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Application of Sustainable Integrated Process Design and Control for Four Distillation Column Systems

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The objective of this paper is to present the application of sustainable integrated process design and control methodology for distillation columns systems. The sustainable integrated process design and control methodology is developed and able to find the optimal solution for a single distillation column to ensure the design is more cost efficient, controllable and sustainable to meet the product quality. The sustainable integrated process design and control problem for a distillation column system is typically formulated as a mathematical programming (optimization with constraints) problem, and solved by decomposing it to six sequential hierarchical sub-problems: (i) pre-analysis, (ii) design analysis, (iii) controller design analysis, (iv) sustainability analysis, (v) detailed economics analysis and (vi) final selection and verification. In the pre-analysis sub-problem, the concept of driving force is used to locate the optimal design-control-sustainable solution targets, which are defined at the maximum point of the driving force diagram. The sustainability analysis sub-problem was analysed by using the three-dimensional sustainability index. The results through separation of n-Pentane, n-Hexane, n-Heptane, n-Octane and n-Decane mixtures with four distillation column systems shows the methodology is capable to find the optimal solution for multiple distillation column systems that satisfies design, control and sustainability criteria in a simple and efficient way.

1. Introduction

The sustainable development is subject of global interest and has attained significant importance because of the growing concern with the preservation of natural resources and the increasing political and social pressure for the adoption of more sustainable practices. A sustainable company must generate profits while protecting the environment and improving the lives of those whom it interacts (Mattioda et al., 2013). The concept of Triple Bottom Line is used to integrate and optimise all the stages and product development design, which is oriented to the sustainability. Mata et al. (2014) had performed the sustainability evaluation in the production of biodiesel. Several sustainability indicators were considered in the sustainability evaluation.

Sustainability is made up from three principles which are environmental, economic and social. From the three principles of sustainability, three different sustainability indexes can be obtained which are one-dimensional (1-D), two-dimensional (2-D) and three-dimensional (3-D) indexes as shown in Figure 1 (Shadiya and High, 2010). Each index is represented with their indicator, use to assess the sustainability performance of a process or a system, in order to evaluate the progress toward enhancing the sustainability. Martins et al. (2010) has list out four indicators to calculate the 3-D sustainability index. Those indicators are material intensity (MI), energy intensity (EI), potential chemical risk (PCR) and potential environmental impact (PEI).

Integrated Process Design and Control (IPDC) methodology was developed and able to obtain an optimal solution for the IPDC problem (Hamid et al., 2010). The IPDC methodology has shown that distillation column design at the highest point of driving force (DF) is the best in term of design and controllability.

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However, the developed methodology for the IPDC did not consider sustainability aspect in the early of design stage. The IPDC methodology was further improved by integrating the sustainability criteria into the IPDC methodology known as Sustainable Integrated Process Design and Control (Sustain-IPDC). It is to ensure that the distillation column design is more cost efficient and controllable, as well as sustainable to meet product quality specifications. Previously, it had been proven that the Sustain-IPDC methodology was able to find the optimal solution for a single distillation column in terms of design, control, economic and sustainability (Nordin et al., 2014). This paper will highlight the capability of the Sustain-IPDC methodology in finding the optimal solution for multiple distillation columns systems.

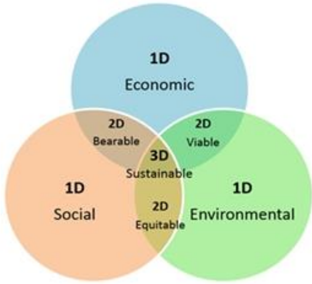

Figure 1: Venn diagram of sustainability criteria.

