Design Guidance for Chemical Processes Using Environmental and Economic Assessments

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Traditionally, process design is focused on the selection of process technologies and optimization of chemical processes based on economic considerations. Increasingly, there is a need to broaden the scope of process design by including environmental impacts. To successfully optimize a process, multiple objective functions must be chosen to consider a variety of economic and environmental process attributes. The objective of this paper is to provide design procedures and guidance for optimizing chemical processes simultaneously based on economic and environmental aspects. Two chemical processes are studied, including a process to recover/recycle VOCs (volatile organic chemicals) from a gaseous waste stream and optimum heat-exchanger network design.

1. Introduction

Typically, traditional process design and optimization are based on economic objectives, such as fixed capital investment, net present value (NPV), operating cost, and payback period. The environmental impacts of process design have been given a lower priority and are generally incorporated into traditional design as end-of-pipe treatment. This design procedure may often overlook the production of large quantities of waste materials and pollution. Over the past decade, as a result of escalating environmental control costs and newly issued environmental regulations, industries are showing increasing interests in minimizing environmental impacts of design.

How does one incorporate environmental perspectives into traditional design and optimization? There are two main ways in which environmental concerns are included. The most common approach is to treat environmental considerations as constraints on economic optimization. For example, Dantus and High[1] developed an economic-based methodology to minimize waste and reduce energy consumption in the chemical industry by modifying existing processes while satisfying all of the environmental, product specification, and profitability constraints. The economic objective, based on the NPV that incorporated both manufacturing and capital costs, was used to select the most profitable technology. Others used annualized profit,[2,3] payback period,[4] or operation cost[5,6] as objectives. Cano-Ruiz and McRae[7] stated that "the main problem with incorporating environmental considerations as constraints...is that the proposed solutions may not address the underlying environmental concerns". This problem was also addressed by El-Halwagi[8] and Srinivas and El-Halwagi.[9] Furthermore, there is no assurance that a more favorable design is not available had the constraints been omitted. The other approach is to treat environmental requirements as objectives together with other objectives such as multiobjective optimization. For example, Ciric and Jia[3] proposed a multiobjective optimization scheme for simultaneously minimizing waste generation and maximizing profits. Chang and Hwang[10] formulated mathematical programming models which took both economical incentives (annualized cost) and environmental penalties (global emission) into account to seek the best design of utility systems. Cano-Ruiz and McRae[7] summarized typical environmental objectives including the "mass of pollutant of concern",[11] "total mass of waste",[12,13] "contribution to specific environmental problems",[14,15] and "overall indicator of environmental impact".[16,17] In the multiobjective optimization, it is often difficult to find an optimum that satisfies both economic and environmental objectives. Also, different environmental objectives may be conflicting or competing; that is, improving one may deteriorate the others. The central point of multiobjective optimization is to reveal the tradeoffs between these two kinds of objectives.

There are several systematic environmental impact assessment methodologies providing environmental objectives appearing in the literature, including life-cycle assessment (LCA),[18] waste reduction algorithm (WAR),[19] methodology for environmental impact minimization (MEIM),[20] and environmental fate and risk assessment tool (EFRAT).[21] All of these methodologies have been incorporated into the design and optimization of chemical processes. For example, Azapagic[22] described an application of LCA for volatile organic chemical (VOC) removal from a dyestuffs manufacturing plant. Four techniques were compared in order to obtain the best practicable environmental option (BPEO). MEIM has been applied to the optimization of continuous and batch processes, for example, the production of vinyl chloride monomer from ethylene[23] and the dairy industry.[24]

Although there are a number of methodologies and tools for environmental assessment of chemical processes that have appeared in the recent literature, most of the commercial process simulation packages can only build simple objective functions, based on economics. In addition, there are few properties in the simulation packages to evaluate environmental impacts, and the simulators do not have the ability to perform decision analysis. As a result, automated tools for environmentally conscious design need further development. Finally, there is a critical need for design procedures and guidance for this integrated design.

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Current design guidance and heuristics were derived with a focus on economics. For example, in the design of distillation columns, the reflux ratio is recommended to be 1.2 times the minimum reflux ratio, based on an economical analysis.[25] Nonetheless, there are efforts leading to preliminary design guidance in environmentally conscious product design. For example, Argonne National Laboratory[26] developed the GREET (greenhouse gases, regulated emissions, and energy use in transportation) model to assist the selection of fuel and transportation technologies to reduce emissions of VOCs, CO_2, NO_X, SO_X, and PM_{10} (particulate matter, less than 10 μm in diameter). Romero-Hernandez et al.[27] developed a framework for evaluating wastewater treatment technologies based on economic and environmental objectives. They investigated the tradeoffs between economic input, such as energy consumption and raw material costs, and environmental impact outputs and derived an optimal degree of pollutant abatement (ODPA). This ODPA can provide process engineers and regulators with guidelines to design treatment processes.

In the next section, two major features of design guidance are reviewed and the objectives of this paper are discussed. Then two typical chemical processes were studied in order to provide some design procedures and guidance for environmentally conscious process design and optimization. These cases include (1) VOC recovery/recycling from a gaseous waste stream using absorption and distillation and (2) optimum heat-exchanger network (HEN) design.

2. Environmentally Conscious Design Guidance

The process by which chemical manufacturing facilities are designed has undergone an evolution over the last 4 decades.[7] Initially, only the reaction and separation processes were designed and optimized with the goal of maximizing profitability. In the 1970s and 1980s, because of the global energy crisis, utility systems were added to the reactor/separator processes in process design and optimization. Today, the scope of design has expanded to include considerations of environmental impacts, other life-cycle stages, and waste treatment. Furthermore, the design process has been adapted for in-process pollution prevention, for example, by including generation of design alternatives using the hierarchy approach of Douglas.[28,29] Methods for evaluating environmental impacts have been applied in a hierarchical fashion, from simple toxicity-based screening assessments of reaction pathways and materials to complex risk assessment approaches that incorporate environmental fate modeling.[30]

Design guidance for environmentally conscious chemical process design has two major features: (a) tools, methodologies, and analysis frameworks that facilitate process synthesis and evaluation for pollution prevention and (b) feedback from detailed process analysis and optimization in the form of heuristics regarding the environmental and economic performance of designs. Many advances in the first area of design guidance have occurred as discussed previously, including the use of documented pollution prevention solutions, hierarchical design and structured thinking methods, pinch analysis, mathematical programming, and artificial intelligence approaches.[7] However, even with these developments, there still exists a broad range of, and therefore a lack in standardization for, environmental impact evaluation

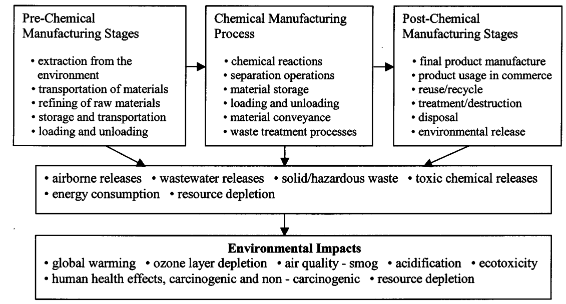

Figure 1. Environmentally conscious design: Life-cycle impacts of chemicals production.

methods. Fewer advances have occurred in the second area of design guidance, that of heuristics. The primary reason for this is that many more process optimization studies have been conducted using only economic assessments, few using only environmental assessments, and fewer still where economic and environmental assessments were conducted together.

