}}^{\text{out}}} B_{W,i}^{\text{out}} + \sum_{i=1}^{NS_{M,\text{waste}}^{\text{out}}} B_{M,\text{waste},i}^{\text{out}} + I \quad (34)$$

The second law of thermodynamics complements and enhances the energy balance by enabling evaluation of both the thermodynamic value of an energy carrier, and the real thermodynamic inefficiencies and losses of processes or systems [17].

## 3.2. Internal and external exergy loss

### 3.2.1. Internal exergy loss

Internal exergy losses, also called “irreversibility” or “exergy destruction” by Tsatsaronis [17], is deduced from the entropy generation and the environment temperature. According to the second law of thermodynamics, irreversibility is always positive.

In practice, for all real processes the exergy input always exceeds the exergy output, this unbalance is due to irreversibilities induced by the thermodynamic imperfection of process operations. The irreversibility phenomena fall in three types: non-homogeneities, dissipative processes and chemical reactions. Non-homogeneities are caused by mixing of two or more systems with different

temperature (T), pressure (P) or concentration (z). Regarding the dissipative effects, mechanical friction can be evoked. Finally, the entropy generated in chemical reactors is proportional to the advancement of the reaction and the affinity of the reaction itself defined using the stoichiometric coefficients and chemical potentials [19]. Although Table 3 is not exhaustive, it enumerates the major sources of irreversibility and gives us some clues taken from literature [2,7,20–23] for process improvement on each class of unit operation. Table 3 can be extended to cover all the unit operations especially using general commandments by Leites et al. [24] for reducing energy consumption.

### 3.2.2. External exergy loss

External exergy loss is associated with material streams rejected into the environment. For example, the flue gas emitted from a fired heater is still hot enough relative to the reference environment temperature (usually 25 °C). By definition, the exergy associated with the flue gas is called external exergy loss of the fired heater.

To see how to reduce external exergy losses, let us take an example of a reactor represented in Fig. 9. Depending on the use of the output byproduct of the reaction, external exergy losses will take different values. In the first case, output byproduct is simply emitted to environment. In this situation, output byproduct must be considered as a waste material and the absolute value of external exergy loss will be equal to the exergy associated with byproduct rejected to the environment. The exergy balance can be written as follows:

$$B_M^{\text{in}} = B_{M,\text{useful}}^{\text{out}} + B_{M,\text{waste}}^{\text{out}} + I \quad (35)$$

and

$$B_{M,\text{useful}}^{\text{out}} = B_{\text{product}} \quad (36)$$

In the second case, on the contrary, the byproduct of the reaction can be valorized in a gasifier as a fuel. In that situation, the byproduct can be considered as a useful stream and the external exergy loss for the control surface inclosing the reactor will be zero:

$$B_{M,\text{waste}}^{\text{out}} = 0 \quad (37)$$

Here, the exergy balance becomes:

$$B_M^{\text{in}} = B_{M,\text{useful}}^{\text{out}} + B_{M,\text{waste},i}^{\text{out}} + I \quad (38)$$

This simple example shows that exergy balance is highly dependent on the utilization of streams. Therefore, systematic calculation of such balances in process simulators such as ProSimPlus® requires a more precise definition of the role of the streams. There are different possible ways to exploit the exergy associated with the waste streams as addressed by Szargut et al. [7]. For example, if the temperature of the waste heat is high enough, waste heat recovery using heat exchanger networks can be an alternative. However, for the low-grade waste heat [25], heat pump [26] or absorption refrigerator [27] can be installed to exploit its physical exergy. To reduce external exergy losses associated with chemical exergy, combustible waste can be used as a fuel for combustion. Utilization of the non-combustible waste as a secondary raw material is an alternative to recuperate wasted chemical exergy [7].

## 3.3. Exergy efficiency

To perform an effective exergy analysis, it seems essential to define indicators measuring the exergetic performance of a process

**Table 3**  
Internal exergy loss and its sources.

Unit operation	Sources of irreversibility	Improvement ways
Reactor	Low conversion	Recycle the non-converted feed
	Exothermic reaction	Raise the temperature
	Endothermic reaction	Reduce the temperature
Distillation column	Temperature difference of cold feed and hot reaction medium	Pre-heating of feed
	Concentration gradients	Increase reaction stages as much as possible
	Mixing of streams	Mixing as uniform as possible
	Concentration gradients	Use intermediate reboiler
	Improper separation sequence	Equal partition of driving force
Heat exchanger	Pressure drop and mechanical friction	Optimize distillation sequencing
	Bubble-liquid mass transfer on the tray [23]	Optimize the hydraulic of the column
	Thermal gradients	Optimize the hydraulic of the column
		Introduce feed in a proper tray [20]
Cold utility	Temperature difference	Splitting feed
	Non-uniform gradient	Use as low as possible driving force
Throttling valve	Pressure drop	Use an uniform gradient
	Low heat transfer	Reduction of number of baffles
	Refrigeration	Optimize the flow velocity [7]
Steam boiler	Thermal difference	Minimize use of sub-ambient system and replace it with cooling water [21]
	Use of external utilities	Use as high level as possible
Compressor	Pressure drop	Maximize process steam generation
	A chemical reaction for oxidation of the fuel [22]	Replacement by a steam turbine (for temperature greater than the ambient)
	An internal heat transfer between high temperature product and the unburned reactant [22]	Preheating of combustion air
	A physical mixing process [22]	Use as low driving force as possible
	A diffusion process where the fuel and oxygen molecules are drawn together [22]	Mix it as uniform as possible
Steam turbine	High heat capacity of combustion products	Make it as gradually as possible
	Isobar combustion	Oxygen enrichment [2]
	Hot inlet streams	Isochoric combustion [2]
Pump	Low temperature of steam	Temperature reduction of inlet streams or between the stages by intercooler
	Hydraulic friction	Use inter-heater (e.g. super-heater) between the stages
Mixer	Temperature difference	Optimize the hydraulic of system
	Pressure difference	Isothermal mixing
	Composition difference	Isobar mixing
		Mixing as close as possible composition

and identifying the unit operations that need to be improved. In the literature, several formulations have been proposed for the exergy efficiency. The simple efficiency [28] is simply the ratio between all exergy inputs and all exergy outputs.

$$\eta_I = \frac{B_{in}^{out}}{B_{in}} = 1 - \frac{I}{B_{in}} \quad (39)$$

Although it is easy to be calculated, the simple exergy efficiency does not provide a clear vision for the cases in which the significant amount of waste (i.e. external exergy loss) is produced.

To solve this problem, coefficient of exergy efficiency taking into account external losses [29] is defined:

$$\eta_{II} = \frac{B_{in}^{out} - B_{waste}^{out}}{B_{in}} = \frac{B_{PRODUCT}}{B_{in}} = \eta_I - \frac{B_{waste}^{out}}{B_{in}} \quad (40)$$

However, this new formulation for exergy efficiency gives a valid evaluation of the performance of a system only when all the components of the incoming exergy flow are transformed to other components of exergy. For example, a hydrocarbon stream heating up in a heat exchanger where only its physical exergy changes, has a high chemical exergy which does not affect at all. In other words, the role of the heater is to heat up the hydrocarbon stream (i.e. physical exergy change) not to change its chemical composition (i.e. chemical exergy change). Although this exergy efficiency gives a value close to unity for the case of this heater, it does not mean the heater is operating perfectly. Therefore, one might deduce the transiting exergy [29] as the unchanged part of exergy which does not participate in the process. This might be the main idea to develop the intrinsic exergy efficiency [29] which deduces the transiting exergy from both the exergy input and the exergy output. However, intrinsic exergy efficiency is not only complicated, but it also does not account for the external exergy losses. Utilizable exergy coefficient [30] might be regarded as the most rigorous exergy efficiency despite its complicated calculation procedure as it can measure the energy efficiency, the waste reduction and the efficient use of raw materials.

Besides these exergy efficiencies, rational efficiency [2] is a ratio of the desired exergy output to the used exergy. It is rigorous enough to evaluate the performance of the most commonly used unit operations if their objective are precisely defined and different components of exergy of material stream (e.g. chemical, thermal and mechanical) are known.

$$\Psi = \frac{\text{Desired Exergetic Effect}}{\text{Used Exergy}} = \frac{\Delta B_{\text{desired output}}}{\Delta B_{\text{used}}} \quad (41)$$

where  $\Delta B_{\text{desired output}}$  is determined by examining the function of the system and of course does not include external exergy loss. The  $\Delta B_{\text{desired output}}$  represents the desired result produced in the system.  $\Delta B_{\text{used}}$  represents the net resources which were spent to generate the product.

