Economic and Controllability Analysis of Energy-Integrated Distillation Schemes

THESIS

(Summary of the Ph.D. dissertation)

by

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December 2002

1. Background

Distillation is the primary separation process used in the chemical processing industries (CPI). While this unit operation has many advantages, one drawback is its significant energy requirements. Appropriate integration of the distillation column with the overall process can result in significant energy savings (Smith and Linnhoff, 1988; Mizsey and Fonyo, 1990) but the scope for this is often limited. Other alternatives are to be investigated.

Conventional distillation schemes are well-known configurations for separation of ternary mixtures by distillation. Due to the higher cost of energy during the last decade, and environmental impacts, there is increasing interest in alternative methods. They include conventional heat-integrated distillation schemes, thermally coupled distillation columns, and complex distillation arrangements which offer alternatives to conventional distillation columns, with the possibility of savings in both energy and capital costs (Petlyuk et al., 1965; Stupin and Lockhart, 1972; Fonyo et al., 1974; Stichlmair and Stemmer, 1989; Annakou and Mizsey, 1996; Agrawal and Fidkowski, 1998; Dunnebier and Pantelides, 1999; Emtir et al., 2001; Becker et al., 2001; Schultz et al., 2002). In practice, the economic potential of such energy-integrated schemes has already been recognised, but their control properties have not been studied to the same degree. Since dynamic behaviour and control of these energy-integrated schemes is also important recent efforts have contributed to the understanding of the dynamic properties of the energy-integrated schemes (Wolf and Skogestad, 1995; Hernandez and Jimenez 1999; Bildea and Dimian, 1999; Jimenez et al., 2001; Serra et al., 2001).

Process design is usually approached by first considering the steady-state performance of the process based on an economic objective and secondly followed the controllability study which include, steady state control indices, open loop and close-loop dynamic simulations.

2. The aims of this work

This work is based on studying and rigorous modeling (design, simulation, optimization, and control aspects) of various conventional and integrated distillation schemes for the separation of ternary mixture at different feed compositions. Economic evaluations of the distillation schemes are founded on rigorous simulation and optimization of each distillation scheme for minimum total annual cost (TAC). Thereafter, the controllability of the optimized schemes is studied, which includes the determination of steady state control indices, the open loop and closed-loop dynamic behavior. Overall evaluation of the best distillation schemes should be based on the combination of economic study, controllability study and environmental aspects. The main aims of this study is outlined below:

1. Design of various conventional and integrated distillation schemes, optimize the investigated alternatives rigorously by steady-state simulation, compare the energy-integrated schemes and the best conventional distillation scheme for better energy utilization of TAC savings.
2. Design and simulation of Petlyuk column for different feed compositions and evaluate its economic features for the given separation. A special emphasis laid on the solution of the internal recycle streams, which represent important design problem by pinpointing the theoretical fractional recovery (β^*).
3. Design and simulation of the complex distillation arrangements (sloppy heat-integrated schemes), applying the theoretical fractional recovery (β^*) concept for designing these complex distillation schemes.
4. Compare the effect of applying different price structures (European and U.S. prices) on TAC savings and the ranking of the schemes.
5. Determine the steady-state control indices of economically optimum distillation schemes at the three different feed compositions and select the best control structure.
6. Study the open loop and closed-loop dynamic behavior of the optimum distillation schemes at equimolar feed composition. Investigate the closed-loop dynamic behavior for different control structures.
7. Estimate the flue gas emissions reductions due to energy-integration.

3. Approach

The Hyprotech's (HYSYS 1.1, 1996) professional simulation package is used for the modelling, steady-state and dynamic simulation of the distillation schemes. Steady-state control indices are determined by the use of MATLAB (Version 5.10.421, 1997).

The following methodological steps are implemented:

a) Shortcut design procedures are used to estimate:
   - the number of theoretical trays,
   - feed location and draw-off trays,
   - and the reflux ratio.
b) Steady-state rigorous simulation is carried out for the desired performance, the rigorous model of the package also used for sizing the different equipment items.
c) Steady-state control indices are determined for the economically optimum schemes at different control structures.
d) Dynamic simulation is carried out for the optimized schemes under feed rate and composition disturbances.

4. The scope and contribution

The scope of this thesis work is to separate a multi-component mixture into pure components by means of continuous distillation. Design, simulation, operation, and control aspects of different distillation arrangements for the separation of ternary mixture are studied. Economic evaluations of distillation schemes are made by rigorous optimization of each distillation scheme for minimum total annual cost (TAC) using steady state simulation. The controllability of the optimized schemes is studied, which include the determination of steady state control indices, the open loop and closed-loop dynamic behavior. Overall evaluation of the optimum distillation schemes are to be made based on the combination of economic study, controllability study and environmental considerations.

This study is devoted to non-ideal alcohol system of (ethanol, n-propanol, n-butanol) with high product purity of 99 % and three different feed compositions (0.45/0.1/0.45), (0.33/0.33/0.33), and (0.1/0.8/0.1).

The economic features of different distillation schemes are investigated including (conventional distillation scheme, conventional heat-integrated scheme, Petlyuk column, and sloppy heat-integrated schemes) and compared to the best conventional distillation scheme.

