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A Modular Approach to Sustainability Assessment and Decision Support in Chemical Process Design

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In chemical and allied industries, process design sustainability has gained public concern in academia, industry, government agencies, and social groups. Over the past decade, a variety of sustainability indicators have been introduced, but with various challenges in application. It becomes clear that the industries need urgently practical tools for conducting systematic sustainability assessment on existing processes and/or new designs and, further, for helping derive the most desirable design decisions. This paper presents a systematic, general approach for sustainability assessment and design selection through integrating hard (quantitative) economic and environmental indicators along with soft (qualitative) indicators for social criteria into design activities. The approach contains four modules: a process simulator module, an equipment and inventory acquisition module, a sustainability assessment module, and a decision support module. The modules fully utilize and extend the capabilities of the process simulator Aspen Plus, Aspen Simulation Workbook, and a spreadsheet, where case model development, data acquisition and analysis, team contribution assessment, and decision support are effectively integrated. The efficacy of the introduced approach is illustrated by the example of biodiesel process design, where insightful sustainability analysis and persuasive decision support show its superiority over commonly practiced technoeconomy evaluation approaches.

1. Introduction

Depletion of nonrenewable resources, global warming, forest depletion, water contamination, air pollution, and many other issues are among the most serious problems today due to decades of unhealthy and mismanaged human activities, especially in economic development. Naturally, development sustainability has become of utmost importance globally. According to Brundtland,[1] development must "meet the needs of the present without compromising the ability of future generations to meet their own needs". The central concept of sustainability, or sustainable development, is so-called "triple bottom line" balance, which is to achieve simultaneously economic prosperity, environment cleanness, and social responsibility. Inherently, leaders in the global business community have begun to realize the effect of sustainability to their business survival and growth, as many CEOs have asserted a belief that sustainable business practices will improve both enterprise resource productivity and shareholder confidence.[2]

"Design for sustainability" is a concept and also a design philosophy. By this, a variety of design methodologies have been developed for improving process design, product design, material design, etc., at different scales of time and length. In chemical engineering, process system engineering (PSE) is perhaps best positioned to address the challenges of design for sustainability, especially in the early design stage, where early sustainability assessment can help ensure a finally selected sustainable design. Conventionally, process design is performed using technoeconomic criteria.[3,4] It becomes more and more obvious that the resulting design may not be sustainable; other aspects of sustainability should also become an integral part in process design selection.[5−12] In recent years, process design sustainability analysis using state-of-the-art process simulators have emerged.[9,13,14] However, the known methodologies are yet to be more systematic and, more importantly, enhanced by incorporating social-aspects-reflected criteria in design selection. In this work, we present (i) a holistic sustainability assessment approach that combines both hard and soft indicators in evaluation of process sustainability performance during the early design stage and (ii) a decision support approach based on an analytical process hierarchy (AHP) method to assist designers in alternative design selection. The approach fully utilizes spreadsheet and process simulation techniques and makes model development, data acquisition and analysis, team contribution assessment, and decision support processes that are effectively integrated in modules. The efficacy of the introduced methodology will be demonstrated by the assessment and selection of biodiesel process alternatives.

2. Sustainability Indicators for Process Design Evaluation

Galileo Galilei once quoted "Measure what is measurable and make measurable what is not." In sustainability assessment, measuring environmental and social impacts of an economic activity is of great importance. In such an endeavor, selection of necessary indicators is critical. Arguably, sustainability assessment indicators can be divided into two groups: hard and soft.

Hard indicators give a *quantitative* evaluation of a process using numerical information and formulas, such as net present value (NPV) and rate of return (ROR) used for economic performance assessment, life cycle assessment (LCA) and waste reduction (WAR) algorithm for environmental performance assessment, and fault tree assessment (FTA) and chemical exposure index (CEI) for safety-related social responsibility assessment. More recent efforts of using hard indicators in biodiesel systems assessment can be found in some recent publications.[15−17]

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Soft indicators, on the other hand, give *qualitative* evaluation, which depends heavily on designers' knowledge and experience (mostly heuristic). The indicators are frequently very subjective because of different interpretations, but eventually they play an important role in obtaining an agreeable solution. Although difficult to be transferred into formulas or equations, this type of soft indicator may be also numerically scaled using appropriate scaling techniques. In sustainability assessment methodology development, several papers[6−8,10,12] applied both types of indicators.

2.1. Economic—NPV and DCFRR. According to Pintarič and Kravanja,[18] process flowsheet optimization frequently uses simple capital and operating costs and profit functions. However, further investigation indicates that NPV and discounted cash flow rate of return (DCFRR) are among those favored by entrepreneurs, as they can provide more appropriate profitability measurement in design alternative evaluation.[3,4] They should be used together. As a note, DCFRR is designed to reflect the highest, after-tax interest or discount rate at which the project can just break even.[19]

NPV can be calculated by summation of the present values of all incomes subtracted by the summation of the present values of all expenditures, as shown below.

$$\mathrm{NPV} = \sum_{m=1}^{n} \frac{C_{\mathrm{A},m}}{(1+r)^m} - C_{\mathrm{TCI}} \qquad (1)$$

where C_A is the total annual income cash flow after the base year for year m, r is the interest rate (%), n is the project lifetime after the base year. C_TCI is the total capital investment before the base year and is the summation of the total fixed capital cost, C_FCC, and the working capital cost, C_WCC. Note that C_FCC is the summation of the total bare module costs of the equipment, the contingency fee, and the auxiliary facility cost. Details on the calculation of NPV will not be covered here, and readers are suggested to refer to process design books[19] for further explanation on calculating NPV.

DCFRR is defined as the discount rate, at which the NPV of a project equals zero (i.e., to set eq 1 to zero). At that point, the values of interest, r, or here denoted as r_ROR, can be readily determined. This so-called internal rate interest is usually determined by corporate management and represents the minimum acceptable rate of return that the company will accept for any new investment. The acceptance of this discount rate depends on many factors, such as economic situation, environmental regulation, and social needs. Obviously, a project that yields DCFRR greater than the internal interest rate is considered to be profitable. Clearly, a combined use of both NPV and DCFRR can reflect a comprehensive economic assessment that include the rate of return and its investment scale.

2.2. Environmental—The WAR Algorithm. The identification of hard indicators for environment impact assessment has been the focus of many researchers. Some of the well-known and widely used methodologies are, to name a few, LCA, WAR algorithm, and exergy and emergy analysis. The adoption of a particular indicator is significantly important, especially in the initial stages of process design such that the indicator presents a direct correlation among flows and impacts and reduces the requirement of complex models.[20] In 1999, Young and Cabezas[21] introduced a so-called WAR algorithm for assessing environmental impact of a chemical process design. It is important to note that in this method the product life cycle is partial, as it covers the stages only from manufacturing to the factory gate (before being transported to consumers). In LCA, this type of assessment is called cradle-to-gate assessment. With

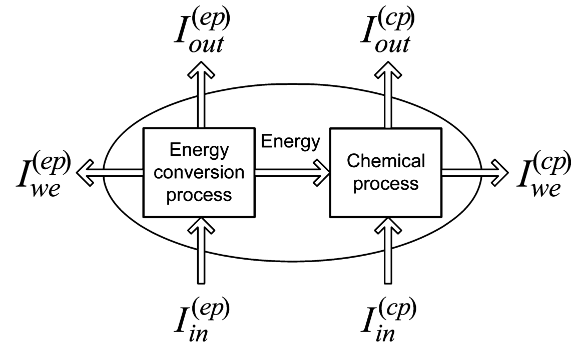


Figure 1. Mass and energy balance for the calculation of the PEI at the manufacturing level.

its simple to use algorithm and easy to find data, WAR algorithm is thus suitable for environmental impact assessment at the design stage.

