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Energy Efficiency Index Applied to Reactive Systems

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***Abstract*—**This paper focuses on the development of an energy efficiency index that will be applied to reactive systems, which is based in the First and Second Law of Thermodynamics, by giving particular consideration to the concept of maximum entropy. Among the requirements of such energy efficiency index, the practical feasibility must be essential. To illustrate the performance of the proposed index, such an index was used as decisive factor of evaluation for the optimization process of an industrial reactor. The results allow the conclusion to be drawn that the energy efficiency index applied to the reactive system is consistent because it extracts the information expected of an efficient indicator, and that it is useful as an analytical tool besides being feasible from a practical standpoint. Furthermore, it has proved to be much simpler to use than tools based on traditional methodologies.

***Keywords*—**Energy efficiency, maximum entropy, reactive systems.

I. Introduction

TRADITIONALLY techniques for evaluating the energy efficiency of a process involves two steps: use of energy balances and calculating efficiency index. Initially, the simple application of the first law of thermodynamics it seemed to be quite satisfactory for solving energy problems. However, it has been shown that only the first law is not suitable for dealing with optimization problems, since it this imposes such restriction, the joint use of both laws can become something indispensable.

In general, we use the ideal state for the development of an energy efficiency index. However, the characterization of such a state has been very difficult, and then in practice, instead is chosen the state close to the ideal. Due to this fact, some observations should be considered about the ideality (or reversibility). For open systems, it is known that the reversible state occurs when the entropy production rate is zero. However, this condition is infeasible, and what really happens is a valuable approximation. Consequently, it must be put aside the idea of perfect ideality, and consider only the nearest of reversibility, i.e. the minimum entropy production rate.

In dealing with reactive systems, in many cases, the energy question cannot be the more essential compared with other demands. In these cases, a clear understanding of what is desired plays a role preponderant. For example, a highly organized system is from reactive standpoint, something strongly desirable, because it minimizes the production of by-products, increasing the performance of the system. It should be emphasized that such requirement is governed by concept of entropy. Hence, the efficiency index based on entropy concepts tends to be consistent, efficient and it can circumvent the problem of ideality.

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II. Theoretical Background

A short review of the existing thermodynamic indicators is necessary for revealing their strong and weak points as realized by [5], [6]. Next, it will be developed a qualitative and quantitative analysis based on the proposed index applied to the reactive system.

A. Thermodynamics Indicators

Energy efficiency has been expressed in a generic form as an energy policy, and not like a single quantitative measure to be able to represent an energy efficiency index. Instead, the energy efficiency index has been defined by a simple relation, normally used in power cycles and given by (1):

$$\gamma = \frac{Useful\ Energy}{Energy\ \ Input} \tag{1}$$

Applied to the Carnot cycle, an ideal cycle, the energy efficiency depends solely on the temperature of the hot and cold sources, being considered as a theoretical reference. However, from practical standpoint, such a measure does not offer gains related to the maximal performance feasible, because it does not measure the distance to such performance. Therefore, an index related to the practical application and addressed to the maximum feasible should be used.

In some cases, the state thermodynamic function has been used to measure the energy efficiency, therefore (1) can be rewritten as shown in (2):

$$\gamma = \frac{\Delta H_{out}}{\Delta H_{in}} \tag{2}$$

where H denotes the enthalpy of the inlet (in) and outlet (out). Such an index is well known as enthalpy efficiency index. The enthalpy index does not differentiate the high quality energy of those of low quality, revealing a classical problem of indices that use solely the first law of thermodynamics.

Another approach is to regard the use of exergy (A) that is defined as the thermodynamic property that quantifies the maximum work. This work is calculated when the system interacts with the environment, moving from its current thermodynamic state (A) to the dead state (A_0). It is worth exploring this concept, because it is based on both the laws of thermodynamics. Equation (3) reveals the behavior of the exergy applied to open systems:

$$\frac{dA}{dt} = \sum_i \left(1 - \frac{T_0}{T}\right)Q_i - \left(\dot{W}_{VC} - p_0 \frac{dV}{dt}\right) - T_0\dot{\sigma} + \sum_{in} \dot{m}\left[(h - h_0) - T_0(s - s_0) + \frac{v^2}{2} + gz\right] - \sum_{out} \dot{m}\left[(h - h_0) - T_0(s - s_0) + \frac{v^2}{2} + gz\right] \quad (3)$$

The terms on the right side of (3) are recognized as a specific exergy. Reference [1] describes some performance indexes based on the exergy analysis, especially in the analysis made by [2], where such index is known as rational efficiency. In this index, the transfers of exergy have been clustered in a required input and a desired output. Thus, (3) can be rewritten in the as shown in (4):

$$\sum_{in} A_{total} = \sum_{out} A_{total} + T\dot{\sigma} \quad (4)$$

Equation (4) expresses the sum of all inlet exergies on the process is equal the sum of all exergies that leave the process added to the amount of exergy destroyed due to irreversibility, which is greater (or equal) to zero. Hence, a rational efficiency index can be established as shown in (5):

$$\gamma = \frac{\sum_{out} A_{total}}{\sum_{in} A_{Total}} \quad (5)$$

At first glance, the rational efficiency seems to be the most appropriated because it takes into account the quality of energy, however, this index presents some practical problems. First, because the 'maximum work' is not always the desired objective in many process. Second, the exergy calculation may not be easy since the environment (dead state) should be defined, depending on local condition and this can be not an easy task. Therefore, the indexes based on ideal conditions, even considering the quality of the energy, can meet restrictions in their applicability to real systems.

