Antonis Kokossis, Michael C. Georgiadis, Efstratios N. Pistikopoulos (Eds.)
PROCEEDINGS OF THE 33rd European Symposium on Computer Aided Process Engineering (ESCAPE33), June 18-21, 2023, Athens, Greece
 http://dx.doi.org/10.1016/B978-0-443-15274-0.50165-7

Synthesis and optimization of NGL separation as a complex energy-integrated distillation sequence

Qing Li,[a,b] Adrian J. Finn,[c] Stephen J. Doyle,[b] Robin Smith,[b] Anton A. Kiss [a*]

[a] *Department of Chemical Engineering, Delft University of Technology, Van der Maasweg 9, 2629 HZ, Delft, The Netherlands*
[b] *Centre for Process Integration, Department of Chemical Engineering, The University of Manchester, Sackville Street, Manchester, M13 9PL, United Kingdom*
[c] *Costain, Costain House, 1500 Aviator Way, Manchester Business Park, Manchester, M22 5TG, United Kingdom*
E-mail: tonykiss@gmail.com

Abstract

The synthesis of heat-integrated distillation sequences for energy-efficient separation of zeotropic multicomponent mixtures is complex due to the many interconnected design degrees of freedom. This paper explores the basis on which reliable screening can be carried out. To solve this problem, a screening algorithm has been developed using optimization of a superstructure for the sequence synthesis using shortcut models, in conjunction with a transportation algorithm for the synthesis of the heat integration arrangement. Different approaches for the inclusion of heat integration are explored and compared. Then the best few designs from this screening are evaluated using rigorous simulations. A case study for the separation of NGL is used to compare options. It has been found that separation problems of the type explored can be screened reliably using shortcut distillation models in conjunction with the synthesis of heat exchanger network designs. Unintegrated designs using thermally coupled complex columns show much better performance than the corresponding designs using simple columns. However, once heat integration is included the difference between designs using complex columns and simple columns narrows significantly.

Keywords: Distillation sequencing; energy efficiency; process synthesis and design; process optimization

1. Introduction

Distillation is by far the most widely applied separation technology but is recognized as the most energy intensive operation in the chemical industries due to its inevitable energy degradation. Therefore, to genuinely enhance the energy efficiency of the distillation system, it is necessary that all the degrees of freedom are manipulated simultaneously (Kiss and Smith, 2020), i.e. the basic separation configuration including thermally coupled complex columns, column pressures, reflux ratios, feed conditions, condenser types and heat integration arrangement. For all but the simplest separation problems an exhaustive search is infeasible. The method most often used to address larger problems is to use short-cut distillation models to screen the large number of structural options and determine the best few potential designs, followed by more detailed examination of the best few designs using rigorous simulation. However, this raises many questions regarding the screening procedure. It is not clear whether short cut distillation models have the necessary accuracy for reliable screening, and whether heat integration must be included in the screening. Moreover, if heat integration is included, it is not clear whether the integration can be represented by the energy targets of pinch analysis, or it is necessary to use detailed heat exchanger network designs for screening. This work addresses the problem of multicomponent separation by distillation sequences, by developing an integral systematic optimization method which simultaneously synthesizes sequences, optimizes simple and complex distillation arrangements, heat integration, operating conditions, as well as closed cycle heat pump for refrigeration systems.

The fractionation of natural gas liquids (NGL) is presented here to demonstrate the developed methodology. NGL fractionation, which demands a sequence of several distillation columns, is one of the most energy-demanding processes in the oil and gas industry, producing marketable products such as ethane, propane, butanes, and heavier hydrocarbons. NGL feed is typically 2.5 million tons per year, and approximately 77 GJ per barrel of NGL feed is required, which is equivalent to 4.65 tons of CO_2 emissions per barrel (Manley, 1998). Several attempts based on process intensification principles have been made on the NGL fractionation process to generate more energy efficient distillation sequence design with better separation performance and lower energy use. However, these previous studies made simplifications to reduce model complexities to achieve the challenging optimization: only simple columns are taken into account (Yoo et al., 2016), column pressures are fixed, relative volatilities of the initial feed stream are used for all sequence columns (Ramapriya et al., 2018), or assume only saturated liquid or vapor-phase feed and product streams (Tamuzi et al., 2020). These simplified assumptions on key operating variables lead to loss of accuracy, and none of the previous works considered all degrees of freedom, which risks missing the promising solutions.