In this paper, we make contributions to both of these design guidance areas. First, we propose a set of guidelines for chemical process environmental impact evaluation. These guidelines should aid researchers and designers in the activities of data gathering and impact analysis. They will also illustrate some of the challenges to be expected when conducting these assessments. Second, we will present results from two detailed process optimization studies where economic and environmental impact assessments were evaluated simultaneously. These results will point to similarities and differences in optimum process configurations based on either economic or environmental performance measures.

2.1. Framework for Environmental Impact Evaluation of Chemical Processes. The chemical manufacturing process is only one step in the life-cycle chain of chemical production leading to many products. Figure 1 shows the relationship between a chemical manufacturing process and other life-cycle stages. Using Figure 1 as a guide, it is apparent that both pre- and post-manufacturing stages need to be included in the impact assessment of chemical manufacturing process designs. Decisions regarding materials utilization within the chemical manufacturing process itself should be made based not only on the properties of these materials but also on the impacts of their manufacturing processes. This is so because materials can differ significantly in their energy and waste generation intensities.[30] In the same way, postmanufacturing stages can pose significant environmental hazards that should be considered during process design. For example, the choice of solvents to use in paint manufacture should be made knowing that the solvent will volatilize during the use stage of the life cycle, causing exposure to users and the environment. Anticipated waste treatment choices should also affect process decisions. A chlorinated solvent that would ultimately be incinerated might generate higher molecular weight chlorinated organics, such as dioxin, that pose significantly greater health threats than the solvent itself.

2.2. Environmentally Conscious Chemical Process Design Heuristics. Design feedback (heuristics) should be based on multiobjective optimization which incorporates both environmental and economic objectives. The environmental impact evaluation should

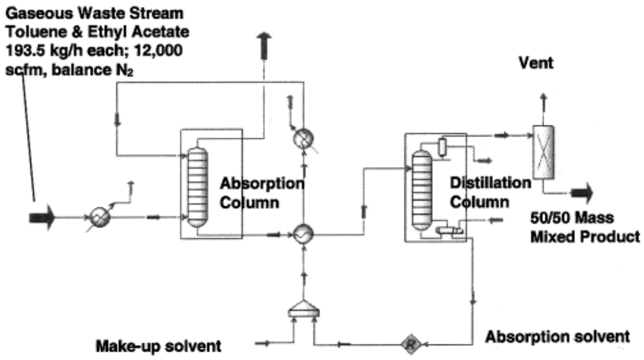

Figure 2. Process flowsheet of VOC recovery/recyling.

include multiple impact categories and include a life-cycle approach. Applications of these design guidance principles for environmentally conscious design are presented next.

3. VOC Recovery/Recycling

3.1. Process Description. Figure 2 is a simplified process flow diagram of an absorption−distillation process to recover and recycle gaseous waste stream VOCs (toluene and ethyl acetate).[31] The gaseous waste stream entering the process is cooled in order to enhance absorption. The absorption solvent flows downward through the absorption column and countercurrent to the gas stream. The mixture of solvent and VOCs is preheated using the recycle solvent stream and then fed into the distillation column to separate solvent from the mixture. The solvent then is recycled back to the absorption column. A small stream of make-up solvent is added in order to compensate for emission loss from the absorption column. The toluene/ethyl acetate mixture is stored in a storage tank prior to recycle to the original process.

The selection of a preferable absorption solvent was conducted by a screening methodology using economic and environmental assessments.[32] The procedure included solubility parameter constraints to screen out incompatible candidates, process specific property constraints (boiling and melting points), total operating cost assessment, and multicriteria environmental impact assessment. Ultimately, diethylene glycol monobutyl ether was the most preferable solvent candidate.

The base case design shown in Figure 2 was arrived at using economic-based rules of thumb. The minimum numbers of trays of absorption and distillation columns were obtained by Kresmer's equation[33] and the Fenske−Underwood equation,[25] respectively. The column diameter was determined from the flooding velocity.[34] The minimum reflux ratio of the distillation column was derived from the relative volatility.[25]

The process shown in Figure 2 was optimized by tuning process parameters. Two decision parameters have been identified based on scaled gradient analysis.[35] These are absorption solvent flow rate and absorption solvent temperature. The range of absorber solvent flow rate was chosen according to the turndown ratio of the two columns to avoid flooding and weeping. In this analysis it was assumed that both the absorption and distillation columns use valve trays having a liquid turndown ratio of 5. Another assumption was that, under normal operating conditions, the internal liquid velocity of each column was between the range of flooding velocity U_f/(turndown ratio) and U_f. Using these process constraints, a flow-rate range of 120−200 kgmol/h for the absorption solvent was obtained. The range of absorption solvent temperature was 26.7−37.8 °C based on the assumption that no additional refrigerant other than cooling water was available for use.

3.2. Process Simulation and Economic and Environmental Assessment. The process was simulated using a commercial simulator HYSYS (Hyprotech ltd., Calgary, Alberta, Canada). Based on material and energy balance results from HYSYS, the integrated assessment tool, SCENE (simultaneous comparisons of environmental and nonenvironmental criteria),[36] was used to evaluate the economic and environmental performance of the process design. The performance was measured using one index for economics and nine for the environment, as discussed below.

The economic assessment covered the purchase, installation, and operating cost of the absorber, condenser, distillation column, reboiler, storage tank, three coolers, and one heat exchanger, purchase cost of the make-up absorption solvent, sales revenue of the VOCs, and utility costs. Cost correlations for major pieces of equipment were generated and incorporated into the software in SCENE.[37] An indicator of profitability was used, NPV.

