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Optimising a Plant Economic and Environmental Performance Over a Full Lifetime

Andreja Nemet*[a], Jiří Jaromír Klemeš[b], Zdravko Kravanja[a]

[a]Faculty of Chemistry and Chemical Engineering, University of Maribor, Smetanova ulica 17, 2000 Maribor, Slovenia
[b]Centre for Process Integration and Intensification - CPI^2, Research Institute of Chemical and Process Engineering MÜKKI, Faculty of Information Technology, University of Pannonia, Egyetem utca 10, 8200 Veszprém, Hungary
nemeta@gmail.com

A significant reduction in energy consumption can be achieved by applying Process Integration methodology. More sustainable process solutions can be achieved both environmentally friendlier (reducing the emissions and pollution) and economically more attractive (reducing utility cost). An improved process design can be achieved by an appropriate trade-off between investment and operating cost. However, the trade-off can only be established correctly if it reflects the future variability, and even unpredictability, of prices for utilities, raw material and products. The objective of this work was to optimise process design for full process lifetime by considering some provisions for future price fluctuations.
Most process synthesis models are single-period models that only consider only fixed cost coefficients. However, prices are fluctuating rather quickly and an optimal process design obtained for one year can be different for another. This work focused on the separation processes as they consume a significant amount of energy. The synthesis of a distillation column sequence integrated with its heat exchanger network was used as a case study for the separation of a multi-component stream into pure component products. In order to consider future price fluctuations, a multi-period mixed-integer nonlinear (MINLP) model was developed. Different projections regarding utility prices based on past prices were derived at due to the uncertainties of forecasting. Maximisation of Net Present Value was chosen as an optimisation criterion, in order to account for future price fluctuations and the time-value of money over a full lifetime.
Trade-off between investment and operating cost, and their distribution between the heat exchanger network (HEN) and the distillation columns were evaluated in the following step. Significant utility savings and a reduction in operational cost can be achieved in this way when compared to those cases where empirical actual-to-minimal ratios within the range of 1.2 - 1.5 is used, especially when future utility prices are considered.
The solution obtained by this novel optimisation methodology seems to be more robust compared to the conventional single–period optimisation as it reflects any forecasted future price fluctuations. Consequently, the probability of meeting the optimal design for each year over a full lifetime of the separation process is thus higher.

1. Introduction

Optimally designing distillation columns in order to ensure energy efficiency is a complex task, which has a significant effect on process profitability, since separation processes require large amounts of utilities. In fact, the energy requirements for separation processes represent quite a high rate of overall

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world energy consumption. Similarly as during the heat integration, there are two main directions for distillation columns synthesis. One direction is the thermodynamic approach. Descriptions about sequencing the distillation columns, and about the heat integration of distillation columns, can be found in different sources (for example Smith, 2005).
An example of retrofit design regarding methanol plant was presented by Demirel (2006) by applying a Column Grand Composite Curve and an Exergy Loss Profile. Soares Pinto et al. (2011) developed a novel approach for temperature-enthalpy profile when determining a target for the usage of side condensers and side reboilers, based on a thermodynamic analysis. They introduced a minimum driving force, which was considered as an exergy loss distribution of the existing column similar to temperature driving force in the case of HEN. By applying the thermodynamic approach, the target for processes is set. However, the rate of integrating the distillation column and HEN depends on the trade-off between the operating cost and the capital cost.
A mathematical programming approach was developed, in order to establish this trade-off. For example, Novak et al. (1996) presented a compact superstructure for the optimisation of distillation column's sequence integrated with its heat exchanger network. A nonlinear short-cut method was applied, in order to overcome the problems with singularities (Yeomans and Grossmann, 1999). A combination of state task network and state equipment network superstructure was suggested for this purpose. A nonlinear disjunctive programming model was proposed for the synthesis of the heat integrated distillation column sequence. Another problem relating to solving MINLP problems is to ensure a feasible initial guess for the optimisation, on which the solution can be highly dependent, not to mention that the objective function and constraints usually have to be continuously differentiable twice. An alternative method for solving these problems is the natural hybrid evolutionary/local search method. Using this approach, the continuous design parameters for the units the local search method are applied, whilst for the optimisation procedure regarding the heat exchanger design an evolutionary optimisation procedure can be used (Fraga and Žilinkas, 2002). Proios et al. (2005) presented a generalised modular framework for the heat integrated distillation column. It is a three-stage systematic procedure that uses logical modelling in order to generate tight and accurate structural models. Grossmann et al. (2005) presented a rigorous model for the synthesis of a complex distillation column. Two models were described - a mixed-integer nonlinear model and a generalised disjunctive programming model. Both models applied tray-by-tray formulation. However, these models are quite complex. A novel approach for obtaining solution for the heat integrated distillation column sequence is the genetic algorithm (Wang and Li, 2010) for the non-sharp separation of the components. Recently Ericco and Rongo (2012) proposed an intensified distillation sequences with only two columns for the separation of four-component mixture. It is possible, when distillation columns are connected with a liquid or a vapour side-stream.
All the models presented considered the fixed current prices for utilities. In order to ensure proper evaluation, any price variations regarding utility requirements should be considered, as this may significantly affect the optimal solution.