The major difficulty in this type of efficiency is the evaluation of  $\Delta B_{\text{used}}$  and  $\Delta B_{\text{desired output}}$ . Contrary to the simple efficiency, it is necessary to define precisely the objective of the operation. This is not straightforward as it will be shown later. It is sometimes possible to define this objective in different ways for a single unit operation. The desired exergy output of the unit operation is defined by the user. After introducing  $B_{\text{used}}$  and  $B_{\text{desired output}}$ , the exergy balance becomes:

$$\Delta B_{\text{used}} = \Delta B_{\text{desired output}} + I + B_{\text{waste}}^{out} \quad (42)$$

Using Eq. (41) in connection with the Eq. (42), the following alternative form of the rational efficiency can also be obtained:

$$\Psi = 1 - \frac{I + B_{\text{waste}}^{out}}{\Delta B_{\text{used}}} \quad (43)$$

Eq. (42) shows that if external exergy losses and desired exergetic effect are known, the exergy balance will allow deducing the  $B_{\text{used}}$ . To illustrate this methodology, let us take the example of a two-stream heat exchanger shown in Fig. 10.



Fig. 9. External exergy loss for a reactor.

Basically the function of a heat exchanger is to change the thermal exergy of one stream at the expense of exergy change of the other stream. Let us assume the function of heat exchanger under consideration to be increase of thermal exergy of cold stream:

$$\Delta B_{\text{desired output}} = B_{\text{cold\_out}}^{\Delta T} - B_{\text{cold\_in}}^{\Delta T} \quad (44)$$

Rewriting the exergy balance around the heat exchanger considering all component of exergy, we obtain:

$$\begin{aligned} & (B_{\text{cold\_in}}^{\Delta T} + B_{\text{cold\_in}}^{\Delta P} + B_{\text{cold\_in}}^{\text{ch}}) + (B_{\text{hot\_in}}^{\Delta T} + B_{\text{hot\_in}}^{\Delta P} + B_{\text{hot\_in}}^{\text{ch}}) \\ &= (B_{\text{cold\_out}}^{\Delta T} + B_{\text{cold\_out}}^{\Delta P} + B_{\text{cold\_out}}^{\text{ch}}) \\ &+ (B_{\text{hot\_out}}^{\Delta T} + B_{\text{hot\_out}}^{\Delta P} + B_{\text{hot\_out}}^{\text{ch}}) + I + B_{\text{waste}}^{\text{out}} \end{aligned} \quad (45)$$

Separating the term that is equal to function of the unit operation, we have:

$$\begin{aligned} B_{\text{cold\_out}}^{\Delta T} - B_{\text{cold\_in}}^{\Delta T} &= (B_{\text{cold\_in}}^{\Delta P} - B_{\text{cold\_out}}^{\Delta P}) + (B_{\text{cold\_in}}^{\text{ch}} - B_{\text{cold\_out}}^{\text{ch}}) \\ &+ (B_{\text{hot\_in}}^{\Delta T} + B_{\text{hot\_in}}^{\Delta P} + B_{\text{hot\_in}}^{\text{ch}}) \\ &- (B_{\text{hot\_out}}^{\Delta T} + B_{\text{hot\_out}}^{\Delta P} + B_{\text{hot\_out}}^{\text{ch}}) \\ &- I - B_{\text{waste}}^{\text{out}} \end{aligned} \quad (46)$$

Canceling out the chemical exergy at the inlet and outlet and rearranging Eq. (45) based on the Eq. (46),  $B_{\text{used}}$  is the right side of the Eq. (47).

$$\begin{aligned} (B_{\text{cold\_out}}^{\Delta T} - B_{\text{cold\_in}}^{\Delta T}) + I + B_{\text{waste}}^{\text{out}} &= (B_{\text{cold\_in}}^{\Delta P} - B_{\text{cold\_out}}^{\Delta P}) \\ &+ (B_{\text{hot\_in}}^{\Delta T} + B_{\text{hot\_in}}^{\Delta P}) \\ &- (B_{\text{hot\_out}}^{\Delta T} + B_{\text{hot\_out}}^{\Delta P}) \end{aligned} \quad (47)$$

Then applying Eq. (41), rational exergy efficiency will be given:

$$\Psi = \frac{\Delta B_{\text{desired output}}}{\Delta B_{\text{used}}} = \frac{B_{\text{cold\_out}}^{\Delta T} - B_{\text{cold\_in}}^{\Delta T}}{(B_{\text{cold\_in}}^{\Delta P} - B_{\text{cold\_out}}^{\Delta P}) + (B_{\text{hot\_in}}^{\Delta T} + B_{\text{hot\_in}}^{\Delta P}) - (B_{\text{hot\_out}}^{\Delta T} + B_{\text{hot\_out}}^{\Delta P})} \quad (48)$$

If pressure drop is negligible, we get the traditional form of exergy efficiency:

$$\Psi = \frac{\Delta B_{\text{desired output}}}{\Delta B_{\text{used}}} = \frac{B_{\text{cold\_out}}^{\Delta T} - B_{\text{cold\_in}}^{\Delta T}}{B_{\text{hot\_in}}^{\Delta T} - B_{\text{hot\_out}}^{\Delta T}} \quad (49)$$

This example shows that for each unit operation, a function needs to first be defined to calculate the rational exergy efficiency. It means that it needs interaction of the user as always one unit operation does not have the same function. Rational efficiency needs to be defined precisely for all unit operations as listed in Table 4. In addition, rational efficiency needs a drastic breakdown of different components of exergy of material stream as chemical, thermal and mechanical.

Having reviewed the different kinds of exergy efficiencies, it can be concluded that the rational exergy efficiency is not complicated as the "exergy efficiency with transiting exergy" and is rigorous enough unlike "simple exergy efficiency". Therefore, the rational exergy efficiency has been chosen to be implemented in ProSimPlus<sup>®</sup> for an adequate exergy analysis.

#### 3.4. ProSimPlus<sup>®</sup> implementation

As pointed out in the previous section, rational exergy efficiency needs a clear function per each unit operation. In addition, the

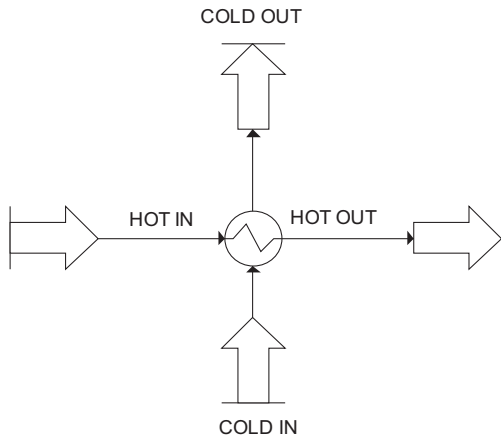
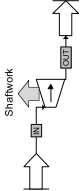
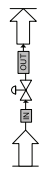
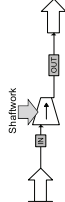
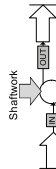
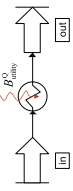
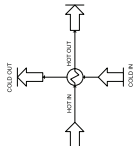
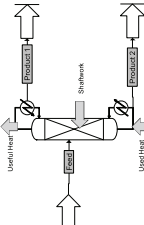


Fig. 10. Two-stream heat exchanger.