B. Indexes Based on the Fundamental Concepts of Entropy

The literature has shown great development potential of such indexes when the entropy is taken into account due to consider the efficiency of chemical process, under the principle of minimum entropy production, how to discussed in [3], [4], where are authors use the entropic approach as the key point for optimization of process. Such developments have become possible approaches in several branches of science, particularly in the context of the pattern recognition.

Reference [8] stated that one way for expressing in a nutshell the essential nature of pattern recognition is to say that it is a conceptual adaptation to the empirical data in order to 'sees a form' in them. That is, pattern recognition has to do with the problem of minimum entropy.

An important result can be drawn from the observation of the concept of entropy based on studies of Boltzmann and Gibbs associated to the index of characterization the degree of organization suitably defined by [8]. The property V defined by [8], called entropy deviation was defined as the degree of deviation of the probability distribution $p(x_i)$ from the normal distribution (non-structured) $w(x_i)$, I = 1, 2, 3, …, n, given by (6):

$$V(p,w) = -\sum_i p(x_i)\log\left[{p(x_i)}/{w(x_i)}\right] \leq 0 \quad (6)$$

Equation (6) reveals the smaller the relative entropy V, larger will be the degree of 'structuredness'. The entropy becomes maximum (V = 0) when $p(x_i) = w(x_i)$, and this means the lowest degree of structuredness. However, since $p(x_i) = 1$ for a particular i for which $w(x_i)$ is the smallest then when $w(x_i) = 1/n$, the minimum of V can be obtained, resulting in (7):

$$V\left(p, {1}/{n}\right) = \underbrace{-\sum_i p(x_i)\log\left[p(x_i)\right]}_{S(P)} - \log n = S(p) - \log n \quad (7)$$

Equation (7) is in according with the physical meaning of entropy, because how much smaller entropy of the system S(p), the greater the degree of structuring. The analysis of (7) shows to be a thermodynamically significant results because it establishes a deviation parameter, i.e., a quantitative measure between the entropy S(p) and the entropy maximum. Thus, the measure of the degree of structuring of a dataset can be used to develop an efficiency index applied to reactive systems, given that the organization of the reactive system is something strongly desired.

If a large number of cases should be considered, the use of minimum entropy concept for developing an energy efficiency index can be inappropriate because it would be necessary to calculate a minimum for each process. To address adequately the formulation of the proposed index, the concept of maximum entropy has been used since the maximum entropy is concerned with a natural tendency for all the process.

It should be emphasized that for a mixing process as a reactive system, the maximum entropy can be given by $\sum w_i \ln(w_i)$ where $w_i = 1/n$, where n denotes the number of chemical species present in the reactive system. In addition, it is interesting to note the strong relation between the maximum entropy and the uniform distribution given by $w_i = 1/n$. Hence, taking into account (7) and the aforementioned considerations, the degree of organization from a reactive system can be calculated by the following index as shown in (8):

$$\gamma = 1 - \sum_{i=1}^{n} \frac{x_i \ln x_i}{w_i \ln w_i} \quad (8)$$

Equation (8) represents the energy efficiency index applied to reactive systems, where x_i is the mole fraction of component i in the final mix and $w_1 = w_2 = w_3 = \ldots = w_n = 1/n$. This index uses the basic principle of maximum entropy to measure how efficient is the reactive effort of a given reaction. It is easy to verify that the level of final organization of the reactive system is maximum (i.e., minimum entropy

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production rate), then the proposed index is γ = 1, otherwise results equal to γ = 0. For example, it is assumed that the realization of a single reaction (aA + bB → cC), when occurs maximum conversion of reactants to products (Xa = 0, Xb = 0, and Xc = 1), substituting this values into (8), yields γ = 1. In this case, the efficiency index applied to reactive systems is 100%.

III. Results and Discussion

To illustrate the performance of proposed index, it was applied to an industrial reactor for the production of cyclic alcohol aiming at to maximize the production of alcohol. The basic procedure was established by [7] using genetic algorithm. The main objective of this application is to compare its effectiveness and simplicity to find the corresponding optimal state with those established by [7], based on a difficult analysis.

Case studies analyzed in this paper, which were carried out by [7], are focused on the condition of the genetic algorithm parameter that optimizes the production of cyclic alcohol. Tables I and II show the analyses where are checked the sensitivity of production cyclic alcohol, when it varies the uniform mutation rat, population size (npz), and crossover rate, to the uniform crossover and the crossover at one point. In this study, we used the efficiency index applied to reactive systems as a criterion for choosing the condition of the genetic algorithm parameters that optimize the process.