The concept of potential environment impact (PEI) in the WAR algorithm is based on the conventional mass and energy balance (see Figure 1). The key formulations of the algorithm are briefly reviewed below. More detailed information can be found in the work of Young and Cabezas.[21]

At the steady state, the algorithm can be expressed as

$$I_{\mathrm{in}}^{(\mathrm{cp})} + I_{\mathrm{in}}^{(\mathrm{ep})} - I_{\mathrm{out}}^{(\mathrm{cp})} - I_{\mathrm{out}}^{(\mathrm{ep})} - I_{\mathrm{we}}^{(\mathrm{cp})} - I_{\mathrm{we}}^{(\mathrm{ep})} + I_{\mathrm{gen}}^{(\mathrm{t})} = 0 \qquad (2)$$

where $I_{\mathrm{in}}^{(\mathrm{cp})}$ and $I_{\mathrm{out}}^{(\mathrm{cp})}$ are, respectively, the mass input and output rates of PEI of a chemical process; $I_{\mathrm{in}}^{(\mathrm{ep})}$ and $I_{\mathrm{out}}^{(\mathrm{ep})}$ are, respectively, the energy input and output rates of PEI of the energy generate process; $I_{\mathrm{we}}^{(\mathrm{cp})}$ and $I_{\mathrm{we}}^{(\mathrm{ep})}$ are, respectively, the outputs of PEI associated with waste energy lost from the chemical process and the energy generation process; and $I_{\mathrm{gen}}^{(\mathrm{t})}$ is the rate of energy of PEI inside the system, representing the creation and consumption of PEI by chemical reactions.

Note that $I_{\mathrm{we}}^{(\mathrm{cp})}$ and $I_{\mathrm{we}}^{(\mathrm{ep})}$ can be neglected since chemical plants usually do not emit large amounts of waste energy and the potential environment impact of mass is much greater than the emission of energy. Thus, the above equation can be simplified as

$$I_{\mathrm{gen}}^{(\mathrm{t})} = I_{\mathrm{out}}^{(\mathrm{cp})} - I_{\mathrm{in}}^{(\mathrm{cp})} + I_{\mathrm{out}}^{(\mathrm{ep})} - I_{\mathrm{in}}^{(\mathrm{ep})} \qquad (3)$$

For the mass expressions,

$$I_{\mathrm{in}}^{(\mathrm{cp})} = \sum_{i}^{\mathrm{EnvCat}} \sum_{h}^{\mathrm{Streams}} M_{h,\mathrm{in}} \sum_{c}^{\mathrm{Comp}} x_{c,h} \psi_{c,i}^{\mathrm{s}} \qquad (4)$$

$$I_{\mathrm{out}}^{(\mathrm{cp})} = \sum_{i}^{\mathrm{EnvCat}} \sum_{h}^{\mathrm{Streams}} M_{h,\mathrm{out}} \sum_{c}^{\mathrm{Comp}} x_{c,h} \psi_{c,i}^{\mathrm{s}} \qquad (5)$$

where M_h is the mass flow rate of the stream h, either input or output stream; $x_{c,h}$ is the mass fraction of component c in stream h; $\psi_{c,i}^{\mathrm{s}}$ is the normalized value of the specific potential environment impact of component c associated with impact category i. The impact categories to measure the affect to environment are based on a study by Heijungs et al.[22] and are generally global atmospheric and local toxilogical. The global atmospheric category involves indicators, such as global warming potential (GWP), ozone depletion potential (ODP), acidification potential (AP), and photochemical oxidation (or smog formation) potential (PCOP). In the local toxilogical level, indicators include human toxicity potential by ingestion (HTPI),

Table 1. Emission Factor for the Coal-Fired Power Plant (US EPA, 1995)

gas pollutants	emission factor (EF), kg/kW h
SO_x	0.00272
NO_x (NO_2 and NO)	0.00181
CO_2	0.3719
HCl	9.0×10^{-5}
methane	0.4763
mercury (Hg)	4.944×10^{-9}

human toxicity potential by inhalation/dermal exposure (HTPE), aquatic toxicity potential (ATP), and terrestrial toxicity potential (TTP).

Potential environmental impact for energy is calculated by summing all the energy requirements of the system, such as the energy used by compressors, reboilers, heat exchangers, cooling and reboiler pumps, refrigeration units, turbines, etc. Typically, the energy source for these can be classified as direct energy (e.g., electricity) and indirect energy (e.g., steam at different pressures and natural gas). Cabezas and Young only considered electrical energy. As an extension this work includes both electrical energy and steam. For the source of energy production in a coal-fired power plant, the amount of emission must be considered, which contains SO_2, NO_x, CO_2, CH_4, and Hg.[23] Some modifications are made to the original equations whereby the input and output energy potential environmental impacts are expressed by

$$I_{\text{in}}^{(\text{ep})} = \zeta_{\text{gas}} \sum_{g}^{\text{Comp}} EF_g^{m,n} \psi_{g,i}^{\text{s}} \tag{6}$$

$$I_{\text{out}}^{(\text{ep})} = \zeta_{\text{gas}} \sum_{g}^{\text{Comp}} EF_g^{m,n} \psi_{g,i}^{\text{s}} + \zeta_{\text{solid}} \sum_{g}^{\text{Comp}} EF_g^{m,n} \psi_{g,i}^{\text{s}} \tag{7}$$

and

$$\zeta_{\text{gas}} = [\sum_{m}^{\text{Streams-gas}} E_{m,\text{in}}^{\text{Direct}} + \sum_{n}^{\text{Streams-gas}} \alpha E_{n,\text{in}}^{\text{Indirect}}] \tag{8}$$

$$\zeta_{\text{solid}} = [\sum_{m}^{\text{Streams-solid}} E_{m,\text{in}}^{\text{Direct}} + \sum_{n}^{\text{Streams-solid}} \alpha E_{n,\text{in}}^{\text{Indirect}}] \tag{9}$$

where $I_{\text{in}}^{(\text{ep})}$ is the potential environment impact of combustion source; $I_{\text{out}}^{(\text{ep})}$ is the potential environment impact of energy output that is used by the process plant; E is the energy requirement of m direct energy streams and n indirect energy streams of the unit operations or facilities; EF is an emission factor for gas pollutants g (in kg g/kW h for coal-fired power plants; see Table 1); α is the ratio of electrical energy to steam energy for plant utilities produced through burning the same amount of coal (this coefficient is used to consider the energy lost from steam that is for generating electrical energy before being used for heating purposes in the plant). Stream-gas and stream-solid are the streams containing gas and solid, respectively. It is assumed that solid compounds are immediate pollutants as the hazardous components are locked in a solid mixture, having no or negligible negative environment impact. Such an assumption makes $I_{\text{in}}^{(\text{ep})}$ approximately zero, since the raw material used (i.e., coal) is in the solid form. This simplifies the calculation of PEI energy to

$$I_{\text{out}}^{(\text{ep})} = [\sum_{m} E_{m,\text{in}}^{\text{Direct}} + \sum_{n} \alpha E_{n,\text{in}}^{\text{Indirect}}] \sum_{g}^{\text{Comp}} \text{EF}_g^{m,n} \psi_{g,i}^{\text{s}} \tag{10}$$

With the assumption, the included PEI indicators are listed below

$$I_{\text{gen}}^{(\text{t})} = I_{\text{out}}^{(\text{cp})} - I_{\text{in}}^{(\text{cp})} + I_{\text{out}}^{(\text{ep})} \tag{11}$$

$$I_{\text{out}}^{(\text{t})} = I_{\text{out}}^{(\text{cp})} + I_{\text{out}}^{(\text{ep})} \tag{12}$$