**Table 4**  
Rational efficiency for the most commonly used unit operations.

Defined by the user		Calculated	
Unit operation	Function	B <sub>Desired Output</sub>	B <sub>Used</sub>
<b>Expander</b> 	Steam turbine: Shaftwork generation in power plants	$B_{Shaftwork}$	$B_{IN} - B_{OUT}$
	Cryo-expander: Reduce temperature in cryogenic systems	$(B_{IN}^{AT} - B_{OUT}^{AT}) + B^O + B_{Shaftwork}$	$B_{IN}^{AP} - B_{OUT}^{AP}$
<b>Throttling valve</b> 	Reduce pressure of steam in power plants	—	$B_{IN} - B_{OUT} = 0$
	Reduce temperature in cryogenic systems	$B_{IN}^{AT} - B_{OUT}^{AT}$	$B_{IN}^{AP} - B_{OUT}^{AP}$
<b>Compressor</b> 	Adiabatic: Increase of exergy	$B_{OUT} - B_{IN}$	$B_{Shaftwork}$
	Non-adiabatic: Increase of pressure	$B_{OUT}^{AP} - B_{IN}^{AP}$	$B_{Shaftwork}$
<b>Pump</b> 	Increase of pressure	$B_{OUT}^{AP} - B_{IN}^{AP}$	$B_{Shaftwork}$
	Heating or cooling by utilities	$B_{OUT} - B_K$	$B_{Utility}^O$
<b>Heater or cooler</b> 	Heating	$B_{cold\_out}^{AT} - B_{cold\_in}^{AT}$	$B_{hot\_in} - B_{hot\_out} + (B_{cold\_in}^{AP} - B_{cold\_out}^{AP})$
	Cooling	$B_{hot\_in}^{AT} - B_{hot\_out}^{AT}$	$(B_{cold\_out} - B_{cold\_in}) + (B_{hot\_in}^{AP} - B_{hot\_out}^{AP})$
<b>Two-streams heat exchanger</b> 	Heating	$B_{cold\_out}^{AT} - B_{cold\_in}^{AT}$	$B_{hot\_in} - B_{hot\_out} + (B_{cold\_in}^{AP} - B_{cold\_out}^{AP})$
	Cooling	$B_{hot\_in}^{AT} - B_{hot\_out}^{AT}$	$(B_{cold\_out} - B_{cold\_in}) + (B_{hot\_in}^{AP} - B_{hot\_out}^{AP})$
<b>Separator</b> 	Separation of product 1 and 2 from feed	$B_{Product\ 1} + B_{Product\ 2} - B_{Feed}$	$B_{Used\ Heat} + B_{Shaftwork}$
	Production of a special product	$B_{product}^{sh} - B_{feed}^{sh}$	$B_{O_{endothermic}}$



waste streams should be specified. Having known the function of the unit operation and waste streams, the  $\Delta B_{\text{used}}$  can be calculated based on the exergy balance around the given unit operation. Therefore, to implement rational exergy efficiency a semi-automated way has to be followed as shown in Fig. 11. As a first step a zone is defined by the user. Then, the simulator automatically provides us with a table (see Table 5) as well as exergy of all streams. Next, the role of each stream (waste vs. useful) is defined by the user in the table given by ProSimPlus®. However, ProSimPlus® can consider all the output streams as waste streams by default. Then the user can change it to the useful. Finally, the process simulator can provide the necessary criteria for analysis such as rational exergy efficiency. To facilitate calculation of the rational exergy efficiency, the desired exergy effect can be automated and embedded in ProSimPlus® for the most commonly used unit operations. In addition, for units which do not have always the same function, a set of possible efficiencies can be proposed by ProSimPlus® which will be finally chosen by the user.

#### 4. Case study

To show the applicability of exergy analysis for energy optimization of a chemical or thermal process in ProSimPlus®, a simple process found in the literature [4] has been enriched and analyzed.

##### 4.1. Process description

Fig. 12 represents ProSimPlus® flowsheet for a stabilization train of natural gas containing traces of oil [4]. To satisfy the specification of marketing, natural gas needs to be stabilized. In this process, the natural gas (C1 to C8 hydrocarbons) is separated into a stabilized condensate (C4 to C8 hydrocarbons) and a saleable gas (C1 to C4 hydrocarbons). As the amount of natural gas in our case is not so high, a full Natural Gas Liquid (NGL) recovery train is not economically justifiable and the simple stabilization scheme shown in the right section of Fig. 12 is chosen [4].

Along of this process, a rich gas is heated in three heaters followed by separators (F101, F102 and F103) where the inlet gas streams are flashed. At each step, the outlet liquid stream is sent to the next flash where the pressure is reduced further. The liquid stream from the last flash is the stabilized condensate. On the other hand, the outlet gas streams from all of the separators (F101, F102 and F103) are mixed together with same pressure to obtain a stabilized gas product stream with the desired specifications [4].

To meet heating requirement of the process, a relative high pressure (HP) steam at 10 bar with 80 °C degree of superheat for all three separation stages is used as shown in Fig. 13. The process streams are heated up by the steam condensation in heat exchangers and condensate is throttled down to 3 bar. The condensate is returned at 3 bar and is mixed with the boiler water makeup to feed the steam boiler. Note that a small portion of steam at 10 bar is used in the deaerator to separate air from return-condensate. As well as steam heating, electricity is required to drive the compressors (C101 and C102) at the second and third stages of stabilization where pressure drop causes the flash separation. The required electricity for the base case is imported from the external electricity grid.

##### 4.2. Simulation

All the required data and specifications for the simulation of the process and the utility system are given in Tables 6–8. As reported in Table 7, the outlet temperature of heater E101, E102 and E103 has to be fixed at 68, 124 and 134 °C. Therefore, splitting ratio of the splitter distributing the steam among the three heaters, and water make-up flowrate will be varied to obtain a converged simulation. In addition, to keep the flue gas temperature equal to 200 °C (higher than the acid dew point), the fuel flowrate will be varied.

To calculate the thermodynamic properties, two different thermodynamic models are defined:

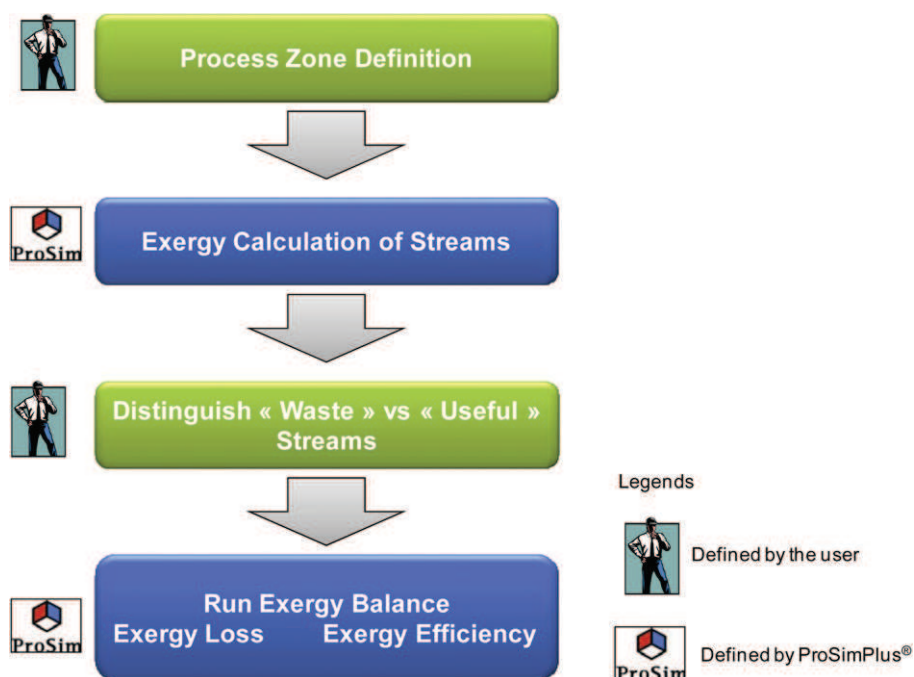


Fig. 11. Exergy balance procedure in process simulator.

**Table 5**

A typical table given by the exergy assistant in ProSimPlus® to distinguish waste vs. useful streams.

Parameter	Stream Type	Stream Name	Unit Operation	Total Exergy (MW)	Chemical Exergy (MW)	Physical Exergy (MW)	Thermal Exergy (MW)	Mechanical Exergy (MW)	Useful	Waste	Desired Exergetic Effect		
											Chemical Exergy (MW)	Thermal Exergy (MW)	Mechanical Exergy (MW)
Input	Material	Feed	Process Feed	306.66	301.63	5.03	1.61	3.42			-		
	Work	W	Compressor	1.68									
	Heat	Q	Heater	3.66									
	Total Input (MW)				312.00								
Output	Material	Liquid Product	Separator	86.65	80.63	6.02	2.34	3.68	√		+		
	Material	Gas Product	Separator	221.90	215.56	6.34	1.36	4.98	√		+		
	Work	—	—	0					0	0			
	Heat	—	—	0					0	0			
	Total Output (MW)				308.55					308.55	0		
Loss	External Exergy Loss (MW)			0	0	0	0	0					
	Internal Exergy Loss (MW)			3.45									
Efficiency	Simple Exergy Efficiency			0.99									
	Rational Exergy Efficiency			0.37									

- The Peng–Robinson equation of state: for the NGL process and the fuel combustion sections.
- The water specific thermodynamic model: for simulation of the utility system.

Note that in this case study, heat losses to the environment has been neglected.

