

OPTIMIZATION OF A DISTILLATION UNIT IN TERMS OF POTENTIAL ENVIRONMENTAL IMPACT AND ECONOMICS

(Pengoptimuman Unit Penyulingan dari Segi Potensi Impak Ekonomi dan Alam Sekitar)

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Abstract

Process energy integration and continuous improvement of process technology are increasing issues to ensure profitability of chemical productions. These objectives are increasingly important due to long-term environmental impact of energy degradation, such as resource depletion, emissions and the release of “waste” heat. The earlier energy conservation, process economics and environmental aspects are integrated into the process development, the easier and less expensive it is to improve the process design. In this work different distillation process design alternatives have been considered with respect to evaluations of process economics and potential environmental impacts. “Optimum design alternatives” are analyzed related to these objectives. A multi-criteria decision making technique such as (Analytic Hierarchy Process) AHP is applied for ranking the alternatives. This method reveals that the heat pump distillation unit which has the highest score of 52 % is the best alternative when compare with base case. In terms of the effluent streams the base case has a less potential environmental impact (PEI) compared with heat pump. The lower total PEI/kg (7.45E-01) of the base case illustrates that the material utilization efficiency of the base case is better than the heat pump whose PEI/kg is 8.14E-01.

Keywords: economic, thermodynamic efficiency, distillation unit, waste reduction (WAR) algorithm

Abstrak

Peningkatan yang berterusan dalam integrasi proses tenaga dan proses teknologi adalah isu-isu yang semakin diperbincangkan untuk memastikan keuntungan dalam pengeluaran kimia. Objektif ini semakin penting disebabkan kesan jangka panjang terhadap alam sekitar akibat kemerosotan tenaga, seperti kehabisan sumber, pelepasan dan pembebasan haba "sisa". Pemuliharaan tenaga yang lebih awal, proses ekonomi dan aspek-aspek alam sekitar disepadukan ke dalam proses pembangunan, lebih mudah dan lebih murah untuk memperbaiki proses rekabentuk. Dalam kejian ini proses rekabentuk alternatif yang berbeza telah dipertimbangkan dalam kombinasi dengan penilaian proses ekonomi dan kesan terhadap alam sekitar yang berpotensi. "Alternatif reka bentuk optimum" telah dianalisis seiring dengan objektif ini. Teknik membuat sesuatu keputusan pelbagai kriteria seperti (Proses Hierarki Analisis) AHP diaplikasikan untuk memperbaharui kedudukan. Kaedah ini mendapati bahawa rekabentuk pam haba yang mempunyai skor tertinggi sebanyak 52% adalah alternatif terbaik. Dari segi asas pengaliran pengeluaran kumbahan ianya mempunyai kesan yang kurang berpotensi terhadap alam sekitar (PEI) berbanding dengan pam haba. Jumlah PEI / kg (7.45E-01) yang lebih rendah dalam penggunaan bahan asas menunjukkan bahawa kecekapan penggunaan bahan asas adalah lebih baik daripada pam haba (PEI / kg 8.14E-01).

Kata kunci: ekonomi, kecekapan termodinamik, penyulingan unit, pengurangan sisa (PERANG) algoritma

Introduction

Currently the chemical process industries rely on distillation processes to separate chemical mixtures into pure products. Due to their high energy-intensive, energy-efficient design and operation are therefore important issues. The importance of alternative energy efficient design distillation columns has become more necessary not only due to the continuous depletion of limited fossil fuel stock but also consideration of better environmental system during

early design or retrofitting stages. Traditionally, chemical process design and optimization are more focus towards economic objective such as total annualized cost (TAC). Less attention has been given to environmental impact of process design; they are generally integrated into traditional design as end-of-pipe treatment [1]. As a result of newly issued environmental regulations, there is a growing interest of minimizing environmental impacts of chemical process design.

