Boundary value design method for complex demethanizer columns

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BOUNDARY VALUE DESIGN METHOD FOR COMPLEX DEMETHANIZER COLUMNS

Muneeb Nawaz and Megan Jobson
Centre for Process Integration, School of Chemical Engineering and Analytical Science, The Mill, Sackville Street, The University of Manchester, Manchester, M13 9PL, UK.
Email: Muneeeb.Nawaz@postgrad.manchester.ac.uk, Megan.Jobson@manchester.ac.uk

Abstract
When a design problem dealing with demethanizer flowsheets is approached in a systematic way, the number of separation alternatives to be studied is generally very large. Repetitive simulation studies to evaluate the economic viability of the process can be facilitated by combining shortcut design models with rigorous optimization. These shortcut models are useful at the initial design stage, when there is little information about the separation tasks beyond the design specifications.

A demethanizer column has many degrees of freedom, including the operating pressure, the location and the order of feeds, the number and duty of side reboilers and the flow rate of the external reflux stream. An appropriate design model for the demethanizer is needed for the development of an optimization framework for process synthesis and evaluation. Such a column design model should be computationally relatively undemanding yet accurate and allow evaluation of both energy demand and equipment requirements. The complexity of the demethanizer column precludes the use of the Fenske–Underwood–Gilliland shortcut design method.

A semi-rigorous boundary value method is proposed for the design of complex demethanizer columns separating multicomponent mixtures. The method has been implemented within MATLAB and linked to HYSYS for prediction of physical and thermodynamic properties. The results of the proposed design methodology are shown to be in good agreement with those of rigorous simulation.

1. Introduction

There is a need to develop a design procedure for demethanizer flowsheets that not only provides reliable process design but also simultaneously generates good initialisation for simulation purposes. The assessment of all possible flowsheets with numerous options is a time consuming task with a large number of simulations required to select the economically best option. Therefore, a systematic approach for synthesis is required to generate effective and economic design of the demethanizer. The demethanizer system is characterized by interactions between the complex distillation column and other flowsheet components, including the turbo-expander, flash units, multistream exchangers and external refrigeration[1].

A shortcut model is necessary for grass-roots design, especially for pre-screening the major design options. Before the detailed sizing and unit operation selection, applying a shortcut model can help to make quick decisions about equipment suitability, approximate size and cost estimates. Short cut design methods are relatively simple to use, at the expense of accuracy. On the other hand, a rigorous design approach may yield an improved result for both screening and initialisation but is computationally more demanding, is more time consuming and requires more parameters to be specified. With this in mind, the aim of this work is to develop a procedure that takes advantage of both approaches.

Conventional short cut approaches to column design such as the Fenske-Underwood-Gilliland method cannot be applied for the design of a demethanizer column. This method assumes constant molar overflow and constant relative volatilities within the column. These conditions are not fully met in a demethanizer, as there is a large difference in the size of the molecules of methane and ethane which also results in a significant difference in the latent heats of vaporization of the two components.

Existing shortcut models cannot be applied to multiple feed columns, or to complex column configurations, e.g. with side reboilers or external reflux streams, such as are used for demethanizer columns. A typical demethanizer column is represented in Figure 1.