2. Methodology

The Sustain-IPDC problem is formulated as a generic optimization problem in which a performance objective in terms of design, control, sustainability and cost is optimised subject to a set of constraints as Eq(1) to Eq(6).

$$\max \quad J = \sum_{i=1}^{m} \sum_{j=1}^{n} P_{i,j} w_{i,j} \tag{1}$$

subjected to:
Process (dynamic and/or steady state) constraint

$$\frac{dx}{dt} = f(u, x, d, \theta, Y, G) \tag{2}$$

Constitutive (thermodynamic) constraint

$$0 = g_1(v, x) - \theta \tag{3}$$

Conditional (process, controllability, sustainability) constraint

$$0 = h_1(u, x) \tag{4}$$

$$0 \le h_2(u, x, d) \tag{5}$$

$$CS = x + uY \tag{6}$$

where:
x = set of process controlled variables
u = set of manipulated (design) variables
d = set of disturbance variables
θ = set of constitutive variables
v = set of chemical system variables
G = set of independent variables
i = category of objective function
j = specific term of each category
Y = set of binary decision variables
w_i = weight factor of each objective term
P_i = objective term

Sustain-IPDC problem for a distillation column system is formulated as a mixed-integer dynamic optimization (MIDO). The design with the maximum value of J is indicated as the best distillation design. The scenarios can be generated as follows:

- To achieve the process design objective, P_1 which is the performance criteria for a distillation design is maximized. To achieve the controller design objectives, $P_{2,1}$ is minimized and $P_{2,2}$ is maximized. $P_{2,1}$ is the sensitivity of controlled variable, y with respect to disturbance, d. While, $P_{2,2}$ is the sensitivity of controlled variables, y with respect to manipulated variables, u.

- To achieve the economic objectives, P_3 which is net profit function are needed to be maximized.
- To achieve the sustainability objectives, $P_{4,j}$ is minimized. There are four indexes used to achieve the sustainability objective which are $P_{4,1}$, $P_{4,2}$, $P_{4,3}$ and $P_{4,4}$. These indexes represent the material intensity, energy intensity, potential chemical risk and potential environmental impact.

Then the multi-objective function can be formulated as Eq(7):

$$\max\ J = w_1 P_1 + w_{2,1}\left(\frac{1}{P_{2,1}}\right) + w_{2,2}P_{2,2} + w_3 P_3 + w_{4,1}\left(\frac{1}{P_{4,1}}\right) + w_{4,2}\left(\frac{1}{P_{4,2}}\right) + w_{4,3}\left(\frac{1}{P_{4,3}}\right) + w_{4,4}\left(\frac{1}{P_{4,4}}\right) \quad (7)$$

The problem is solved by decomposing it into six stages: (i) pre-analysis, (ii) design analysis, (iii) controller design analysis, (iv) economic analysis, (v) sustainability analysis and (vi) final selection and verification, as shown in Figure 2. In this way, the solution of the decomposed set of sub-problem is equivalent to the original problem. As each sub-problem is being solved, a large number of feasible solutions within the search space is identified and hence eliminated. Therefore, while the problem complexity may increase with every subsequence stage, the number of feasible solution is reduced at every stage.

