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Operational Optimisation for Hybrid Membrane-Distillation Systems

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Hybrid membrane-distillation systems are reported to be an energy-efficient separation processes compared to conventional distillation process; especially for separating close-boiling mixtures. However, several optimization methods are available and can be applied to find a cost-effective design and operation of hybrid membrane-distillation systems. This work evaluates the hybrid system design in terms of energy and compares the performance (i.e. the accuracy and computational efficiency) of stochastic optimisation method (Simulated Annealing) and deterministic method (Pattern search method) for optimisation of process operating conditions. The parallel hybrid membrane-distillation system for the separation of ethylene-ethane mixture is selected for analysis. The decision variables manipulated for the optimisation are the stage cut and permeate pressure. Results show that pattern search is faster than Simulated Annealing but that is more able to find the close-global results. The difference between the optimal result found by Simulated Annealing and pattern search is about 0.02 % for the total operating costs, 0.3 % for the stage cut and 5 % for the permeate pressure. These findings suggest that it is possible to use deterministic method for optimisation complex system. However, to locate an optimal solution and increase confidence in the result, a variety of initial points should be tested.

1. Introduction

The separation of ethylene from ethane, in the cold-end process of an ethylene plant, represents a significant challenge due to their approximate close molecular weight, boiling point, and low relative volatilities. Cryogenic distillation, which is currently implemented for this separation, can produce extremely high purity ethylene at high capacities but it is highly energy and capital intensive (Zimmermann and Walzl, 2012). In the literature, hybrid processes have been proposed as a viable alternative to traditional intensive separation method. To realise the full potential of hybrid process technology, it is important that all available degree of freedom are explored systematically by process optimisation. In the literature, various approaches have been proposed for the design and optimisation of hybrid membrane-distillation processes.

Marquardt et al. (2008) present a framework for the design of separation flowsheets, which include hybrid membrane-distillation separations. In the proposed framework, different flowsheets are generated and then evaluated with shortcut methods. Finally, the most energy-efficient alternatives are rigorously optimized using mixed integer non-linear programming (MINLP) to calculate detailed information and obtain the most cost-effective design. A similar approach to Marquardt et al. (2008) has been employed by Caballero et al. (2009) for the design of hybrid membrane-distillation systems. The approach proposed by Caballero et al. (2009) was applied to optimise and retrofit design of ethylene-ethane separation. Caballero et al. (2009) formulated and solved the optimisation problem as MINLP, the objective of optimisation was to maximise the annualized cost saving. They concluded that the parallel hybrid system can lead to an energy saving of 30 % in the condenser compared to the conventional column. The main drawback is the methodology that is used to solve the MINLP. In their method, some form of integer relaxation is used (i.e. binary variables are relaxed to continuous variables that lie between 0 and 1). Such an approach might result in numerical problems, as stated by Caballero et al. (2007). Etoumi et al. (2014) extend the design and optimisation approach of Caballero et al. (2009) and modify it in order to make it applicable to a heat-integrated hybrid distillation-vapour membrane separation system. The opportunity for heat recovery was taken into account to minimise the utility demand of the separation system. In

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their work, the entire process simulation and optimisation are performed by MATLAB which has been connected with HYSYS through an active client-server application for the calculation of thermodynamic and physical properties. Pattern search algorithm was applied for solving the resulting nonlinear optimisation problem. Case study results show that parallel hybrid scheme can reduce energy cost by 11 %, compared to distillation.

The opportunity to apply a stochastic optimisation method (genetic algorithms) for design and optimisation of hybrid pervaporation-distillation processes has been investigated by Barakat and Sørensen (2008), whereby optimal process configuration, design and operation using a superstructure representation was obtained simultaneously based on trade-offs between capital investment, production revenue and operating costs. The parallel hybrid continuous distillation- pervaporation process is found to produce the highest overall profit that encapsulates capital and operating costs as well as production revenues. For an equimolar acetone-water mixture, Barakat and Sørensen (2008) reported reductions of 14 % in capital costs and 4 % in operating costs compared to the optimal distillation process. The shortcoming of the mathematical programming methods is that it restricts design considerations to the proposed superstructure (i.e., to total column condensation and above ambient temperature). Also, the optimisation algorithm requires long computational time and early convergence to a local optimal is possible.

