

Modeling of distillation column for C3 fraction for multiple pressure levels

Introduction

In modern world, plastic products have become an inseparable part of everyday life. Their production has grown rapidly in recent times, partly due to their various applications [1]. There are many different types of plastics, one significant class being thermoplastics such as polypropylene. Polypropylene is manufactured by processing almost pure propylene (99.5 %) [2]. Achieving such purity level is very challenging, since propylene in refineries is present in the same material stream as propane. Separating propylene from propane is difficult because the two substances have very similar boiling points. To reach the required propylene purity, it is necessary to employ tall columns and large reflux ratio. This causes high energy demands on the process. There are two main ways to address the energy demands of rectification when processing propane-propylene mixtures. The first, traditional approach supplies the necessary heat to the reboiler via a heating medium and removes heat from the condenser using cooling water (Fig. 2). The second approach employs a distillation column with an integrated heat pump (Fig.1), which uses vapor recompression of the overhead vapors to provide reboiler heating [2,3].

Object of study

To choose the most cost-effective C₃-splitting approach, start by sizing and rating the core equipment like column number of stages and feed-tray location, the heat-exchanger duties and surface areas, and the compressor power. Once these design points are established, compute each scheme capital and operating expenses and identify the set of parameters that yields the lowest total annual cost [4]. Before starting the mathematical modeling, it is essential to analyze the feedstock to be separated. Available data were collected for the mixture coming from the Fluid Catalytic Cracking (FCC) unit of a Slovak refinery, from which propylene of the required purity must be obtained. From these, the data corresponding to steady-state operating conditions were selected. Since the model should address the most demanding scenario, we focused on the case with the highest feed rate (10.3 t/h) with the following molar composition: propane 17.69 %, propylene 82.10 %, isobutane 0.16 %, and isobutene 0.05 %. The feed temperature and pressure (44.1 °C, 2.11 MPa) were obtained directly from the operational data.

Thermodynamic analysis

Because the distillation column operates at high pressures, it is appropriate to conduct thermodynamic analysis. We constructed P-x-y diagrams for the binary propane-propylene system at 30 °C to compare vapor-liquid equilibria predicted under the ideal gas assumption with those calculated using the Peng-Robinson equation of state. Both sets of computed data were plotted against experimental VLE measurements taken from the literature, all at the same 30 °C conditions in Fig. 3. The ideal-solution approximation deviates markedly from the published data, whereas the Peng-Robinson model closely follows the experimental points. As a result, the Peng-Robinson equation of state was adopted for all subsequent simulations.

Mathematical modeling

The mathematical model of the column for both operating pressures was constructed in MATLAB using MESH equations [5]. Mass and enthalpy balances, summation relationships, and equilibrium calculations were performed for each stage of the mathematical model [3, 5]. Subsequently, the results were utilized to compute the necessary data for determination of investment and operating costs. The output of the mathematical modeling was the dependence of the reflux ratio on the number of stages and the feed stage location.

Tab. 1: Comparison of the parameters for the optimized operating points.

Parameter	Real process	Modeled process
Number of stages	165	165
Feed stage	110/120	110
Column diameter [m]	2.8	2.87
Power duty of the compressor [kW]	1250	1147
Flash drum volume [m ³]	34	30.3
Area of E-01 [m ²]	1340	1549
Area of E-02 [m ²]	297	300.5

Aknowledgments

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References

- [1] Hervé Millet et al., The Nature of Plastics and Their Societal Usage, *Issues in Environmental Science and Technology*, vol. 47, p. 1-20, 2019, doi: 10.1039/9781788013314-00001.
- [2] Hendrik A. K., Taylor R., Distillation of Bulk Chemicals, *Distillation*, p. 191-253, 2014, doi: 10.1016/C2010-0-67739-X.
- [3] Digner R., Dreux H. et al., Process for heating the column for distillation of the C₃ fraction from an FCC unit by means of a circuit of water heated by streams belonging to units placed upstream and/or downstream of the FCC unit, Munich: Europea Patent Office, 2014. P. n. EP3016728B1.
- [4] Furda, P. et al., C₃MR LNG process design: Novel approach to optimization for feedstock variability and multi-criteria analysis including economics, safety and environmental impact. *Energy*, vol. 322, 2025, doi: 10.1016/j.energy.2025.135194.
- [5] Perry R. H., Green W. D., *Perry's Chemical Engineers' Handbook*, 7th. ed. New York: McGraw-Hill, 1997, ISBN: 9780070498419.