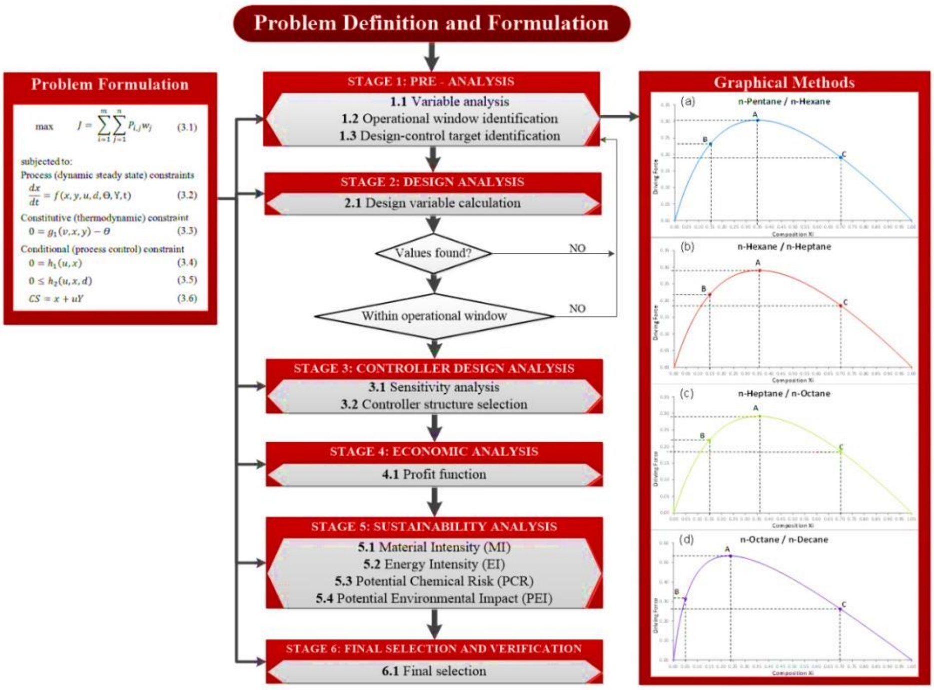

Figure 2: Sustainable Integrated Process Design and Control methodology for distillation columns systems.

3. Application

The Sustain-IPDC methodology is illustrated with the separation of five components mixture with four distillation columns systems. The feed composition considered and the product purity specifications are reported in Table 1 (Errico et al., 2014). It is required to design the distillation sequence reported in Figure 3.

Stage 1: Pre-analysis. The objective of this stage is to define the operational window where the optimal solution is located. The operational window is identified based on bottom and top product quality. Step-by-step algorithm for a simple distillation by Bek-Pedersen and Gani (2004) is implemented in this step. The driving force diagrams are drawn as shown in Figure 4. The target for optimal sustainable process-control-sustainable design solution for each distillation column is identified at the maximum point of driving force (Point A). Two other points are identified as alternative designs (Points B and C).

Table 1: Feed composition and product purity.

Components		Feed molar fraction	Product molar purity
n-Pentane	C_5H_{12}	0.35	0.999
n-Hexane	C_6H_{14}	0.10	0.989
n-Heptane	C_7H_{16}	0.10	0.990
n-Octane	C_8H_{18}	0.40	0.988
n-Decane	$C_{10}H_{22}$	0.05	0.979

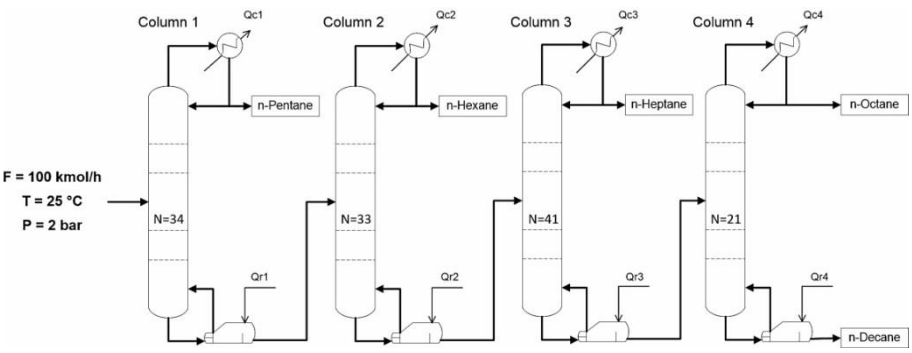

Figure 3: Operating point and sequence considered for the distillation columns design.