### 4.3. Exergy analysis

By offering the possibility to make automatic calculation of exergy of material and heat streams and to present the result of exergy balance in different forms such as pie or bar diagram for the given process or utility zone in an automated way, ProSimPlus® simulator facilitates exergy analysis on the process [31].

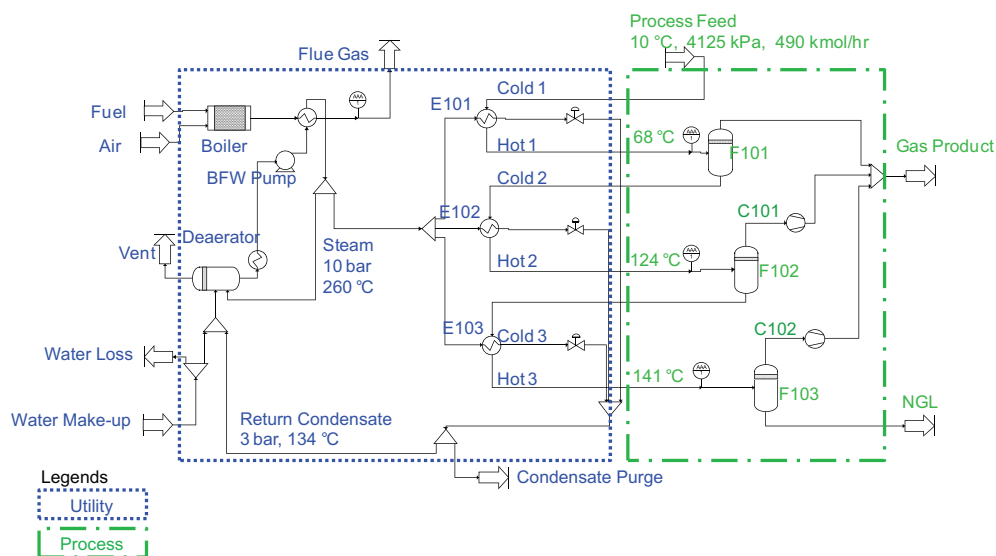
As demonstrated earlier, the exergy analysis requires the definition of the utilization of streams (i.e. waste or useful) by the user. In this case study, all the material streams leaving the process are useful whereas all the material output streams in the utilities system are considered as waste streams as they are directly rejected

into the environment. As a consequence, in this specific case study, external exergy loss will only be associated with the utility system.

#### 4.3.1. Internal/external losses

By representing the external and internal exergy losses occurring in each of the unit operations on a bar diagram (see Fig. 14), one can identify technical solutions to improve the performances of the process. While the internal exergy losses (or irreversibilities) can be reduced through development of the process or technology improvement, reduction of external exergy losses requires a thermal, mechanical and chemical treatment of effluents.

As can be seen in Fig. 14, the largest irreversibilities occur in the steam boiler. Intrinsic irreversibility due to the combustion is unavoidable; however, according to Table 3 solutions exist to reduce the internal exergy loss such as preheating of combustion air through an economizer. The second-largest irreversibility occurs in the heat exchanger network because of the large temperature difference between hot and cold streams. As listed in Table 3, to reduce exergy losses, as low as possible driving force between the hot (steam) and cold (process) streams have to be used. In addition,



**Fig. 12.** Natural gas stabilization.

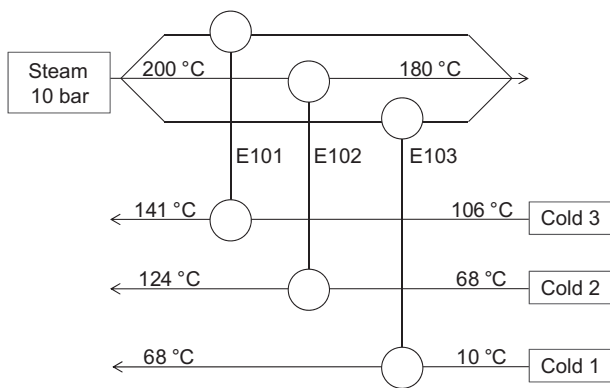


Fig. 13. Grid diagram of heat exchanger network for the base case.

throttling valves cause relatively high irreversibilities that could have been easily avoided by their replacement with steam turbines as reported in Table 3.

The external exergy losses associated with the steam boiler is due to its flue gas. To reduce this external loss chemical recuperation of flue gas [32] can be applied. To exploit the thermal component of exergy of hot streams such as the vent of dearetor and condensate purge, a waste heat exchanger might be a solution.

Exergy analysis of this flowsheet has so far identified and quantified the available thermal energy in a process that could have been potentially exploited to meet energy demands elsewhere on the process or even on the industrial site. At this point, however, exergy analysis cannot deal with the energy integration of the process. Coupling of exergy analysis with a pinch analysis [33] could be helpful to provide solutions relevant to the reduction of exergy losses in the process.

#### 4.3.2. Exergy efficiency

Figs. 15 and 16 represent the simple and the rational exergetic efficiencies of each unit operation. Whereas simple exergy efficiencies are very easy to calculate (see Eq. (39)), a desired exergetic effect has to be defined for calculation of rational exergy efficiency. For example, the major desired exergetic effect for the three heaters is to heat up the process streams. Concerning the NGL process as a whole, its desired effect relies on the chemical exergy change between input and output. The part of chemical exergy which remains unchanged between the input and the outputs of the process is not included in the rational exergetic efficiency calculation. As shown in Fig. 15, the simple exergy efficiency is quite restrictive for this case where the major part of exergy input consists in the chemical exergy which remains unchanged. As can be seen from comparison between Figs. 15 and 16, rational exergy efficiency is much more informative. Fig. 15 shows that most units

Table 6 Specifications and variables of action for the base case.

Specification	Variable of action
Outlet temperature of heater E101 = 68 °C	Splitting ratio of the splitter 1 and 2
Outlet temperature of heater E102 = 124 °C	Splitting ratio of the splitter 1 and 2
Outlet temperature of heater E103 = 134 °C	Water makeup flowrate
Flue gas temperature = 200 °C	Fuel flowrate

Table 7 Composition of feed.

Compound	Mole fraction
Methane	0.316
Ethane	0.158
Propane	0.105
<i>i</i> -Butane	0.105
<i>n</i> -Butane	0.105
<i>i</i> -Pentane	0.053
<i>n</i> -Pentane	0.053
<i>n</i> -Hexane	0.027
<i>n</i> -Heptane	0.026
<i>n</i> -Octane	0.026
<i>n</i> -Nonane	0.026

operations are operating with efficiency close to unity, but rational exergy efficiency in Fig. 16 gives a real thermodynamic picture by presenting the imperfection occurring in the unit operations. The units which suffer from thermodynamic imperfection can be identified and improved to obtain a better performance. For example, comparing the heater E101, E102 and E103, the lowest rational exergy efficiency belongs to heater E101 where a relative high pressure steam is used to heat up the process stream of the first stage. Working with a low pressure steam can significantly reduce irreversibility by reduction of minimum approach temperature.

The advantage of analysis of exergy efficiencies rather than the exergy losses relies on the possibility to quantify the potential for improvement of each unit operations [34]: the lower exergy efficiency, the higher will be the potential for improvement. For example, although BFW pump has the same exergy efficiency as E103, its small exergy losses do not justify its revamping for exergy loss reduction. On the other hand, E101 has lower exergy efficiency, but it has higher exergy losses which means its small potential for improvement can finally reduce significantly the total exergy losses.

Comparing the absolute exergy losses with exergy efficiency, the order of unit operations is different. In addition, two unit operations with the close exergy efficiency can have different exergy losses. For example, exergy efficiency of BFW Pump is the same of E103, but it has 0.5 kW exergy losses which is very small compared to E103 with 36.6 kW exergy losses. This is mainly due to the properties of flow coming into and out of the given unit operation such as temperature, pressure, composition and flowrate. As boiler feed water in the liquid state does not carry high quantity of exergy, 73% exergy efficiency cannot cause significant exergy losses. On other hand, exergy input of E103 is very high as the high exergetic steam (relative high pressure and temperature) are entering into the E103. Therefore, 73% exergy efficiency for E103 causes 36.6 kW exergy losses.

Table 8 Input data for simulation of process.