The environmental assessment for this case study includes a "gate-to-gate" assessment of impacts from the facility releases and energy consumption. After presenting these facility impacts, the effects of premanufacturing life-cycle stage impacts on raw materials and equipment will be compared and contrasted. Sources of pollutant release include the absorber and distillation column vents, storage tank, fugitive emission sources, and emission from utility consumption. The impact assessment methodology applied here, EFRAT,[21] integrates all steps of environmental assessment into a single software package. These steps include (1) process release estimation, (2) pollutant fate and transport calculation, (3) assessment of exposure potential, and (4) relative risk assessment. The relative risk index of chemical i for impact category k relative to a benchmark compound is represented by ($I^*_{i,k}$). The cumulative environmental impact for n chemicals emitted from the process for environmental impact category k (kg/yr) is

$$I_k = \sum_{i=1}^{n} (I^*_{i,k} E_i) \tag{1}$$

where E_i (kg/yr) is the emission rate of chemical i.

Nine categories of environmental impacts are included: fish toxicity (I_{FT}), human inhalation toxicity (I_{INH}), human ingestion toxicity (I_{ING}), human carcinogenic inhalation toxicity (I_{CINH}), human carcinogenic ingestion toxicity (I_{CING}), smog formation (I_{SF}), acid rain (I_{AR}), ozone depleting (I_{OD}), and global warming (I_{GW}).

A single process composite index is developed to aggregate these nine environmental indices. It is constructed by applying a normalization factor for each impact category index using national emissions data followed by a valuation step.[21] A normalization step is performed using eq 2 by dividing each environmental index, which is calculated using eq 1, by the output of environmental impact based on national emissions data,

$$I^k_N = I_k/\hat{I}_k \tag{2}$$

where I^k_N is the normalized environmental index for

Table 1. Weights, Average Index, and U.S. Annual Emissions for the VOC Recovery Case

environmental impact category	$\hat{E}_k$	weight	$\langle I^* \rangle_k$
global warming	5.50×10^{12} kg of CO_2/yr	2.5	1.0
smog formation	1.90×10^{10} kg of VOC/yr	2.5	0.39
acid rain	1.80×10^{10} kg of SO_2/yr	10	1.0
human noncarcinogenic inhalation toxicity	1.30×10^{9} kg/yr of TRI releases	5	121
human noncarcinogenic ingestion toxicity	1.30×10^{9} kg/yr of TRI releases	5	1329
fish toxicity	1.30×10^{9} kg/yr of TRI releases	10	0.83

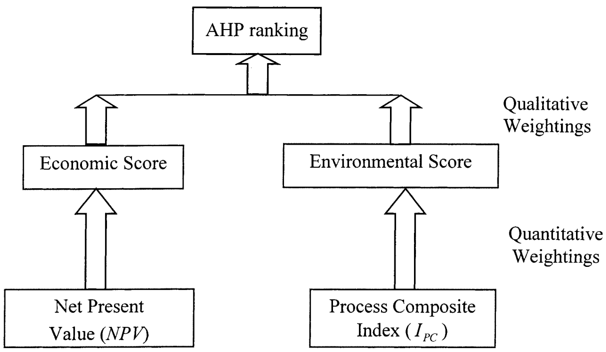

Figure 3. AHP hierarchy structure.

impact category k and $\hat{I}_k$ is the national output of environmental impact for category k (kg/yr), given by the following equation:

$$\hat{I}_k = \hat{E}_k \langle I^* \rangle_k \tag{3}$$

In eq 3, $\hat{E}_k$ is the national emission of chemicals representing impact category k (kg/yr) and $\langle I^* \rangle_k$ is, in general, the average relative risk index for these chemicals of importance to the national inventory obtained from the chemicals in the EFRAT database. The valuation step involves application of weighting factors to each environmental impact category based on their "distance to target" (EcoIndicator 95 method), where the target value is sufficiently low to ensure adequate protection of human and ecosystem health.[17]

The process composite index is calculated using eq 4, where the summation is taken over all impact

$$I_{\mathrm{PC}} = \sum_k I_{\mathrm{N}}^k W_k \tag{4}$$

categories k and W_k is the impact category k weighting factor.[17] A summary of this method for calculating the process composite index I_{PC} is also found in work by Shonnard and Hiew.[21] Table 1 shows the values of $\hat{E}_k$, $\langle I^* \rangle_k$, and W_k for each impact category k used in this study.

The economic and environmental objectives were aggregated into a single objective function using the analytic hierarchy process (AHP).[38] Figure 3 demonstrates the hierarchy structure for this study. At the bottom of the hierarchy are an economic index (NPV) and the process composite environmental index (I_{PC}). These indices are normalized by a maximum value over the parameter space, and the results are converted to quantitative scores.[39] The qualitative weightings of economic and environmental attributes are provided by Dechanpanya,[40] who carried out a survey. The final weighting factors are 0.82 and 0.18 for economics and environment, respectively.

The AHP score of the process design equals the sum of the products of the average process score for a given attribute and the weighting for that attribute, that is,

$$AHP = (\underset{\substack{\uparrow \\ \text{Economic}}}{Weight} * Score + \underset{\substack{\uparrow \\ \text{Environment}}}{Weight} * Score) \tag{5}$$

The process was optimized using a "brute force" methodology; that is, a number of process simulations were performed using HYSYS, and the corresponding environmental and economic assessments were carried out sequentially using the SCENE software. The range of the absorption solvent flow rate was divided into 8 equal segments, while that of the absorption temperature was divided into 10 equal segments. A total number of 99 simulations and assessments was conducted. The AHP scores of these 99 cases were compared to achieve a final ranking of the process parameters.

3.3. Premanufacturing LCA. As stated earlier, the environmental assessment for this case study includes a "gate-to-gate" assessment of impacts from facility releases and from facility energy consumption. Besides these impacts, the effects of other life-cycle stages are also investigated. Because the products from this process are recycled to the original process, the postmanufacturing stages are not included in the analysis. Only the effects of premanufacturing stages on raw materials and equipment are considered.

The premanufacturing life-cycle impacts from this process are quantified using the economic input−output LCA (EIOLCA)[41] developed by Carnegie Mellon University. This method estimates the environmental impacts from the emission of specific pollutants based on the purchase and installation costs of equipment and the purchase cost of materials. Purchase costs and installation costs were estimated for each major piece of equipment in the process using the DORT (design options ranking tool) software within SCENE. In addition, life-cycle emissions from the materials used in the process (natural gas and absorption solvent) were also estimated using EIOLCA. The EIOLCA method is a "cradle-to-gate" impact assessment, up to the facility gate. The EFRAT assessment described earlier contributes the operational impacts of using the equipment and materials in the process shown in Figure 2. Together EFRAT and EIOLCA provide a complete assessment from cradle to facility gate (out).