Energy efficient design process can help reduce the quantity of pollution or waste generated during operation of a manufacturing process. However, a design with less waste does not necessarily have lower impacts on the environment, since the wastes may have a higher contribution to the potential environmental impacts than another design with a larger amount of waste but a lower environmental effect [2]. Hui et al. [1] suggested that there are two ways of integrating environmental perspectives into traditional design and optimization, the most popular method is to treat environmental considerations as constraints, for example Dantus et al. [3] did developed a methodology based on economic to minimise waste and reduce energy consumption, however Cano-Ruiz [4] stated that “the main problem with incorporating environmental considerations as constraints is that the proposed solutions may not address the underlying environmental concerns”. The other alternative is to treat environmental requirement as objective. Among the most recent systematic methods for the assessment of environmental impacts of chemicals processes includes, life cycle assessment (LCA) [5], the environmental fate and risk assessment tool [6], thermodynamic analysis method (emergy and exergy) [7] and waste reduction (WAR) algorithm introduced by Hilaly and Sikdar [8]. Later Young and Cabezas [9] extended the PEI balance to include the consumption of energy of the process into the environmental evaluation. Morais et al. [10] did study the potential environmental impacts (PEIs) and economic potentials of alkali-catalysed trans-esterification process; they apply the Waste Reduction algorithm (WAR) to evaluate the potential environmental impacts (PEIs) of process alternatives. More recent studies on environmental impact assessment of chemical process plants can be found in [11, 12].

In this paper, the evaluation of energy related optimization of a technical multi-component distillation unit is presented. For every design alternative, the optimum solution is identified based on cost objective function. Environmental performance index based on WAR algorithm is used to evaluate environmental effects. Finally, a multi-criteria decision making technique such as (Analytic Hierarchy Process) AHP is applied for ranking the alternatives. The analysis is based on steady state simulation using Aspen PlusTM. A case study of a Hydrocarbon Recovery (HCR) plant is discussed to highlight the proposed methodology.

Methodology

As a first step in the design methodology, the design starts with framing of the problem (see Figure 1). This step consists of gathering thermodynamic data of the process flow sheet (base case) model. The process is modelled using Aspen PlusTM simulator. Mass and energy data from the Aspen PlusTM model are used to compute the exergy of the streams and thermodynamic efficiency. The process data from Aspen PlusTM are entered into the WAR Graphical user interface (GUI) in order to compute environmental criteria of the base case model. The process data information includes the chemicals used, the flow rates of the streams entering and leaving the process, and the energy usage of the process. The successive quadratic programming algorithm (SQP) in Aspen PlusTM is used for economic optimization. The next step is the generation and evaluation of alternatives which includes identifying energy saving alternatives. Finally, in the last step a multi-criteria decision making technique such as AHP is applied for ranking the alternatives.

Case study

This paper concentrates on the stripping column which is part of a Hydrocarbon Recovery (HCR) unit. Figure 2 provides a simple schematic illustration of the distillation unit (steam stripping column) unit from a real chemical plant. The main components of the feed stream are water, acetone, methanol, and acetic acid etc. The feed stream, which is close to its bubbling point enters the stripping column on tray 17. The column has a diameter of 0.728 m and 35 trays, where the rectifying section includes trays 1-15 and the stripping section 16-35. The column is operated with steam (550 - 650 kg/hr, 140°C and 3.75 bars) injection into the bottom below stage 35. The top pressure is 1.01 bar with reflux ratio of 0.7 (operating plant) and feed flow rate of 4000 kg/hr.

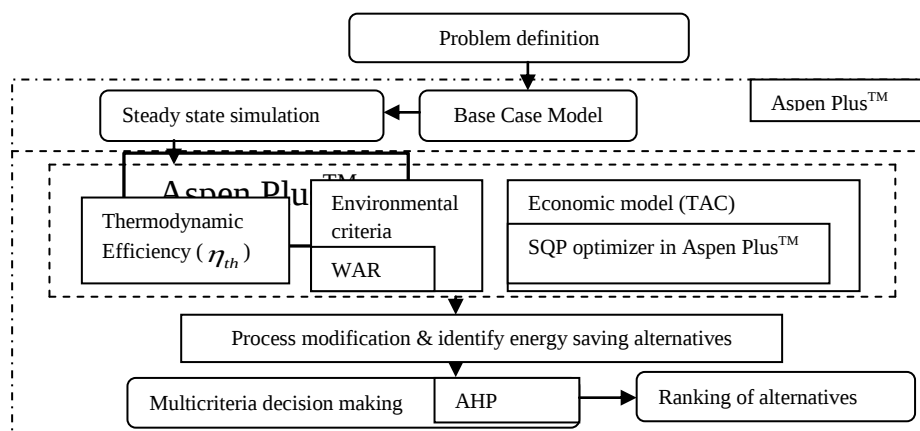


Figure1. Procedure of the integrated methodology.