2. Methodology

The aim of this work was to optimise distillation columns sequence when integrated with their heat exchanger network over an entire lifetime. A multi-period mixed-integer nonlinear programming (MINLP) model was applied based on the single-period model developed by Novak and Kravanja (1996). The superstructure applied was a compact distillation superstructure, where each separation task is represented by a distinct distillation column. As the role of optimisation is to optimise the sequence of separation tasks, the solution for the optimisation is the optimal path of the distillation sequence. For the integration of a heat exchanger network (HEN), a one-stage HEN superstructure developed by Yee and Grossmann (1990) was integrated within the distillation superstructure. In this model each hot stream, representing condensation at the top of the distillation column, can be potentially matched with each cold stream, representing evaporation at the bottom of the column. The overall model's superstructure was presented in Novak et al. (1996).
As highlighted earlier, the utilities prices vary quite quickly. In order to account for these variations, future utility price projections, based on past price fluctuations, were forecast. The past price profiles

for utilities were determined by applying the data and methodology described in Ulrich and Vasudevan (2006), INDEX MUNDI (2012), and Chemical Engineering (2012). There are 5 scenarios due to the uncertainty of the projections, Figure 1. The neutral scenario 3 is based on the average utility prices; a more pessimistic scenario is 4, which is determined as the average of the utility prices above the overall average; a more optimistic scenario is 2, which is obtained as the average of the utility prices below the overall average; and the extreme scenarios (1 and 5) are determined as the averages above the scenarios 4 and 2.

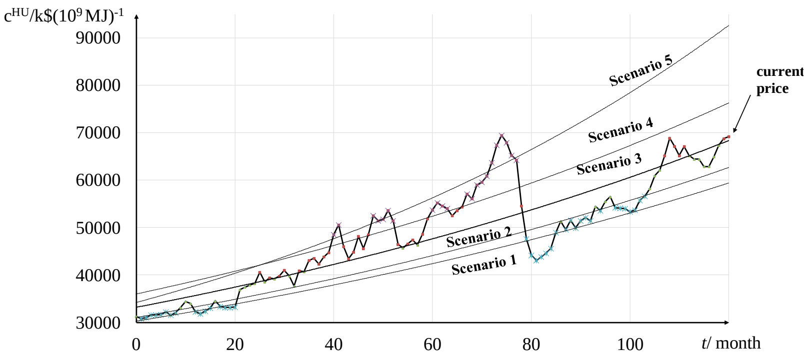


Figure 1: Basis of price-projection

The distillation sequence synthesis model previously developed by Novak et al. (1996) and the single-period model for the synthesis of HEN (Yee and Grossmann, 1990) were merged together and converted into a multi-period optimisation model, in order to account for utility prices variations. The synthesis of distillation column sequence, integrated within its heat exchanger network, was thus performed simultaneously.

$$
\begin{array}{lcl}
\max \quad Z = cy^T + f(x) & & \max \quad NPV(d, x_i, y) \\
\text{s.t.} & & \text{s.t.} \\
Ay + h(x) = 0 & \xrightarrow{\text{Disaggregation into periods}} & A_i y + h_i(x_i) = 0 \\
By + g(x) \le 0 & & B_i y + g_i(x_i) \le 0 \\
x_i \in X_i = \{x_i \mid x_i \in X,\ x_i^L \le x_i \le x_i^U\} & & d \ge d_i^e(x) \\
y \in \{0,1\}^m & & (x_i, d) \in X = \{(x_i, d) \mid (x_i, d) \in X,\ x_i^L \le x_i \le x_i^U,\ d^L \le d \le d^U\} \\
 & & y \in \{0,1\}^m \\
\text{Single-period model} & & \text{Multi-period model}
\end{array}
\qquad (1)
$$