Feed conditions	10 °C and 4125 kPa
Outlet temperature of Heater E101	68
Outlet temperature of Heater E102	124
Outlet temperature of Heater E103	134
Feed flowrate	490 kmol/h
Stage 1 pressure drop	0 kPa
Stage 2 pressure drop	2075 kPa
Stage 3 pressure drop	1700 kPa
Gas Product pressure	4125 kPa
C101 adiabatic efficiency	75%
C102 adiabatic efficiency	75%

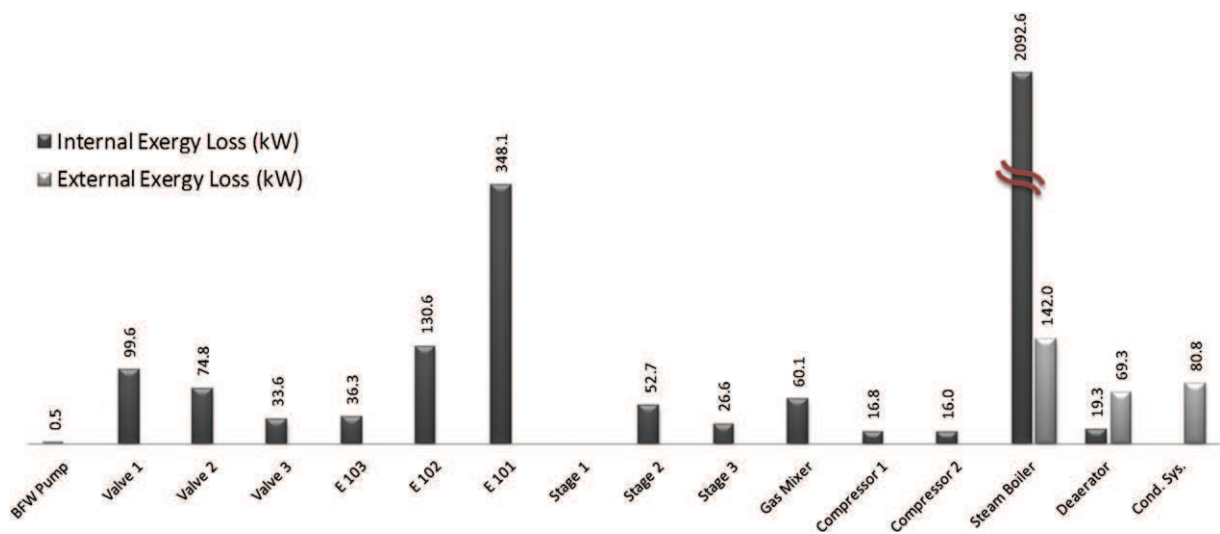


Fig. 14. Internal and external exergy losses (kW) for the base case.

#### 4.3.3. Proposal of a retrofit scheme

Having pinpointed the sources of exergy losses, the next step consists in determining a retrofit scheme based on the analysis of sources of irreversibilities. Although external exergy losses contribute in total exergy losses as well as internal exergy losses, reduction of internal exergy losses which originate from the heart of thermal and chemical process can consequently reduce external exergy losses. In other word, if the internal exergy losses are reduced, consequently the external exergy losses will be reduced as well.

The analysis of Fig. 16 permits to identify the less efficient unit operations that need to be improved:

- *Steam boiler*: Preheating of combustion air though an economizer as pointed out earlier.
- *Compressor*: Although the temperature reduction of inlet stream can reduce exergy losses (see Table 3), there is a risk of condensation of natural gas liquid in the compressor.

Therefore, the temperature of inlet stream has to be kept as it is in the base case.

- *Heat exchanger*: To reduce its irreversibilities, it is necessary to reduce the driving force between hot and cold stream. For obvious reasons, the process streams cannot be modified; thus, it is decided to reduce the inlet temperatures of the steam by its expansion. For that purpose, steam turbines are preferred over the simple expanding valves as the steam turbines can provide the required shaft power for stages 2 and 3. To keep the steam hot enough to meet the heating demand of the process, the steam is expanded to 4.5 bar for the last stage and 3 bar for the first and second stages. Note that compared to the base case, the degree of superheat of steam generated by the boiler, is fixed to be 80 °C to avoid the steam condensation in the steam turbine which can damage the machine.

The improved configuration of the process and its grid diagram are presented in Figs. 17 and 18. To simulate the modified flowsheet,

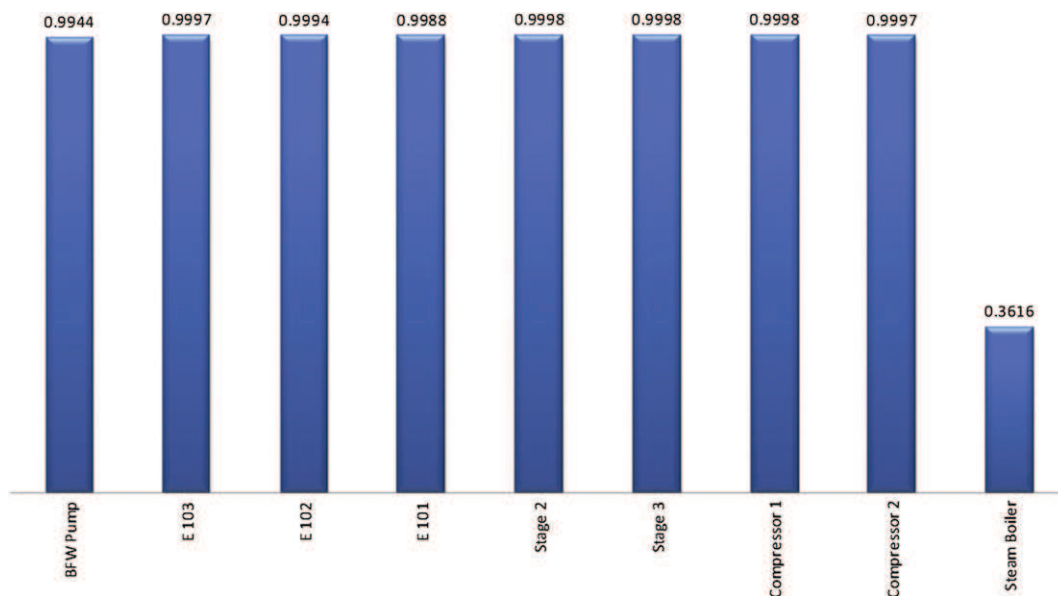


Fig. 15. Simple exergy efficiency for unit operations.

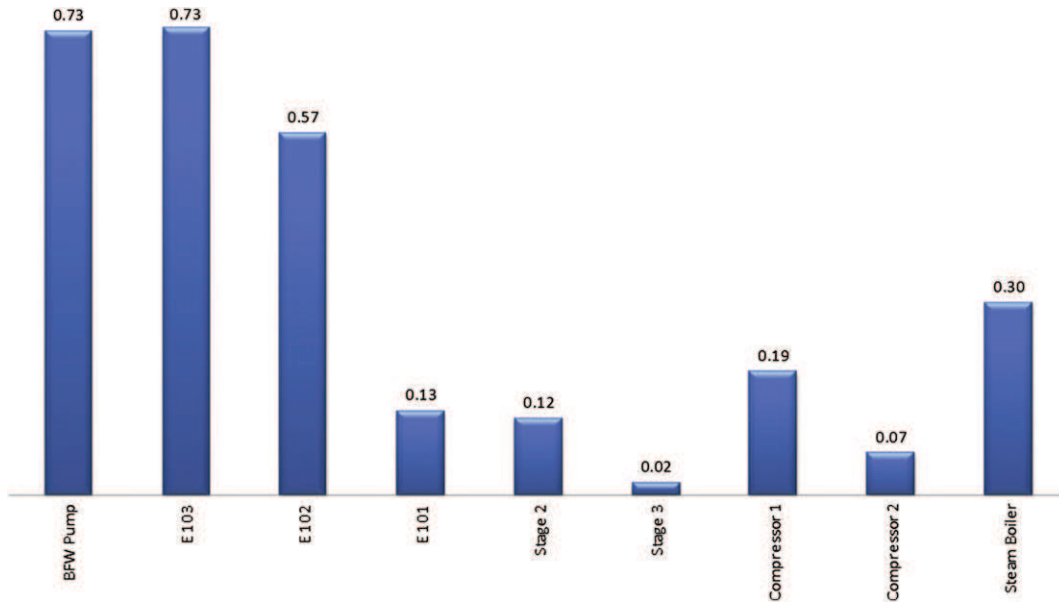


Fig. 16. Rational exergy efficiency for unit operations.

as reported in Table 7, the outlet temperature of process streams in heater E101, E102 and E103 has to be fixed to 68, 124 and 134 °C. Therefore, splitting ratio of the splitter 1 and 2 distributing the steam among the heaters, and water make-up flowrate will be modified by the simulator. In addition to keep the flue gas temperature equal to 200 °C (higher than the acid dew point), the fuel flowrate will be modified as listed in Table 6.