3.4. Results and Discussion. First, a gate-to-gate environmental impact assessment and economic analysis of the process shown in Figure 2 will be presented. Afterward, the contributions of premanufacturing life-cycle stages will be presented and compared to the gate-to-gate analysis. The reason for conducting the assessment in this fashion is because the impact indices from EFRAT and EIOLCA are inherently incompatible and not easily combined into a more encompassing analysis.

In the feasible ranges of these two operating parameters, toluene is almost completely recovered. Figure 4 shows the variation of ethyl acetate recovery due to the absorption solvent flow rate and absorption temperature. The recovery of ethyl acetate increases dramati-

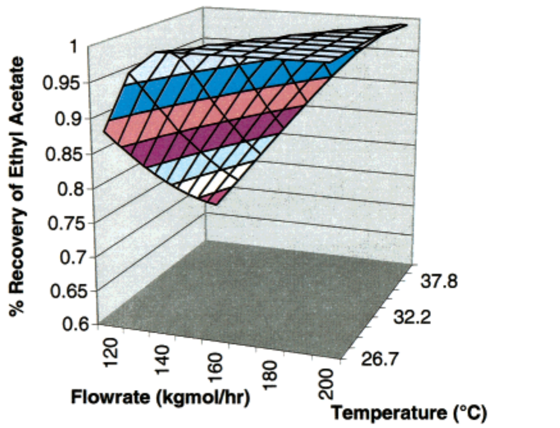

Figure 4. Variation of percent recovery of ethyl acetate due to absorption solvent flow rate and temperature.

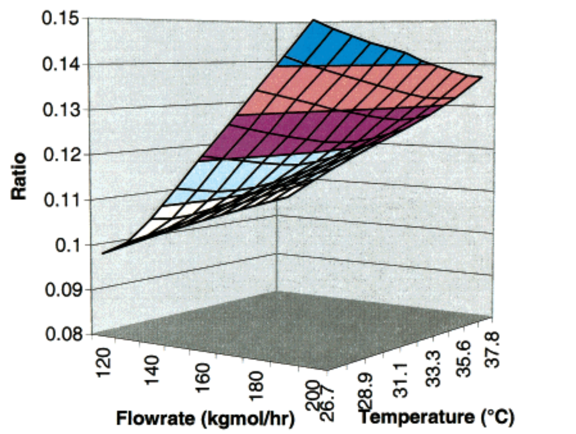

Figure 5. Variation of the ratio of natural gas usage to the VOCs recovered due to absorption solvent flow rate and temperature.

cally as the absorption solvent flow rate increases and the absorption temperature decreases. However, the rate of change for ethyl acetate recovery is very small within a narrow range of parameter space when ethyl acetate recovery exceeds 95%.

Figure 5 shows the effect of the absorption solvent flow rate and absorption temperature on the ratio of the natural gas usage rate to the total recovery rate of VOCs. Natural gas provides the energy for the distillation reboiler. This index is an indicator of resource utilization efficiency in the process and ranges from about 0.1 to 0.15 over the range of parameters. A higher value of this index means a less efficient process with regard to materials utilization. The materials utilization efficiency of the process decreases as more ethyl acetate is recovered, especially at high absorption solvent flow rates.

The values of the fish toxicity index (I_{FT}) are shown in Figure 6. The human ingestion toxicity index (I_{ING}) and smog formation index (I_{SF}) have response surfaces similar to that of the fish toxicity index. These indices decrease with increasing absorption solvent flow rate and with decreasing temperature as more VOCs are recovered from the waste stream. These indices, to various degrees, are influenced mostly by the emission of VOCs, carbon monoxide, and absorption solvent. Almost 100% recovery of the VOCs is needed to minimize these environmental indices. The human inhalation toxicity index (I_{INH}) has a surface similar to that of the fish toxicity index. It decreases with decreasing temperature but decreases dramatically, reaches the

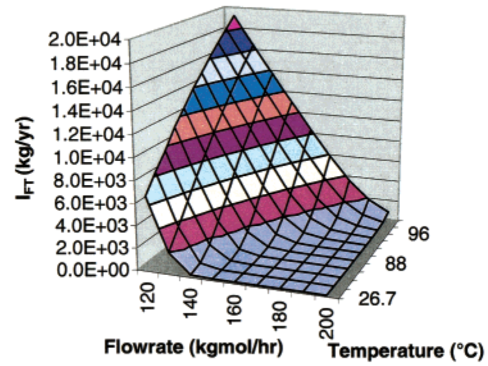

Figure 6. Variation of I_{FT} due to absorption solvent flow rate and temperature.

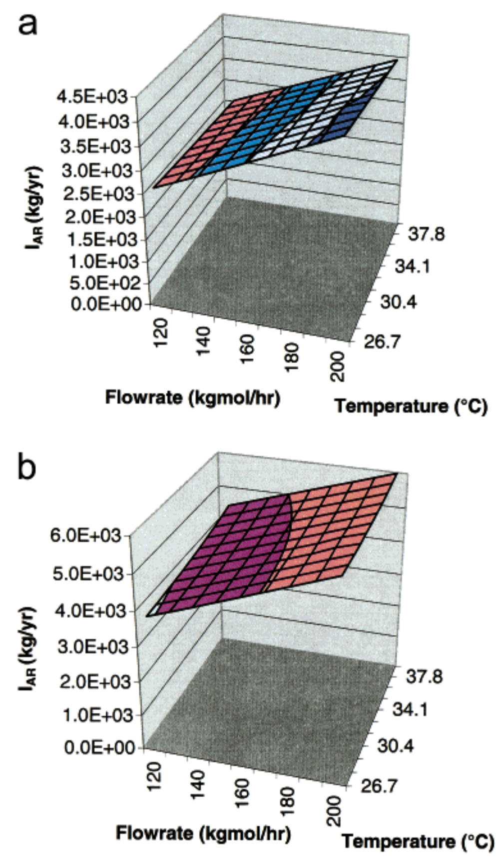

Figure 7. (a) Variation of I_{AR} due to absorption solvent flow rate and temperature. (b) Variation of total I_{AR} including operational impact and life-cycle impact due to absorption solvent flow rate and temperature (the emission of SO_2 from the premanufacturing stage is in the range of $8.41 \times 10^5 - 1.30 \times 10^6$ kg/yr).

minimum, and then slightly increases with increasing absorption solvent flow rate.

The acid rain index (Figure 7a) is influenced only by the emissions from utility consumption. Utility usage is the least when the temperature is highest and the absorption solvent flow rate is lowest, that is, 37.8 °C and 120 kgmol/h. The global warming index (Figure 8a) is dominated by both VOC emissions and utility consumption. As the absorption solvent flow rate increases, the global warming index decreases first and then increases. At absorption solvent flow rates lower than the minimum, the index is dominated by the emissions of VOCs, while at higher flow rate, utility consumption dominates the index.