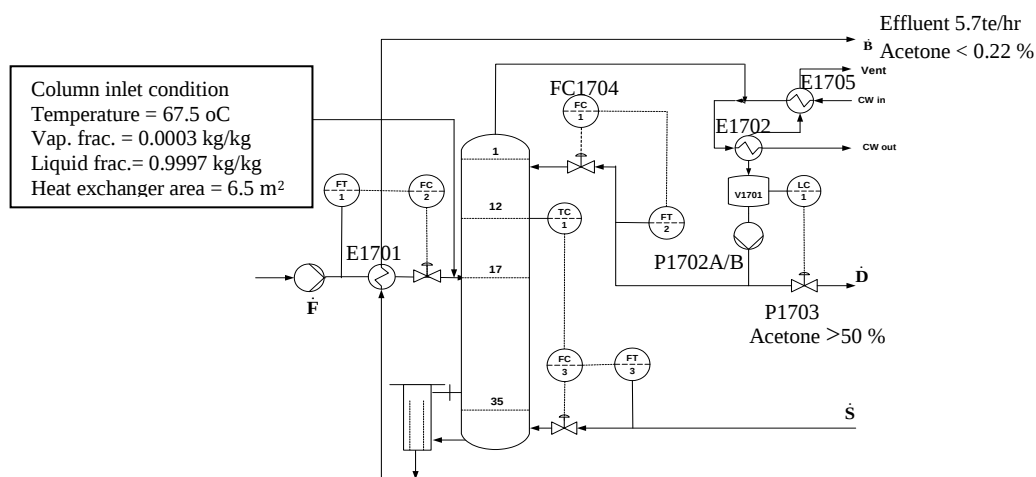


Figure 2. Base case flow sheet of a hydrocarbon recovery (HCR) unit.

The operating targets are as shown below:

Distillate: $x_{\text{Water}} < 10 \%$ (percentage of water by mass at distillate should be less than 10%), $x_{\text{Acetone}} > 50 \%$
 Bottom: $x_{\text{Acidity}} < 3 \%$, $x_{\text{Acetone}} < 0.22 \%$, $x_{\text{Methanol}} < 2 \%$

The acidity is the sum of the mass fraction of the acids i.e. acetic acid, formic acid and propionic acid. Acetone is the key component for the bottom and distillate qualities. The design alternative studied in this work is the heat pump distillation unit (see Figure 3). The head product is condensed in heat exchanger E1702 with the vent passing through heat exchanger E1705 to the atmosphere and the liquids are collected by reflux drum V1701. Using pump P1702A/B the reflux is transferred under flow control back into the column on stage 2. Since the feed flow rate changes continuously the set point of reflux control valve (FC1704) is fixed to high rates to prevent hydrocarbon from slipping through the base at different feed rates. The remaining crude acetone is pumped through product

control valve (P1703) and sent to the acetone recovery storage unit. The liquid level in V1701 is set to 50% under normal operating conditions. The base product passes the heat exchanger E1701 for cooling and is then discharged into the in-plant effluent pit.

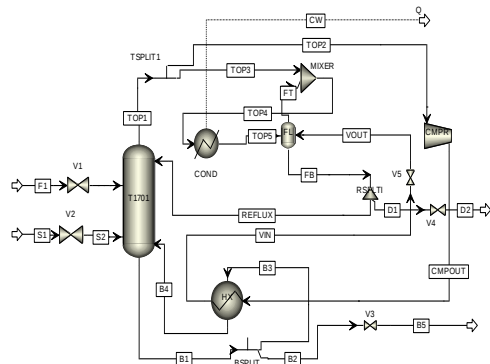


Figure 3. Aspen model for heat pump design alternative.

