

# Integrated environmental performance assessment of chemical processes

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## Abstract

A method for environmental performance assessment is presented in this paper. The proposed method considers the procedure for environmental performance comparison of design alternatives as a multi-criteria decision-making (MCDM) problem. Integrated assessment model based on analytic hierarchy process (AHP) is presented for solving MCDM problem. An integrated environmental index (IEI) for chemical processes is proposed to combine resource conservation, energy consumption and potential environmental impacts associated with releases. This paper presents IEI as an environmental performance comparison index. As a case study, two alternatives of ethanol production are assessed by means of the proposed method.

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## 1. Introduction

Nowadays the consideration of environmental problems plays an ever-increasingly important role in chemical process design. In order to eliminate or reduce negative environmental problems, environmental performance of chemical process should be identified and quantified at the early stage of process design. Therefore, the new method is required to enable the comparison of process alternatives.

The quantitative analysis of environmental performance of process alternative is an ongoing task and remains a controversial topic (Pennington, Norris, Hoagland, & Jane Bare, 2001). Although various methods are available in the literature, (Dechapanya, Rogers, & Baker, 1999; Miettinen & Hämäläinen, 1997; Spengler et al., 1998) a generalized method is not established yet. An effective linkage between process modeling and environmental performance assessment, as well as an integrated environmental index are required.

A new method for environmental performance assessment is presented in this paper. The conceptual framework of the process environmental performance assessment is introduced. An integrated environmental index is proposed for the environmental decision-making. Then the paper presents the detailed procedure for environmental performance assessment based on the analytic hierarchy process. In the end, a case study is used to illustrate the proposed method.

## 2. Method

### 2.1. Process environmental performance assessment (PEPA)

To obtain the environmental information during the process design, the quantitative analysis of environmental performance is highlighted. The integration between the process design and the performance assessment is the aim of the tool developed in this work. PEPA is such a tool to select the environmentally friendly process alternative by evaluating the environmental performance. PEPA comprises the steps

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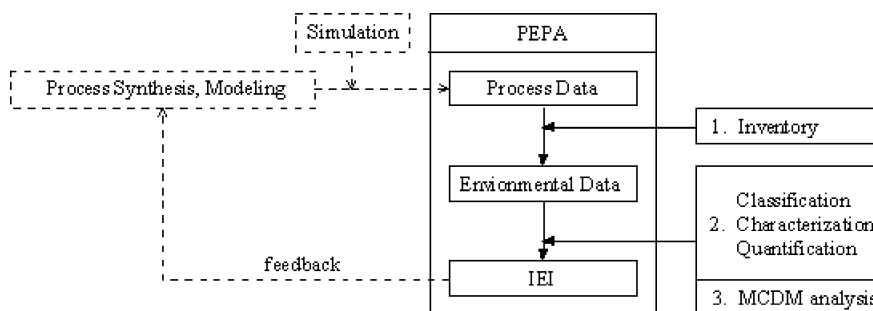


Fig. 1. Conceptual framework for PEPA.

of classifying, characterizing, and quantifying the environmental data as shown in Fig. 1. A short description of the procedure is addressed as follows.

At the first stage of the assessment, the process data are inventoried. According to the environmental impacts categories, environmental data are classified, characterized and quantified at the second stage. Finally, an integrated environmental index is obtained by utilizing multiple criteria decision-making (MCDM) analysis.

## 2.2. Integrated environmental index

Several comprehensive surveys of current research work to develop indices that describe the process environmental performance are available according to different professional background and research fields of the individual researchers (Cano-Ruiz & McRae, 1998; Youqi & Lei, 2000). Sharratt listed a collection of such indices as atom efficiency, BOD, LC<sub>50</sub>, etc. (Sharratt, 1999). Riverto introduced exergy analysis (Riverto, 1997). Considering regional toxicological impacts, Pennington et al. proposed the concept of relative impact potentials to assess design alternatives (Pennington et al., 2001). Bakshi developed a framework based on thermodynamic concepts of emergy and exergy (Bakshi, 2002).

Actually, the process environmental performance has many criteria due to the complexity of environmental problem. Krottscheck et al. measured the potential impact of processes using the concept of the sustainable process index, which combines resources and emissions to multi-compartment (Krottscheck & Narodslawsky, 1996). Cabezas et al. quantified the potential environmental impact of a process alternative as the screening indices (Cabezas & Douglas, 1999). Wang and Feng (2000) developed the concept of system negative effect factor using exergy analysis to aggregate resource utilization and environmental influence. Vassiliadis et al. suggested a global environmental impact vector representing the environmental performance of a process alternative (Vassiliadis, Stefanis, & Pistikopoulos, 2001). These work described environmental impacts as several criteria. And all of them showed implicitly the benefit of integrated index to support decision-making. However, a holistic approach to represent environmental problems is required and a systematic method to integrated assessment is

required as well. Therefore, this paper will give hierarchical criteria and present a multi-criteria decision-making method.