The indices presented to this end are in terms of rate PEI/h. To evaluate on a product basis (PEI/kg), a simple transformation can be made to the index by

$$\hat{I}_{\text{gen}}^{(\text{t})} = \frac{I_{\text{out}}^{(\text{cp})} - I_{\text{in}}^{(\text{cp})} + I_{\text{out}}^{(\text{ep})}}{\sum_{p}^{\text{prodStreams}} P_p} \tag{13}$$

$$\hat{I}_{\text{out}}^{(\text{t})} = \frac{I_{\text{out}}^{(\text{cp})} + I_{\text{out}}^{(\text{ep})}}{\sum_{p}^{\text{prodStreams}} \dot{P}_p} \tag{14}$$

where P_p is the mass flow rate of product p. Using eqs 11−14 allows us to measure the environmental impact of a chemical process. The value of the total rate of PEI output, $I_{\text{out}}^{(\text{t})}$, enables us to identify an appropriate site for a plant (a plant with low $I_{\text{out}}^{(\text{t})}$ should be located in an ecologically sensitive area). $\hat{I}_{\text{out}}^{(\text{t})}$ measures the efficiency of material utilization by a specific process per unit mass of products; it decreases when the mass rate of PEI, $I_{\text{out}}^{(\text{t})}$, is reduced or the production rate is increased. This means that improving material utilization efficiency through process modification/innovation tends to lower the PEI output per unit mass of products. This suggests that engineers design process systems through a careful selection of process operating conditions, which directly affects the magnitude of $I_{\text{gen}}^{(\text{t})}$ (an indicator useful in comparing processes based on how fast they generate impact). On the other hand, $\hat{I}_{\text{gen}}^{(\text{t})}$ is used for comparing processes and products based on the amount of new potential environmental impact generated in product manufacturing. Obviously, the lower the PEI, the more desirable the process.

The equations considered above count for all products and nonproducts streams (such as intermediate products, byproduct, waste, etc.), because all of them may have potential environmental impacts. In some cases, however, when the product of one process is an intermediate of a downstream process, there is a high demand on the product, and the analysis objective is to reduce waste, then the product stream should be excluded from the analysis. This is to ensure that a user or producer is not directly penalized for producing chemical that has a high PEI value.[21]

2.3. Social—Soft Quality Indicators. IChemE introduced 20 quantitative social indicators for assessing social performance that reflected the company's attitude to treatment of its own employees, suppliers, contractors, and customers and also its impact on society at large.[24] However, using these indicators for evaluating social criteria is irrelevant at an early design stage. When defining the term social and to define explicitly its relevant indicators most of the research focuses on safety aspects of the chemical plant and its effect on human safety. However, there are other aspects besides safety that should be considered during the early process design evaluation. In 1998, Herder and Weijnen[25] conducted a study to define explicitly quality indicators for early design decision making. They observed industrial practice case studies and conducted interviews with expert panels and professionals from industry and from academia and formulated their top ten quality indicators. These qualitative

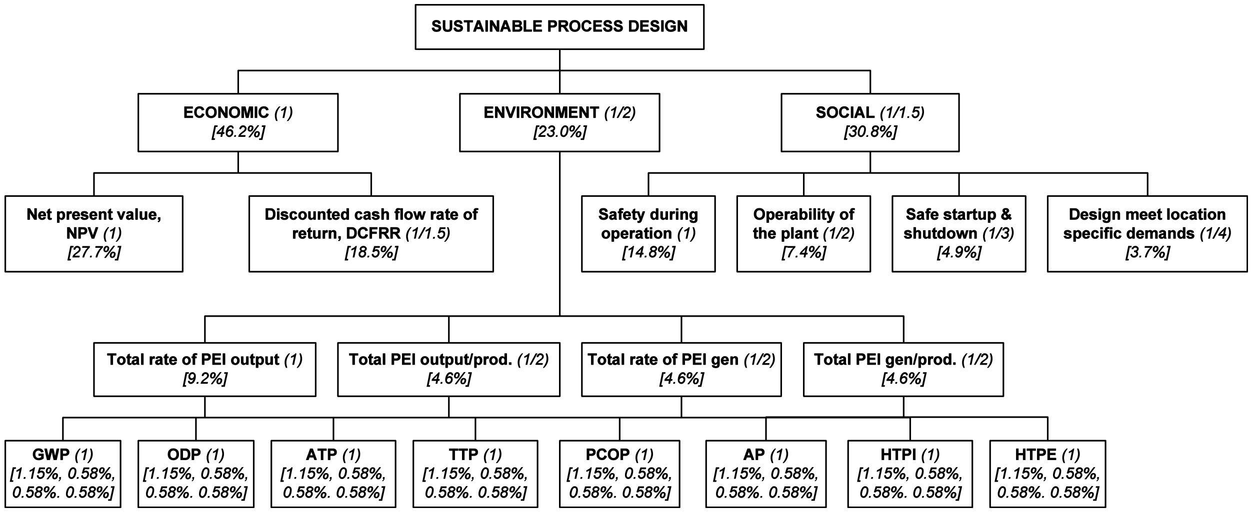


Figure 2. Decomposition of MCDM for sustainable process design, weights setting, and its corresponding normalized vector for each indicator.

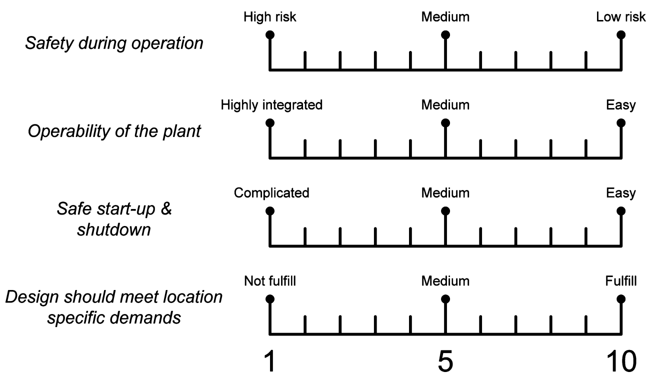


Figure 3. Scaling systems for the social indicators.

indicators are suitable to assessing a good quality design as they utilize the heuristics knowledge of assessors in process design evaluation. Furthermore, they provide a rapid assessment that is hoped to be close to the best possible evaluation without the need for extensive data search. In this work, four of them are adopted (see Figure 2) and categorized under the social-related criteria. Note that these soft-based indicators are difficult to measure and formulate, but generally they can be converted to numbers using appropriate scaling systems. A scaling system proposed is shown in Figure 3. Although not very specific, it acts as a general guideline to assess various types of chemical processes. This type of approach is widely used in process safety engineering. Note also that to conduct an appropriate evaluation of process design, the indicators to be used should be explicitly defined to avoid confusion. As a guideline, each of the indicators is defined in Table 2. Although not very rigid, they should be useful to guide decision makers.

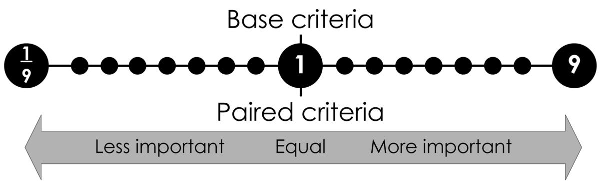
2.4. Decision Support—The AHP Methodology. Design screening requires a systematic decision-making method. Decision making relies first on effective assessment of design alternatives. Saaty[26] developed a multicriteria decision making (MCDM) methodology, called the analytical hierarchy process (AHP), performing decision trade-off between multiple objectives in a hierarchically organized structure. It accepts any particular constitutive criterion for inclusion and allows individual decisions to be aggregated into overall criteria, which allows other members to review and participate in that aspect of the decision-making process at an appropriate level of detail.

Table 2. Standard Definition of the Social Indicators

indicators	definition
safety during operation	The condition or state of being safe; free from danger or hazard; exemption from hurt, injury, or loss. Evaluation of hazards and risks associated with, but not limited to, chemical compounds, reactions, unit operations and equipment, and operating conditions should be included in the assessment.
operability of the plant	The condition where the plant is able to operate feasibly. Assessment should consider the operation feasibility by workers and also control systems of the plant, especially if tightly integrated and also in the presence of process variations and uncertainties.
safe start-up and shutdown	Start-up means the act or process of setting into operation or motion, while shutdown means cease to operate or cause to cease operating. The degree of difficulties of the procedure depends on the system complexity and workers' capability.
design should meet location specific demands	Local demands may include technology transfer, employment, affect to other related industries, local regulations and policies, legal proceedings, etc.