In conclusion, the literature reviews show that few researchers have applied stochastic optimisation methods to explore the optimisation of design and operation of hybrid systems. Stochastic optimisation methods can find a close global optimum solution for non-convex functions. Simulated Annealing for example is able to escape local optima because it uses a probabilistic acceptance scheme, which accepts solutions that increase the objective function value in the case of minimization. The present work aims to apply and compare a deterministic and a stochastic optimisation algorithm for their efficiency of solving the resulting optimisation problem. To achieve this goal, the systematic design and optimisation approach proposed by Etoumi et al. (2014) will be applied to simulate and optimise a case study for ethylene-ethane separation. The optimisation framework presented by Etoumi et al. (2014) is selected because the optimisation algorithm and the aspect to be optimised are completely decoupled. Such feature allows exploring a diverse set of algorithms that can be used to solve the optimisation problem.

2. Simulation and optimisation method

This section describes the proposed method for the operational optimisation of a hybrid membrane-distillation process. In this work, the optimisation aims to minimise the total operating cost (TOC) of the hybrid separation system. The optimisation problem formulated as a non-linear programming (NLP) and then solved either by the ‘Pattern Search’ method or the ‘Simulated annealing’ algorithm. The principle of the pattern search algorithm is simple. It generates a set of mesh points around an initial guess point in an attempt to find one that yields a lower objective function than the initial guess point. The algorithm stops when termination conditions are met. For more details on pattern search algorithms and simulated annealing, the reader can refer to The Math Works Global Optimisation Toolbox User's Guide (2013). The optimisation algorithm uses established models for the distillation column (Nikolaides and Malone, 1987), the membrane unit (Shindo et al., 1985) and refrigeration cycle (Etoumi et al., 2015). To improve the column performance, energy balance is included in the calculation of minimum reflux ratio (Suphanit, 1999). The vapour flow is only assumed constant in the pinch zone, and the minimum vapour flow in the top section of the column is calculated by performing an enthalpy balance. All of the aforementioned models are used to simulate and design the hybrid system, and to allow the performance (in terms of TOC) of the process to be determined.

The input to the optimisation algorithm is the initial guess of the most important parameters that affecting the process performance, such as the column pressure, the ratio of reflux ratio, the membrane permeates pressure and the stage cut or membrane area. The output of optimisation is the optimum operating conditions that minimizes the objective function, Eq. (1).

$$\mathrm{TOC} = \mathrm{W}.\mathrm{C}^{\mathrm{elec}} + \sum_{\mathrm{I}=1}^{\mathrm{n}_{\mathrm{sourse-m}}} \frac{\mathrm{Q}_{\mathrm{evap}_\mathrm{I}}}{\mathrm{COP}_\mathrm{I}} \left(\mathrm{C}^{\mathrm{elec}} + \mathrm{C}^{\mathrm{cw}}\right) + \sum_{\mathrm{j}=1}^{\mathrm{n}_{\mathrm{sink}}} \mathrm{Q}_{\mathrm{H}_\mathrm{j}}.\mathrm{C}_\mathrm{k}^{\mathrm{steam}} + \mathrm{C}^{\mathrm{cw}}.\left(\sum_{\mathrm{I}=1}^{\mathrm{n}_{\mathrm{source-m}}} \mathrm{Q}_{\mathrm{evap}_\mathrm{I}} + \sum_{\mathrm{I}=1}^{\mathrm{m}} \mathrm{Q}_{\mathrm{C}_\mathrm{I}}\right) \tag{1}$$

Subject to the following constraints:

$$\mathrm{P}_{\mathrm{MR}} = \mathrm{P}_{\mathrm{MF}} \tag{2}$$

$$\mathrm{P}_{\mathrm{MF}} = \mathrm{P}_{\mathrm{C}} \tag{3}$$

$$\mathrm{P}_{\mathrm{MP}} < \mathrm{P}_{\mathrm{MF}} \tag{4}$$

$$\mathrm{P}_{\mathrm{C}}^{\mathrm{L}} \le \mathrm{P}_{\mathrm{C}} \le \mathrm{P}_{\mathrm{C}}^{\mathrm{U}} \tag{5}$$

$$\mathrm{RR^L \leq RR \leq RR^U} \tag{6}$$

$$\mathrm{P_{MP}^L \leq P_{MP} \leq P_{MP}^U} \tag{7}$$

$$\theta^{\mathrm{L}} \ \leq \theta \quad \leq \theta^{\mathrm{U}} \tag{8}$$

$$\mathrm{F_M^L \leq F_M \leq F_M^U} \tag{9}$$

$$\mathrm{y}_{\mathrm{MF},i}^{\mathrm{L}} \leq \mathrm{y}_{\mathrm{MF},i} \leq \mathrm{y}_{\mathrm{MF},i}^{\mathrm{U}} \tag{10}$$

