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General Methodology for Exergy Balance in ProSimPlus®

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Introduction

In the context of sustainable development, energy issue is one of the major problems. Therefore, optimization of process energetic efficiency appears to 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 enegy that can be practically recovered.

Definition of Exergy

The most natural and convenient standard as a measure of the energy quality is called exergy. The energy quality is synonym with the capacity of a given form of energy to cause changes in a process. (Kotas, 1985).

Exergy of Material Stream

Key Definitions

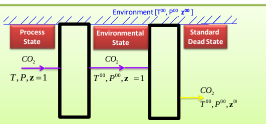
Exergy for Material Stream is defined as *"The amount of work obtainable when a material stream is brought to a state of thermodynamic equilibrium with the common components of the natural surroundings by means of reversible processes, involving interaction only with the abovementioned components of nature"*. (Szargut *et al.*, 1988).

To calculate exergy of a material stream, a reference medium, called *Reference Environment (RE),* is necessary. It is defined as "*an idealization of the natural environment which is in stable equilibrium. It is characterised by a perfect state of equilibrium with no gradients or differences involving pressure, temperature, chemical potential, kinetic or potential energy. This means that there is no possibility of producing work from any form of interaction between parts of the environment. The exergy of reference environment is zero. The exergy of a system in equilibrium with reference environment is zero too*".

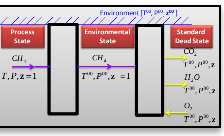
The material stream heading to Reference Environment needs to pass through different states, starting with *process state* and ending with *standard dead state*. These states by order are defined as follows:
***Process State* (T, P, z)**: The initial state of the given material stream is called *process state.*
***Environmental State* (T^{00}, P^{00}, z)**: The state of the given material stream when it is in thermal and mechanical equilibrium with the reference environment, i.e., at pressure P^{00} and temperature T^{00} of the reference environment.
***Standard Dead State* (T^{00}, P^{00}, z^{00})**: The state of a system when it is in thermal, mechanical and chemical equilibrium with a conceptual environment (having intensive properties pressure P^{00}, temperature T^{00}, and chemical potential μ^{00}) for each of the reference substances in their respective dead states).

To calculate exergy of a material stream with respect to a specified RE, the properties of the Process Substances (PS) of the material stream must be referred to the properties of Reference Substances (RS) (Szargut et al., 1998) in that RE.

If the PS is a RS, a change in pressure and temperature, is required to bring this PS to RE.

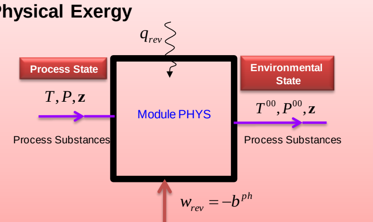


On the other hand, if the PS is a Non-RS, a reversible chemical reaction is needed to transform the Non-RS under consideration into one or more RS with the aid of RS brought from the RE.



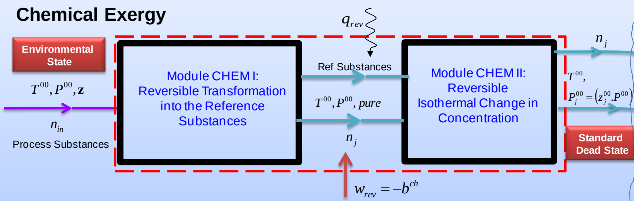
Calculation

Physical Exergy



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

Chemical Exergy

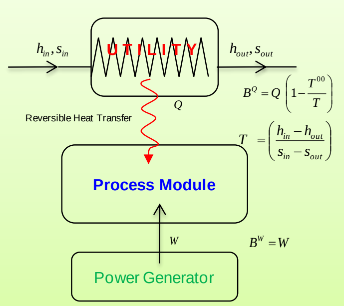


Reference Environment:
T^{00}= 25°C
P^{00}= 101,325 kPa
CO_2 = 0,0335 kPa
H_2O= 2,2 kPa
N_2 = 75,78 kPa
O_2 = 20,39 kPa
Ar = 0,9 kPa
D_2 = 0,000 342 kPa
He = 0,000 485 kPa
Kr = 0,000 485 kPa
Ne = 0,001 77 kPa
Xe= 0,000 000 09 kPa