Development of AHP for decision making in process design could involve the steps for problem decomposition, weighting, ranking, and evaluation. Figure 2 shows the problem decomposition adopted in this work with four levels in the hierarchy. It starts with the first level indicating the decision objective. The criteria for design selection are then expanded into the second level decision hierarchy, which are economy-, environment-, and social-related. Each of these criteria is then broken into the third level criteria. The fourth level is only defined for the environment criteria that consider the eight environmental impact categories. This is useful especially when a certain category is of a special focus.

In the weighting stage, each criterion is assigned with a weight based on its perceived importance or relevance through a pairwise comparison. It can be done through consistency matrix formulation approach, which can provide a simple calculation and generate accurate and consistent results.[27] Figure 4 shows a scaling system based on the work by Saaty[26] and also a general guideline to the weights setting. It is used for aiding weighting selection to each indicator based on consistency matrix formulation. Using this scaling system, one needs to identify a criterion that acts as a basis of comparison and pairs it with other criteria to measure its relative importance. A value greater than 1 indicates that the paired criterion is relatively more important than the base criteria, whereas a value less than 1 indicates its unimportance compared to the base case. Assigning weights to indicators is subjective. Decision makers' knowledge, experience, and judgment ability are critical in weight assignment.



Quantitative scale	Qualitative indicator	Explanation
1	Equal Importance	Two activities contribute equally to the objective
2	Weak or slight	
3	Moderate importance	Experience and judgement slightly favour one activity over another
4	Moderate plus	
5	Strong importance	Experience and judgement strongly favour one activity over another
6	Strong plus	
7	Very strong or demonstrated importance	An activity is favoured very strongly over another; its dominance demonstrated in practice
8	Very, very strong	
9	Extreme importance	The evidence favouring one activity over another is of the highest possible order of affirmation
2, 4, 6, 8	Intermediate values	
1/3	Weakly less important	May be difficult to assign the best value but when compared with other contrasting activities the size of the small numbers would not be too noticeable, yet they can still indicate the relative importance of the activities.
1/5	Moderately less important	
1/7	Strongly less important	
1/9	Absolutely less important	
1/2, 1/4, 1/6, 1/8	Intermediate value etc.	

Figure 4. Pairwise comparison and weighting scale for consistency matrix formulation.

3. m-SAS Framework

A modular-based sustainability assessment and selection (m-SAS) framework is proposed for systematic assessment and selection of sustainable process design alternatives. Figure 5 shows an overview of the framework. It includes four modules that are commonly a part of design stages and are systematically integrated to assist case model development, data acquisition and analysis, team contribution assessment, and decision support process. The first module is the process simulation (PS) module, where process model development takes place. A commercial process simulator, Aspen Plus, provides the flexibility to model, modify, or optimize processes but at the same time keeps the data updated, accurate, and consistent for further evaluation processes. Furthermore, it provides reliable results with computational ease. The other three modules are developed using an Excel spreadsheet. The main advantage of the spreadsheet is its capability of integration with other programs, i.e. Visual Basic, SQL, which is suitable for integrated task applications. The main function of the equipment and inventory acquisition (EIA) module is to acquire and deposit inventory data. It includes the data concerning equipment design specifications, streams information, and economic, environmental, and operational parameters. The acquired data is obtained from the user's definition and the process simulator. While the former is obvious, the latter involves an automated acquisition using Aspen Simulation Workbook (ASW). Applying ASW offers a huge advantage, as the interface in Excel allows direct communication with the Aspen Plus simulation engine that is running in the background, thus allowing an automated customized data exchange. Consequently, it enables the development of Excel interfaces to process models in Aspen Plus without writing VB programs, enabling it to extend its application capabilities. The third module, the sustainability assessment (SA) module, calculates the hard indicators using the inventory data deposited in the EIA module. Separating this module and developing it as a stand alone allows a rapid calculation despite any data changes in the EIA module, thus aiding users to focus on the real issues in process design development. The last module, the decision support (DS) module, is developed to support team contribution in decision making. It calculates the weighting vectors, normalized vector, scores, normalized scores, and also the final results provided that the decision makers define the scaling margin and criteria weights of each level and also the evaluation score of the social indicators.

3.1. m-SAS Algorithm. The m-SAS algorithm is shown in Figure 6. The left-hand side shows the flow diagram, while the right explains the details about how to execute a specific task block. It starts with a definition of the problem by providing a design flowsheet and the information on product type and quality. The production scale or the problem could also assess the feasibility of any intensification or modification on the existing design flowsheet. Once the problem is defined, the next step is to model each identified flowsheet in Aspen Plus. The modeling includes the definition of chemical components, the selection of thermodynamic models and methods, the flowsheet design setting, and process specifications and input parameters setting. Once modeling is completed, a process flowsheet is selected, and equipment and inventory acquisition are performed with the assistance of the EIA module. The user defined data, which includes the economics parameters and the component-specific potential environment impact, is provided by the users,

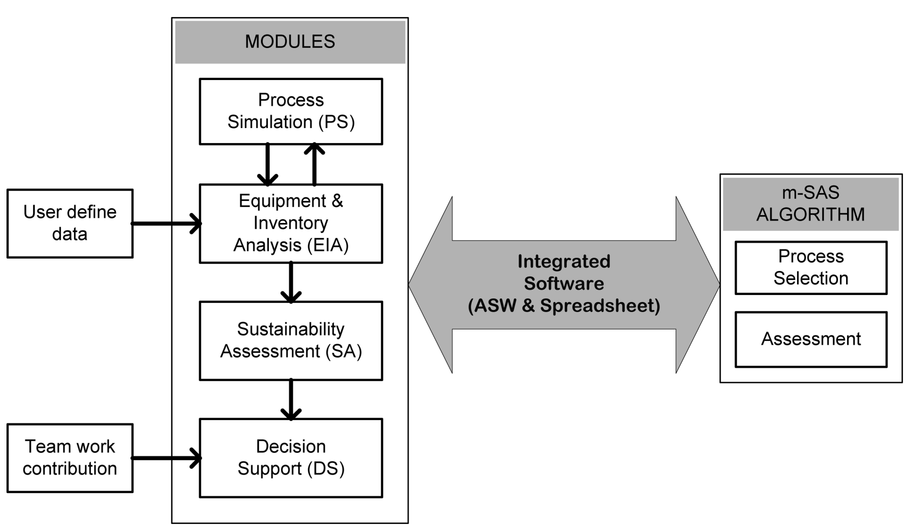


Figure 5. m-SAS framework.