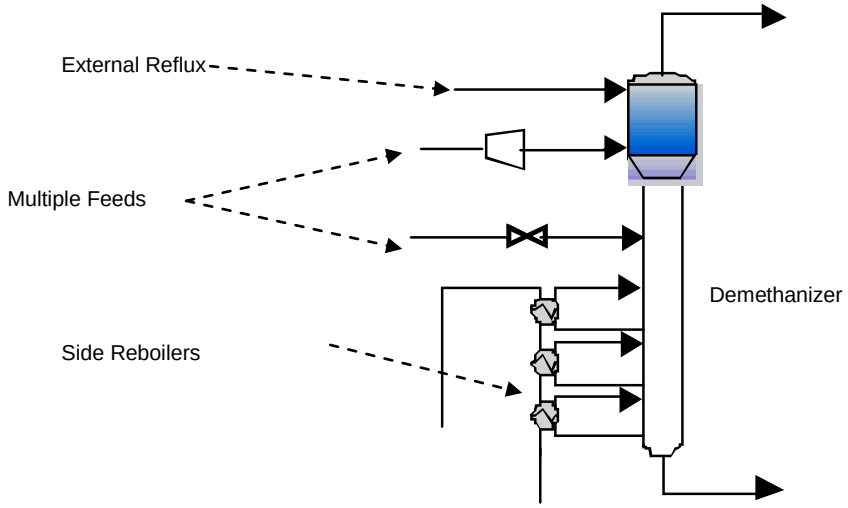

Figure 1. A typical demethanizer column

2. Demethanizer Design by Modified Boundary Value Method

A new shortcut design procedure is developed based on the boundary value method that has been applied previously to the azeotropic distillation design[2,3]. This design method assumes constant molar overflow and a constant pressure across the column. For a column with one feed and two products, this design method requires the specification of feed and product compositions and a feed condition. The liquid composition profiles are calculated starting from the fully specified product compositions by applying material balance and vapour-liquid equilibrium equations. The specified separation is identified as feasible if the two composition profiles intersect each other. The number of theoretical stages can be counted from the composition profiles and the feed location is indicated from the intersection between the two composition profiles. The minimum reflux ratio, which can be used as an indicator for evaluating column designs[4], can be determined by varying the reflux ratio until the two composition profiles just touch each other.

2.1. Model Development

The boundary value model is coded in MATLAB 2007b with a link to HYSYS 2006.5 for vapour-liquid equilibrium and enthalpy calculations using the Peng-Robinson equation of state. The composition of the bottom product is given by the overall material balance.

$$x_{B,i} = x_{F,i} - \frac{x_{F,i} - x_{D,i}}{x_{F,i} - x_{D,1}}\left(x_{F,1} - x_{B,1}\right) \tag{1}$$

In the column, the boil-up ratio is not an independent variable, as the boil-up and reflux ratio are connected via the overall mass and energy balance equations[5]:

$$s = (r+q)\left(\frac{x_{B,i} - x_{F,i}}{x_{F,i} - x_{D,i}}\right) + q - 1 \tag{2}$$

Existing boundary value methods are limited by the constant molar overflow assumption. This limitation may be overcome by including an energy balance when computing the composition profiles.

2.2. Model Modification for Multicomponent Mixtures

Composition profiles of a ternary mixture are conveniently represented using triangular diagrams[6]. Although the boundary value method is applicable to multicomponent mixtures, for more than three components, the visualisation of the intersection is difficult because the lines must intersect in higher-dimensional space. Furthermore, in a multicomponent system, profile intersection is much less likely

and much more sensitive to the product specifications. To approximate the intersection between the stripping and rectifying profiles, a 'minimum distance' criterion is employed[7]. The rectifying and stripping profiles are constructed in the normal way from the product compositions for the given reflux or reboil ratio. The intersection of profiles is assessed by calculating the shortest distance in the mole fraction space between the two profiles (eq. 3). If any two points on a pair of lines lie within this specified minimum distance, the lines are considered to 'intersect':

$$\text{Minimum distance} = \sqrt{\sum_{i=1}^{j}\left(x_{i,n_{rec}} - x_{i,n_{str}}\right)^2} \qquad (3)$$

The stripping stage giving the minimum difference is taken to correspond to the feed stage. The number of stages can be counted from the data points (stages) in each profile with one data point (stage) removed to account for the overlap at the feed stage.

2.3. Double-feed Column Design by Boundary Value Method

The demethanizer is a double-feed column with feed streams entering at different locations in the column. The boundary value method maybe modified to accommodate two feeds. In this case, the column is divided into three sections, namely the rectifying, middle and stripping sections [1]. The composition profiles of the rectifying and stripping section are calculated in the usual way. The composition profile of the middle section can be calculated in two ways: top-down; where the middle section profile starts from a specified stage of the rectifying profile, or bottom-up, where the lower feed stages is specified and the profile continues upwards from the stripping section.