In order to convert the model to multi-period, the following performance and operational variables x were disaggregated and indexed over a set of periods $i \in I$ so that they may vary throughout a lifetime: minimum number of trays $N_{DIST,i}^{\min}$, theoretical number of trays $N_{DIST,i}^{t}$, minimum reflux ratio $R_{DIST,i}^{\min}$, actual reflux ratio, $R_{DIST,i}^{ac}$, average volatility, $\alpha_{DIST,i}^{av}$, temperature of the hot stream $T_{H,k,i}$, temperature of the cold stream $T_{C,k,i}$, heat surplus of hot stream $Q_{H,k,i}$, heat demand of cold stream $Q_{C,k,i}$, amount of heat exchanged between hot and cold stream $Q_{H,C,k,i}$, temperature difference between hot and cold streams at stage k $\Delta T_{H,C,k,i}$, temperature difference between hot and cold stream at stage k+1 $\Delta T_{H,C,k+1,i}$, mass flow F_i, mass flow of component FC_i, temperature T_i, pressure P_i, vapour pressure VP_i, cold utility demand Q_i^{cool}, hot utility demand Q_i^{heat}, heat capacity flow-rate of hot stream $FCP_{H,i}$ heat capacity flow-rate of cold stream $FCP_{C,i}$, heat duty of reboiler $Q_{HP,i}$, and heat duty of condenser $Q_{CP,i}$. As these variables would be changing throughout the periods, the optimal design may be different from one year to another. However, in practice, once the distillation columns and the HEN are installed, the design variables d (distillation column diameters, numbers of trays, reflux rates, and heat exchanger areas) are constant over the entire lifetime. In order that these variables suit all the future periods, their maximal values have to be selected and minimised within the objective function:

$$R_{DIST,i}^{ac} \geq R_{DIST,i}^{\min} \tag{2}$$

$$N_{DIST}^{ac} \geq \frac{N_{DIST,i}^{t}}{E_{DIST}} \tag{3}$$

$$D \geq \sqrt{\frac{4 \cdot F_{out,DIST,i} \cdot (1 + R_{DIST,i}^{ac})}{1.61 \cdot \pi} \sqrt{\sum_{comp} (M_{comp} \cdot \frac{FC_{out,DIST,comp,i}}{F_{out,DIST,i}}) \cdot \frac{R \cdot T_{out,DIST,i}}{p}}} \tag{4}$$

$$A_{H,C,k} \geq \frac{Q_{H,C,k,i}}{U_{H,C} \cdot 0.5 \cdot (\Delta T_{H,C,k} + \Delta T_{H,C,k+1})} \tag{5}$$

The Net Present Value was selected as the objective function, in order to consider utility price variations and the value of money.

3. Case Study

In the case study the separation sequence of four component system - benzene (38.585 %), toluene (29.230 %), O-xylene (21.973%) and diphenyl (10.212 %) - was synthesized simultaneously with the heat integrated HEN. The sharpness of the distillation was set at 0.995. The inlet flow of the mixture was 0.05 kmol/s at a temperature of 374 K and the inlet pressure was 0.1 MPa. The efficiency of the distillation was 0.85. There were two available utilities: hot utility at 700 K with the heat transfer coefficient h = 4500 J/(s m^2 K) and cold utility at 299K with h = 1200 J/(s m^2 K). There were two types of heat exchangers. Double pipe exchangers were used to exchange heat between the heat excess regarding the condensation of one column, with the heat requirement regarding evaporation of the other column. The fixed cost coefficient for these exchangers was 59.8 k$ and the variable cost 3.565 k$/m^2. Shell-and-tube exchangers were assumed for the utility to distillation heat exchange. The fixed cost coefficient of these exchangers was 157.8 k$ and the variable cost was 0.251 k$/m^2.
The actual-to-minimum reflux ratio was set at 1.35 as can be found in the literature (Tham, 2009). The optimal scheme obtained is presented in Figure 2. It follows the sequence where separation of the most volatile component always occurs first. Heat exchange takes place between the condenser of the third column and the evaporator of the first column.

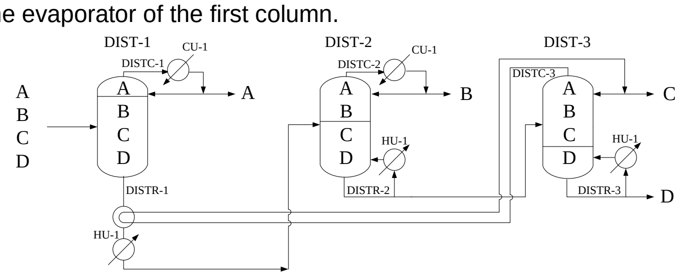


Figure 2: Distillation column optimal design with its HEN

The solution obtained with an actual-to-minimum reflux ratio of 1.35 was compared to the solution obtained, where the actual reflux ratio was optimised. The solution yielded a ratio what was 0.01 greater than the minimum reflux ratio. Table 1 presents the NPV of the mentioned optimisations at different future forecasted price scenarios.