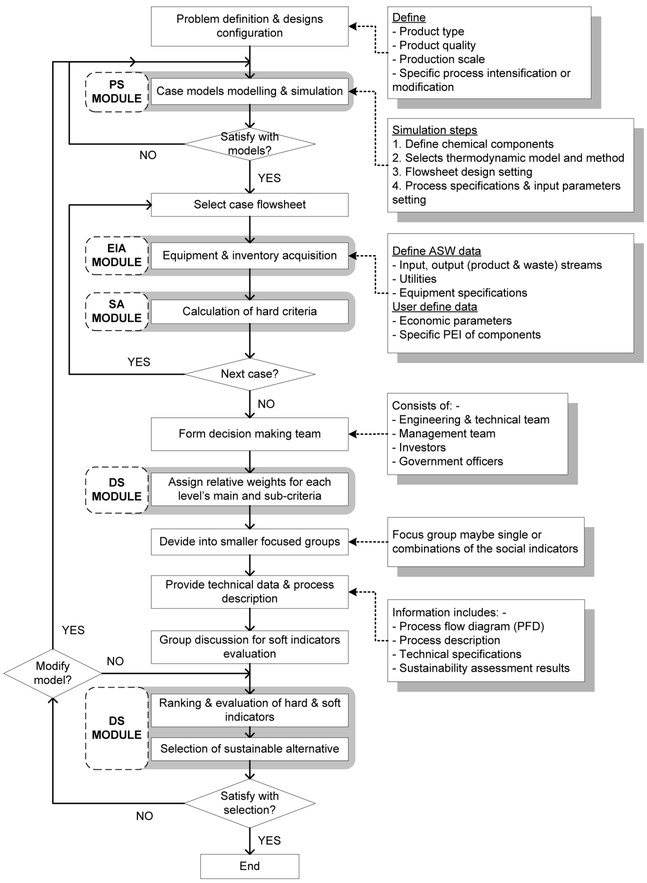


Figure 6. Flowchart of the m-SAS algorithm.

whereas simulation data is acquired using ASW. These data are then analyzed by the SA module to calculate the hard indicators, such as NPV, DCFRR, and the four environmental indicators. This step is repeated for all modeled flowsheets. The next step involves a group participation. A good blend of a decision group should involve members within the organization and also external partners, e.g. investors, top managers, engineers, technicians, and government officers so that a holistic and in-depth evaluation can be conducted. Once the group is formed, it needs to assign weights to each level and its indicators. They are then grouped accordingly on the basis of their expertise to either a single or combination of social indicators. With provided information concerning the design, they perform a thorough discussion to finally set the scores to the designated social indicators assigned to each specific group. Once the results are obtained, it is inserted into the DS module for elicitation of the final ranking and selection solution.

4. Biodiesel Process: Alkali-Based Catalyst vs Supercritical Methanol

To demonstrate the applicability of the proposed approach, two biodiesel processes will be investigated. The first process, namely case 1 in Figure 7a, is to use a conventional method to produce biodiesel using alkali-based catalyst, while the second process, namely case 2 in Figure 7b, is using supercritical methanol. Alkali-based catalyst for producing biodiesel is mostly preferred in the industry, as it is more efficient, less corrosive, and operated at low temperature and pressure with a high conversion yield. One limitation of alkali-catalyzed process, however, is its sensitivity to the purity of reactants, e.g., water content and free fatty acid (FFA). Too much water can lead to the formation of emulsion through ester saponification under alkaline conditions, while too much FFA will cause a reaction with alkali catalyst to form soaps and water. This competing reaction consumes the catalyst and hinders the transesterifation reaction. Moreover, the formation of emulsions can cause difficulties in downstream recovery and biodiesel purification.

In recent years, researchers began to investigate producing biodiesel at supercritical condition. Applying such conditions offers several advantages, including a noncatalytic process, insensitive to both water and FFA, and simultaneous esterification of FFA in oil.[28] Recent studies on supercritical methanol, however, show that it is technologically and economically promising.[29,30] On the basis of these facts, supercritical methanol can be an alternative to the conventional method of producing biodiesel. Although the method can compensate for problems associated with the alkali-based process, it requires a high operating cost due to its high operating temperature and pressure. Consequently, a consumption of too much energy leads to more pollutants resulting from high consumption of energy resource. No research thus far has assessed and selected these cases from the sustainability point of view, although there is an effort that focuses solely on the environment impact.[31] Thus, it will be interesting to assess and compare these two cases based on economic, environment, and social criteria.

4.1. Process Modeling. Simulating the actual content of vegetable oil is complex because it is a mixture of oils with different fat content. Because oleic acid is a major fatty acid in rapeseed oil with composition of 64.4%,[32] triolein is chosen to represent rapeseed oil. Methyl oleate is taken as the resulting biodiesel product. In real application, however, new vegetable oil actually contains 0.05 wt % FFA,[33] but this is not considered in this work. The simulated capacity of both cases is 8000 ton/yr with an oil feed input of 1050 kg/h. The biodiesel purity of more than 99.6 wt % is assumed according to the ASTM specification. Additionally, to optimize the plant profitability, glycerol is further refined to meet the pharmaceutical standard of more than 92 wt %. The economic feasibility of the biodiesel industry is much more affected by plant capacity, vegetable oil price, and price of biodiesel and thus requires a government subsidy for positive net profit.[34] In this work, the total biodiesel selling price is assumed to be \$1.30/kg, with inclusion of a government subsidy.

In biodiesel production, both methanol and glycerol are highly polar components. Therefore, both NRTL and UNIQUAC models are recommended for predicting the activity coefficients of the components in a liquid phase.[35] In this simulation, NRTL is used as the main thermodynamic method. For the modeling of decanter and mixer, the Redlich–Kwong–Soave (RKS) thermodynamic properties are used following the approach by Myint and El-Halwagi.[33]

Case 1—Alkali-Based Process. The modeling for case 1 is based on the work of several researchers.[29,33,35] The flowsheet configuration is shown in Figure 7a. The reaction is carried out with a 100% excess of methanol to oil or 6:1 molar ratio with 1 wt % sodium hydroxide based on oil. The catalyst and methanol feed flow rates are 10 and 110 kg/h, respectively. The reaction yield is assumed to be 95%, the temperature is set at 60 °C, and the pressure is at 1 bar. The reaction product then enters a methanol recovery unit with six theoretical stages and the reflux ratio of 0.05. The distillation column is kept below the atmospheric pressure in order to maintain the bottom product temperature under 250 °C, which will prevent decomposition of biodiesel and glycerol. The bottom product is then sent to a water washing column. It is mixed with 10 kg/h water before