Clearly, there are tradeoffs observed in Figures 6−8 in terms of the optimum absorption solvent flow rate

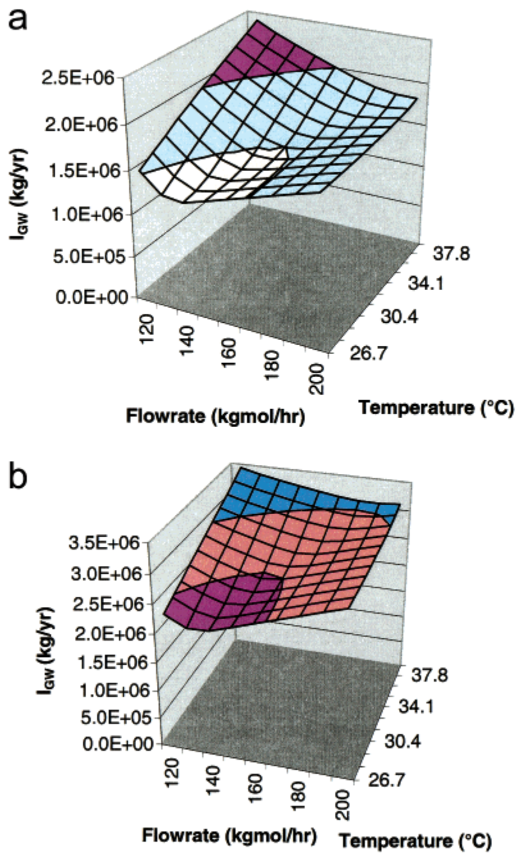

Figure 8. (a) Variation of I_{GW} due to absorption solvent flow rate and temperature. (b) Variation of total I_{GW} including operational impact and life-cycle impact due to absorption solvent flow rate and temperature (the emission of CO_2 from the premanufacturing stage is in the range of $1.24 \times 10^3 - 2.05 \times 10^3$ kg/yr).

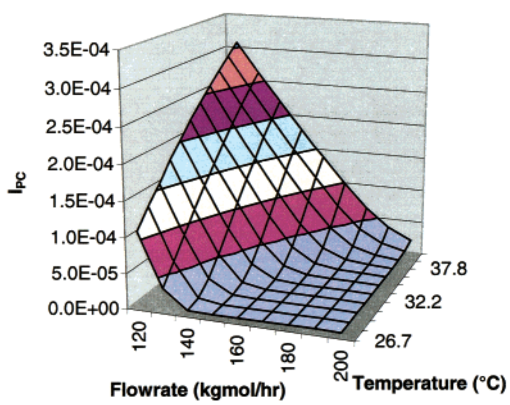

Figure 9. Variation of I_{PC} due to absorption solvent flow rate and temperature.

and absorption temperature. For example, high flow rate and low temperature are optimum to reduce toxicity but low flow rate and high temperature are required to minimize acidification impacts, and at low temperature and medium flow rate the process performs best for global warming impact. Figure 9 shows the process composite environmental index (I_{PC}), which is minimized at an absorption solvent flow rate of 150 kgmol/h and a temperature of 26.7 °C. This index is mainly dominated by I_{FT}, I_{INH}, I_{SF}, and I_{AR}. At high absorption temperature or low absorption solvent flow rate, the fish toxicity is the major contributor to I_{PC}. At other points in the parameter space, those four indices contribute nearly equally.

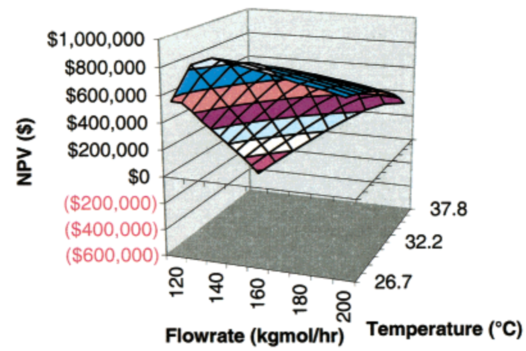

Figure 10. Variation of NPV due to absorption solvent flow rate and temperature.

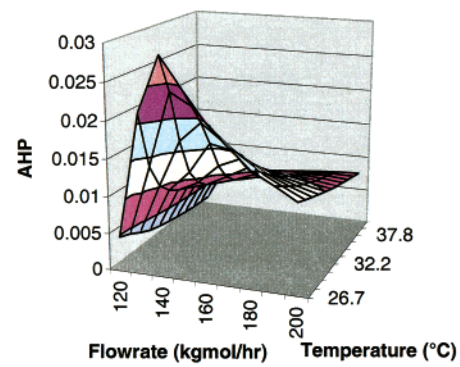

Figure 11. Variation of AHP score due to absorption solvent flow rate and temperature.

A sensitivity study of the multiplification factor of each index, $W_k/\hat{I}_k$, was conducted by varying each multiplification factor up 20% and down 20% around the base value. The shape of the I_{PC} response surface changes very little. The minimum environmental impact point remains the same (150 kgmol/h and 26.7 °C), and the value is between 7.22×10^{-6} and 1.04×10^{-5}. The process has the best performance at the same parameter configuration even though the uncertainties of the normalization and weighting factors are considered. Therefore, the decisions regarding the process configuration could be made with a good degree of confidence.

Figure 10 shows NPV as a function of the absorption solvent flow rate and the absorption temperature. The optimum configuration to maximize NPV is 140 kgmol/h and 26.7 °C. NPV is determined by the revenue of the VOC product, which is related to the recovery of VOCs, and the utility consumption. As the flow rate increases, NPV increases first and then decreases. At lower flow rates, NPV is enhanced by significant gains in recovery of VOC product, while at higher rates, NPV is diminished by negligible gains in product recovery and by increasing rates of utility consumption. Figure 11 shows the variations of AHP scores with the absorption solvent flow rate and the absorption temperature. These optimization results show that the process has the best performance based on an aggregation of environmental and economic considerations at the absorption solvent flow rate of 140 kgmol/h and the absorption temperature of 26.7 °C. Other sets of weightings to economic and environmental aspects were investigated, such as equal weights and larger environment weights (environment, 0.82; economics, 0.18). The process still has the best performance at 140 kgmol/h and 26.7 °C.