In this paper, environmental performance criteria consist of potential environmental impacts associated with releases (PEI), resource conservation (RC) and energy consumption (EC).

RC refers all needed raw materials. EC refers utilities including vapor steam and electricity. These two items are converted into money. PEI is somehow complex which refers the potential impacts produced by releases. According to the literature (Cabezas & Douglas, 1999; Pennington et al., 2001), potential impacts are classified into nine categories, including global warming potential (GW), photochemical oxidation potential (PO), ozone depletion potential (OD), acidification potential (AP), eutrophication potential (EP), human toxicity potential by ingestion (HI), human toxicity potential by either inhalation or dermal exposure (HE), aquatic toxicity potential (AT), and terrestrial toxicity potential (TT).

As mentioned above, aggregating criteria into IEI is considered as a hierarchical MCDM problem. Analytic hierarchy process (AHP) is suitable to solve this problem.

## 2.3. Analytic hierarchy process

The AHP is a powerful and flexible multi-criteria decision-making method for complex problems, and has been used in many governmental and industrial applications. These applications include multi-criteria decision-making problems in the areas of environmental protection, scheduling, project evaluation, and strategic planning (Saaty, 1980). The AHP combined qualitative and quantitative aspects of complex problem by means of a hierarchical structure. The AHP is used to (a) break down a complex and unstructured problem into its component parts, (b) use facts and judgements of key individuals to relate and prioritize the components, and (c) synthesize the results.

IEIs for process alternatives are calculated by four stages:

- *Step 1*: Criteria analysis and identification. Integrated assessment model is viewed as a hierarchical structure as shown in Fig. 2, in which the top level of the hierarchy specifies the goal, intermediate levels specify criteria and subcriteria which reflect suc-

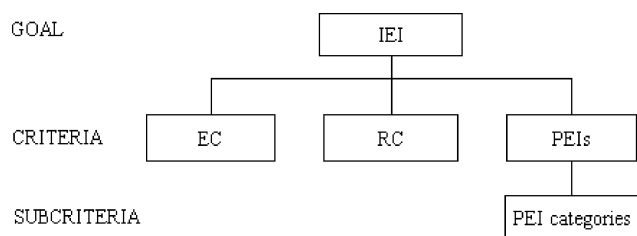


Fig. 2. The hierarchical structure for environmental performance decision-making.

Table 1  
The structure of judgement matrix

	$B_1$	$B_2$	...	$B_n$
$B_1$	$b_{11}$	$b_{12}$	...	$b_{1n}$
$B_2$	$b_{21}$	$b_{22}$	...	$b_{2n}$
...	...	...	...	...
$B_n$	$b_{n1}$	$b_{n2}$	...	$b_{nn}$

Table 2  
Numerical comparison scale suggested by AHP method

1	Two impacts contribute equally to the objective
3	Experience and judgement slightly favor one impact over another
5	Experience and judgement strongly favor one impact over another
7	One impact is favored very strongly over another, its dominance demonstrated in practice
9	The evidence favoring one impact over another is of the highest possible order of affirmation
2, 4, 6, 8	When compromise between values of 1, 3, 5, 7, and 9, is needed

cessive categorizations of environmental performance. The lowest level corresponds to the inputs associated with particular process alternatives. Based on different levels, criteria and subcriteria are prioritized.

- *Step 2*: Pair-wise comparison matrix is constructed according to the relative importance of each criterion as shown in Table 1.  $B_i$  ( $i = 1, \dots, n$ ) represents criterion  $i$ .  $b_{i,j}$  ( $i, j = 1, \dots, n$ ) represents numerical comparison scale that is assigned to  $B_i$  relative to  $B_j$ . At this stage, numerical comparison scales are assigned to each pair of criteria or sub-criteria. The AHP method suggests numerical comparison scale as shown in Table 2.

- *Step 3*: Relative weights are calculated based on the judgement matrix. The consistency measure is used.
- *Step 4*: IEIs are calculated. Then the different alternatives are ranked according to their IEIs. For each branch of the hierarchy, weights along the branch are multiplied with the input value of the lower level to obtain the contribution of the processes. A case study will be presented in Section 3.

### 3. Case study

Two alternatives for ethanol production are investigated in this paper: ethylene-derived feedstock process and straw cellulose-derived feedstock process.