Where TOC : is the total operating cost
W : is the compressor shaft power
Q : is the duty (evap: evaporator; H: heater; C: cooler)
COP : is the coefficient of performance of refrigeration system
C : is the units of cost per unit of energy (elec: electricity; cw: cooling water)
$\mathrm{C_k^{steam}}$: is the steam cost in the range of temperature k
m : is the number of streams cooled using ambient cooling utility (e.g. cooling water or air)
n_{source} : is the number of source streams
n_{sink} : is the number of sink streams
I : is a counter for cold streams
j : is a counter for hot streams
P : is the pressure (MP: permeate; MR: retentate; MF: feed; C: column)
Θ : is the stage cut
RR : is the ratio of reflux ratio to minimum reflux ratio
F_{M} : is the membrane feed flow rate
y_{MFi} : is the membrane feed mole fraction of component i
L : is the lower bounds
U : is the upper bounds

It should be mentioned that for the hybrid design and operational optimisation, the retentate stream pressure, P_{MR}, is set equal to the membrane feed stream pressure, P_{MF}, because of a very slight drop in pressure on the feed-side of the membrane is usually assumed. Moreover, this constraint is introduced to avoid recompressing the retentate stream to the column pressure, in turn reducing the operating cost. Also, the membrane feed pressure is set equal to the column pressure, P_{C}. The permeate stream pressure is set to be less than the membrane feed pressure to achieve the pressure gradient and obtain a separation.

3. Case study: comparison of ‘Pattern Search’ versus ‘Simulated Annealing’ for operational optimisation of a hybrid separation system

This case aims to compare the performance of the two mathematical optimisation methods for the operational optimisation of a hybrid separation system on ethylene-ethane system. The objective of optimisation is to minimise TOC. In this work, the hybrid flowsheet shown in Figure 1 is considered for investigation. The feed flow rate to the column is 100 kmol/h and it contains 54 mol% ethylene and 46 % ethane. The required distillate and bottom purity are 99.9 mol% ethylene and 99.5 % ethane respectively. The membrane is cross-flow vapour permeation type, in which the solution-diffusion model is used to describe transport mechanism in the membrane (Pinnau and Toy, 2001). The membrane selectivity to ethylene is 54 at a feed pressure and temperature of 20 bar and 23 °C (experimental conditions), respectively. The cooling requirement for the column condenser is supplied by the refrigeration system. The ambient temperature at which the condensing heat may be rejected from the refrigeration cycle is set at 20 °C. The minimum temperature approach is assumed to be 5 °C. Soave-Redlich-Kwong is the equation of state that is used to determine vapour-liquid equilibrium behaviour and thermophysical properties such as enthalpies. This is because of its accurate prediction for a relatively ideal mixture (Ploegmakers et al., 2013).