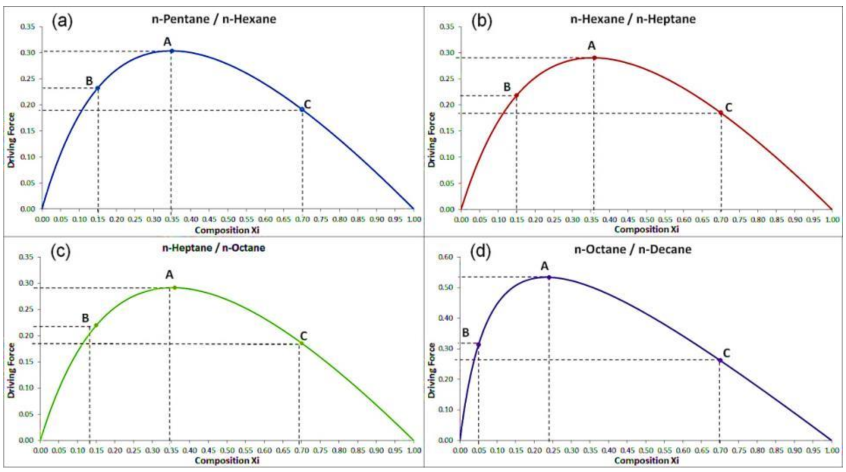

Figure 4: Driving force diagram for each distillation columns: (a) Column1, (b) Column 2, (c) Column 3 and (d) Column 4.

Stage 2: Design Analysis. All targets identified in Stage 1 are validated by finding the acceptable values of controlled and manipulated variables. Each point is analysed by applying the methodology proposed by Bek-Pedersen and Gani (2004). Then, from the results, other design-process variables of distillation column are obtained by using the Aspen HYSYS steady-state process simulator. From the process simulator, the energy required by the condenser (Q_c) and reboiler (Q_r) were taken and the results are summarized in Table 2. It is noted that design A corresponds to the lowest energy consumption (Q).

Stage 3: Controller Design Analysis. At this stage, the controllability performance of each of the feasible candidates is evaluated and validated for the selection of controller structure. There are two criteria that were analysed. Firstly, Table 3 shows the derivative value of energy (condenser and reboiler) with the respect to feed flowrate (F) and temperature (T) which are the disturbance. A smaller derivative means that the process sensitivity is lower, hence, from process control of view, distillation column design A is less sensitive to the effect of disturbance thus make it more robust in maintaining its controlled variable in the presence of disturbances. The controller structure is selected by calculating the derivatives values of the potential controlled variables (x_{D1}, x_{B1}, x_{D2}, x_{B2}, x_{D3}, x_{B3}, x_{D4}, x_{B4}) with respect to manipulated variables (V and L), in a constant step size. The values of the derivatives are tabulated in Table 4. Higher gain in process control means the process will require smaller control action to maintain the controlled variable at the optimal set point value. So, it can be concluded that to maintain the purity of the product in the distillation column can be done by directly manipulating the value of V and L.

Table 2: Values of total condenser and reboiler energy for different design alternatives.

Design	Total Q_c (kW)	Total Q_r (kW)	Total Q (kW)
A	1,367.07	1,973.32	3,340.39
B	7,592.55	8,229.84	15,822.39
C	2,358.84	2,996.08	5,354.91

Table 3: Derivative values of energy with respect to disturbances.

Design	dQ/dF	dQ/dT	Total Derivative
A	37.2479	1.5994	38.8473
B	157.9332	4.1095	162.0427
C	54.1459	4.2646	58.4105

Table 4: Derivative values of composition with respect to V and L.

Design	dx_{D1}/dL_1	dx_{B1}/dL_1	dx_{D1}/dV_1	dx_{B1}/dV_1	dx_{D2}/dL_2	dx_{B2}/dL_2	dx_{D2}/dV_2	dx_{B1}/dV_2
A	0.3048	0.0186	0.0059	0.7201	0.7115	0.0021	0.1714	21.7749
B	0.1737	0.0007	0.0065	0.1915	0.2323	0.0003	0.0510	0.2556
C	0.2565	0.0141	0.0002	0.4632	0.4025	0.0133	0.1248	0.6678
Design	dx_{D3}/dL_3	dx_{B1}/dL_3	dx_{D3}/dV_3	dx_{B3}/dV_3	dx_{D4}/dL_4	dx_{B4}/dL_4	dx_{D4}/dV_4	dx_{B4}/dV_4
A	0.8059	0.0010	0.0932	0.2130	0.2585	0.1400	0.2087	4.1542
B	0.2525	0.0001	0.0271	0.0642	0.1671	0.0018	0.0700	1.2371
C	0.4783	0.0120	0.0081	0.1509	0.2204	0.0174	0.0011	3.7474

Stage 4: Economic Analysis. The distillation designs will be analysed using profit function in order to analyse the design that will provide the maximum profit. There are four criteria used to calculate the profit function, which are profit of product (C1), cost of material (C2), depreciation cost (C3) and operating cost (C4). The economic analysis is calculated by assuming that the distillation column is operating in 5 years and 340 days per year. The result of the calculation is summarized in Table 5. From the results, distillation design at Point A has the highest profit and this verified that the best design in terms of economic criteria.

