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General Methodology for Exergy Balance in a Process Simulator

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Abstract

This paper presents a general methodology for exergy balance in chemical and thermal processes in order to be integrated in a process simulator. In this work, as well as using the general expressions for heat and work streams, a new general expression for calculating exergy of material stream in process simulators has been developed. The applicability of the computer-aided exergy balance in a ProSimPlus[®] is shown through a simple scheme of Natural Gas Liquids (NGL) recovery process from raw natural gas.

Keywords: Exergy, Process design, Process integration, Process simulator

1. Introduction

In the context of sustainable development, energy issue is one of the major problems. Therefore, optimization of process energetic efficiency appears to be a challenging task for industries and society. In order to tackle this challenge, exergy analysis has been shown by Kotas (1985) to be a useful tool as it considers the idea of energy quality to quantify the portion of energy that can be practically recovered. The energy quality is synonym with the capacity of a given form of energy to cause changes in a process. The most natural and convenient standard as a measure of the energy quality is called exergy (Kotas, 1985). 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. All these will be presented in the following sections.

2. Exergy Calculation

2.1. Exergy of Material Stream

According to Szargut *et al.* (1988) exergy of a material stream is defined as “*the amount of work obtainable 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 abovementioned components of nature*”. Exergy of material stream is calculated with respect to a Reference Environment (RE), defined by temperature T^{00} , pressure P^{00} and composition \mathbf{z}^{00} of Reference Substances (RS). In this study, the widely accepted RE defined by Szargut *et al.* (1988) is used. The total exergy of a material stream is the sum of chemical exergy and physical exergy.

2.1.1. Physical Exergy

According to Kotas (1985) physical exergy is defined as “the maximum amount of work obtainable when a given system is brought from its *process state* (P, T, \mathbf{z}) to the *environmental state* ($P^{00}, T^{00}, \mathbf{z}$)”. With reversible heat transfer (q_{rev}) the reversible work (w_{rev}) delivered by the Module PHYS shown in figure 1 is equal to the molar physical exergy of the material stream (b^{ph}). A combination of the First & Second Laws of Thermodynamics leads to the following expression for the physical exergy:

$$b^{ph} = -w_{rev} = h(T, P, \mathbf{z}) - T^{00} s(T, P, \mathbf{z}) - [h(T^{00}, P^{00}, \mathbf{z}) - T^{00} s(T^{00}, P^{00}, \mathbf{z})] \quad (1)$$

2.1.2. Chemical Exergy

According to Kotas (1985) chemical exergy is defined as “the maximum work obtainable when a given system is brought from *environmental state* ($P^{00}, T^{00}, \mathbf{z}$) to the *standard dead state* ($P^{00}, T^{00}, \mathbf{z}^{00}$)”. To calculate exergy of a material stream with respect to a specified RE, the properties of the material stream (Process Substances PS) must be referred to the properties of the environment (Reference Substances RS) (Szargut *et al.*, 1998). Applying the mass conservation together with the First & Second Laws of Thermodynamics for the Modules CHEM I & II (see figure 2), the following expression for chemical exergy of the material stream (b^{ch}) can be derived:

$$b^{ch} = -w_{rev} = h(T^{00}, P^{00}, \mathbf{z}) - T^{00} s(T^{00}, P^{00}, \mathbf{z}) - \sum_{j=1}^{N_{RS}} \left(\frac{n_j}{n_{in}} \right) [h_j(T^{00}, P^{00}, \mathbf{z}^{00}) - s_j(T^{00}, P^{00}, \mathbf{z}^{00})] \quad (2)$$

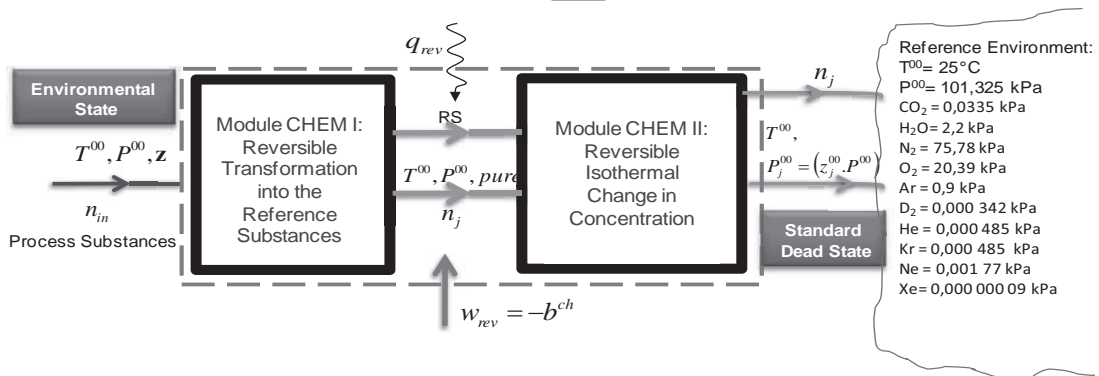


Figure 2. Modules CHEM I and Module CHEM II for chemical exergy

In the underlined term of equation (2), n_j refers to the number of moles of RS leaving the module CHEM II. The underlined term refers to the number of moles of j -th RS at the outlet of Module CHEM II per one mole of material stream. This term is resulted from conservation of *chemical elements* to handle the transformation of PS to RS in the Module CHEM I & II. General form of the *element balance* for one mole of material stream (i.e. $n_{in}=1$) is:

$$\forall = 1 \dots N_{\text{REL}} \quad \sum_{i=1}^{N_{\text{C}}} \alpha_{k,i} \cdot z_i = \sum_{j=1}^{N_{\text{RS}}} \left(\frac{n_j}{n_{\text{in}}} \right) \alpha_{k,j} \quad (3)$$

where $\alpha_{k,i}$ and $\alpha_{k,j}$ are the number of element “k” in i-th PS and j-th RS, respectively. In addition, N_{REL} and N_{RS} are number of reference elements (REL) and number of reference substances (RS), respectively, in RE. Unlike the existing exergy calculation methodologies in literature (e.g. Hinderink *et al.* 1996; Montelongo-Luna *et al.* 2007), the proposed method is not based on *Standard Chemical Exergy Tables* (Szargut *et al.*, 1998). This will guarantee a consistent exergy values as the only external data is the concentration of chemical RS not their chemical exergy values. Note that to obtain the exergy values equal to those in the standard tables, the enthalpy and entropy of formation should be chosen as the enthalpy and entropy bases, respectively.

2.2. Exergy of Work Stream (Shaftwork)

Exergy is defined as the equivalent work of a given energy form. Consequently, shaft-work by definition (either mechanical or electrical work) is equivalent to exergy (Dincer and Rosen, 2007).

2.3. Exergy of Heat Stream

Exergy associated to heat stream Q is the maximum work W_{max} obtainable from it by using the environment as a reservoir of zero-grade thermal energy:

$$B^Q = W_{\text{max}} = W_{\text{A Reversible Heat Engine}} = Q\tau = Q \left(1 - \frac{T^{00}}{T^{\text{Utility}}} \right) \quad (4)$$

For a given utility supplying the heat stream Q, T^{Utility} is obtained by the equation (5) (Tsatsaronis, 1993).

$$T^{\text{Utility}} = \frac{Q}{\Delta S^{\text{Utility}}} = \frac{H_{\text{out}}^{\text{Utility}} - H_{\text{in}}^{\text{Utility}}}{S_{\text{out}}^{\text{Utility}} - S_{\text{in}}^{\text{Utility}}} \quad (5)$$

3. Exergy Balance

Suppose a system that transform inputs material, heat and work into output ones as shown in figure 3. To keep exergy in balance, the exergy destroyed in the system (i.e. irreversibility, internal exergy loss) will be added to the exergy output:

$$B^{\text{in}} = \underline{B_{\text{useful}}^{\text{out}}} + \underline{B_{\text{waste}}^{\text{out}}} + I \quad (6)$$

where underlined term is external exergy loss and I represents the internal exergy loss.

To apply equation 6 on a process zone or a unit operation in process simulator, a distinction between the waste vs. useful output streams by the user is necessary.

4. Case Study

To show the applicability of computer-aided exergy balance in a process simulator, a simple process from the literature (Montelongo-Luna *et al.*, 2007) with some modifications is analyzed. Figure 4 shows a simple stabilization scheme to recover Natural Gas Liquids (NGL) from raw natural gas. As shown in figure 4b, in this configuration 10 bar steam is used as hot utility.

Table 1 summarizes the results by presenting the external and internal exergy losses occurring in each of the unit operations. As expected the largest irreversibilities occur in steam boiler. Although there are some ways (e.g. air pre-heater) to reduce its exergy loss, but its intrinsic irreversibility due to combustion is unavoidable.

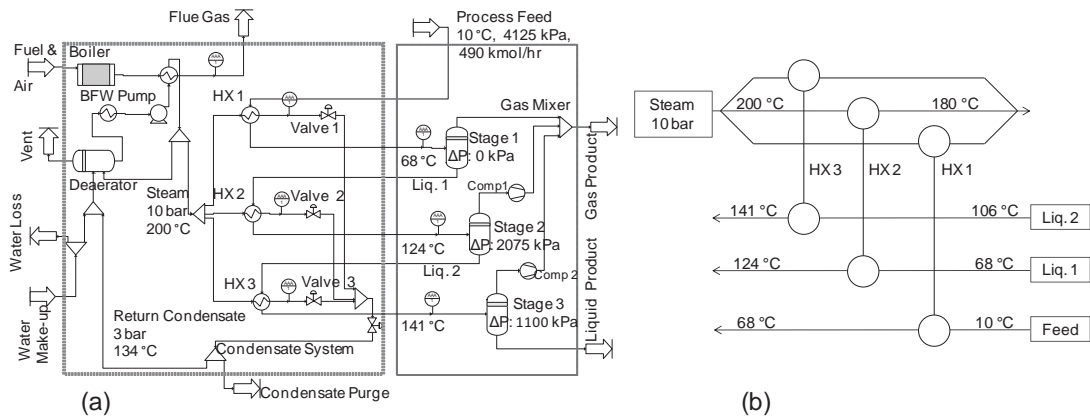


Figure 4. Base case: a) process & utility flowsheet, b) grid diagram of heat exchanger network

The second-largest irreversibility occurs in the heat transfer in the heat exchanger network. This is due to the finite temperature difference for heat transfer. The higher the temperature difference, the higher is the exergy loss. In addition, throttling valves cause relatively high irreversibilities that could be easily avoided.