Table 10 shows that use of low-pressure steam for heating reduces both fuel and water demand while increases cogeneration potential as more latent heat can be taken from the condensation of steam in the lower pressure. As listed in Table 9, performance improvement of the integrated process is noticeable based on several criteria which makes analysis of the process very complex. To fill this gap and facilitate further optimization of the process, the rational exergy efficiency proposes an aggregated criterion including all the aspects listed in the Table 9. As the process cannot undergo any modification, therefore it is left out of the optimization. The exergy efficiency will be defined only for the utility system where the 'desired effect' of the utility can be defined as heating of the three process streams (Cold 1, Cold 2 and Cold 3) and production of shaft power required for compression of the streams coming out of stages 2 and 3:

$$\Psi = \frac{\left( B_{\text{Cold 1}}^{\Delta T} - B_{\text{Hot 1}}^{\Delta T} \right) + \left( B_{\text{Cold 2}}^{\Delta T} - B_{\text{Hot 2}}^{\Delta T} \right) + \left( B_{\text{Cold 3}}^{\Delta T} - B_{\text{Hot 3}}^{\Delta T} \right) + W_{\text{Turbine}}}{B_{\text{Fuel}} + B_{\text{Water Make-up}} + W_{\text{Pump}} - \left( B_{\text{Flue Gas}} + B_{\text{Vent}} + B_{\text{Water Loss}} + B_{\text{Condensate Purge}} \right)} \quad (50)$$

where the underlined terms in the nominator represent the process, and the rest is standing for the utility system. The desired exergetic effect is taken to generate shaft power and heat up the process streams at the expenses of exergy supplied by the difference between input material (i.e. fuel of steam boiler, water make-up, required shaft power of pump) and effluents (i.e. flue gas, vent, water loss and condensate purge). As noted earlier, this term

includes the excess shaft power available for the electricity grid, the consumption of all natural resources (e.g. fuel, water) and the wastes rejected to the environment (e.g. flue gas, steam vent) in a single criterion which is useful for analysis of performance of the system as a whole.

#### 4.4. Estimation of the capital cost of the retrofit schemes

Reducing the provided stream pressure necessarily results in a reduction of the minimum temperature approach and of course an increasing of the required surface area of heat exchangers E101, E102 and E103. To complete the analysis of the process, estimation the capital cost (CAPEX) of heat exchanger network (HEN) as a function of surface area needs to be performed. For that study, the costing law proposed by Hall et al. [35] has been adapted:

$$\text{Cost(USD)} = 30800 + 750A^{0.81} \quad (51)$$

where A represents total heat transfer area. To use this costing law it is assumed that plant life is 6 years and capital interest is 10% per year. The heat exchangers are assumed to be made of carbon steel and operate under 10 bar in both sides of shell and tube.

Note that use of ProSimPlus® simulator permits to implement very easily the cost calculation. The use of another law more relevant for the considered case study would not be difficult to be implemented.

Using Eq. (51), investment cost of economizer will be 32 822.32 USD. Taking into account a profit from fuel saving, the installation of economizer results in 22% return on investment.



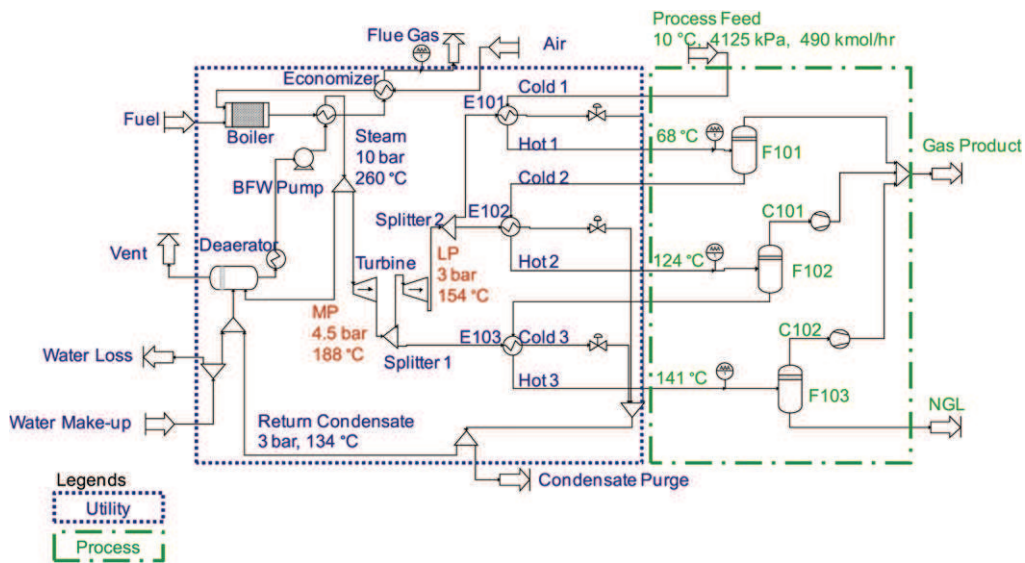


Fig. 17. Improved process & utility flowsheet.

#### 4.5. Sensitivity analysis for exergetic optimization of the process

As shown earlier, to reduce the exergy losses occurring in the steam distribution system, throttling valves have been replaced by steam turbines. The exhaust pressure of steam turbine have been fixed arbitrary to 4.5 and 3 bar to keep the steam hot enough to meet the heating demand of the process. The choice of steam levels in the design of utility systems is critical to ensure cost-effective generation of heat and power, and its distribution to the process. In a new design, pressures of steam levels can be readily optimized.

The results of a sensitivity analysis of the rational exergy efficiency and capital cost with the exhaust pressures of steam turbines are presented in Figs. 19 and 20. When fixing medium pressure (MP) steam level, the decrease of low pressure (LP) steam level results in an increase of the rational exergy efficiency: indeed in these conditions, the shaft power increases and the fuel demand decreases. The lower pressure of LP steam level, the higher is the potential for steam to be expanded in the turbine for power generation. In addition, the lower pressure the higher will be the latent heat taken from condensation of steam, consequently less

fuel is required to be fed to the steam boiler. As shown in Fig. 19 the rational exergy efficiency has the same trend when pressure of MP steam changes under the fixed conditions of LP steam main. Furthermore, as a consequence of pressure reduction, temperature of steam is reduced which leads to less minimum temperature approach in heat exchangers. Consequently, more area is required to exchange the fixed amount of heat which finally leads to higher capital cost of the heat exchangers.

As shown in Figs. 19 and 20, both HEN cost and rational exergy efficiency are more sensitive to the pressure of LP steam level compared to the MP steam level due to use of LP steam in two out of the three stages. Therefore, minimum and maximum limit for LP steam main as a variable of optimization should be chosen with more precaution.

Note that this sensitivity analysis serves as a necessary step to create the required data for construction of Pareto frontier curve which will be used in an exergetic optimization described in the following section.

#### 4.6. Bi-criteria optimization

In addition to the sensitivity analysis and due to the difficult interpretation of some results in rational exergy efficiency (Fig. 19) in terms of steam levels, a bi-criteria optimization task has been performed by ProSimPlus<sup>®</sup> to offer a decision support in retrofitting steps. However, it should be kept in mind that for retrofitting of existing systems, opportunities to change the steam level conditions are limited. The mechanical limitation for the steam mains limits a significant increase in steam pressure. Indeed, long term investment with a proper optimization of the steam levels may be economically viable, in spite of the fact that the short term investment cannot be justified [21].

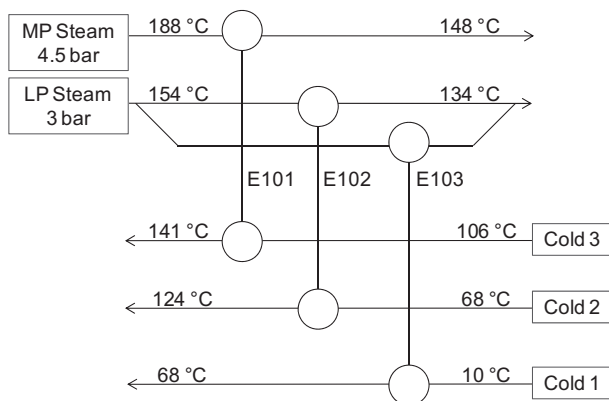


Fig. 18. Grid diagram of heat exchanger network for the retrofit scheme.