Table 1: Expected NPV for the optimisations at different future forecasted price scenarios.

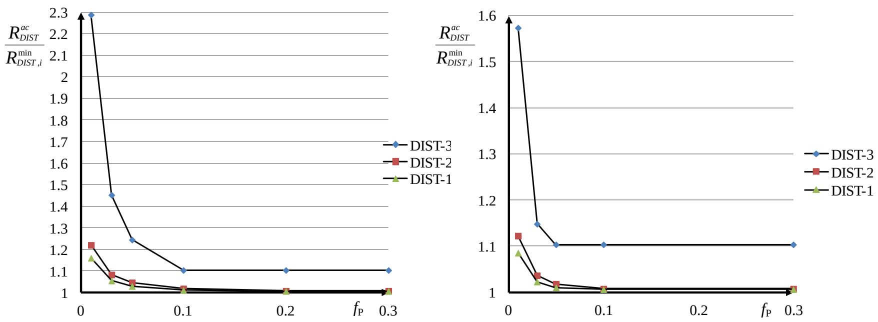
Optimisation	NPV	NPV1	NPV2	NPV3	NPV4	NPV5
Current prices (R_{ac}=1.35 R_{min})	1.220	-48.002	-65.241	-84.314	-114.298	-237.746
Price projection (R_{ac}=R_{min}+0.01)		-19.905	-34.553	-50.759	-76.229	-181.131
ΔNPV		26.097	30.688	33.555	38.078	119.615

Table 2: Comparison between solutions obtained by optimisation when considering the current prices of utilities and R_{Dist}^{ac} =1.35 $R_{Dist}^{\min}$ with the solution, when future utility prices are considered with the $R_{Dist}^{ac} = R_{Dist}^{\min}$ +0.01

Optimisation	Q^{heat} MJ/s	Q^{cool} MJ/s	N_{Dist}^{ac}	R_{Dist}^{ac}	$A_{H,C,k}$ /m^2	C_{DIST} /k$	C_{HEN} /k$
Current prices (R_{ac}=1.35 R_{min})	3.821	3.427	N_{Dist-3}^{ac} = 23 N_{Dist-2}^{ac} = 27 N_{Dist-1}^{ac} = 27	R_{Dist-3}^{ac} = 0.131 R_{Dist-2}^{ac} = 1.910 R_{Dist-1}^{ac} = 2.377	$A_{DISTC-3,DISTR-1,k}=51.9$ 9 $A_{DISTC-2,CU-1,k}=31.1$ 7 $A_{DISTC-1,CU-1,k}=68.9$ 4 $A_{HU-1,DISTR-3,k}=4.89$ $A_{HU-1,DISTR-2,k}=5.58$ $A_{HU-1,DISTR-1,k}=5.65$	462.89	1,063.32
Price projection (R_{ac}=R_{min}+0.01)	3.224	2.830	N_{Dist-3}^{ac} = 27 N_{Dist-2}^{ac} = 52 N_{Dist-1}^{ac} = 53	R_{Dist-3}^{ac} = 0.107 R_{Dist-2}^{ac} = 1.425 R_{Dist-1}^{ac} = 1.771	$A_{DISTC-3,DISTR-1,k}=50.8$ 9 $A_{DISTC-2,CU-1,k}=25.9$ 7 $A_{DISTC-1,CU-1,k}=56.5$ 7 $A_{HU-1,DISTR-3,k}=4.83$ $A_{HU-1,DISTR-2,k}=4.65$ $A_{HU-1,DISTR-1,k}=4.41$	677.355	1,054.42

A comparison between the solutions obtained by different optimisation is presented in Table 2. As can be seen from Table 2, the utility consumption was significantly reduced when the reflux ratio was optimised and future utility prices were considered. As the reflux ratio decreased, the number of trays in the columns had to be increased in order to maintain the same sharpness of separation. As the reflux ratio was decreasing the amounts of the distillate and condensate returned to the distillation were decreasing, which led to a decrease in the heating/cooling requirements and, therefore, smaller areas of the heat exchanger were appropriate. As a consequence, the HEN cost was reduced whilst the investment in the distillation columns due to a higher number of trays was increased.