2. Problem statement

The optimization of the NGL fractionation system is motivated by the benefits of energy savings in reducing costs and CO_2 emissions. Its design requires many interconnected design degrees of freedom, as well as column arrangement possibilities (simple column or complex column arrangements), which lead to a challenging optimization problem. The present study solves this problem through a novel and systematic optimization approach to evaluate all the complex energy integrated NGL fractionation sequence alternatives simultaneously, eliminating simplifications on key design variables. The best sequences can be ranked based on techno-economic analysis.

3. Methodology and optimization approach

For a given multicomponent mixture, a superstructure is initially created that contains all possible sequences using simple columns, and then the superstructure is extended to merge any two simple columns in series to form different complex column arrangements, including side draw columns, side stripper, side rectifier, prefractionator, Petlyuk and dividing wall column, as illustrated in Figure 1 (a) (Smith, 2016). Therefore, based on the same starting defaults of each simple column sequence, the modified superstructure generates complex column sequences accordingly. Shortcut Fenske-Underwood-Gilliland models are used to design the columns in this task, which can screen the very many options and avoid dramatic computational difficulties created by nonlinear, large tray-based combinations of rigorous design formulation. The sequences screened by shortcut models are then evaluated by Aspen Plus rigorous simulations.

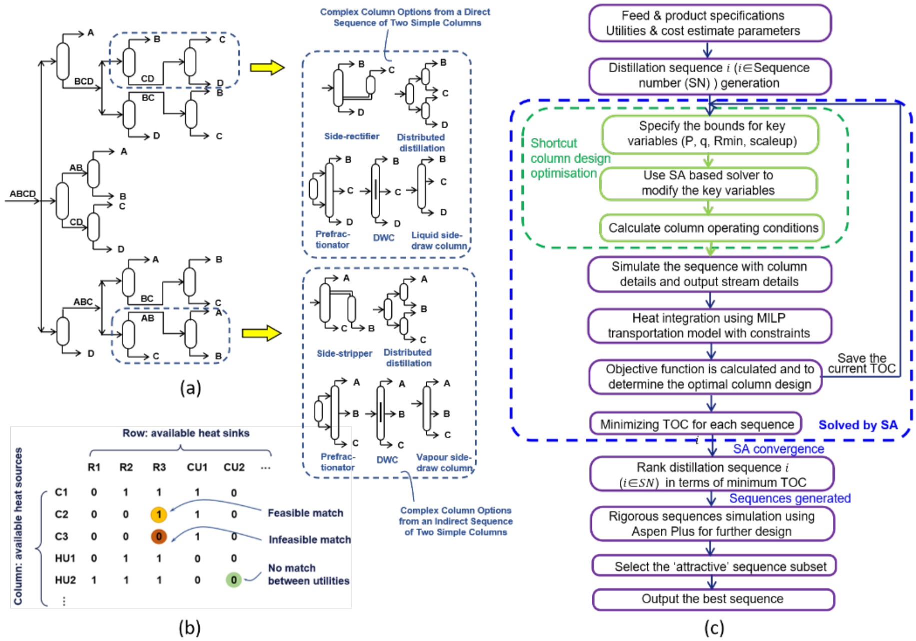

Figure 1 Extended superstructure for sequence synthesis (a), heat integration matrix (b) and the overall methodology flowchart (c)

Heat integration opportunities including feed preheating or precooling and column to column heat recovery are optimized with sequence synthesis and sequence design simultaneously. All heat sinks and heat sources are compiled into an incidence matrix (as shown in Figure 1 (b)) and solved by the MILP transportation method. Binary variables are introduced to make discrete decisions for each match between rows and columns of the matrix. The optimal heat exchanger network structure to minimize operating costs is determined. Liquids and gases are pressurized by pumps and multistage-compressors and depressurized by valves and turbo expanders. The separation is assumed to be sharp split.