#### 3.1. Process statement

Ethanol production via the direct hydration of ethylene process produces 95% (v/v) ethanol product as shown in Fig. 3. Ethylene gas and water vapor are fed into the reactor at 250 °C and 70 atm pressure for hydration. The ethylene conversion is only of 4% per passage. The reaction gas is recycled many times to increase the total efficiency. The ethylene has to be of high purity to avoid inert gases concentration. The reaction gas is cooled to condense the liquid products. The liquid product is separated for further purification to ethanol product (Ullmann's Encyclopedia of Industrial Chemistry, 2002).

Fig. 4 shows ethanol production via separate saccharification and fermentation process (Hatzis, Riley, & Philippidis, 1996). In this process, the mulled straw and steam at the temperature of 220 °C are fed into the pretreatment unit where hemicelluloses are converted into xylose and furfural. The effluent from pretreatment unit removes the steam in the flash vessel and is fed into vacuum filter, and liquid and solid components are separated. In the liquid phase, xylose is isomerized into xylosone by the isomerase in the fermentor. The xylosone is converted into ethanol that is sent to the distiller. Glucose is converted from the solid components in the zymohydrolysis. The liquid phase produced from rotary

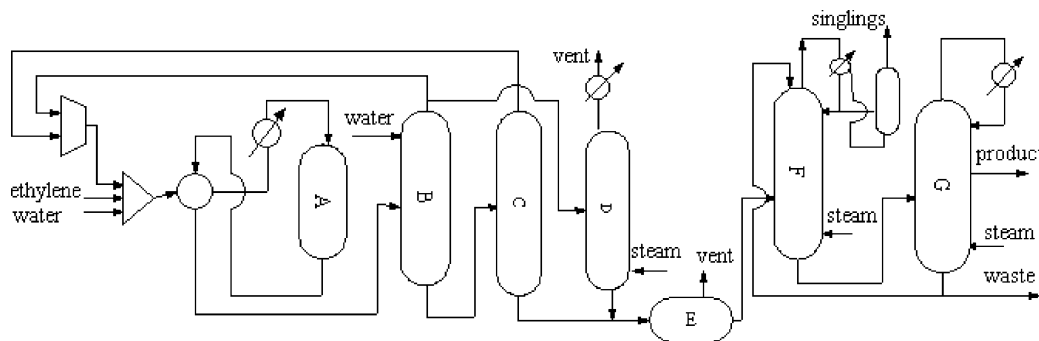


Fig. 3. The simplified flowsheet of ethylene-derived process: (A) reactor; (B) absorption tower; (C) flash; (D) ethylene tower; (E) crude ethanol vessel; (F) extractor; (G) ethanol tower.

vacuum filter is fermented into ethanol and some by-products are separated for further purification to 95% ethanol in the distiller.

### 3.2. Simulation results

Two processes are simulated by the simulator PRO/II. (We denote ethylene-derived process as P1 and straw cellulose-derived process as P2.) Because of the limited space, resource inventory and energy inventory of P1 and P2 are omitted. RC and EC of P1 are RMB1858.05 yuan and RMB363.71 yuan per ton of product, respectively. RC and EC of P2 are RMB1406.78 yuan and RMB442.03 yuan per ton of product, respectively. The values of PEIs categories for P1 and P2 are calculated by ECSS (Engineering Chemical Stimulation System developed by the group of Prof. Fang-yu Han) as shown in Tables 3 and 4.

In order to calculate each environmental impact category for the entire process, we multiply each chemical's environmental potential with its emission rate from the process and sum these for all chemicals emitted. The equation is

$$I_j^* = \sum_{i=1}^N I_{j,i} m_i \quad (1)$$

where  $I_j^*$  is the impact value for each category  $j$ .  $I_{j,i}$  the impact score of the emitted chemical  $i$  in the category  $j$ ,  $m_i$  (kg) is the quantity of the chemical  $i$  emitted.

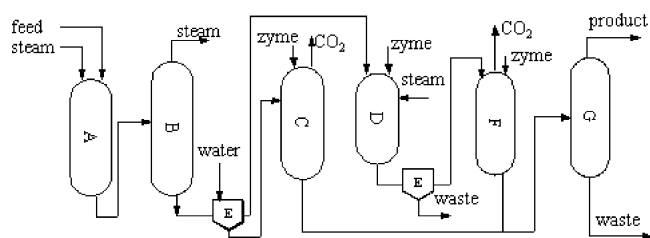


Fig. 4. The simplified flowsheet of straw cellulose-derived process: (A) decrepitation vessel; (B) flash; (C) zylose fermentation; (D) converter; (E) filter; (F) pentose fermentation; (G) product tower.