Environmental Criteria

The potential environmental impacts (PEI) of each alternative are evaluated using the waste reduction (WAR) algorithm developed by Young and Cabezas [12]. These environmental impact scores reflect the potential environmental harm of each chemical in the effluent stream (bottom stream) of the distillation column. These PEI categories are human toxicity by ingestion (HTPI) and by dermal/inhalation exposure (HTPE), terrestrial toxicity potential (TTP), aquatic toxicity potential (ATP), photo oxidation chemical potential (POCP), acidification potential (AP), global warming potential (GWP) and ozone depletion potential (ODP). The chemical PEI of each impact category is given by:

$$PEI_i = \sum_i^{Envt\ cat} w_i \cdot \dot{M}_b \cdot \sum_j^{comps} X_{kj} \cdot \psi_{ki} \quad (PEI/kg\ product) \quad (1)$$

PEI_i = PEI of category i,

w_i = weighting factor associated with PEI for each category I,

$\dot{M}_b$ = mass flow rate of effluent (bottom stream),

X_{kj} = mass fraction of chemical (component) k in base stream,

ψ_{ki} = Normalized impact score of chemical component k for category i.

The weighting (w_i) factors are used to combine PEI categories into a single PEI index. They represent the relative or site-specification concerns of the user. For instance, Douglas et al. [13] did mentioned that, if a user was evaluating a process that was located in the Los Angeles area the weighting factor for smog formation (PCOP) would probably receive a high value. Whereas, if the user was evaluating a process in the Northeast the weighting factor for acid rain (AP) would probably receive a high value, they concluded that since their case study has no specific site in mind, they assigned a weighting factor of unity for all the categories. This paper also follows this procedure of assigning a weighting factor of unity for all the categories. This gives the basis for assigning each category a weighting factor of unity in this paper.

Economic Model

In all stages of design process, estimation of Total annualized cost (TAC) is very important for the evaluation of process alternatives. In this section both the base case and heat pump distillation structures were investigated. Optimal operating conditions are determined for these distillation structures. TAC (Operational cost + Annualized

capital investment cost) is considered in this paper as the economic objective function. The estimation of the purchase cost of the distillation column, trays, condenser, compressor heat exchanger and the cost of their installation is considered as the Capital investment cost. The bare-module concept introduced by Seider [14] was used in the estimation of capital investment cost of each equipment. The total Capital investment ($\dot{C}_{TCI}$) cost is given by:

$$\dot{C}_{TCI} = (C_{cond} + C_{col} + C_{tray} + C_{comp} + C_{HX} + C_{flushdrum}) \cdot \dot{d} \quad (2)$$

C_{cond} =cost of condenser (\$),
 C_{col} =cost of distillation column (\$),
 C_{tray} =cost of tray (\$),
 C_{comp} =cost of compressor (\$),
 C_{HX} =cost of heat exchanger (\$),
 $C_{flush\ drum}$ =flush drum (\$),

where $\dot{d}$ is the depreciation or capital recovery factor and normally varies from 15 to 20% of the total fixed capital investment.

Operating cost

Operating cost is estimated in terms of utility cost of cooling water, steam and electrical energy consumption. The operating cost is formulated according to Douglas [15] as follows:

$$\dot{C}_{utility} = c_s \cdot \dot{M}_s \cdot (8000\text{ hr} / \text{yr}) + c_{cw} \cdot \dot{M}_{cw} \cdot (8000\text{ hr} / \text{yr}) + c_{el} \cdot \dot{P}_{el} \cdot (8000\text{ hr} / \text{y}) \quad (3)$$

$\dot{C}$ = cost per year (\$/yr),
 c_s =cost of steam (\$/kg),
 c_{cw} =cost of cooling water (\$/kg),
 c_{el} =cost of Electricity (\$/kW),
 $\dot{M}_s$ =Mass flow rate of steam (kg/hr),
 $\dot{M}_{cw}$ =Mass flow rate of cooling water (kg/hr),
 $\dot{P}_{el}$ =electrical power (kW).

The operating cost is estimated using the following utility prices in Table 1. For the examples studied in this paper, low pressure steams as well as cooling water costs data are taken from Douglas [15] and are assumed to be available as shown in Table 1.