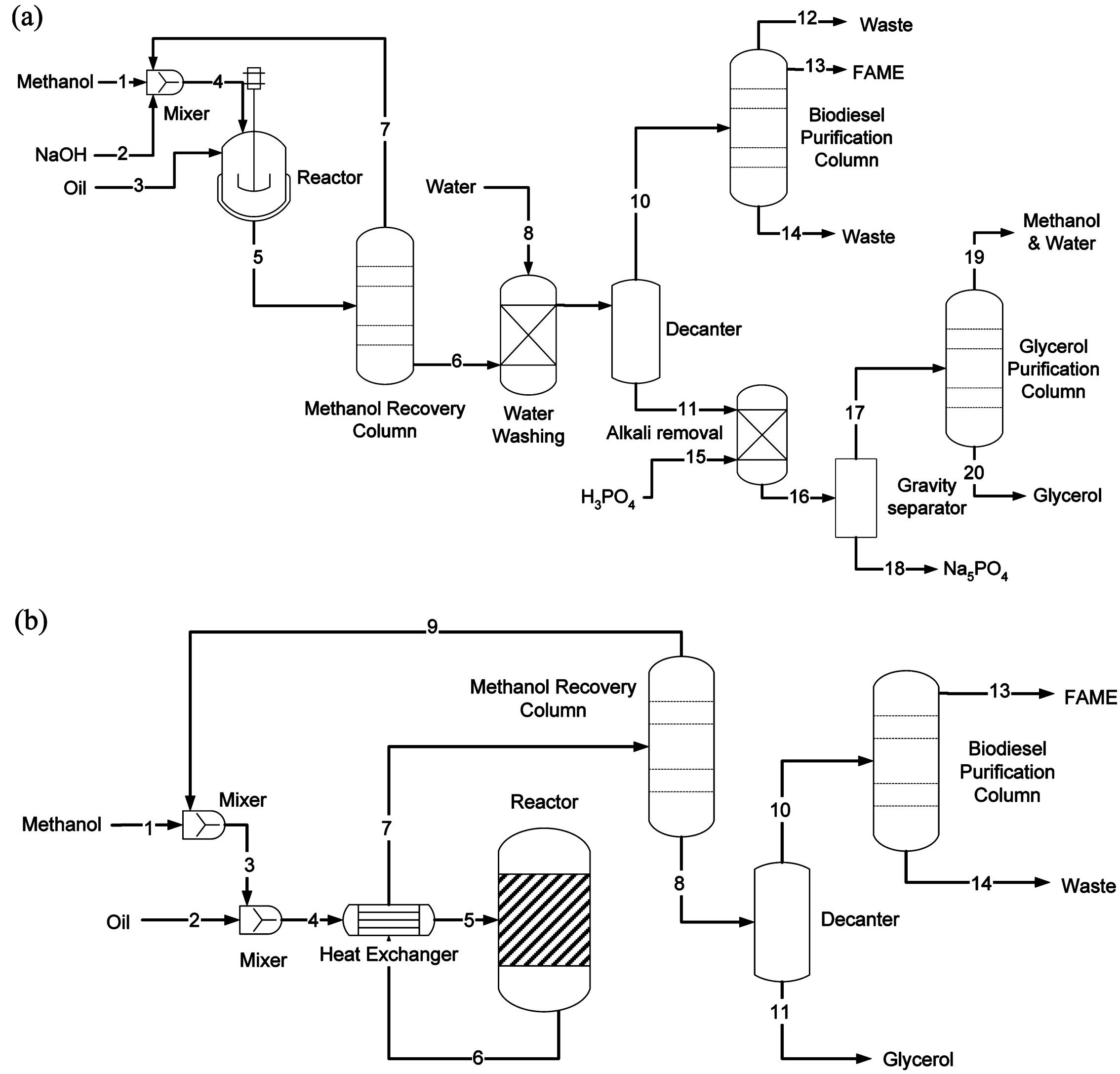


Figure 7. Biodiesel process flowsheets: (a) alkali-based and (b) supercritical methanol.

being settled down in a decanter to separate the main products, i.e., biodiesel and glycerol. On the basis of the component density, the upper part, which contains 97% biodiesel, is sent to a biodiesel purification column. Using six theoretical stages with a reflux ratio of 2 and being operated under vacuum to maintain product temperature below 250 °C, biodiesel is further purified to meet the product specifications of 99.6 wt %. The bottom stream of the decanter contains 82% glycerol and the rest is a mixture of methanol, water, and sodium hydroxide. To further purify glycerol, the stream is first passed through a catalyst neutralization reactor. Phosphoric acid at 8.33 kg/h is added to neutralize the sodium hydroxide. The output stream is then sent to a gravity separator to separate the solid sodium phosphate salt. The liquid stream is then sent to a glycerol purification column. Using four theoretical stages, at the reflux ratio of 1 and being operated under vacuum, the bottom product stream is able to achieve a glycerol purification of above 92 wt %. The summary of the main unit operation specifications for case 1 is listed in Table S1 in the Supporting Information. Table S2 in the Supporting Information gives the simulation results of the input and output streams.

Case 2—Supercritical Methanol. Modeling of case 2 is based on the work of several researchers.[28−30] The flowsheet configuration is shown in Figure 7b. The reaction conditions vary in the literature, but generally excess methanol with a temperature of over 300 °C and pressure above 300 bar are used. In this work, the reaction conditions with 42:1 methanol to oil molar ratio, temperature of 350 °C, and pressure of 430 bar are used. According to Lim et al.,[30] at this condition, the reaction takes only 4 min with a yield of 95%. Because of the high temperature of the reactor output stream, the heat is utilized to preheat the reactor input stream using a heat exchanger. The reaction product then enters the methanol recovery distillation column with 12 theoretical stages and the reflux ratio of 0.5. Nearly 99.6% of the excess methanol can be recovered with the purity nearly 99.9%. This recycled methanol is mixed with the fresh methanol feed of 114 kg/h before being fed again, together with oil, to the reactor. The bottom stream of the column is then cooled down before being sent to a decanter. On the basis of the component density, the upper part contains 94.7% biodiesel and the rest is unreacted oil and other impurities. The bottom stream contains over 92% of glycerol and the rest is mostly methanol. As the purity of glycerol meets the commercial standard, no further purification step is needed. The biodiesel rich stream still needs to undergo further purification. The stream is fed to a biodiesel purification column using eight theoretical stages with the reflux ratio of 0.05 and under vacuum. The biodiesel purity at the distillate stream achieves the product specifications of more than 99.6 wt %. The summary of the main unit operation specifications for case 2 is listed in

Table 3. Economics Parameters

specifications	value
Feed Input Price, $/kg	
soy oil (crude, degummed)[a]	0.5
methanol (99.85%)[a]	0.18
NaOH[a]	0.34
H_3PO_4[a]	4
Product Price, $/kg	
biodiesel (with subsidy)	1.3
glycerol (92 wt %)[a]	1.2
Utilities Price, $/kg	
electricity, $/kWh[a]	0.062
LP steam (5 barg, 160 °C)[b]	0.00608
MP steam (10 barg, 184 °C)[b]	0.0068
HP steam (41 barg, 400 °C)	0.1164
process water[b]	6.7×10^{-5}
Disposal Cost, $/kg	
solid waste[a]	0.15
liquid waste[a]	0.037
discount factor, %r	10
annual depreciation, %	10
tax, %	34
salvage value recovery %	5
plant life cycle, yrs	15
construction duration, yrs	1
working weeks/yr	49
working hours/yr	8000

[a] Value from Zhang et al.[34] [b] Value from Turton et al.[19]

Table S1 in the Supporting Information. Table S3 in the Supporting Information summarizes the simulation results of the input and output streams.

Data Acquisition. As previously mentioned, the data is provided by the users and the process simulator. Tables 3 and 4 show, respectively, the economics parameters and the component-specific potential environment impact. The values for the latter are obtained from the MSDS datasheet and classification factor published in Heijung et al.[22] The data from the process simulator is exported to the EIA module using ASW. These include stream flow rates, compositions, process utilities parameters such as heat duty and utility type, mass of cooling water and steam, and operating temperature, pressure, and design specifications of unit operations and equipments. Once defined, any modification to the designated process model is automatically updated in the EIA module.

4.2. Assessment Results. Table 5 shows the economic performance of both cases. Case 1 has a lower total capital investment (TCI) value as compared to case 2. Since case 2 is operated at an extremely high pressure and temperature, the equipment cost increases especially for the transesterification reactor and methanol recovery column, because of expensive material and a huge heat transfer area for heat exchangers, reboilers, and condensers. Furthermore, the huge requirements for recirculation of large amounts of methanol into the process increases the pump load, eventually increasing its price due to expensive material and high energy consumption. On the other hand, case 2 has a lower total production cost (TPC). Because case 2 requires no catalyst, acid, and also water, it manages to cut down the overall production costs, despite of a high demand of utility. For a plant life cycle of 15 years, case 1 has a shorter payback period than case 2 with a higher percentage of DCFRR. However, since case 2 has a lower production cost, it is able to compensate a high initial investment and obtained a higher NPV at the end of the plant life cycle. In the long run, case 2 is economically feasible. This economic trend agrees with the work by West et al.[29] It seems that in the economic point of view, supercritical methanol is a promising alternative. But when it comes to sustainability, this criterion alone is not enough for process design decision.