The effects of premanufacturing life-cycle stages will be presented next. To compare the premanufacturing

Table 2. Data of the HEN Case

stream	source temp T_s (°C)	target temp T_t (°C)	heat capacity flow rate C (kW/°C)	heat load Q (kW)
C1	60	160	7.62	762
C2	116	260	6.08	875.5
H1	160	93	8.79	588.9
H2	249	138	10.55	1171
cooling water (cw): $T_s = 38$ °C, $T_t \leq 82$ °C				
steam (satd, s): $T = 270$ °C cost of cw = 0.00034 $/kg				
cost of $s = 0.015$ $/kg				
capital cost of heat exchangers				
double pipe: $K_1 = 3.0238$, $K_2 = 0.0603$, $K_3 = 0$				
fixed tube sheet or U-tube: $K_1 = 3.2138$, $K_2 = 0.2688$, $K_3 = 0.079\ 61$				
annualized factor: $r = 0.23852$ yr^{-1}, $r' = 0.3221$ yr^{-1}				
equipment operability: 8500 h/yr				

life-cycle impacts with operational impacts, the emissions of equivalent CO_2 and SO_2 are calculated because they are the only indices that are compatible with EFRAT (I_{GW} and I_{AR}). Figures 7b and 8b show the variations of total I_{GW} and I_{AR} (including both manufacturing and premanufacturing life-cycle impacts). The shape of either I_{GW} or I_{AR} changes only slightly, and the minimum of I_{GW} is shifted to lower absorption solvent flow rate, 130 kgmol/h in Figure 8b vs 140 kgmol/h in Figure 8a. The impacts from the manufacturing life-cycle stage contribute 58−70% to I_{GW} and 57−75% to I_{AR}, with the remainder contributed by the premanufacturing life-cycle impacts. Although this life-cycle assessment is limited to the premanufacturing and operational stages and to only two environmental indices, we conclude that both premanufacturing and operational impacts contribute significantly both to the magnitude of the impact and to the location of the optimum.

Based on these results, there are a number of useful lessons for design guidance. First, the optimum parameter values for operating this separation process were *similar but not identical* for both the economic and environmental assessments of the design. The economic optimum configuration requires a lower recovery of VOCs compared to the environmental optimum. Second, the most striking differences in the optimum process configuration were among the various environmental impact categories. There is a critical need to reconcile these sorts of tradeoffs among competing environmental impact objectives. To accomplish this, in this study a methodology of normalization and valuation was implemented to derive a single aggregated environmental index (I_{PC}). Third, there exist many challenges for incorporating all life-cycle impacts of materials, energy, and products into chemical process design. Whereas a number of impact assessment tools are available that link effectively with commercial process simulators, such a linkage with pre- and postmanufacturing life-cycle stages is not as easy. In addition, there are several incompatibilities in the methods of impact assessment between chemical process design assessment tools such as WAR and EFRAT and life-cycle assessment tools such as EcoIndicator 95 and -99 and EIOLCA that need to be addressed before environmentally conscious chemical process design using commercial process simulators can be fully realized.

4. Heat-Exchanger Network (HEN)

4.1. Process Description. Heat exchangers are important unit operations in chemical processes and also for many other manufacturing processes. Optimum design of HENs can reduce energy consumption and improve the economic performance of the processes. One important element in the design of HENs is the establishment of an optimum minimum approach temperature for streams entering and leaving the exchangers (ΔT_{min}). Previous work for establishing ΔT_{min} has focused on economic tradeoffs between capital and operating costs. The case study presented here, taken from Linnhoff and Flower,[42,43] is a multiobjective optimization problem in which environmental assessments were included with traditional economics in the evaluation of optimum ΔT_{min}. In this case study, a network of heat exchangers is to be synthesized for two hot and two cold streams. The stream data are listed in Table 2. There are four steps in this work: HEN synthesis, economic evaluation, environmental impact assessment, and establishment of an optimum minimum approach temperature.

4.2. HEN Synthesis. Generally, there are two approaches to the HEN synthesis: the graphical method and the algorithmic method. The algorithmic approach[25,44] is applied here.

There are many papers describing algorithms for HEN synthesis. Given a minimum approach temperature (ΔT_{min}) of hot and cold process streams and the input information about the streams and utilities, the temperature intervals of the HEN are defined. With these temperature intervals, the heat transfer and residual enthalpy in each interval are calculated by an enthalpy balance. The minimum external energy duty of the HEN is calculated by solving the linear program (LP).[25] Based on the minimum utilities, the stream matching of the HEN is performed with the objective to minimize the number of heat exchangers.[45] Although the minimum number of heat exchanger does not mean minimum capital cost, the result is close to the absolute optimum and is regarded as one of the important HEN design methods. The heat exchangers can be positioned by solving the mixed-integer LP (MILP).[45] The Lindo software[46] was used in this research to perform the LP and MILP calculations.

4.3. Economic Evaluation. The economic evaluation is based on annualized purchase and operating costs. The purchase cost of heat exchangers is the arithmetic mean of the results obtained from four different sources. The purpose is to get a more credible capital cost, leading to more credible economic and environmental evaluation results.

(1) Correlation from Turton, et al.[47]

$$\log C_p = K_1 + K_2 \log A + K_3(\log A)^2 \qquad (6)$$

where C_p is the purchase cost of the equipment ($) and A is the heat-transfer area (m^2). The correlation coefficients K_1, K_2, and K_3 are given for double pipe and fixed tube sheet or U tube, respectively, and those yielding the smaller C_p in our selection of heat exchangers were chosen.

(2) Vendor's quote, provided by SEC heat exchangers, Canada.[48] These shell and tube heat exchangers use stainless steel AISI 316L, their working pressure is 250 psi at 406 °F, and their working temperature is −4 to +406 °F: model C-8.19.90 (0.761 m^2), $400; model P-43.06.50 (4.0 m^2), $1400; model C-188.37.50 (17.5 m^2), $3900.

Using eq 7 to calculate capital cost for the heat exchangers with similar areas,

$$\frac{C_{p1}}{C_{p2}} = \left(\frac{A_1}{A_2}\right)^{0.6} \tag{7}$$

where C_{p1} and C_{p2} are the purchase costs of the heat exchangers 1 and 2 ($) and A_1 and A_2 are the heat-transfer areas of the heat exchangers 1 and 2 (m^2).

(3) Results from one equipment capital cost estimate website, Matches.[49]

(4) Results from the DORT software within SCENE.