### 3.3. Determining IEIs

#### 3.3.1. Constructing judgement matrix

The comparison scale can be considered by the guideline of field experts or authoritative findings. In this paper, the relative importance of nine categories of potential environmental impacts (or sub-criteria) are determined under the guideline of US EPA Science Advisory Board study (United States Environmental Protection Agency, 1990). The SAB classified global warming, ecological toxicity, human toxicity, ozone depletion, and smog as relatively high-risk problems, acidification and eutrophication as relatively medium-risk problems. Impacts associated with solid waste are neglected. In this paper, the pair-wise comparison scale between high-risk and medium-risk is assumed to be 3. The relative importances of criteria are assumed to be equal. Therefore, the judgement matrices are constructed as shown in Tables 5 and 6.

Table 3  
Environmental impact of P1 (per ton of ethanol)

Emission	C <sub>2</sub> H <sub>4</sub>	N <sub>2</sub>	C <sub>4</sub> H <sub>10</sub> O	Acetald	Butanol	Ethane	Total
Flow rate (kg/h)	1.04	0.004	185.14	13.671	48.559	17.187	–
GW	0	0.000327	0	0	0	0	0.000327
PO	0	0	0	0	0	0	0
AP	0	0.000163	0	0	0	0	0.000163
EP	0.174676	0.017	125.345	8.60706	43.63828	12.42176	190.2039
HI	0.87109	0	40.0819	115.302	4.550549	7.278650	168.084176
HE	0.001458	0.000024	0	8.51994	0.060525	0	8.581945
TT	0.871092	0	40.0819	115.302	4.550549	7.278650	168.084176
AT	0.016152	0.000366	0.85999	0.35829	0.029128	0.012183	1.276103

Table 4  
Environmental impact of P2 (per ton of ethanol)

Emission	Acetic acid	Glycerin	FururoI	CO <sub>2</sub>	Total
Flow rate (kg/h)	25.00	48.208	8.575	197.207	–
GW	0	0	0	0	0
PO	0	0	0	0	0
AP	0	0	0	0	0
EP	9.237723	78.3484	5.05422	114.858	207.498
HI	7.304593	25.11663	0	37.5641	69.9853
HE	0.056089	0	0	1.78405	1.84014
TT	7.304593	25.11663	0	37.5641	69.9853
AT	0.374141	0.25715	0	10.5888	11.2201

Table 5  
Pair-wise comparison of PEIs categories

	GW	PO	AP	EP	HI	HE	AT	TT	$w_i$
GW	1	1	3	3	1	1	1	1	0.15
PO	1	1	3	3	1	1	1	1	0.15
AP	1/3	1/3	1	1	1/3	1/3	1/3	1/3	0.05
EP	1/3	1/3	1	1	1/3	1/3	1/3	1/3	0.05
HI	1	1	3	3	1	1	1	1	0.15
HE	1	1	3	3	1	1	1	1	0.15
AT	1	1	3	3	1	1	1	1	0.15
TT	1	1	3	3	1	1	1	1	0.15

Table 6  
Pair-wise comparison of PEI, RC and EC

	PEI	EC	RC	$w_i$
PEI	1	1	1	0.333
EC	1	1	1	0.333
RC	1	1	1	0.333

### 3.3.2. Calculating the IEIs

Based on the judgement matrices, the relative weights ( $w_i$ ) of criteria and sub-criteria are obtained as shown in Tables 5 and 6. Then integrated environmental performance indices are calculated based on the step 4 in Section 2.3. IEI of P1 is 760.32, while IEI of P2 is 648.94. Finally from the point view of environmental performance, P2 is more environmentally friendly.

## 4. Conclusion

Environmental performance assessment can be served as a decision-supporting tool to improve process performance. A proper representation of environmental impact is a hard task. The goal of this paper is to develop an integrated environmental index that will help process designers to screen environmentally friendly process alternatives.

Two alternatives for ethanol production are used as the illustrative case study, and the procedure of AHP is presented. The results suggested that the environmentally friendly processes could be obtained. Compared to ethanol production of ethylene-derived feedstock, that of straw cellulose-derived feedstock is more environmentally friendly.

It should be noted that process environmental performance assessment remains an ongoing topic. More work of uncertainty and variation associated with assessment index were beneficial (Pennington et al., 2001). It should also be noted that the conclusions for comparison was limited to the processing stage. Consideration of the alternatives in terms of their full life cycle may result in different conclusions (Pennington et al., 2001).

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