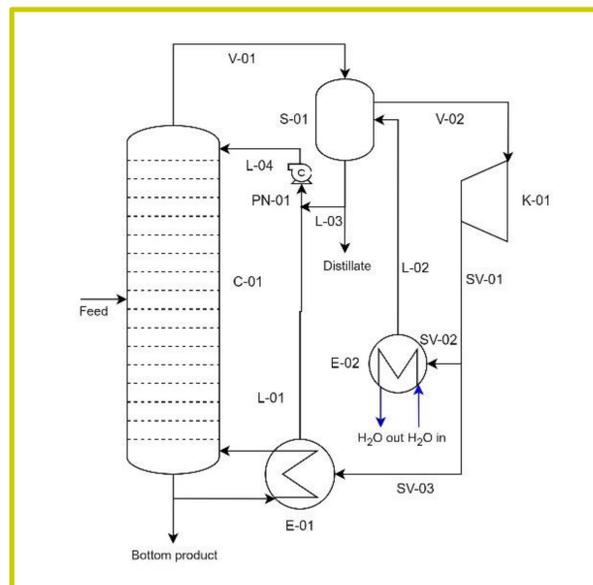


Fig. 1: Process-flow diagram of the modeled system with a heat pump operating at 11 bar.

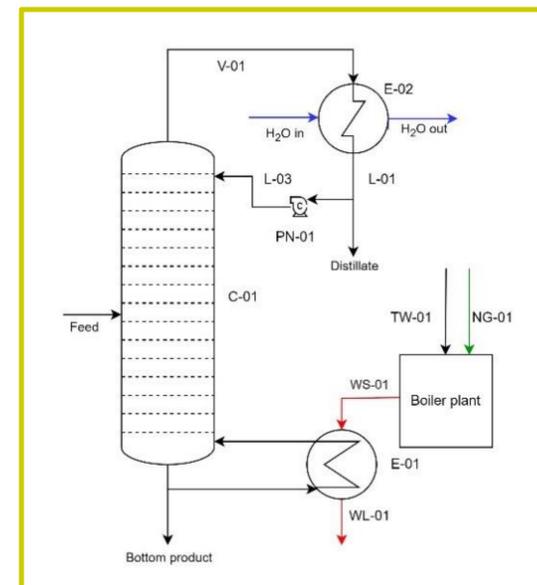


Fig. 2: Process-flow diagram of the modeled system operating at 20 bar.

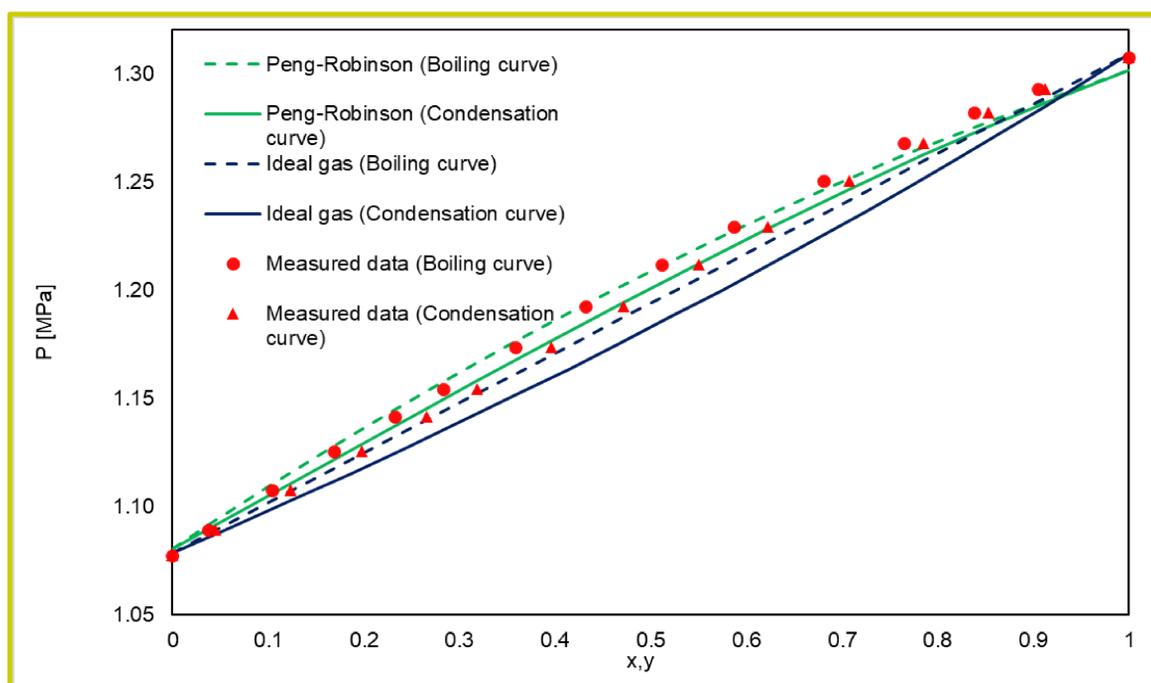


Fig. 3: Comparison of equilibria of ideal gas, real gas, and measured data using the P-xy diagram.