The installed cost and annualized cost are calculated by eqs 8 and 9 using the purchase cost taken from the arithmetic mean of the above four methods.

$$C_c = 3.5C_p \tag{8}$$

$$C_A = rC_c + sF_s + (\mathrm{cw})F_{cw} \tag{9}$$

where C_p is the purchase cost of the equipment ($), C_c is the installed capital cost ($), C_A is the annualized cost ($/yr), and r is the annualized factor (0.238 52 yr^{-1}), assuming that a 10-yr project life and a minimum acceptable rate of return of 0.2 are chosen. F_s and F_{cw} are the annual flow rates of steam and cooling water, respectively (kg/yr), and s and cw are the unit costs of steam and cooling water, respectively ($/kg).

4.4. Environmental Assessment. The environmental assessment for this case study also includes the impacts both from the premanufacturing stages and from the impacts of the manufacturing process (the HEN operation). Because a HEN has no product other than internal energy exchange and the environmental impacts from disposal of the heat exchangers are small relative to the premanufacturing and manufacturing stages, the postmanufacturing stages are not included in this analysis.

The premanufacturing life-cycle impacts from this process were quantified using the EIOLCA[41] method. Using this method, the environmental impacts from the emission of specific pollutants based on the purchase and installation costs of heat exchangers were estimated. In addition, the premanufacturing life-cycle emissions from the materials used in the process (natural gas) were also estimated using the EIOLCA method. The cost of natural gas was calculated from the energy requirement of the HEN auxiliary duty considering an efficiency factor of 0.8.

In the manufacturing stage (the operation of the HEN), the life-cycle impacts were also quantified using the EIOLCA method. The environmental indices for the operation of the HEN were based on calculated external (auxiliary) utilities. Given the external energy duty of the HEN and the emission factors[50] of specific chemicals from the combustion of natural gas, the emission rates of criteria and toxic pollutants were developed. These indices are as follows: global warming index (CO_2 equivalent release), total toxic release (TTR), VOC, PM_{10}, SO_2, NO_X, and RCRA (Resource Conversation and Recovery Act) hazardous waste release, all in units of metric tons of annual release (Table 3).

Table 3. Weights and U.S. Annual Emissions of Environmental Indices for the HEN Case

environmental index	weight	U.S. annual emission (metric tons/yr)
CO_2 equivalent release	2.5	5.50×10^9
TTR	5	1.30×10^6
VOC release	2.5	1.90×10^7
PM_{10} release	2.5	2.76×10^7
SO_2 release	10	1.80×10^7
NO_X release	2.5	2.14×10^7
RCRA hazard release	5	2.58×10^8

Like the annualized cost, the annual environmental indices were calculated by integrating the indices of premanufacturing and manufacturing stages using eq 10. E'_i is the emission rate of each index listed in Table 3 (metric tons/yr), $E'_{i,\mathrm{equ}}$ is the emission from the purchase and installation of equipment (heat exchangers) in the premanufacturing stage (metric tons/yr), $E'_{i,\mathrm{mat}}$ is the emission from production of the material (natural gas) in the premanufacturing stage (metric tons/yr), $E'_{i,\mathrm{opr}}$ is the emission from the operation of heat exchangers in the manufacturing stage (metric tons/yr), and r' is the environmental annualization factor (0.1 yr^{-1}). This factor allows the emission of the premanufacturing stage to be "spread out" over the life of the project, in a manner similar to that of capital costs. The seven environmental indices were combined into a single normalized and weighted environmental index using the methods of eq 4.

$$E'_i = r'(E'_{i,\mathrm{equ}}) + E'_{i,\mathrm{mat}} + E'_{i,\mathrm{opr}} \tag{10}$$

Once the economic and environmental indices were calculated for a given $\Delta T_{\min}$, this parameter was changed and the indices were recalculated.

4.5. Establishment of an Optimum Minimum Approach Temperature. The economic and environmental results were aggregated into a single-objective function using the AHP.[38] The economic index (annualized cost) and the process composite environmental index (I_{PC}) were normalized by a value from the process that is not likely to be exceeded (a maximum value over the parameter space), and the results are converted to quantitative scores.[39] Qualitative weightings for economic and environmental attributes are generated by pairwise comparisons. The final weighting factors are 0.82 and 0.18 for economics and environment.

4.6. Results and Discussion. Figure 12 shows that the minimum in the annualized cost occurs at approximately a $\Delta T_{\min}$ of 8 °C. Prior work[42−44,51] shows that the optimum $\Delta T_{\min}$ varies with process conditions and depends on the complexity of the case study, the cost correlations for equipment, and cost parameters of streams and utility consumption. However, the value determined in this study, 8 °C, is within the range determined in other studies.

Figure 13 shows that the $\Delta T_{\min}$ of the normalized and weighted environmental index (I_{PC}) is 5 °C, which is less than the economic optimum $\Delta T_{\min}$ but is similar.

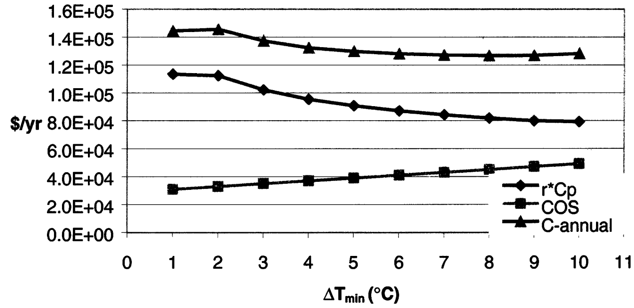

Figure 12. Variation of annualized cost due to minimum approach temperature ($\Delta T_{\min}$).

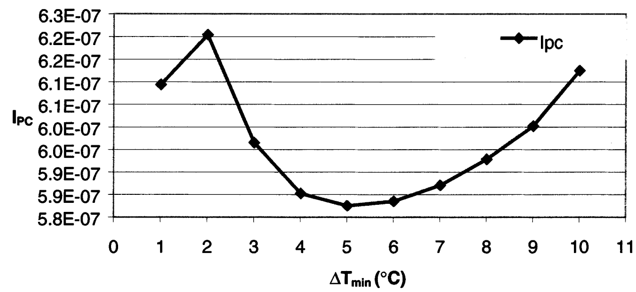

Figure 13. Variation of I_{PC} due to minimum approach temperature ($\Delta T_{\min}$).

Because there are environmental penalties associated with energy use, a lower approach temperature saves energy and reduces impacts but at the expense of larger equipment. The existence of the similar minimum point is primarily due to only two indices that are the most significant contributors to I_{PC}: TTR and CO_2 equivalent release. TTR decreases with increasing $\Delta T_{\min}$ as do the capital equipment costs in Figure 12 and is dominated by premanufacturing life-cycle stage releases. CO_2 equivalent release increases with increasing $\Delta T_{\min}$ as do the operating costs in Figure 12 and is dominated by the releases from the manufacturing life-cycle stage (HEN operation). Contributions to I_{PC} from each environmental index in descending order are TTR > CO_2 equivalent release > SO_2 > RCRA hazardous waste > NO_X > VOC > PM_{10}.

