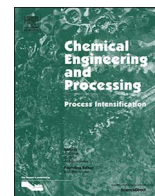




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# Chemical Engineering & Processing: Process Intensification

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## Eco-efficiency evaluation of acetone-methanol separation processes using computational simulation



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### ABSTRACT

The evaluation of environmental parameters of industrial processes plays a fundamental role in reducing not only their ecological impacts but also the costs associated with plant operations. In this regard, this work aims to evaluate, through eco-indicators and with the aid of computational simulation, the energy consumption, the CO<sub>2</sub> emissions and the water consumption of three different acetone-methanol separation plants, namely, Pressure Swing Distillation, Conventional Extractive Distillation and Energetically Integrated Extractive Distillation. Said processes were compared to one another in terms of their environmental efficiencies by means of the Eco-efficiency Comparison Index (ECI) method, which demonstrated that the integrated process is the most ecologically friendly.

### 1. Introduction

Notwithstanding the current concerns related to global warming, the world has been facing an alarming increase in greenhouse gases emissions, especially when it comes to industrial activities. In addition, the inappropriate raw materials exploitation, together with other environmental burdens such as the excessive consumption of water and energy, has compelled the companies and governments to seek alternatives for mitigating such ecological impacts.

The development of new technologies has become necessary to provide industrial processes with a better “eco-efficiency”, that is, the efficiency related to raw material consumption, product quality and environmental effects, in addition to the traditional financial income.

Eco-efficiency is a common object of industries that aim at sustainability, since it represents a direct relationship between economic development and its corresponding ecological impacts [1] and is based on the evaluation of the so-called “eco-indicators”. An eco-indicator is generally represented by the ratio of an environmental variable (e.g. energy consumption, CO<sub>2</sub> emissions, wastewater generation, water consumption, among others) to an economic variable (either net

income or production rate) [2,3,12].

One of the main purposes of eco-indicators is to improve decision-making procedures by providing guidelines for assisting safe economic and environmental decisions. Eco-indicators also enable the prediction of the environmental impacts resulting from economic activities, which can be taken into consideration during the design phase of a new process, thus allowing the selection of more eco-efficient routes/configurations or improving an existing process.

In order to demonstrate the usefulness of eco-indicators as a convenient tool for predicting and comparing the eco-efficiency of industrial processes, three different acetone-methanol separation technologies were evaluated, namely, Pressure Swing Distillation (PSD), Conventional Extractive Distillation (CED) and Energetically Integrated Extractive Distillation (EIED). The analysis was carried out by quantifying their respective CO<sub>2</sub> emissions, as well as their water and energy consumption, with the aid of computational simulation.

### 2. Literature review

The increase in greenhouse gases emissions and the excessive

*Abbreviations:* CAPEX, capital expenditure; CED, conventional extractive distillation; CW, cooling water; CWP, cooling water pump; CWR, cooling water return; CWT, cooling water tower; ECI, eco-efficiency comparison index; EIED, energetically integrated extractive distillation; ESCAP, economic and social commission for Asia and the Pacific; FW, feed water; FW.R, feed water to reactor; FWP.B, feed water Pump to boiler; FWP.R, feed water pump to reactor; hps, high pressure steam; IPCC, Intergovernmental Panel on Climate Change; lps, low pressure steam; MCTI, Brazilian Ministry of Science, Technology and Innovation; mol, molar; mps, medium pressure steam; OPEX, operating expenditure; PSD, pressure swing distillation; UNIQUAC, universal quasi chemical; WBCSD, World Business Council for Sustainable Development

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**Nomenclature***Symbols*

$l$	Side of the triangle
$n$	Number of eco-indicator
$Q1$	Pump P-100 energy (MW)
$Q_{cond1}$	Condenser E-101 energy (MW)
$Q_{cond2}$	Condenser E-102 energy (MW)
$Q_{reb1}$	Reboiler E-103 energy (MW)
$Q_{reb2}$	Reboiler E-104 energy (MW)
$S_a$	Minor triangle area
$S_T$	Major triangle area
$S_T^*$	Largest possible area

*Greek Symbols*

$\theta$	Angle formed between two sides of the triangle
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*Sub- and superscripts*

*	Largest possible
$A$	Side a
$a$	Minor area
$B$	Side B
$i$	Minor triangle
$T$	Major area

consumption of water and energy, along with other environmental burdens, have brought forth critical concerns related to the effects on the environment. Zhou and coworkers [7] stated that approximately 40% of the global CO<sub>2</sub> emission result from the processing industry, which is responsible for one third of the global energy use. This industry also stands out on water expending account, corresponding to approximately 23% of the global water consumption.