The procedure for the middle profile calculation according to the bottom up approach can be summarized as:

- A stage in the stripping profile is arbitrarily chosen as the lower feed location e.g. stage M in Figure 2. The location of the stage is an additional degree of freedom.
- The vapour composition of stage M is determined by bubble point calculation from the liquid composition of stage *M* ($\boldsymbol{x}_M$). The value of $\boldsymbol{x}_M$ is already known from the stripping composition profile calculated earlier.
- The liquid composition of the stage above, *M+1*, is calculated from the material and energy balances (equations 4 and 5).
- The calculation is continued by solving the material, energy and vapour-liquid equilibrium calculations.
- The intersection between the middle and rectifying section composition profiles is identified, giving the upper feed location.

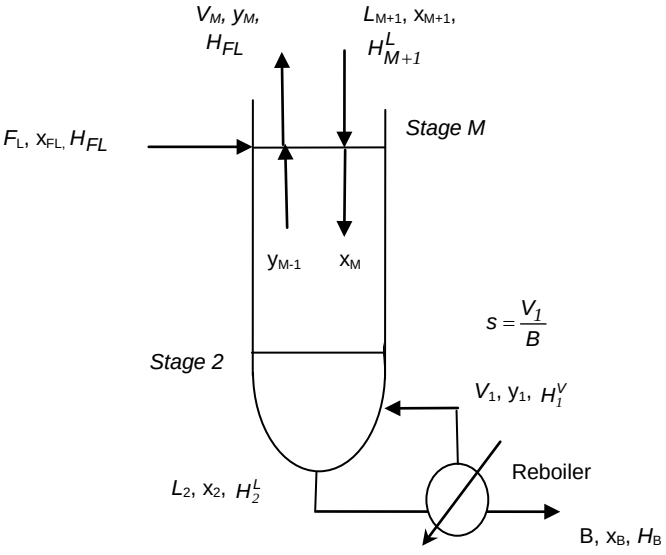

Figure 2. Schematic representation of the stripping section

$$(V_M + B - F_L)x_{i,M+1} - V_M y_{i,M} - Bx_{i,B} - F_L x_{i,FL} = 0 \quad (4)$$

$$(V_M + B - F_L)H^L_{M+1} - V_M H^V_M - BH_B + F_L H_{FL} + Q_{reb} = 0 \quad (5)$$

where $Q_{reb} = (sH^V_1 - (s+1)H^L_2 + H_B)B$ (6)

The middle section composition profile can be calculated when the column pressure (assumed constant), feed flow rates and compositions, lower feed stage quality and location, bottom flow rate and stripping section composition profile are known. These variables give additional degree of freedom for double-feed column compared to the conventional column with a single feed. In this work, the lower feed location is specified, rather than the lower feed quality, Many feasible designs are generated, as several middle section profiles are obtained corresponding to various lower feed locations. For a given reflux and boil-up ratio pair, the design with the fewest total stages is selected, to minimize capital cost. The feed stage location can also be selected such that the number of stages of the column is minimized.

2.4. Extended Boundary Value Method for Column with Side Reboilers

Side reboilers in low-temperature distillation columns are particularly important because they can provide cost-effective refrigeration at temperatures lower than that of the column reboiler. They are used to precool the feed in the multistream exchanger, thus reducing the external refrigeration requirements. The side reboilers are modelled as side heaters in the column design model. The duty and location of these heaters are specified. The energy balance for the stripping section incorporates the heat introduced by the side reboiler on a specified stage.

2.5. Extended Boundary Value Method for a Reboiled Absorption Column Design

Liquid in the upper section of the column is provided by an external reflux stream at the top tray in the column. The top product from the demethanizer, methane, is taken as a vapour product; most commercial flowsheets do not have a conventional condenser. This reflux stream is normally produced by a flash separator or turbo expander.