A decomposed optimization methodology is created and illustrated by a flowchart shown in Figure 1 (c). The overall model is formed as an MINLP problem and solved by simulated annealing (SA). The shortcut distillation models equations are built into the optimizer, acting as a 'simulation' section to eliminate the non-linearity in the optimization. For a given mixture, the SA creates 'moves' in the optimization that allow for changes in the distillation structure, for example, changing two adjacent simple columns to be a complex column, and the operating variables in their permitted bounds. The values are then sent to the objective function which uses them as inputs for the simulation model. After each move, the sequences are simulated, heat exchanger network designed, and the corresponding total operating cost (TOC) is evaluated by the current column design details and then by the heat integration. The objective value is then returned to the optimizer. The operating variables can subsequently be changed by the optimizer and the process repeated until convergence. This optimization methodology can be carried out within the ColSeq software developed and available at the Centre for Process Integration, The University of Manchester (CPI Suite, 2022).

4. Results and discussion

The conventional configuration of the NGL fractionation uses a train of 4 simple distillation columns: deethanizer (30.98 bar), depropanizer (17.50 bar), debutanizer (5 bar) and deisobutanizer (6.50 bar) to generate 5 products (Manley, 1998; Long et al., 2018). In this work, the NGL fractionation is optimized by applying the developed optimization model to enhance its energy benefits. Multiple utilities considered for heating, cooling and refrigeration and their prices are taken from Turton et al., (2018). The corresponding details of feed and products are taken from Long et al., (2016). For heat exchangers, the minimum temperature difference between hot streams and cold streams (including utilities) is assumed to be 10 K for above ambient heat transfer, whereas for sub-ambient it is assumed to be 4 K (Kiss and Smith, 2020). The optimization is carried out using a desktop with CPU - *Intel$^{(R)}$ Core i7-10700 CPU 2.90 GHz* with 8 cores, and the average time resource is 16 hours.

By optimization, a total of 14 simple sequences using 4 simple columns, and the corresponding 14 complex column sequences are generated. These sequences are developed by two optimization routes for the NGL fractionation: sequences without heat integration and integrated sequences with detailed heat exchanger network design.

4.1. Optimization results evaluation and analysis

Firstly, the developed approach is validated demonstrating by non-heat integrated simple column sequences. Figure 2 (a) shows sequence rankings in terms of the total operating cost. The ranking top 5 sequences (Zone-I) shown in Figure 2, with relatively small differences in TOC (less than 5%), are considered as the most economically attractive sequence family identified by the screening method based on shortcut models. To evaluate the optimized sequences based on shortcut models, the short-cut design details (reflux ratio, trays, condenser temperatures and distillate rate) are extracted as the initialization parameters, and then all optimized sequences are rigorously simulated using Aspen Plus rigorous distillation models. The sequences S7, S6, S4 are the top ranked sequences identified by rigorous simulations in terms of total operating costs, which have all been preselected in the attractive families by the developed pre-screening approach. These results indicate that despite the deviation between shortcut and rigorous models, the developed fast screening method using shortcut models is validated and comparable. Compared to the conventional distillation sequence (Manley, 1998), the optimized operating conditions based on the same separation structures lead to lower column pressure for all four columns without changing the refrigerant level of the deethanizer, and lower condenser and reboiler duties with 2.37 M$/yr TOC savings.