Table 5. Economic Performance

	case 1	case 2
NPV, $ $\times 10^3$	2028	2736
DCFRR, %	28.69	23.46
payback period, yr	6.2	7.8
total capital investment (TCI), $ $\times 10^3$	1856	3550
total production cost (TPC), $ $\times 10^3$	10693	10373

In this paragraph, the results on the environment and social aspects will be discussed. The environmental assessment results for both cases are shown in Figure 8. Figure 8a gives the potential environmental impact for the process material input streams. It is found that case 1 has a higher PEI input value than case 2, which is caused by the presence of catalyst for the transesterifation reaction and acid for neutralization of the catalyst. Although case 2 does not use any other components besides the reaction reactants, it does consume 9% of higher methanol than case 1. This increases significantly the PEI value, but it is still lower than case 2. Apparently, this result seems to influence the PEI value of the process material output streams. Note that the output stream assessment excluded the biodiesel and glycerol product streams as to avoid unnecessary penalization for producing chemical with high demands. As indicated in Figure 8b, the PEI for the output stream of case 2 is more environmentally friendly than case 1. Given that case 2 requires no catalyst and acid or water washing step, the amount and type of raw materials is reduced, as is the amount of effluents and

Table 4. Specific Potential Environmental Impacts of Components

components	HTPI[a] (mg/kg)	HTPE[b] (ppm)	ATP[c] (ppm)	TTP[a] (mg/kg)	GWP[d]	POCP[d]	AP[d]	ODP[d]	EF
oil	–[e]	–	–	–	–	–	–	–	–
methanol	5628	200	29400	5628	–	0.123	–	–	–
NaOH	–	2	–	–	–	–	–	–	–
glycerol	12600	10	58.5[f]	12600	–	–	–	–	–
biodiesel	–	–	–	–	–	0.223	–	–	–
water	–	–	–	–	–	–	–	–	–
H_3PO_4	1530	1	–	1530	–	–	–	–	–
Na_3PO_4	4150	15	220[g]	4150	–	–	–	–	–
SO_x	1.2	–	–	1.2	–	–	1	–	2.7×10^{-3}
NO_x	0.78	–	–	0.78	–	–	1.77	–	1.8×10^{-3}
CO_2	–	–	–	–	1	–	–	–	3.7×10^{-1}
HCl	–	–	–	–	–	–	0.88	–	9.0×10^{-5}
methane	–	–	–	–	35	0.007	–	–	4.8×10^{-1}
mercury	–	0.025	–	–	–	–	–	–	4.9×10^{-9}

[a] LD_{50} (oral, rat). [b] TWA-TLV (CGIH). [c] LC_{50} (fathead minnow). [d] Classification factors published by Heijung et al.[22] [e] Denotes either nonapplicable or nondetermined data. [f] LC_{50} (trout). [g] LC_{50} (bluegill sunfish).

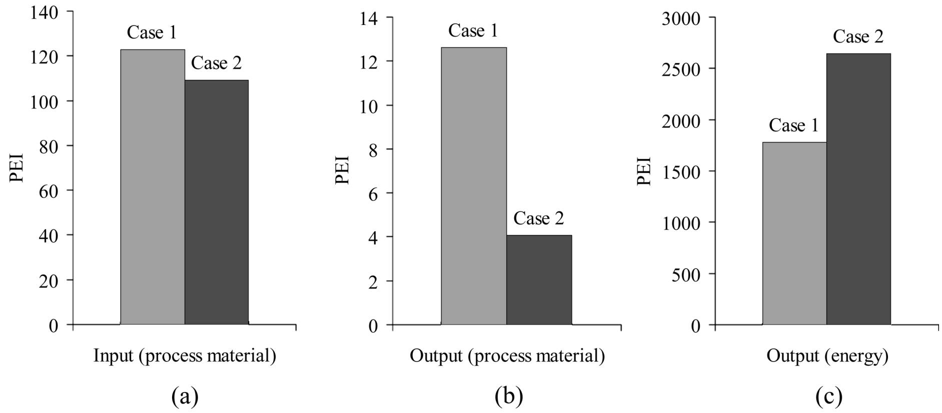


Figure 8. Total rate of the PEI: (a) the input (process material), (b) the output (process material), and (c) the output (energy).

Table 6. Social Criteria Assessment Results

soft indicators	score case 1	case 2	justification
safety during operation	5	3.5	Case 2 operates at very high pressure and temperature, thus exposing workers to a higher risk.
operability of the plant	5	6	Case 2 involves integrated equipment, e.g., heat exchanger and reactor. This may create difficulty in process control because of the influence of disturbances from other equipment. On the other hand, case 2 is able to compensate for the high amount of FFA in the feedstock, therefore enabling the use of used cooking oil as feedstock. Furthermore, exclusion of water and catalyst eliminate saponification and soap formation effect.
safe start-up and shutdown	5	3	Operation at very high pressure and temperature usually requires tedious and complicated start-up and shutdown procedures.
design should meet location specific demands	10	10	Criteria met.

waste generated. Overall, as far as the process material is concerned, case 2 performs better than case 1. However, a contrary result is found when energy usage is taken into consideration. Figure 8c shows the PEI output energy of both processes, which indicates that case 2 has a higher value. This result is expected, since case 2 operates at a very high pressure and temperature, and thus, it consumes a large amount of energy. Furthermore, the requirement for recirculation of a large amount of methanol to the process also contributes significantly to energy consumption. This finding agrees with the study conducted by Kiwjaroun et al.[31] For the social criteria, the evaluation of both processes is heuristic, due to the soft type indicators whose score is indicated in Table 6. Justification for each indicator is also provided in the table.

4.3. Decision Making. Weight Assignment and Ranking of Indicators. Figure 3 shows the weights assigned to the indicators in parentheses and the corresponding normalized vectors in square brackets. Note that the economic criterion is taken as the basis for comparison in the second level, whereas NPV, total PEI output, and safety during operation are the basis for comparison in the third level, representing the economic, environmental, and social criteria, respectively. Weight assignment is subjective. Nevertheless, justification for such decision is important. As previously mentioned, the economic feasibility in the biodiesel industry is vital for its survival. Although there have been increasing awareness to the environment, biodiesel production generally uses and produces nontoxic and nonpollutant materials. Therefore, a weight of 1/2 is assigned to the environment criterion, which indicates an intermediate value, less important than the economic criterion. On the other hand, a comparison between economy and social criteria is assigned by a value of 1/1.5, which shows near equal importance. Overall, for the second level, the economy and social criteria influence 46.1% and 30.9% of the total decision, respectively, while the environment influence is 23%. The remaining weights and normalized vectors for the third and fourth levels are shown in Figure 3. Note that the weights assigned to the normalized vectors indicate the percentage importance of the criteria in the overall decision of its parent level. Performing evaluation in AHP requires the assessors to be aware of the contradictory behavior between the value desirability of the indicators that are sometimes overlooked. Arguably, this behavior can be categorized as *higher-value—higher-desirability* (HVHD) and *lower-value—higher-desirability* (LVHD). While the HVHD is obvious, such as profits, the LVHD refers to the inverse behavior, which prefers a lower value. This type of behavior is closely related to the environmental indicators, such as CO_2 emission and the PEI. Such proportional and inverse value desirability behavior could create confusion, especially for the ranking purpose. Therefore, in order to make the evaluation consistent, a score-based approach is proposed. The approach works by converting the indicator value into a score of 1−10. For an indicator with the HVHD behavior, a high value is assigned to a high score. Inversely, for a LVHD indicator, a low value is assigned to a high score (see Table 7). The conversion from the initial indicator value, v, to its corresponding score, S, is shown below.

For HVHD,

$$S_{\mathrm{HVHD}}^{ij} = \frac{v^{ij}}{a_{\mathrm{u}}^{ij}}(b_{\mathrm{u}}^{ij}) \tag{15}$$

and for LVHD,

$$S_{\mathrm{LVHD}}^{ij} = \frac{a_{\mathrm{u}}^{ij}}{v^{ij}}(b_{\mathrm{l}}^{ij}) \tag{16}$$

where v^{ij} is the initial value of ith indicator for jth criteria. a_{u}^{ij} is the value for the upper value margin of the indicator. b_{u}^{ij} and b_{l}^{ij} correspond to the upper and lower score margin for the designated indicators, respectively. Once the corresponding score has been defined, the procedure for calculation of the normalized value remains the same and variation of the value margin does not affect the normalization value. Note that the calculation

Table 7. Conversion Parameters for the Proposed Score-Based Approach

		scores			
		value margin, a		score margin, b	
criteria	indicator	upper, a_u	lower, a_l	upper, b_u	lower, b_l
econ	NPV, $	10^6	0	10	1
	DCFRR, %	100	0	10	1
env	total rate PEI output	3000	0	1	10
	total PEI output/prod.	3	0	1	10
	total rate PEI gen	3000	0	1	10
	total PEI gen/prod.	3	0	1	10
social	safety during operation	10	1	10	1
	operability of the plant	10	1	10	1
	safe start-up and shutdown	10	1	10	1
	design should meet location specific demands	10	1	10	1

procedure is not shown here. Interested readers could refer to Marsh et al.[27] for details.