The rectifying section uses the external reflux to remove the heavier components from the overhead product. For the purposes of design using the boundary value method the demethanizer rectifying section is treated as a reboiled absorber, with the external reflux stream analogous to the absorbent. It is assumed that no rectification takes place on the top feed stage. Some of the volatile components in the top feed will exit the column with the overhead product.

In a reboiled absorption column model, the feed and recovery specification of the light and heavy key components are the input parameters. Composition profiles are calculated in the usual manner, starting from the top stage. An initial estimate of the flow rate of the components in the external reflux stream that leave in the overhead product is given by an adiabatic flash calculation for the feed gas and external reflux stream. For an external reflux stream with a flow rate L_o, composition x_o and enthalpy H^L_0, the material and energy balance at the top of the column are given by:

$$y_1 V_1 - x_o L_o = y_2 V_2 - x_1 L_1 \quad (7)$$

Similarly, from the energy balance:

$$H^v_1 V_1 - H^L_0 L_o = H^v_2 V_2 - H^L_1 L_1 \quad (8)$$

As the net product flow is given by $V_1 - L_o$, the reflux ratio can be written as:

$$R = \frac{L_o}{V_1 - L_o} \quad (9)$$

The composition profiles of the rectifying, stripping and middle sections are calculated as discussed before.

3. Case Study

The demethanizer column design procedure is demonstrated by example: a five-component mixture of mixture of methane, ethane, propane, i-butane and n-butane is to be separated in a demethanizer column. The upper feed flowrate is 2200 kmol/h while the lower feed flow rate is 800 kmol/h; feed compositions are given in Table 1. The separation is carried out at a constant pressure of 30 bar in the column. The recovery of ethane in the bottom product is specified as 98%, while the mole fraction of methane in the top product is specified as 99.5%. The side heaters are specified to be at the fourth and eighth stage from the reboiler with duties of 900 kW and 600 kW, respectively. A column with a partial condenser is employed in HYSYS for validation of the boundary value model results. The composition profiles and flow profiles shown in Figures 3 and 4 demonstrate that the new model can adequately represent complex demethanizer column.

Table 1. Molar feed compositions

Component	Upper Feed	Lower Feed
Methane	0.865	0.65
Ethane	0.06	0.16
Propane	0.04	0.09
i-Butane	0.02	0.06
n-Butane	0.015	0.04

Table 2. Comparison of results from new model with those of HYSYS simulations (* indicates model inputs)

	Boundary Value Model	HYSYS
Number of Stages	24	24*
Upper Feed Location	6	6*
Lower Feed Location	12	12*
Reboiler Duty (kW)	4210	4145