Table 1. Economic data considered

Utility	cost
Cooling water, c_{cw}	0.07 \$/10 ³ kg
Low-pressure steam (5-10bar), c_s	8.8 \$/10 ³ kg
Electricity, c_{el}	0.04 \$/kWhr
Operating hours per year	8000 hr/yr

Thus total annualized cost is

$$\dot{C}_{TAC} = \dot{C}_{utility} + \dot{C}_{TCI} \quad (5)$$

Results and Discussion

In chemical processes, the operating conditions are often varied due to influence of market needs and price variations. It is therefore important to know what extent the distillation unit will tolerate to changes in its nominal operating condition and still maintain lower cost (TAC). Figure 4 shows the variation of steam flow rate with acetone recovery at the distillate. It can be observed that the target percentage of acetone recovery (55 % by mass) at the distillate is achieved with steam flow rate of 550kg/hr. Further increase in steam flow rate does not result in any significant increase in the acetone recovery instead it increases the operating cost which leads to increase in TAC (see Figure. 5). TAC can however be at it's minimum of 351×10^3 (\$/yr) at steam rate within the range of 550 to 560kg/hr.

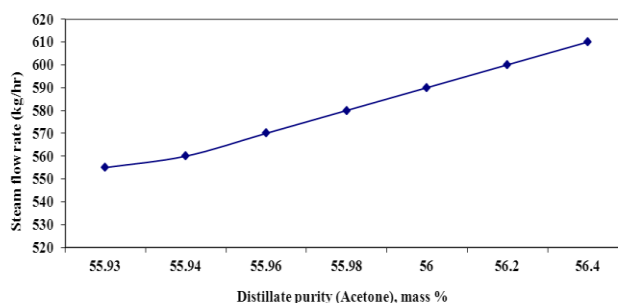


Figure 4. Variation of acetone recovery due to steam flow rate.

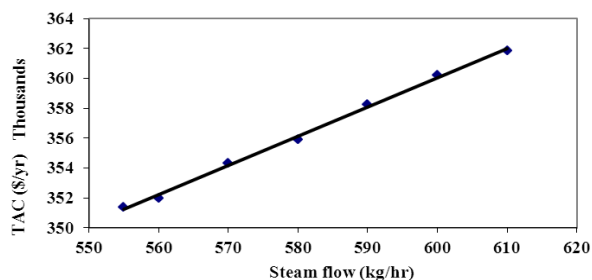


Figure 5. Variation of TAC due to steam flow rate

Environmental assessment

The contribution to the total potential environmental impacts (see Table 2) due to energy consumption decreases as the level of energy integration increases because energy consumption (steam) decreases. This result shows that the energy consumption of the heat pump has 30% decrease in total PEI when compared to the base case. Table 3 shows the comparison of PEI for both design alternatives on the basis of effluent stream discharge. A higher value of this index means a less efficient process with regard to materials utilization. The lower total PEI/kg (7.45×10^{-1}) of the base case illustrates that the material utilization efficiency of the base case is better than the heat pump (PEI/kg 8.14×10^{-1}).

Table 2. Normalized PEI score associated with the energy generation process.

Case	HTPI	HTPE	TTP	ATP	GWP	ODP	PCOP	AP	TOTAL
Base Case	5.94E-01	9.26E-03	5.94E-01	2.01E+00	1.46E+00	1.54E-05	5.36E-04	4.54E+01	5.01E+01
Heat Pump	3.25E-01	5.07E-03	3.25E-01	1.10E+00	8.02E-01	8.43E-06	2.94E-04	2.48E+01	2.74E+01

Table 3. Normalized Total PEI of effluent stream (bottom stream) per mass of products (PEI/kg product).

Case	HTPI	HTPE	TTP	ATP	GWP	ODP	PCOP	AP	TOTAL
Base Case	1.53E-01	1.98E-03	1.53E-01	7.32E-03	1.59E-03	1.67E-08	3.79E-01	4.92E-02	7.45E-01
Heat Pump	1.73E-01	2.23E-03	1.73E-01	7.15E-03	9.78E-04	1.03E-08	4.28E-01	3.03E-02	8.14E-01

Optimal operating conditions of base case model

Each potential environmental impacts category are caused by energy consumption and effluent streams. An optimization study was conducted for the base case model and the results show that as energy consumption (steam flow rate) increases the effluent streams decreases but the environmental impact due to energy and TAC increases. An optimum steam rate that satisfies both the environment and the TAC for base case model was reached as shown in Figure 6.