Scoring. Figure 9 illustrates the normalized scores for the criteria and the final solution. The normalized score for the economic criteria in Figure 9a shows that case 2 has its advantage over case 1. As previously mentioned, case 2 has a lower production cost, which contributes to a long-term profit, despite having a higher initial investment cost. However, for the environmental criterion, case 1 is environmentally more friendly than case 2 (see Figure 9b), which is due to its large energy consumption. Note than the environmental score is an inverse of the indicators value. Figure 9c depicts the normalized score for the social indicators. Case 1 has the advantage over case 2, as reflected by a larger area. Mainly, a process that is operated at a lower temperature and a lower pressure is more preferable due to safety concerns and the simplicity of operation, start-up, and shutdown procedures. But the main advantage of case 2, however, is the capability of processing oil feed materials with a high content of FFA. Thus, it is able to provide better plant operability despite the variation in oil FFA content. This crucial attribute manages to close up the social advantage gap between these two processes. Overall, the normalized score of the criteria is summarized in Figure 9d. It is found that case 2 is more economically desirable, but the other two criteria prefer case 1. Unlike any other decision-making methodology, AHP considers a quantitative evaluation of indicators, which makes the decisions made more justified. Adding all the scores for the criteria, the final result prefers case 1 with a score 12.8% higher than that of case 2. This difference is very much influenced by the modifications made to the process models and the weights in the AHP procedure. For the latter, an analysis on the effect of weight modifications to design selectivity is discussed below.

Effects of Decision Weights to Decision Result. Sensitivity analysis is performed by changing the weight of the selected criterion while fixing the others to 1. The percentage difference, %Diff, of the final normalized score between each case can be readily calculated by the equation

$$\%\text{Diff} = \left[\frac{S^{N^\circ} - S_i^{N}}{S^{N^\circ}}\right] \times 100\% \quad i = 1,2,3... \tag{17}$$

where S^{N° is the base case normalized score that acts as a reference value; S_i^N is the normalized score for the ith case. A positive percentage difference indicates that the base case

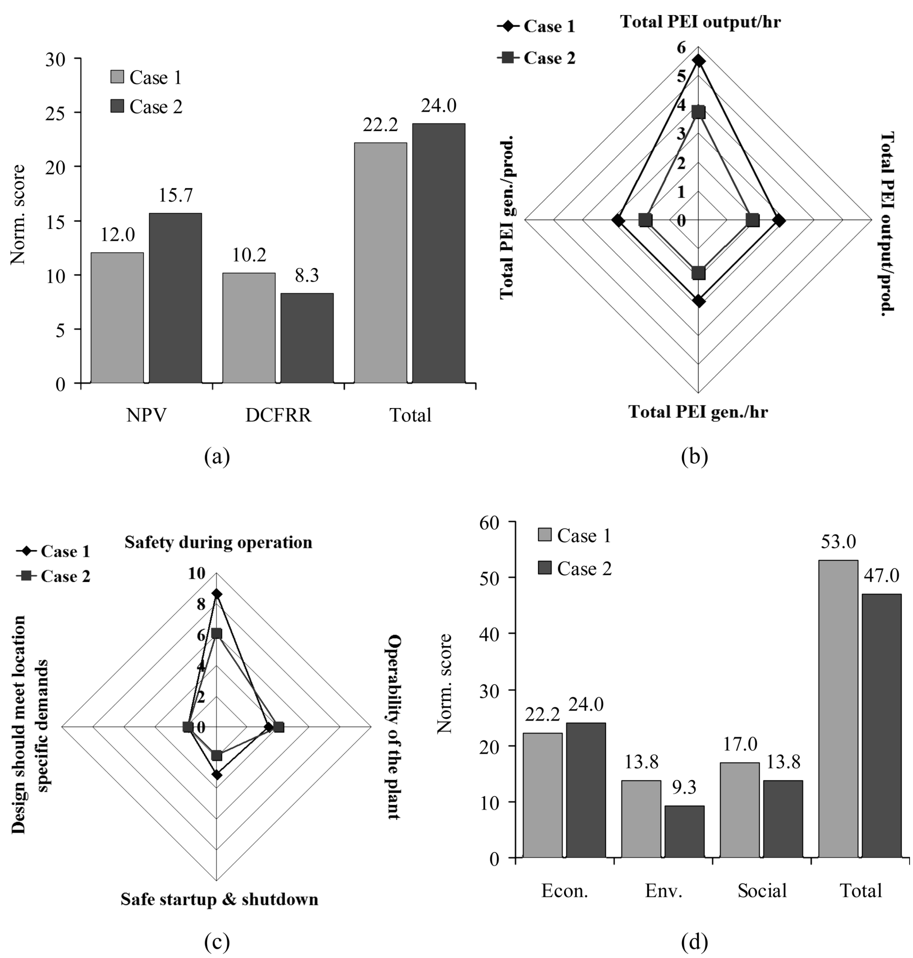


Figure 9. Normalized scores for (a) the economic criteria, (b) the environmental criteria, (c) the social criteria, and (d) the overall score and final result.

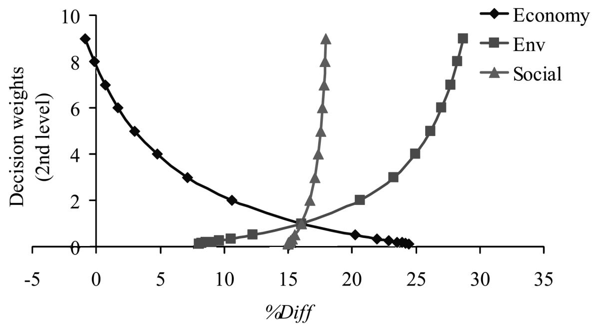


Figure 10. Sensitivity analysis of the decision weights at the second level decision hierarchy.

is more preferable, whereas a negative percentage indicates otherwise. Figure 10 shows the sensitivity analysis of the second level decision hierarchy; economic, environment, and social decision weights toward the final selection of the alternatives. It clearly shows that modifications of the decision weights significantly affect the final decision selection. Increasing weights for the environment and social criteria increases the selectivity toward case 1. This is consistent with the high score achieved by case 1 (shown in Figure 9) in the environment and social criteria, which leads to these preferences. On the other hand, increasing the economic weights decreases the selectivity of case 1 and the preferability moves toward case 2. This effect corresponds to the high score in economics achieved by case 2. Figure 10 also indicates that, if all the weights were equal, the selection result prefers case 1, shown at the intersection point of the three curves with the difference margin of 16.1%.

5. Concluding Remarks

In this work, we have presented a systematic and modularized framework for sustainability assessment and selection of chemical process design alternatives. The framework of the assessment methodology utilizes specifically defined indicators that consider both hard and soft performance of process design. This not only offers a quantitative evaluation but also imparts a knowledge-based solution, thereby providing the decision makers with important and holistic information for achieving sustainable design. A multicriterion decision hierarchy is also established to embed the indicators, and the AHP methodology is adopted for performing trade-offs among the economic−environment−social criteria in solution derivation. The assessment and decision support methodology is built in four modules with an integrated function utilizing the integration capabilities of process simulators and a spreadsheet. With its structured form, the assessors are able to focus on the real issues involving process design development. Furthermore, it allows the involvement of a multidisciplinary team in process design evaluation. The case study on biodiesel process evaluation shows the methodological effectiveness in assessing sustainable conscious process design and supporting persuasive decision making, thus showing its pre-eminence over commonly practiced technoeconomy evaluation approaches.

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