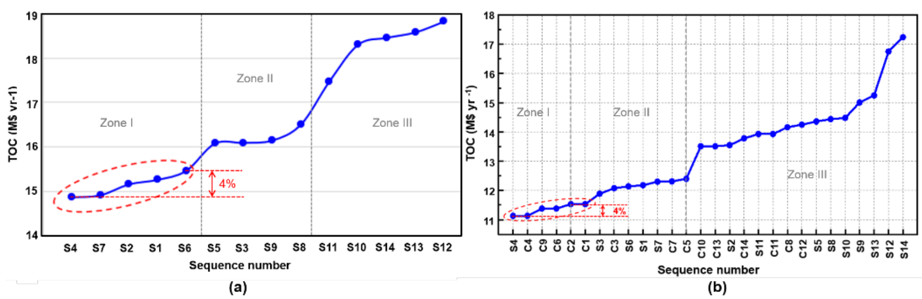

Figure 2 Total operating costs ranking of non-heat integrated simple column sequences (a) and heat integrated sequences (b)

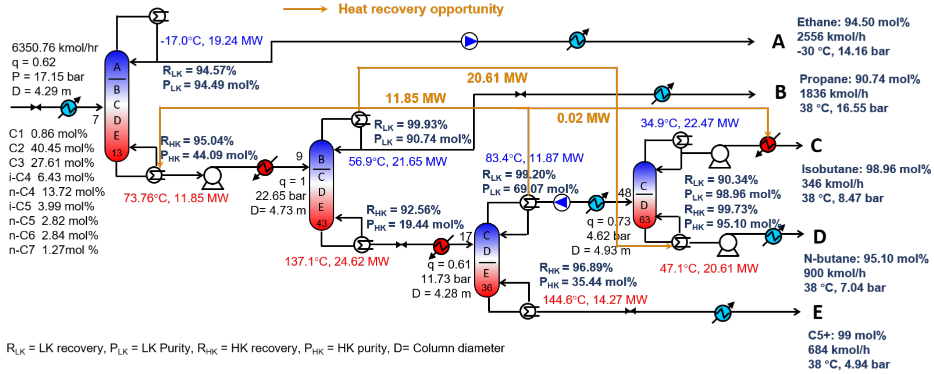

Figure 3. Design details of heat integrated simple column sequence S4

4.2. Energy integrated distillation sequences

Energy intensified sequences using complex columns can bring energy savings. For the non-heat integrated sequences, introducing complex columns can achieve up to 21% operating cost savings compared with the simple column sequences. The conventional sequence (which is the same structure as the simple sequence S4 in this case) that is ranked as the most economical sequence in a simple column sequence, is ranked 11 out of 28 taking into account complex column sequences. The best sequence is now the complex sequence 6, which separates isobutane by a side rectifier, followed by two simple columns separating C2 / C3 and n-butane / C5+, with the TOC of 12.78 M$/yr.

To achieve further energy savings, heat integration is adopted, achieved by optimizing heat exchanger network with column operating conditions simultaneously for both simple and complex sequences. Figure 2 (b) shows the overall rank of heat integrated simple and complex column sequences. The total operating cost saving brought by heat integration on the optimized non-heat integrated simple columns is up to 26%, and the operating cost saving from optimizing both heat integration and complex columns can achieve up to 38%. The top 6 sequences are considered as the most economically attractive sequences family with a relatively small operating cost difference. Further designs can be taken within this attractive families based on different requirements.