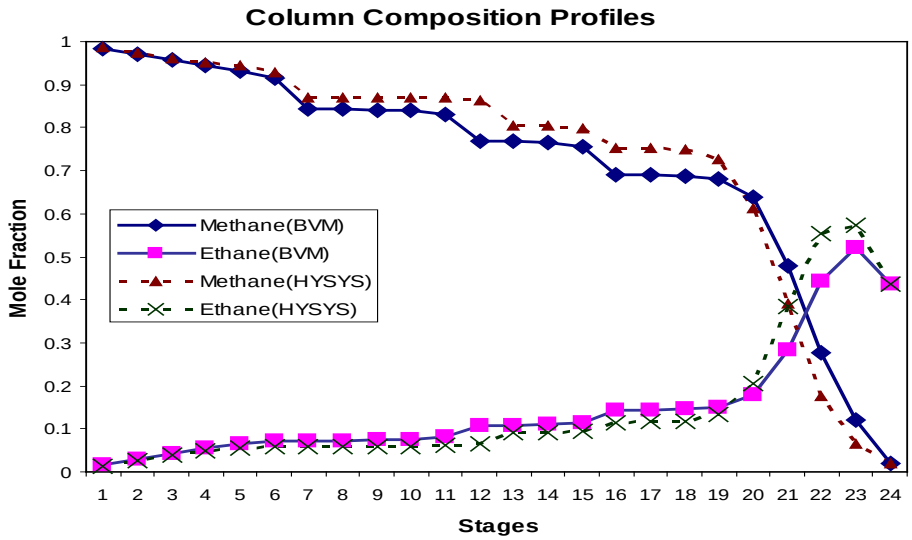

Figure 3. Composition profiles for key components: new model (BVM) vs. HYSYS

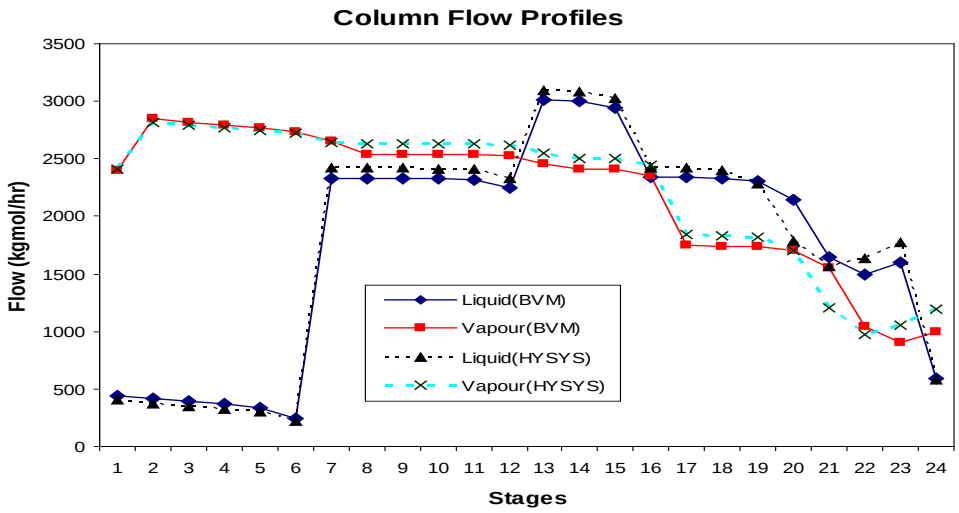

Figure 4. Molar flow profiles: new model (BVM) vs. HYSYS

4. Conclusions

This work presents a new design method for demethanizer columns. The boundary value method is employed for generating column designs, establishing separation feasibility and calculating column energy requirements. Existing boundary value methods are extended to accommodate multicomponent mixtures, two column feeds, side reboilers and an external reflux stream. The feed and product compositions, column pressure and reflux or reboil ratio must be specified.

The new boundary value method is validated by comparison with more rigorous simulation results obtained using HYSYS. The column design parameters obtained from the boundary value method are used for initialising the simulation. The simulation results are in good agreement with those of the boundary value method. The flow and composition profiles of the key component are in good agreement. The model can therefore be used for assessing the feasibility of a proposed specification, for generating preliminary designs (i.e. number of stages, feed locations and reboiler and condenser duties) and for evaluating design alternatives.

References:

1. L. Bai, R. Chen, J. Yao and D. Elliot, *GPA Annual Convention Proceedings* (2006) 300-314.
2. M. F. Doherty and G. A. Caldarola, *Ind. Eng. Chem. Fund.,* 24(1985) 474-485.
3. S. G. Levy and M. F. Doherty, *Ind. Eng. Chem. Fund.* 25(1986) 269-279.
4. J. Koehler, P. Poellmann and E. Blass, *Ind. Eng. Chem. Res.,* 34(1995) 1003-1020.
5. V. Julka and M. F. Doherty, *Chem. Eng. Sci.,* 45(1990) 1801-1822.
6. D. Y. C. Thong et.al, *Chem. Eng. Process.: Process Int.,* 43(2004) 239-250.
7. K. A. Amminudin et.al, *Chem. Eng. Res. Des.,* 79(2001) 701-715.