Table 1. Internal and External exergy losses (kW) for base case and retrofit

Unit Operation	Base Case		Retrofit	
	Internal	External	Internal	External
BFW Pump	0.5	0.0	0.4	0.0
Valve 1	99.6	0.0	0.0	0.0
Valve 2	74.8	0.0	0.0	0.0
Valve 3	33.6	0.0	9.5	0.0
HX 3	36.3	0.0	17.2	0.0
HX 2	130.6	0.0	65.8	0.0
HX 1	348.1	0.0	261.8	0.0
Stage 1	0	0.0	0.0	0.0
Stage 2	52.7	0.0	52.7	0.0
Stage 3	26.6	0.0	26.6	0.0
Gas Mixer	60.1	0.0	60.1	0.0
Compressor 1	16.8	0.0	16.8	0.0
Compressor 2	16.0	0.0	16.0	0.0
Turbine 1a	-	-	30.9	0.0
Turbine 1b	-	-	12.8	0.0
Steam Boiler	2092.6	142.0	2040.7	139.2
Deaerator	19.3	69.3	17.4	20.4
Cond. System	0.0	80.8	0.0	10.8
Total	3007.6	292.1	2628.7	170.4

Table 2. Utility data for base case and retrofit

	Fuel demand (kg/hr)	Water makeup (t/hr)	Degree of superheat of steam from boiler	Electricity Requirement
Base Case	224.6	1.03	20 °C	191 (kW)
Retrofit	220.1	0.63	80 °C	0

Having pinpointed the sources of exergy losses, a retrofit scheme is proposed. First, to exploit the pressure component of physical exergy and provide the required shaft power for compressors of stages 2 and 3, a pass-out turbine is used to expand steam down to 4.5 and 3 bar. Then, the exhaust of steam turbine is used to heat up the process streams. As the utility temperature is decreased in the heat exchangers, the irreversibilities are decreased. The improved configuration of the process is presented in figure 6. Table 2 shows that use of low-pressure steam for heating reduces both fuel and water demand (i.e. natural recourses) while increases cogeneration potential.

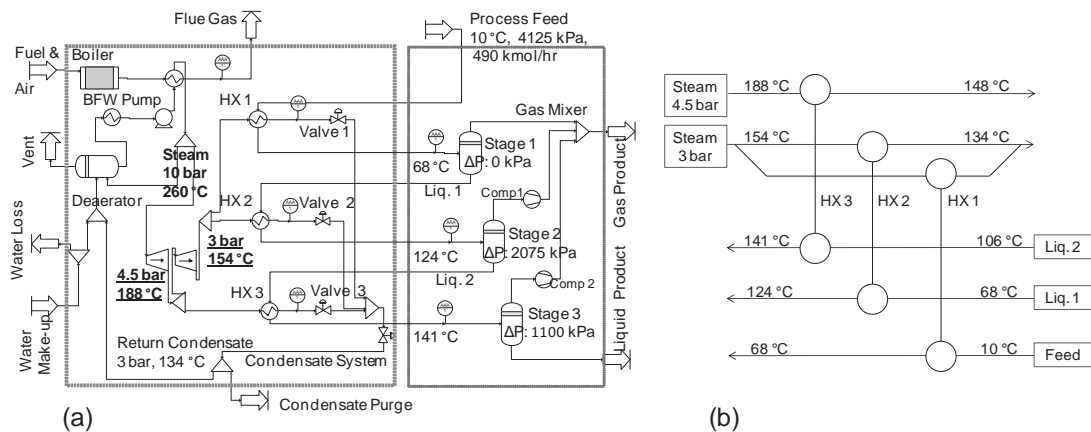


Figure 5. Retrofit data: a) process & utility flowsheet, b) grid diagram of heat exchanger network

5. Conclusions

As a first step of computer-aided exergetic analysis, this paper presents a general methodology for implementing exergy balance in process simulators like ProSimPlus[®] using the parameters and functions which are supposed to be features of most process simulators. In this work, as well as using the general expressions for heat and work streams, a general formula for calculating exergy of material stream has been developed. These are generic and totally independent of thermodynamic model used. Presently, the only limitation is due to the Reference Environment (RE) which should theoretically be extended to include all the chemical elements.

Through a case study the contribution has also shown how integration of exergy balance in process simulator can be a useful tool to identify the process areas in which heat recovery project must be defined. In the future, an exergetic multi-criteria optimization will be implemented to find the optimum configuration and operating conditions.

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