Table 5: Economic analysis value for the distillation columns systems.

Design	C1 ($)	C2 ($)	C3 ($)	C4 ($)	ϕ ($)
A	13,527,242,607	2,767,016,083	15,315,728	12,359,998	10,732,550,798
B	13,527,242,607	2,767,016,083	15,315,728	58,616,393	10,686,294,403
C	13,527,242,607	2,767,016,083	15,315,728	19,824,705	10,725,086,091

Stage 5: Sustainability Analysis. The purpose of this stage is to analyse the optimal design of distillation column in terms of sustainability. The sustainability of each distillation design is assessed by using 3-D sustainability index. There are four indicators of 3-D sustainability index used to assess the sustainability analysis which are material intensity, energy intensity, potential chemical risk and potential environmental impact (Martins et al., 2007). In order to fulfil the sustainability criteria, it must have low impacts to the economic losses as well as environmental impacts. The values of all sustainability metric are tabulated in Table 6. It can be seen that Point A has the lowest energy intensity compared with other designs, while other indicators has the same values for all the designs. It proves that the distillation design at the maximum point of driving force will have the best objective function in term of sustainability.

Table 6: Sustainability analysis value for the distillation columns systems.

Design	MI	EI	PCR	PEI
A	1.0000	1.2443	0.0003	0.0724
B	1.0000	5.8905	0.0003	0.0724
C	1.0000	1.3597	0.0003	0.0724

Stage 6: Final Selection and Verification. The objective of this stage is to select the best candidate by analysing the value of the multi-objective function. The multi-objective function is calculated by summing up the objective function value using Eq(7) where the $w_{i,j}$ is assumed equal which is equal to 1.0. Each objective value is normalized with respect to the highest value since the range of the objective function can be different. From the result tabulated in Table 7, it is clearly seen that the multi-objective function, J for distillation column design A is the highest compared to other designs due to it has the best value for design, controller design, sustainability and economic. Therefore, it is verified that the distillation column design at the maximum point of driving force is an optimal solution for Sustain-IPDC of multiple distillation columns systems which satisfies the design, controller design, sustainability and economic criteria.

Table 7: The values of multi-objective function calculation. (The best candidate is in bold)

Design	$P_{1,1}$	$P_{2,1}$	$P_{2,2}$	P_3	$P_{4,1}$	$P_{4,2}$	$P_{4,3}$	$P_{4,4}$	
A	0.3551	38.8473	14.4715	10,732,550,798	1.0000	1.2443	0.0003	0.0724	
B	0.2462	162.0427	1.2870	10,686,294,403	1.0000	5.8905	0.0003	0.0724	
C	0.2061	58.4105	3.1935	10,725,086,091	1.0000	1.3597	0.0003	0.0724	
	$P_{1,1s}$	$P_{2,1s}$	$P_{2,2s}$	P_{3s}	$P_{4,1s}$	$P_{4,2s}$	$P_{4,3s}$	$P_{4,4s}$	J
A	1.000	0.240	1.000	1.000	1.000	0.211	1.000	1.000	**14.905**
B	0.693	1.000	0.089	0.996	1.000	1.000	1.000	1.000	6.778
C	0.580	0.360	0.221	0.999	1.000	0.231	1.000	1.000	11.907

4. Conclusion

As a conclusion, a systematic-based methodology has been developed for Sustain-IPDC for a distillation column system. This methodology has been applied and verified for a single distillation column. The presented case study of Benzene-Toluene separation process has shown that the optimal design with respect to design, control, sustainability and economic criteria can be obtained in an efficient and systematic way.

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