In view of such alarming scenario, the industries have been developing new studies and techniques associated with the economic and environmental performance of their activities in order to mitigate the resulting ecological impacts. In this regard, the concepts of eco-efficiency and eco-indicators play a crucial role because they can be utilized for evaluating the ecological performance of economic activities through a relationship between an environmental variable and an economic variable [4].

ESCAP (2009) [5] defined eco-efficiency as “a link between business and sustainable development”, being usually evaluated through the determination of eco-indicators and related to carrying out industrial operations in parallel to environmental preservation.

The analysis of eco-indicators provides information on the environmental performance of an industrial process that is related to its financial performance and improves the prediction of economic and ecological impacts [2]. Eco-indicators are generally defined as shown in Eq. (1). For evaluation purposes, the lower the value of the eco-indicator the more eco-efficient the process.

$$\text{Eco-indicator} = \frac{\text{Environmental Variable (unit)}}{\text{Economic Variable (production rate)}} \quad (1)$$

Regarding industrial operations, the environmental variable may represent several categories such as energy consumption, CO<sub>2</sub> emissions, water consumption and wastewater generation, among others. The economic variable, in turn, is usually related to production rate [6–9]. However, when the objective is maximizing the economic variable, generally the eco-indicator is determined by the inverse ratio of Eq. (1) [10,40].

There are several other methodologies that have been applied to eco-efficiency analysis of chemical processes. Ecoindicator-99 [40], for instance, is a method which has been also applied for the sustainability evaluation of industrial processes. Hofstette et al. [40] applied Ecoindicator-99 for a life-cycle assessment (LCA) of two case studies: a waste solvent incineration plant and a batch distillation column. Such methodology was also applied by Luis et al. [41] in the analysis of batch and continuous distillation for the treatment of four waste-solvent mixtures typically produced in the chemical industry. Furthermore, five environmental indicators, namely Eco-indicator 99, UBP-97, global warming potential (GWP), cumulative energy demand and CO<sub>2</sub>-balance, were applied by Amelio et al. [42] to analyze the production of solvents. The authors showed that said indicators led to the same conclusions for the evaluated mixtures, with some exceptions for UBP-

97. Sánchez-Ramírez et al. [43], in turn, showed that eco-efficiency analysis can be applied to optimization studies of chemical plants. The authors have proposed the optimization of a biobutanol production plant by using the Ecoindicator-99 as one of the objective functions.

Eco-efficiency has also been widely studied in the literature for several industry fields such as iron [11], steel [6], petrochemical [10], separation of acetone-methanol [13], among others. Most studies regarding industrial eco-indicators relate to both energy consumption and CO<sub>2</sub> emissions, since the former is directly associated with the latter. This is due to both the highly perilous ecological impact resulting from greenhouse gases emissions and the connection between energy consumption and economic potential [14].

In the following sections we describe the main eco-indicators used in this study.

## 2.1. Eco-indicators

### 2.1.1. Energy consumption eco-indicator

Energy consumption is inextricably associated with ecological impacts since, in many cases, fossil fuel combustion is necessary to generate electricity and vapor energy, for example. Particularly in relation to industrial operations, the current energy demand from industrial processes is not only extremely high but also expected to grow. Therefore, process optimization techniques (e.g. thermal integration) have become a crucial strategy for reducing energy use and thus the consequent environmental impacts [15].

The joint evaluation of the energy consumption of a process and its economic performance can be carried out by determining the respective eco-indicator:

- Energy Consumption Eco-indicator – Ratio of the total energy (including electricity) used in a certain period to the total equivalent production rate (GJ/t).

### 2.1.2. CO<sub>2</sub> emissions eco-indicator

As previously stated, the CO<sub>2</sub> emissions eco-indicator is the most highlighted among the environmental indicators evaluated for industrial processes due to the notorious concern in relation to global warming. In fact, Adams [16] indicated that in the last decades there has been an increase in carbon dioxide emissions, especially from industrial activities. Such increase – approximately 500% between 1950 and 2012 – corresponds to about 9.74 million tons of CO<sub>2</sub> emitted.

The joint evaluation of the CO<sub>2</sub> emissions of a process and its economic performance can be carried out by determining the respective eco-indicator:

- CO<sub>2</sub> Emissions Eco-indicator – Ratio of the total CO<sub>2</sub> emissions (combustion, indirect and fugitive) in a certain period to the total equivalent production rate (tCO<sub>2</sub>/t).

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