A trade-off between the investment and operating cost was established by applying maximisation of the net present value. The investment was calculated for the distillation columns and their heat exchanger network. The operating cost was defined as the cost for utilities only. The solution, when considering current utility prices and the 15 y lifetime of the process, yielded to NPV of 21,920 k$, which corresponded to the 113,556 k$ for annual operating cost and the 1,730 k$ for investment: 677 k$ for distillation columns, and 1,053 k$ for HEN.



a) b)

Figure 3: Optimal-to-minimum reflux ratio as a function of a multiplication factor regarding the current utility price, f_P, for the lifetimes of the distillation columns a) 5 y and b) 15 y.

As can be seen, that proportion of the operating cost relative to the investment was very high. It resulted in a high level of integrating of the process with very small reflux ratios already in the distillation columns when considering current utility prices. The difference between the minimal reflux ratio and the optimal reflux ratio was quite small. In most of the cases it almost hit the lower bound. It can be concluded, that for this case study, even at significantly decreased utility prices the proportion of the operating costs relative to investment remained high. This affects the optimal-to-minimum reflux ratio, being significantly smaller than suggested in most of the literature (1.2 to 1.5).

4. Conclusions

Synthesising the distillation column sequence simultaneously with its HEN was optimised over the whole lifetime of the process by applying a multi-period mixed-integer nonlinear programming model. The degree of integration depends on the trade-off between the operating costs and the investment. The presented case study reflected the need for optimising the reflux ratios separately for each column. Applying an empirical actual-to-minimal ratio within the range of 1.2 - 1.5 is problematic, as it does not even reflect the optimal trade-off at the current prices for utilities. It can also be concluded that when the proportion of operational cost with respect to investment is low, the trade-off between the operating cost and the investment is more sensitive to utility prices and, hence, future utility prices also, and shifts more towards smaller utility consumption and higher investment than in those cases when the proportion is high, as was the case during the example problem.

References

Chemical Engineering. Economic indicators, <www.che.com/business_and_economics/economic_indicators.html>, accessed 12.04.2012.

Demirel Y., 2006, Retrofit of Distillation Columns Using Thermodynamic Analysis. Separation Science and Technology 41, 791-817.

Errico M, Rong B.-G., 2012, Modified simple column configurations for quaternary distillations, Computers and Chemical Engineering, 36, 160-173.

Fraga E.S., Žilinskas A., 2002, Evaluation of hybrid optimization methods for the optimal design of heat integrated distillation sequences. Advances in Engineering Software 34, 73-86.

Grossmann I.E., Aguirre P.A., Barttfeld M., 2005, Optimal synthesis of complex distillation columns using rigorous models. Computers and Chemical Engineering 29, 1203–1215.

INDEX MUNDI, <www.indexmundi.com/commodities/?commodityĽgasoline&;monthsĽ360>, accessed 12.04.2012.

Novak Z., Kravanja Z., Grossmann I.E., 1996, Simultaneous synthesis of distillation sequence in overall process schemes using an improved MINLP approach. Computers and Chemical Engineering 20, 1425-1440.

Proios P., Goula N.F., Pistikopoulos E.N., 2005, Generalized modular framework for the synthesis of heat integrated distillation column sequences. Chemical Engineering Science 60, 4678-4701.

Smtih R., 2005, Chemical process design and integration. John Wiley and Sons Ltd, Chichester, West Sussex, England.

Soares Pinto F., Zemp R., Jobson M., Smith R., 2011, Thermodynamic optimisation of distillation columns. Chemical Engineering Science 66, 2920–2934.

Tham M.T., 2009, Distillation an introduction, <lorien.ncl.ac.uk/ming/distil/distil0.htm>, accessed 14.06.2012.

Ulrich G.D., Vasudevan P.T., 2006, How to Estimate Utility cost? Chemical Engineering, April <www.che.com/technical_and_practical/2798.html> accessed 12.04.2012.

Wang X.-H., Li Y.-G., 2010, Stochastic GP synthesis of heat integrated nonsharp distillation sequences. Chemical Engineering Research and Design 88, 45-54.

Yee T.F., Grossmann I.E., 1990, Simultaneous optimization of models for heat integration - heat exchanger network synthesis. Computers and Chemical Engineering 14, 1151-1184.

Yeomans H., Grossmann I.E., 1999, Nonlinear disjunctive programming models for the synthesis of heat integrated distillation sequences. Computers and Chemical Engineering 23, 1135 -1151.