As in the previous case study for VOC recovery and recycle, this HEN design study indicates a close correspondence between the economic and environmental optimum configuration of the process. The life-cycle impacts from the premanufacturing stages become a dominant factor in I_{PC} when the exchanger size increases dramatically at low values of $\Delta T_{\min}$. Finally, the environmental optimum $\Delta T_{\min}$ is a function of the weighting and normalization steps and also the way that emissions from the premanufacturing life-cycle stage are "spread out or amortized" over the life of the project. Choosing different weightings for each impact index will affect the outcome, as will be shown next.

The most dominant environmental indices are CO_2 equivalent release and TTR. The weights of these two indices were changed, and the effects are shown in Figures 14 and 15. The environmental optimum $\Delta T_{\min}$ decreases from 8 to 1 °C with respect to the change of weight of CO_2 equivalent from 0.5 to 10, while keeping the weight of TTR and other indices constant. The environmental impacts of the operation of the network are dominant when the weighting of CO_2 equivalent release increases; thus, the optimum $\Delta T_{\min}$ decreases. Similarly, the environmental optimum ΔT_{min} increases from 1 °C to 8 °C with respect to the change of weight

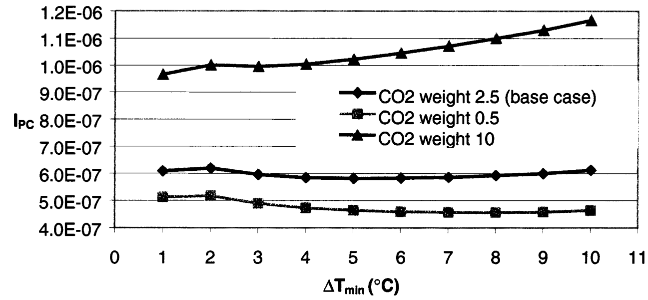

Figure 14. Variation of I_{PC} due to the weight of CO_2 equivalent release.

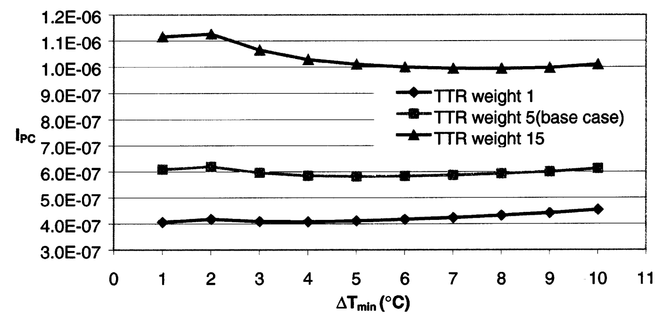

Figure 15. Variation of I_{PC} due to the weight of TTR.

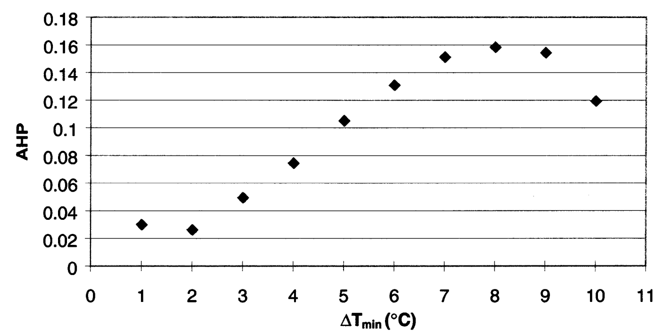

Figure 16. Variation of AHP score due to minimum approach temperature ($\Delta T_{\min}$).

of TTR equivalent from 1 to 15, while keeping the weight of CO_2 and other indices constant. Thus, the manner of weighting environmental indices to create a single aggregate index has a significant effect on the outcome of the optimization.

Figure 16 shows the variations of AHP scores with the optimum minimum approach temperature ($\Delta T_{\min}$). These optimization results show that the process has the best performance based on both environmental and economic considerations at the optimum minimum approach temperature ($\Delta T_{\min}$) of 8 °C, which is identical as the economic optimum.

In this HEN case study, the environmental indices used for the premanufacturing stages were identical to the indices used for the HEN operation stage (manufacturing stage). Thus, there were no incompatibilities between the indices from different life-cycle stages (in the VOC recovery study, there were incompatibilities). However, the disadvantage in using the EIOLCA indices is that environmental transport and the fate of pollutants are not incorporated. Thus, although the EIOLCA method provides a comprehensive inventory of releases by the relevant industrial sectors of the economy, the impact assessment is not as sophisticated as other impact assessment methods (see the Introduction). The design guidance from this case study regarding the optimum $\Delta T_{\min}$ for the HEN should be regarded as preliminary because of the uncertainties in the environmental and economic assessments and the need to analyze many more case studies.

5. Conclusion

This paper describes two major features of environmentally conscious chemical process design guidance: (1) tools and methodologies and (2) heuristics. This paper contributes to both of these design guidance areas. First, we proposed a set of guidelines for chemical process environmental impact evaluation and multicriteria analysis. These guidelines should aid researchers and designers in the activities of data gathering and impact analysis. Second, process design evaluations were conducted for two important classes of unit operations in chemical processes: separations and heat exchange. The assessments for each case included both environmental and economic indices of performance. Although it is difficult to state generally applicable design guidelines from such a small number of studies, there are a few useful insights that have emerged.

A. In all cases both the environmental and economic assessments provided similar optimum design configurations. This might suggest that performing only economics-based optimization is sufficient to minimize environmental impacts of design.

B. In both the VOC recovery and HEN case studies, the environmental assessment leads the decision maker to design these processes for a higher degree of mass and energy recovery compared to the economic assessment.

C. In the VOC recovery, premanufacturing life-cycle impacts for global warming and for acidification are less important compared to the manufacturing stage impacts, although both stages contributed significantly to I_{PC}.

D. The environmental assessment is complex, and it yields a number of indices for different environmental impact categories. The methods of combining these various indices and the uncertainties in the factors for normalization and weighting have a significant influence on the outcome.

E. Including premanufacturing life-cycle stages can have a profound effect on the environmental assessment and optimization, as shown in the HEN study.

F. Finally, incompatibilities exist in the methodologies for environmental impact assessment used for various life-cycle stages of chemical processes. It is recommended that a standard set of indicators be adopted to facilitate the assessment of manufacturing and pre- and postmanufacturing life-cycle impacts of chemical process designs.

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