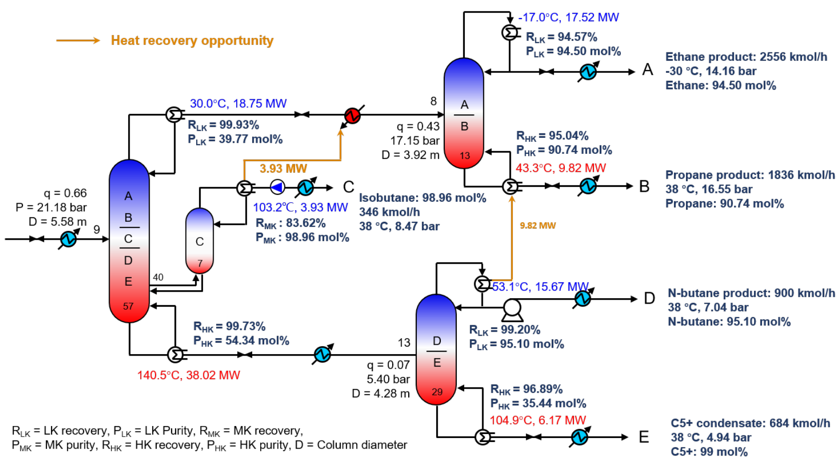

Figure 4. Design details for heat integrated complex column sequence C9

It is shown that when heat integration is adopted, the simple sequence 4 is ranked the best (with the detailed design in Figure 3), followed by the complex sequence C9 (as shown in Figure 4). Simple column sequences benefit to a larger extent from heat integration compared to complex column sequences; simple column sequences can achieve an average energy saving of 16% by introducing heat integration, but complex columns gain an average 11% energy saving by introducing heat integration. This is because complex columns could lose potential heat integration possibilities when constraining the combination of heat sinks and sources during the merging, so that the number of design degrees of freedom of complex columns decrease. The complex sequence C9 may get more benefits when taking into account capital costs due to the reduced equipment sizes. The capital cost is not considered at this stage, as capital costs may not be reflected accurately using approximate capital cost calculation methods.

5. Conclusions

The systematic screening approach developed in this study was successfully used for simultaneously optimizing sequence structures, accounting for all design degrees of freedom and heat integration in the distillation sequences. By optimizing the whole sequencing process, new NGL fractionation sequences have been explored and ranked techno-economically. The generated economically attractive sequences (ranked by the operating costs) are shown to be comparable with those of rigorous simulations using the Aspen Plus RadFrac model. For a given feed composition and product requirements, the ranking of the detail designed energy integrated complex sequences for NGL fractionation are listed, and the most energy efficient and economically attractive sequences family have been selected. These results demonstrate that screening of the search space of energy-efficient distillation sequences, considering synthesis and optimization of the many design degrees of freedom, is achievable with the newly proposed approach.

References

CPI Suite, 2022, The University of Manchester, Centre for Process Integration, Online: https://www.ce.manchester.ac.uk/cpi/research/resources/software/

A.A. Kiss, R. Smith, 2020, Rethinking energy use in distillation processes for a more sustainable chemical industry, Energy, 203, 117788

N.V.D. Long, L.Q. Minh, T.N. Pham, A. Bahadori, M. Lee, 2016, Novel retrofit designs using a modified coordinate descent methodology for improving energy efficiency of natural gas liquid fractionation process. Journal of Natural Gas Science and Engineering, 33, 458e68.

D. Manley, 1998, Thermodynamically efficient distillation: NGL fractionation, Latin American Applied Research, 28, 211-216

G.M. Ramapriya, A. Selvarajah, L.E. Jimenez Cucaita, J. Huff, M. Tawarmalani, R. Agrawal, 2018, Short-cut methods versus rigorous methods for performance-evaluation of distillation configurations, Industrial & Engineering Chemistry Research, 57, 7726-7731

R. Smith, 2016, Chemical process design and integration, Chichester, West Sussex, United Kingdom, John Wiley & Sons, Inc

A. Tamuzi, N. Kasiri, A. Khalili-Garakani, 2020, Design and optimization of distillation column sequencing for NGL fractionation processes, Journal of Natural Gas Science and Engineering, 76, 103180

R. Turton, R.C. Bailie, W.B. Whiting, J.A. Shaeiwitz, 2008, Analysis, synthesis and design of chemical processes, Pearson Education

H. Yoo, M. Binns, M.G. Jang, H. Cho, J.K. Kim, 2016, A design procedure for heat-integrated distillation column sequencing of natural gas liquid fractionation processes, Korean Journal of Chemical Engineering, 33, 2, 405-415