Table 9  
Input data for simulation of utility.

Stack temperature	200 °C
Degree of superheat of HP steam	80 °C
Temperature of return condensate	134 °C
Pressure of return condensate	3 bar
For revamped case: steam turbine isentropic efficiency (stage 1 and 2)	75%



**Table 10**

Comparison of performance of the base case and integrated retrofit configurations.

	Fuel demand (kg/hr)	Water makeup (t/hr)	Degree of superheat of steam from boiler	Electricity requirement	Internal exergy losses (MW)	External exergy losses (MW)
Base case	224.6	1.03	20 °C	191 (kW)	3.007	0.292
Retrofit	220.1	0.63	80 °C	0	2.628	0.170

#### 4.6.1. Optimization framework

In this study, optimization tool of ProSimPlus® is used to perform a bicriteria (exergetic efficiency/investment cost) optimization. The details of the optimization model are as follows:

**4.6.1.1. Objective function.** The purpose is to maximize the exergetic efficiency calculated by Eq. (50) and minimize the HEN cost calculated by Eq. (51). It should be noted that minimizing the HEN cost does not correspond to minimum overall cost of utility systems. However, it is extremely difficult to generalize the capital investment to be required in the conceptual stage of process design, and the current study focuses on the maximizing exergy efficiency for the utility systems, which provides sufficient information and reliable guidance for achieving an effective design in the later stage of detailed design. Two steam mains (MP and LP) are used in the current optimization model based on the needs and operating characteristics on the plant. An  $\epsilon$ -constraint procedure is carried out and a Pareto frontier curve [36] is constructed for support of decisions making.

**4.6.1.2. Model constraints.** In order to maintain feasibility of heat recovery across steam mains, a set of constraints is needed.

Temperature of all hot streams (steam) should be always greater than temperature of all cold streams (process) as follows:

$$T_{LP \text{ Steam(in)}} - T_{Hot 1} \geq 10 \quad (52)$$

$$T_{LP \text{ Steam(in)}} - T_{Hot 2} \geq 10 \quad (53)$$

$$T_{MP \text{ Steam(in)}} - T_{Hot 3} \geq 10 \quad (54)$$

$$T_{LP \text{ Steam(out)}} - T_{Cold 1} \geq 10 \quad (55)$$

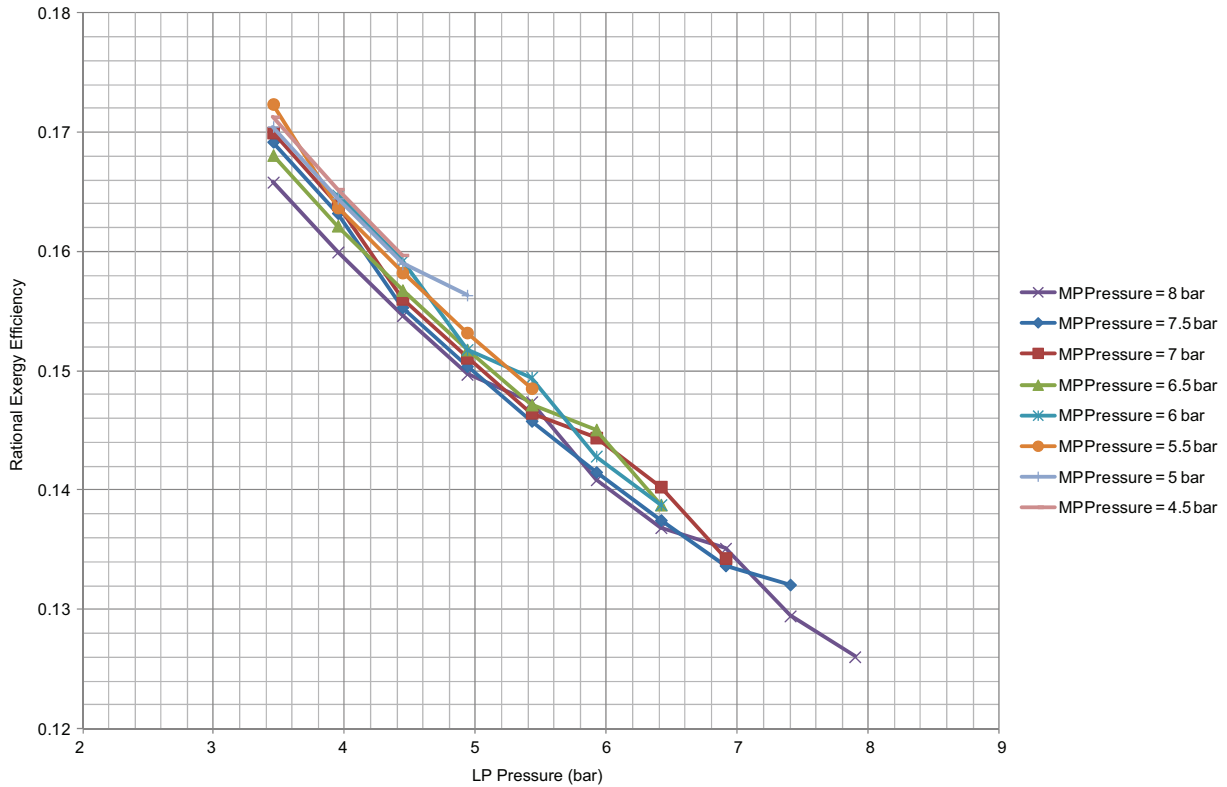
$$T_{LP \text{ Steam(out)}} - T_{Cold 2} \geq 10 \quad (56)$$

$$T_{MP \text{ Steam(out)}} - T_{Cold 3} \geq 10 \quad (57)$$

Obviously, the exhaust pressure of second stage of turbine should be lower than the first stage:

$$P_{MP \text{ Steam(in)}} - P_{LP \text{ Steam(in)}} > 0 \quad (58)$$

**4.6.1.3. Equality constraints.** The utility system has only one equality constraint which is to fix the flue gas temperature to a temperature higher than the acid dew point (473 K).

**Fig. 19.** Rational exergy efficiency.

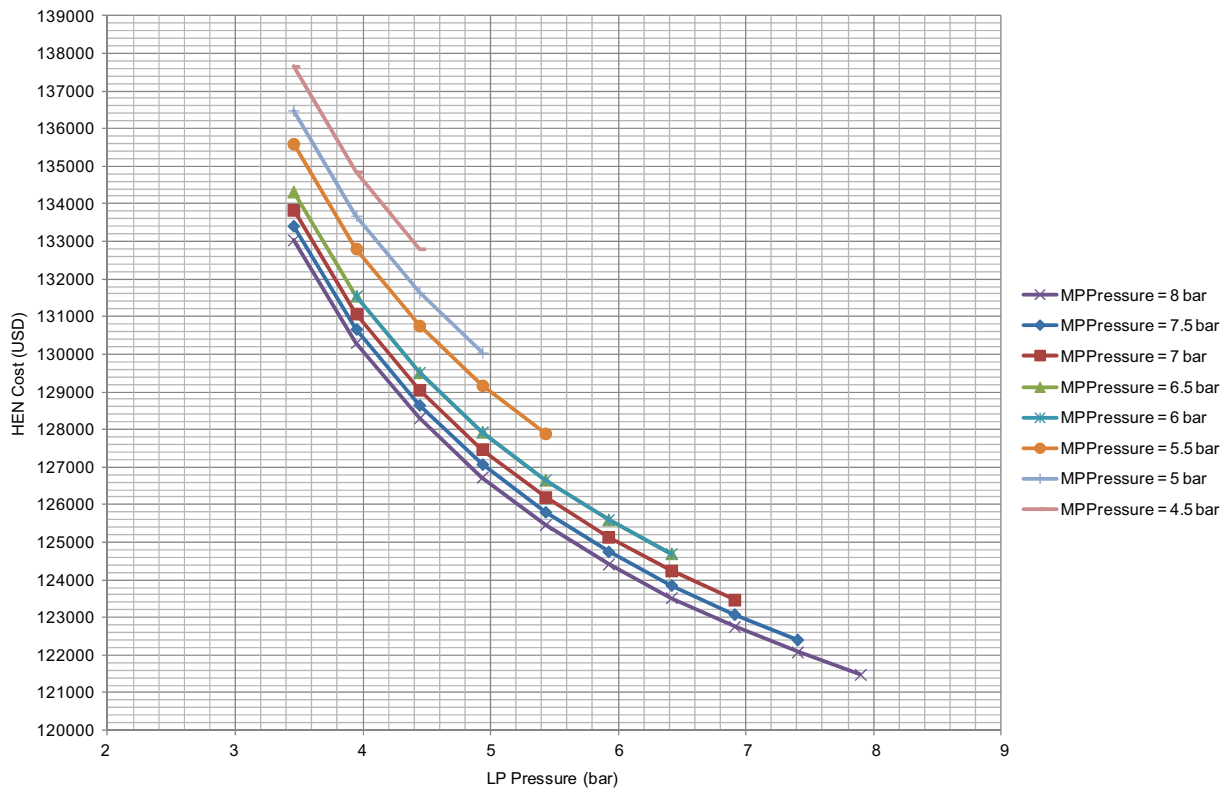


Fig. 20. HEN cost (USD).