Results and conclusions

In Fig. 4 -7, the outcomes of the mathematical model at both pressure levels are compared. The assessment of the minimum Total Annual Cost (TAC) indicated that integrating a heat pump and running the C₃ splitter at reduced pressure is more cost-effective. Ultimately, the model results were compared with the design specifications of an actual industrial C₃ splitter. As illustrated in Tab. 1, a high degree of agreement was observed across various parameters.

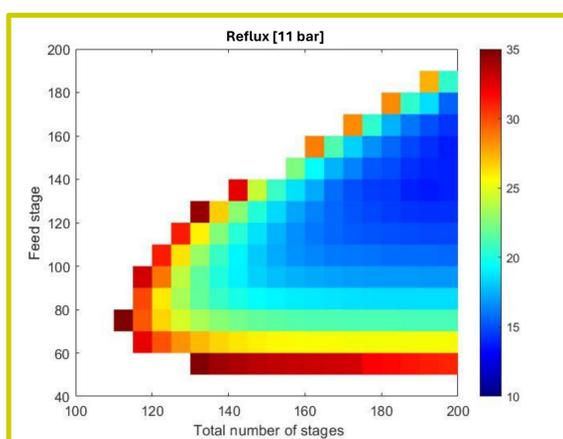


Fig. 4: Reflux ratio at 11 bar as a function the total number of stages and the position of feed stage

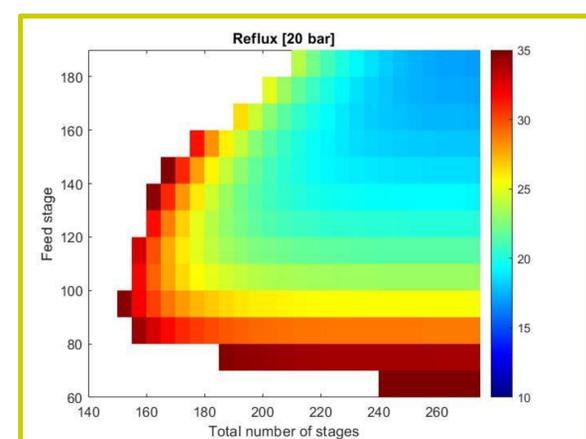


Fig. 5: Reflux ratio at 20 bar as a function the total number of stages and the position of feed stage.

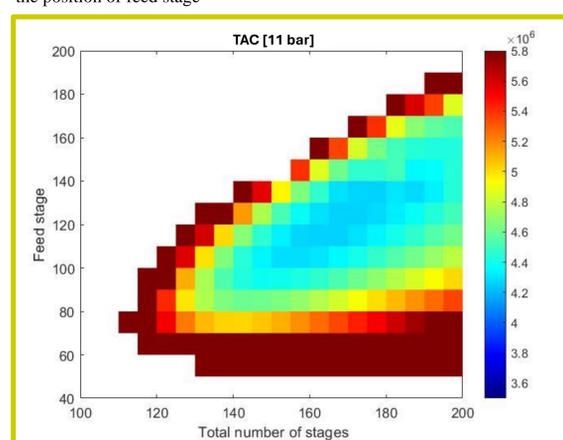


Fig. 6: TAC at 11 bar as a function the total number of stages and the position of feed stage.

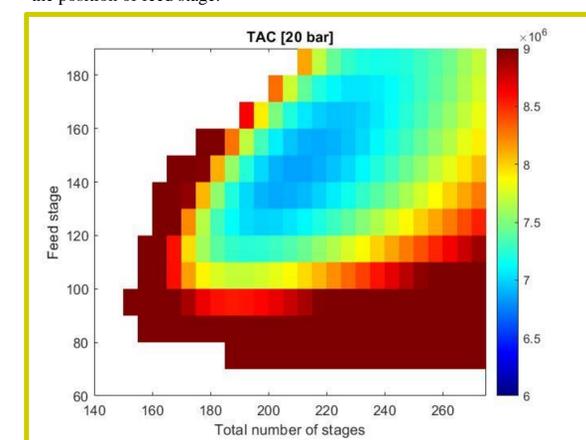


Fig. 7: TAC at 20 bar as a function the total number of stages and the position of feed stage.