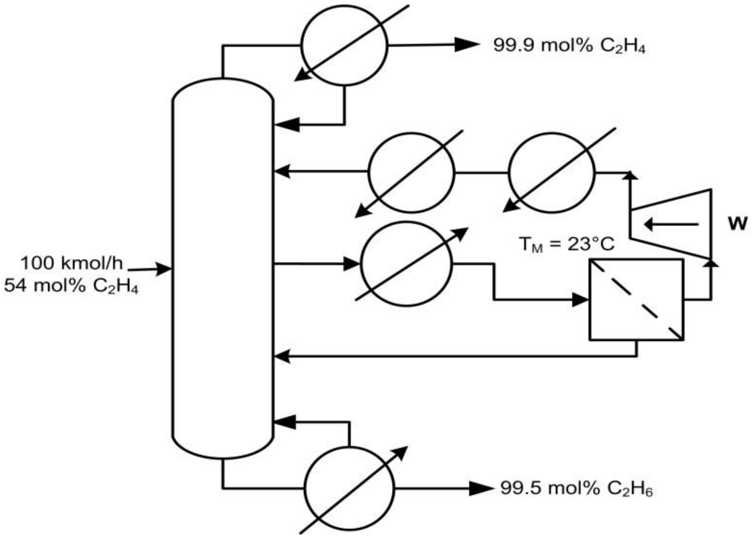

Figure 1: Parallel hybrid membrane-distillation scheme

In the present work, the optimisation problem will be solved by the pattern search and the simulated annealing algorithm available in the MATLAB's global optimisation Toolbox. Before running the optimiser for the given objective function, an initial starting point is specified, as well as bound, equation constraints and termination criterion, etc. The upper and lower bounds for the variables permeate pressure and stage cut is specified as follows: A lower bound for stage cut is set to 0.01and the upper bound to 0.75. A lower bound of permeate pressure is set to the atmospheric pressure and the upper bound value is set to 0.4 of the membrane feed pressure; according to the sensitivity results (Figure 2). The ratio of the reflux ratio (R/R_{min}) is set to 1.05, as recommended by Ray et al. (1998) for sub-ambient distillation. For the purpose of simplicity and to reduce the power consumption of the refrigeration system, the column pressure is set to be constant to 20 bar. Also, the column pressure drop is assumed to be negligible. This assumption is acceptable because the simulation results from HYSYS considering a pressure drop of 1 bar over the column show that the condenser and reboiler duty vary by less than 1 % (data not shown). The molar flow rate fed to the membrane unit can be varied between 20 % (Ayotte-Sauve et al., 2010) and 80 %(Caballero et al., 2009) of the vapour flow rate in the column. Also, the membrane feed purity, which usually provides the minimum condenser duty, is equal or very close to the column feed purity (Caballero et al., 2009). In the present work, the amount of side draw that is fed to the membrane is set to 100 kmol/h (about 35 % of the vapour flow rate inside the rectifying section of the conventional column), and its mole fraction set to 0.54 for ethylene.

To fine tune the optimisation parameters, several runs are performed for the given objective function. In each run, different options are specified using the optimisation function option. In pattern search, poll and search methods and other key parameters such as the initial mesh size, the mesh expansion and contraction factors are examined, as shown in Table 1. In simulated annealing, different initial annealing temperature and annealing schedules are examined as shown in Table 1.

Results in Table 1 show that the most efficient poll is GPS positive basis NP1 with complete poll and search method set to off, 1 mesh size, 0.5 mesh contraction and 2 of mesh expansion. It can be seen that the minimum total operating cost is 146,208 £/y at the optimal variables value, which comprises a permeate pressure of 6.69 bar and a stage cut value of 0.606. The comparison of the results of the pattern search with several inputs shows insignificant difference between the optimal results. The optimal solution deviates from the average optimal solution (a permeate pressure of 7.34 bar and a stage cut value of 0.609) by around 10 % for a permeate pressure and by around 0.5 % for a stage cut. Table 1 shows also that setting the reannealing interval at 100 with the combination of Boltzman annealing and temperature exponential results in the lowest TOC value (146,176 £/y). The lowest elapsed time is 216 s for pattern search and about 1,800 s for simulated annealing. Comparing simulated annealing with pattern search it can be concluded that pattern search is faster than simulated annealing but that simulated annealing is more close to the optimal result. The important observation here is that, in this case, both methods can find the minimum value of the objective function, but with a different starting point for the pattern search method.

Table 1: Influence of 'Pattern Search' parameters and 'Simulated Annealing' parameters on optimisation performance of the parallel hybrid system

a) Pattern search

Starting point					Optimisation results		
Θ	P_P, bar	Poll method/ Complete poll	Search method	Mesh size/ Contraction/Expansion	Θ	P_P, bar	TOC, £/y
0.3	4	GSSNP1/On	Off	1/0.5/2	0.611	8	146,544
0.3	4	GSSNP1/On	MADSNP1	1/0.5/2	0.609	7.34	146,255
0.3	4	GPSNP1/Off	Off	1/0.5/2	0.609	7.34	146,255
0.3	4	GPSNP1/Off	Off	0.5/0.5/1	0.609	7.34	146,255
0.3	4	GPS2N/Off	Off	1/0.5/2	0.610	7.68	146,344
0.2	3.5	GPSNP1/Off	Off	1/0.5/2	0.606	6.69	146,208

b) Simulated annealing

Starting point						Optimisation results		
Θ	P_P, bar	Annealing function	Temperature updated function	Reannealing interval	Initial temperature	Θ	P_P, bar	TOC, £/y
0.3	4	Fast annealing	Exponential	100	100	0.59	3.81	150,855
0.3	4	Boltzman annealing	Exponential	100	100	0.608	6.95	146,207
0.3	4	Boltzman annealing	Exponential	300	100	0.605	6.33	146,304
0.3	4	Boltzman annealing	Logarithmic	100	100	0.611	7.95	146,586
0.3	4	Boltzman annealing	Exponential	100	200	0.608	7.04	146,176

GPS: Generalized Pattern Search; GSS: Generalized Set Search; MADS: Mesh Adaptive Direct Search; 2N: 'pattern positive basis' set with a double number of variable vectors; NP1: 'pattern positive basis' set with a number of vector equal to the number of variables plus one.