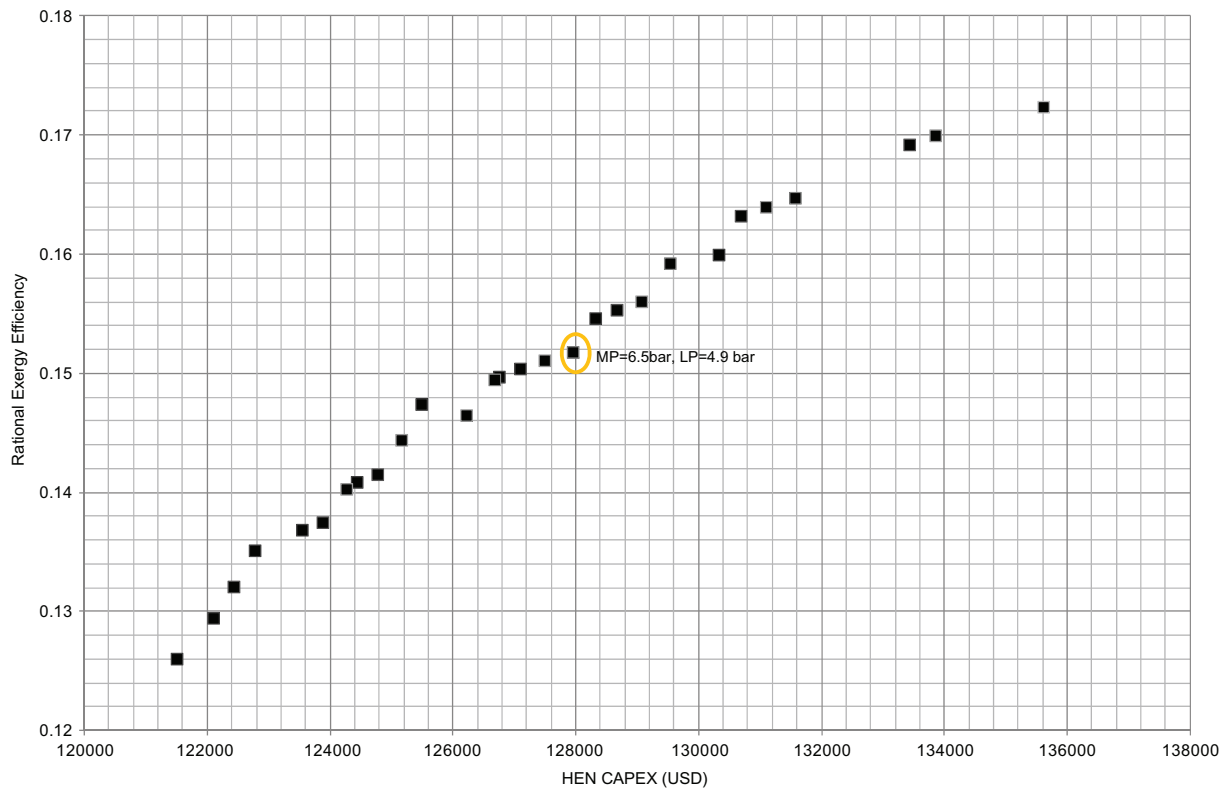


Fig. 21. Pareto frontier curve.

$$T_{\text{FLUE GAS}} = 473 \quad (59)$$

The process streams have to be heated enough to make separation of NGL possible from the natural gas. The feed entering into the first separator (F101), the stabilized gas coming from the second separator (F102) and the third separator (F103) have to be heated up to 341, 397 and 414 K.

$$T_{\text{Hot 1}} = 341 \quad (60)$$

$$T_{\text{Hot 2}} = 397 \quad (61)$$

$$T_{\text{Hot 3}} = 414 \quad (62)$$

#### 4.6.2. Results

The Pareto frontier curve is shown in Fig. 21. It exhibits all the non-dominated points, i.e. the points where the exergy efficiency cannot increase without an increase in capital cost. Then, the decision maker is able to choose the "solution" in this Pareto frontier curve. A maximum value of capital cost can be put and then the maximum expected exergy rational efficiency can be deduced. Alternatively, efficiency can be targeted and then the minimum available capital cost to achieve the target can be deduced. Therefore, this kind of representation based on cost and exergy calculations in the process simulator constitutes the first steps of a decision support system for plant retrofitting. For example, as listed in Table 11, for available capital cost of 127 940 USD, maximum exergy efficiency that can be achieved is 0.15 which corresponds to 6.5 and 4.9 bar for pressure of MP and LP steam mains. Other key data such as fuel demand, water makeup, splitting ratio for Splitter 1 and Splitter 2 are listed in Table 11.

#### 4.7. Conclusion of the case study

In the base process flowsheet, the pressure component of the exergy was simply destroyed in throttling valve to meet the required steam pressure on process-utility heat exchangers. Among a number of unit operations, exergy analysis as a scoping and screening tool identifies quickly the sources of inefficiency occurring in the system. Then, the expertise of the user and exergy assistant can come together to find a way to exploit the mechanical component of exergy by expanding the steam in the steam turbine. This is not of course the case for all the ways of improvement on the flowsheet where several alternatives can be taken into account. Even for our study, exhaust pressure of steam turbine can be fixed with trading-off between the capital cost of heat exchanger and rational exergy efficiency.

Moreover, through this case study it has been shown that based on exergy as a universal value, a comprehensive meaningful criterion can be defined to include the most important process and utility variables. The exergy efficiency not only include operating cost but also environmental aspects including in the external exergy losses (waste streams including emitted CO<sub>2</sub> as well as fuel

and fresh water). Moreover, contrary to a traditional operating cost, it does not depend on the actual market prices.

## 5. Conclusion

This papers has presented a methodology which has been become a part of ProSimPlus<sup>®</sup> to perform exergy balance like the traditional enthalpy balance, without further needs to any external subroutines interacting with process simulators. The applicability of the new exergy calculator has been illustrated through a case study. This tool does not only provide the user with necessary exergetic criteria to pinpoint the source of exergy losses, but it also helps the user to find a way to reduce the exergy losses by the guidelines listed in panel of solutions. Ultimately, each case study tackled with ProSimPlus<sup>®</sup> will enable to enrich these guidelines. Moreover, integration of exergy in ProSimPlus<sup>®</sup> can allow performing exergetic optimization in which exergy efficiency is used as a criterion.

In addition, exergy analysis which pinpoints the sources of inefficiency in the given system, can serve as a preliminary step for defining the set of hot and cold streams for thermal pinch analysis which ultimately screens streams for maximum heat recovery. As shown through a recent case study on a pulp and paper process [33], exergy analysis and pinch analysis can be combined in a sequential strategy. First, exergy analysis permits to obtain a diagnosis of the existing process and suggests technical ways to improve the process. Depending on the contribution of thermal exergy losses compared with other exergy components, the streams can become hot or cold streams for pinch analysis. Then, starting from the list of hot and cold streams, pinch analysis proposes different solutions to reduce the energy consumption. Finally, calculation of the exergetic efficiency of the different retrofit options can help the process manager to choose the one which is more likely to yield the greatest benefits. This combined approach and its implementation in ProSimPlus<sup>®</sup> is currently under development at the Laboratoire de Génie Chimique and will be subject of a future contribution.

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**Table 11**

A typical data automatically given by ProSimPlus<sup>®</sup> for a point in Pareto frontier curve.

MP pressure (bar)	6.5
LP pressure (bar)	4.9
Fuel demand (kg/s)	46.9
Water makeup (kg/s)	7.8
Splitting ratio for Splitter 1	0.83
Splitting ratio for Splitter 2	0.57
Rational exergy efficiency	0.15
HEN CAPEX (USD)	127 940

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