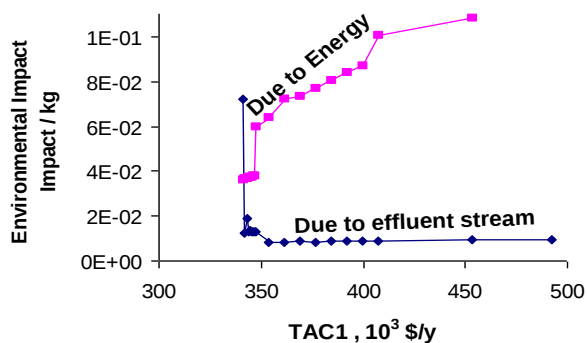


Figure 6. Effect of process variable (steam) on environment and TAC for base case.

The result also shows that steam consumption has more influence on PEI due to energy than due to effluent stream (see Figure 6). In terms of the effluent streams the base case has less PEI compared with heat pump (see Table 4). The lower total PEI/kg (7.45E-01) of the base case illustrates that the material utilization efficiency of the base case is better than the heat pump (PEI/kg 8.14E-01). The total exergy loss in the column decreased from 49.90kW for base case to 45.31kW for heat pump. The lower exergy loss of the heat pump model accounts for its higher thermodynamic efficiency (18.47%) (see Table 4). The product purity was within the target range as shown in Table 5.

Table 4. Cost and exergy analysis

Alternatives	Base case	Heat pump
Steam rate kg/hr	550.0	315.56
Reflux ratio	0.586	0.620
TAC [\$ /y]	351, 000	402, 000
η_{th} %	14.30	18.47
Exergy loss kW	49.92	45.31
PEI/kg	7.45E-01	8.14E-01

Table 5. Product purity

Product purity	Base case	Heat pump
Distillate compositions mass %		
$X_{\text{water}} < 10 \%$	2.19	2.75
$X_{\text{acetone}} < 50 \%$	55.9	63.20
Bottom compositions mass %		
$X_{\text{methanol}} < 2 \%$	1.48	1.67
$X_{\text{acidity}} < 3 \%$	2.49	2.69

Ranking of alternatives

The economic and environmental results were aggregated into a single-objective function as stated by Hui et. al. [1] (see equation 7). The economic index (TAC) and the process composite environmental index were normalized and the results are converted to quantitative scores. As part of the AHP method, the values of the pairwise comparison are determined by using a scale proposed by Satty [16]. The numerical values of this scale are used to calculate the priority weights of each criteria (economic or environment). The result of the pairwise comparison shows that economic, environment and thermodynamic efficiency (η_{th}) criteria have the following weights; 0.57, 0.29 and 0.16 respectively. The weighting results closely agree with the result of Hui et. al. [1], who computed the qualitative weighting factors of 0.82 and 0.18 for economic and environment respectively. According to Satty [16], the best alternative is indicated by:

$$A_{\text{AHP-score}} = \max_i \sum_{j=1}^n a_{ij} \cdot w_j, \quad \text{for } i = 1, 2, 3, \dots, m \quad (6)$$

The entry a_{ij} , represents the relative value of alternative A_i (base case or heat pump) when it is considered in terms of criteria C_j (economic or environment). Equation 6 was further modified by Hui et. al. [1]:

$$A_{\text{AHP-Score}} = (\underset{\substack{\uparrow \\ \text{Economic}}}{\text{Score}} \cdot \underset{\substack{\uparrow \\ \text{Environment}}}{\text{Weight}}) + \text{Score} \cdot \text{Weight} \quad (7)$$

When equation 7 is applied, the following scores were obtained for each alternative A_1 , $A_{\text{HP-score}} = 0.48$, A_2 , $A_{\text{HP-score}} = 0.52$

Therefore the best alternative is alternative A_2 (heat pump) because it has the highest AHP score; 0.52. This value is achieved because of low operating cost of the heat pump and also because of the higher thermodynamic efficiency of the heat pump.