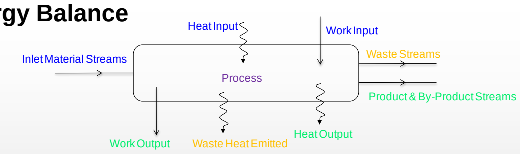
$$b^{ch} = -w_{rev} = h(T^{00},P^{00},\mathbf{z}) - T^{00}s(T^{00},P^{00},\mathbf{z}) - \sum_{j=1}^{N_{\text{CompRef}}} \left(\frac{n_j}{n_{in}}\right)\left[h_j(T^{00},P^{00},\mathbf{z}^{00}) - s_j(T^{00},P^{00},\mathbf{z}^{00})\right]$$

$$\forall k = 1 \ldots N_{\text{ElRef}} \qquad \sum_{i=1}^{NC} \alpha_{k,i} . z_i . n_{in} = \sum_{j=1}^{N_{\text{CompRef}}} \alpha_{k,j} n_j$$

Exergy of Work and Heat Stream



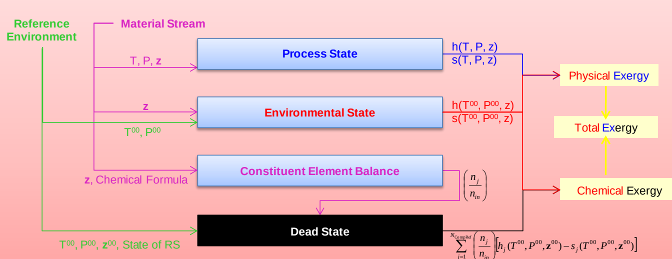
Exergy Balance



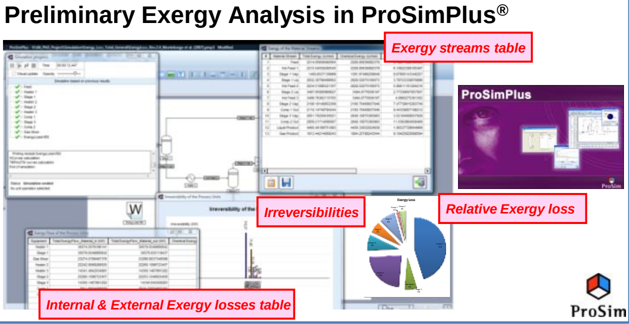
E n e r g y B a l a n c e
Energy Input of (Product + Heat + Work) = (Energy Output of (Product + Heat + Work))+ (Energy Lost of Wastes)

E x e r g y B a l a n c e
Exergy Input of (Material + Heat + Work) = (Exergy Output of (Material+ Heat + Work))+ (Exergy Lost of Wastes) + (Exergy Destruction or Irreversibility)
U s e f u l E x e r g y O u t p u t | External Exergy Loss | Internal Exergy Loss
T o t a l E x e r g y L o s s

Implementation: Material Stream Exergy Calculator



Preliminary Exergy Analysis in ProSimPlus®



Summary and Perspectives

As a first step of computer-aided exergetic analysis, this work presents a general methodology for implementing exergy balance in ProSimPlus® using the parameters and functions which are supposed to be features of ProSimPlus®. In this work, as well as using the general expressions for heat and work streams, a general formula for calculating exergy of material stream comprising $C_\alpha H_\beta N_\gamma O_\delta$ components has been developed. Unlike the existing calculation methodologies [1, 2, 3, 4, 6 and 7] ease of application and generality of the proposed approach make it preferable in process simulators. These are all 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 rather than C, H, N and O. Beside of exergy calculation of material stream, to go further in diagnosis of processes, exergetic criteria (e.g. exergetic efficiencies) can be integrated in ProSimPlus.

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