TABLE I
Results of Simulations for Level 1 of Production, Considering the Following Parameters: Population Size (npz) 20; Uniform Crossover Rates 0.6 and 0.8; Uniform Mutation Rates Ranging from 0.001 to 0.1

npz = 20	mutation rate of drag = 0,00				
rate crossover = 0,6	uniform mutation rate	AC	AB	C	Efficiency index (γ)
Uniform	0.001	0.949279	4.64124E-06	0.0507	0.817334
	0.005	0.950169	2.42435E-06	0.0498	0.819732
	0.01	0.950232	7.70371E-06	0.0497	0.819858
	0.05	0.949683	6.84226E-06	0.0503	0.818394
	0.1	0.948927	6.3983E-06	0.0510	0.81638
rate crossover = 0,8	uniform mutation rate	AC	AB	C	Efficiency index (γ)
Uniform	0.001	0.95056	9.31474E-06	0.0494	0.820726
	0.005	0.950883	8.51731E-06	0.0491	0.821602
	0.01	0.95129	6.87455E-06	0.0487	**0.822715**
	0.05	0.949778	6.85042E-06	0.0502	0.818648
	0.1	0.948687	7.67516E-06	0.0513	0.815731

[Molar Compositions of Cyclic Alcohol (AC), Benzyl Alcohol (AB), and Cycloalkane (C), and Energy Efficiency Index (γ)], Considering the Following Parameters: Population Size (npz) 20; Uniform Crossover Rates 0.6 and 0.8; Uniform Mutation Rates Ranging from 0.001 to 0.1

By assessing the results for the efficiency index (γ) of Table I, the parameters of the genetic code that maximizes the production of cyclic alcohol are given by: uniform crossover rate 0.8 and uniform mutation rate 0.01 for which the efficiency index is γ = 0.822715.

TABLE II
Results of Simulations for Level 1 of Production When Considered the Following Parameters: Population Size (npz) 20; Point Crossover Rates 0.6 and 0.8; Uniform Mutation Rates Ranging from 0.001 to 0.1

npz = 20	mutation rate of drag = 0,00				
rate crossover = 0,6	uniform mutation rate	AC	AB	C	Efficiency index (γ)
Uniform	0.001	0.94999	2.34458E-06	0.0500	0.819253
	0.005	0.951131	5.67824E-06	0.0488	0.822296
	0.01	0.951511	6.89053E-06	0.0484	0.823314
	0.05	0.951042	8.31008E-06	0.0489	0.822034
	0.1	0.949515	5.86869E-06	0.0504	0.817952
rate crossover = 0,8	uniform mutation rate	AC	AB	C	Efficiency index (γ)
Uniform	0.001	0.950142	2.3765E-06	0.0498	0.81966
	0.005	0.951127	9.53819E-06	0.0488	0.822255
	0.01	0.951244	6.44388E-06	0.0487	0.822594
	0.05	0.951231	8.97997E-06	0.0487	0.82254
	0.1	0.949324	7.44816E-06	0.0506	0.817431

[Molar Compositions of Cyclic Alcohol (AC), Benzyl Alcohol (AB), and Cycloalkane (C), and Energy Efficiency Index (γ)] When Considered the Following Parameters: Population Size (NPZ) 20; Point Crossover Rates 0.6 and 0.8; Uniform Mutation Rates Ranging from 0.001 to 0.1

It is easy to note from Table II that the parameters of genetic code which maximize the production of cyclic alcohol are given by: crossing rate at one point 0.6 and uniform crossover rate 0.01, corresponding to the efficiency index equal to γ = 0.823314.

The results obtained between the best and worst index related to the crossover at a point (Table II) shows a significant increase in productivity of cyclic alcohol in 7.56 tons per month and a reduction of unwanted product (cycloalkane) of 6.708 tons per month. From analytical point of view, it can be clearly seen the power and sensitivity of the proposed index, since a very small variation between the best and the worst case of 0.005883 denotes a substantial increase in the production of cyclic alcohol.

Finally, all results found were identical those obtained by [7] when it considered a large number of factors in his analytical procedure. This shows that the proposed index is also efficient for extracting the key information about the optimization process.

IV. Conclusions

An index based on the first and second law of thermodynamics was developed, by considering in particular the concept of maximum entropy. This is concerned with the more realistic concept of than the reversible state.

The results showed that the measure of the efficiency index determined with (8) presents a very good agreement with the results obtained by [7], for which a large set of data was taken for analysis of the optimal point, besides being laborious procedure. It should also be emphasized that the index proposed reveals how far the process from their optimal conditions is, and consequently, it can be considered a metric in the general sense. The result allows the conclusion to be drawn that the energy efficiency index applied to reactive systems is efficient, consistent by extracting the expected information, being useful as an analytical tool, by considering also the feasible implementation from a practical point of view. Moreover, it has been shown to be also easier to understand and to handle when compared to traditional methods, having a low operating cost.

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