Conclusion

There were a number of tradeoffs found in this study. As the level of energy integration increases the PEI increases. On the other hand as the level of heat integration increases, the column performance increases due to the higher thermodynamic efficiency of the heat pump (18.47 %) compared with the base case (14.30 %), which is evidence from the lower exergy loss of the heat pump distillation. The TAC of the heat pump was greater compared with the base case, this is due to the integration of process equipment such as heat exchanger and process machinery such as compressor to the heat pump design. With these trade-offs, the application of AHP method shows that the heat pump is the better alternative.

References

1. Hui Chen, Ya Wen, Michelle D. Waters, and David R. Shonnard. (2002). Design Guidance for Chemical Processes Using Environmental and Economic Assessments. *Ind. Eng. Chem. Res.*, 41, 4503-4513.
2. Teresa M. Mata, Raymond L. Smith, Douglas M. Young, Carlos A.V. Costa. (2003). Evaluating the environmental friendliness, economics and energy efficiency of chemical processes: heat integration, *Clean Techn Environ Policy* 5, 302-309.
3. Dantus, M. M.; High, K. A. (1996). Economic Evaluation for the Retrofit of Chemical Processes through Waste Minimization and Process Integration. *Ind. Eng. Chem. Res.*, 35, 4566.
4. Cano-Ruiz, J. A.; McRae, G. J. (1998). Environmental Conscious Chemical Process Design. *Annu. Rev. Energy Environ.* 23,499.
5. Lou, H.H., Kulkarni, M.A., Singh, A. and Hopper, J.R. (2004). Sustainability assessment for industrial systems. *Ind Eng Chem Res*, 43(15): 4233-4242.
6. Achour, M.H., Haroun, A.E., Schult, C.J., et al. (2005). A new method to assess the environmental risk of a chemical process Gasem. *Chem Eng Process*, 44(8): 901-909.
7. Hau, J.L., Yi, H.S. and Bakshi, B.R., (2007). Enhancing life cycle inventories via reconciliation with the laws of thermodynamics. *J Ind Ecol*, 11(4): 1-21
8. J. Rafael Alca'ntara-Avila, Manabu Kano, Shinji Hasebe. (2012). Environmental and economic optimization of distillation structures to produce anhydrous ethanol, *22nd European Symposium on Computer Aided Process Engineering*, 30: 712-716.
9. Wang, M., Shi, Y., Xia, X., Li, D., Chen, Q. (2013). Life-cycle energy efficiency and environmental impacts of bioethanol production from sweet potato. doi: [http:// dx.doi.org/10.1016/j.biortech.01.067](http://dx.doi.org/10.1016/j.biortech.01.067).
10. Gomez-Castro, F. I., Rico-Ramirez, V., Segovia-Hernandez, J. G., Hernandez-Castro, S., & El- Halwagi, M. M. (2013). Simulation Study on Biodiesel Production by Reactive Distillation with Methanol at High Pressure and Temperature: Impact on Costs and Pollutant Emissions, *Computers and Chemical Engineering* doi:10.1016/j.compchemeng.01.007.
11. Hilaly AK, Sikdar SK. (1994) Pollution balance: a new method for minimizing waste production in manufacturing processes. *J Air Waste Manag. Assoc* 44:1303-1308.
12. Young DM, Cabezas H. (1999). Designing sustainable processes with simulation: the waste reduction (WAR) algorithm. *Comput Chem Eng* 23:1477-1491.
13. Douglas Young, Richard Scharp, Heriberto Cabezas. (2000). The waste reduction (WAR) algorithm: environmental impacts, energy consumption, and engineering economics *Waste Management* 20 (2000) 605-615.
14. Seider, W. D., Seader, J.D., Lewin, D.R., 2003, *Product and Process Design principles, Synthesis, Analysis and Evaluation*, John Willey & Sons, Inc., New York. Pg. 142-145.
15. Douglas, J. M., (1988). *Conceptual Design of Chemical Processes*. McGraw-Hill Book Company, New York, pg.425-432.
16. Satty, T. (1980). *The Analytic Hierarchy Process*; McGraw-Hill: New York, pg. 560-601.