The investigated schemes are:

i. Direct separation sequence without heat integration (**D**)
ii. Direct separation sequence with forward heat integration (**DQF**)
iii. Direct separation sequence with backward heat integration (**DQB**)
iv. Indirect separation sequence without heat integration (**I**)
v. Indirect separation sequence with forward heat integration (**IQF**)
vi. Indirect separation sequence with backward heat integration (**IQB**)
vii. Thermally coupled sloppy separation sequence (Petlyuk column) (**SP**)
viii. Sloppy separation sequence with forward heat integration (**SQF**)
ix. Sloppy separation sequence with backward heat integration (**SQB**)

The above mentioned schemes are designed, simulated rigorously, and then optimized for minimum total annual cost and compared with the best conventional distillation scheme for better energy utilization and saving in total annual cost (TAC). A particular emphasis is given to the question of fractional recovery of the middle component in the prefractionator and as a consequence to the internal recycles streams in the complex distillation arrangements (Petlyuk column and sloppy heat-integrated schemes). The effect of using higher and lower utility prices (European and U.S. prices) on the energy and total annul cost (TAC) saving are investigated for different types of energy-integrated schemes.

The controllability features of the distillation schemes that indicate better economic feature are investigated by determining their steady state control indices. According to the calculated steady-state control indices, open loop and closed-loop dynamic simulations have been carried out for the equimolar feed to investigate its dynamic behavior. The time constants, controller settings, overshoots, and the settling times are determined to characterize the controllability features of the schemes.

Finally, flue gas emissions of the optimum schemes are estimated for two different types of fuels (natural gas and petroleum oil).

This work is a contribution to the evaluation of the various distillation arrangements for the separation of multicomponenet mixtures considering their economic and controllability features. The work provides a better knowledge for the conventional and energy-integrated schemes. Energy requirements and controllability are the most emphasized design aspects. The complex distillation arrangements (Petlyuk column and sloppy heat-integrated schemes) are very attractive from energy point of view but their complexity makes them rare processes. The study of their properties has become principal parts of this work. This study can be considered as an extension to the previous studies in the area of energy-integration and controllability of distillation columns.

5. Major new results

Thesis 1. For the studied ternary mixture, heat-integrated conventional-schemes show the best economic features in case of equimolar feed (0.33/0.33/0.33) and very competitive to Petlyuk column at lower concentration of middle component **B** in the feed (0.45/0.1/0.45).

Thesis 2. The economic applications of the Petlyuk arrangement are constrained to a very small range of feed composition and relative volatility ratio. Since it is situated around balanced ratio of relative volatility **A/B** to **B/C**, small amount of the middle component **B**, and balanced presence of the two swing components **A** and **C** in the feed.

Thesis 3. Sloppy heat-integrated schemes (complex arrangements) have the highest TAC savings only at high concentration of middle component B (0.1/0.8/0.1).

Thesis 4. The optimum fractional recovery ($\boldsymbol{\beta_o}$) of the middle component in the prefractionator column is found close to the theoretical values ($\boldsymbol{\beta^*}$) in most of the cases. The selection of the theoretical fractional recovery ($\boldsymbol{\beta^*}$) as an initial design parameter is very important in determining the internal recycle streams in the Petlyuk arrangement and its extended for sloppy separation sequence and found to be valid also. The TAC is very sensitive to the optimum fractional recovery parameter ($\boldsymbol{\beta_o}$).

Thesis 5. A general rule governing the ranking of the optimized schemes is that the priority for heat-integrated schemes to achieve higher savings in energy and TAC increases with higher middle component **B** concentration in the feed. The reason of this effect is that the heat requirement for the separation increases drastically with increasing concentration of the intermediate boiling substance **B** in the feed.

Thesis 6. At the price structure valid for the time being, the utility costs proved to be dominating the economic scheme selection. This explains the superiority of the conventional and sloppy heat integrated schemes in both price structures (European and U.S. utility prices).

Thesis 7. Open loop transient behavior of the studied schemes (conventional, conventional heat-integrated, Petlyuk column, and sloppy heat-integrated) show similar order of magnitude for the time constants except for sloppy sequence with backward heat integration (**SQB**). **SQB** shows significantly slower dynamic behavior compared to the other schemes and its time constant is the highest.

Thesis 8. The results of closed-loop dynamic behavior studies show that complex distillation schemes (Petlyuk column and sloppy heat-integrated schemes) have worse controllability features by showing longer settling time and higher overshoots compared to conventional heat-integrated schemes. These results indicate that the interactions due to the control of three-product column, and flow direction of materials and energy plays important role on the transient dynamic behavior of the schemes. The schemes which have material and energy going in the same direction always faster than that having materials and energy flows in opposite direction. This phenomena becomes much more significant in the case of sloppy sequence with backward heat integration (**SQB**), due to interactions inside the column and the opposite directions of materials and energy. The effect of these obstacles on the heat-integrated conventional schemes is not significant.

Thesis 9. Petlyuk arrangement shows slower dynamic behavior in closed-loop compared to the conventional heat-integrated schemes and shows longer settling time due to the interactions inside the main column.

Thesis 10. The savings in gas emissions are proportional to the savings in energy of the energy-integrated schemes and a reduction of the flue gas emissions can be achieved in the range of 36-57 % compared to the conventional distillation schemes. The percentage of savings increases in the direction of increasing middle component **B** in the feed.

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