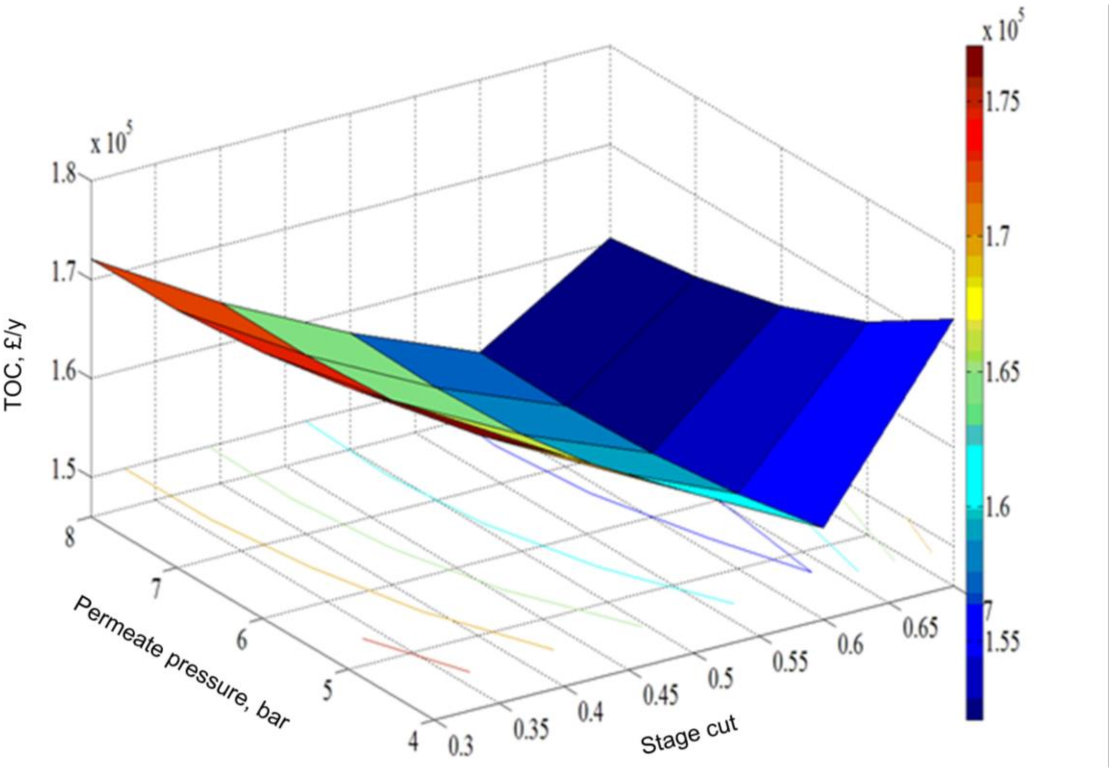

Figure 2: Influence of permeate pressure and stage cut on the total operating cost of the parallel hybrid membrane-distillation scheme for ethylene-ethane separation system. Membrane feed purity 54 mol% of C_2H_4, membrane feed pressure 20 bar and membrane feed flow rate 100 kmol/h

4. Conclusions

The performance of ‘Simulated Annealing’ and ‘Pattern Search’ method for the operational optimisation of the ‘parallel’ hybrid membrane-distillation separation system has been explored. The results of the two optimisation algorithms show that the pattern search algorithm with a GPS positive basis NP1 poll method is competitive to the simulated annealing, and that needs less computation time for reaching the optimal solution. However, in order to guarantee a close optimal result, different starting points for pattern search should be tested. The deviation between the optimal results of the simulated annealing and pattern search is about 5 % for the permeate pressure, 0.3 % for stage cut and 0.02 % for the total operating cost. Future work should consider optimising the total annualised cost which considers the trade-off between the operating costs and the capital costs.

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