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Specialization Project

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PROJECT TITLE:

Operation of Energy-efficient Divided Wall (Petlyuk) Column

By

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Abstract

Distillation alone accounts for the significant amount of world's energy consumption. Operating the column at minimum energy is always a favorable condition both for economics as well as reducing CO_2 emissions. The project deals with a real plant situation which is explained below:

"There is a known design of Divided Wall (Petlyuk) Column. The required energy usage to run the column is V_0 but when actually the column is run the vapor split ratio R_v is found to be non-optimal. The value of V_0 is actually lower than what is required for the separation."

This situation is likely to happen in industrial operation and a situation may be that the available energy to run the column is even lower than the minimum energy required for optimal operation of the column. This project evaluates and analyzes the effect on product compositions in case the column is operated with the energy lower than the minimum energy required for running the column at optimal conditions. The analysis is typically useful when the price of product is dependent on its purity.

Optimization was done to maximize purity such that products' specifications were not given. The optimization was done in Matlab using fmincon NLP solver.

To start with and get an insight into the topic, firstly the task was done for conventional two-product distillation column and then the work was further extended to Divided Wall (Petlyuk) Column.

Preface and Acknowledgement

This Project had been started with two goals: a) Preliminary- Operation of Energy- efficient Divided Wall (Petlyuk) Column and b) Main-Simple and Robust Control Structure Design for Energy-efficient Divided Wall (Petlyuk) Column. The work on previous one has been done as a part of specialization project and has been presented in this report. The work on latter one will be done in the Master Thesis.

I would like to express my heartiest gratitude to my project supervisor Sigurd Skogestad for his immense support and continuous guidance throughout the project period. Even though he had many Master students to supervise still he managed to take out time to clear my doubts.

I would also like to thank Vladimir L. Minasidis for helping me out even though he was officially not associated with this project.

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Publications

1. Ambari Khanam, M. Shamsuzzoha, Skogestad, S, “Operation of energy efficient divided wall column”, 23rd European Symposium on Computer Aided Process Engineering – ESCAPE 23 June 9-12, 2013, Lappeenranta, Finland (manuscript submitted for presentation and publication, 6 pages for review)
2. Ambari Khanam, M. Shamsuzzoha, Skogestad, S, “Design and operation of energy efficient divided wall column”, 9th European Congress of Chemical Engineering –21-24 April, 2013, The Hague, The Netherlands (Extended Abstract submitted)
3. Working to prepare the manuscript for journal publication “Operation of energy efficient divided wall column”

Introduction

Divided wall column or Petluyk column are more suitable for multi-components product separation because of their potential contribution to energy saving and capital cost saving. It is proven that a typical three product petlyuk column gives potential energy saving in the range of 20-30% Triantafyllou and Smith (1992). The more complex and fully coupled thermal arrangements have even larger potential, but operation and control remains still challenging in the present scenario Halvorsen and Skogestad (2011)

Further different people and groups (Wolff and Skogestad (1995); Mutalib and Smith (1998), Mutalib, Zeglam et al. (1998), Niggemann, Gruetzmann et al. (2006); Olujic, Jödecke et al. (2009); Niggemann, Hiller et al. (2010) have conducted rigorous experimental and simulation studies to conduct dynamic studies related to startup as well as normal operation of such systems.. Halvorsen and Skogestad (2003) presented the idea of the V_{min} diagram for analyzing the energy consumption for separation of feed components in distillation column. The graphical tool V_{min} diagrams can be utilize to check the minimum energy requirement for sharp and non–sharp separations in both the conventional and thermally coupled columns. V_{min} diagrams can be created for any mixture assuming a column with a large number of theoretical stages and it is based upon the Underwood equations.

Recently, Dwivedi et al.(2012) have studied the three-product Petlyuk (divided-wall) column with an objective to achieve desired product purities with minimum use of energy (V_{min}). They have mainly focused on the control structure selection and considered four alternate control structures with and without the vapor split as a degree of freedom.

Ghadrdan et al. (2012) have extended the concept of three products DWC to four product Kaibel distillation column. They worked for two different objectives, first minimizing energy requirement at fixed product purities, and second maximizing product purities with a fixed boilup rate.

It is clear from the above literature survey that none of the study has focused on the operation of the divided wall column at energies lower than minimum energy required for optimal operation of the column. Therefore, this study is focused on the operation of dividing wall column at energies lower than minimum energy (V_{min}). This could be the usual case in the operation of the divided wall column. The results and analysis of this study can be quite useful in the real plant where sometimes the available energy (boilup) is less than the energy needed for optimal operation. It could also give some insight when the column is not operating at optimal R_V.

In cases when R_V is not optimal how should impurities be minimized and which streams of the main column should contain more impurities. Earlier work on optimal operation of Petlyuk Column have shown more impurities directed to the side stream S Ghadrdan et al. (2012). It should be noted that a non-optimal value of R_V affects the product specifications. Since specification for energy is given but products' specifications are not given the price of all three products will depend on the purity of the product streams. Energy price and Energy supply are factors affecting products' specification.

Chapter A

Binary-Product Distillation Column

1. Background

As a preparatory part of main goal of the project on Divided Wall (Petlyuk) Column, the Binary Product Continuous Distillation Column has also been studied. The process modeling {used the one studied by Skogestad and Postlethwaite (1996)} as well as optimization has been done using matlab interactive environment and programming language. The constrained non-linear solver Fmincon has been used for optimization. Firstly optimization has been done with the objective function to minimize the energy so as to obtain the minimum energy for optimal operation. Once this energy has been achieved for optimal operation optimization has been done with the objective function of minimizing the sum of impurities in the product streams. The following subsections provide the basic information of the conventional binary product column.

1.1 Binary-Product Column Model

Binary Product Distillation Column model for this study is same as Skogestad and Postlethwaite,(1996). The column model is non-linear with NT-1 theoretical stages including a reboiler (stage1) plus a total condenser ("stage" NT). This means that the stage counting is started from reboiler. The liquid flow dynamics are modeled by a simple linear relationship. The Binary Product Column diagram is shown in fig.1, all the notations and nomenclatures are given in table 1 and matlab codes for the model and optimization are given in appendix.

The simplified model assumptions are:

- Two components (binary separation).
- constant relative volatility
- Equilibrium on all stages.
- no vapor holdup
- one feed and two products
- constant molar flows (same vapor flow on all stages)
- total condenser

1.2 Binary Column Design

Separation becomes easier with increase in relative volatility between the components but for given components separation can still be increased by either increasing the number of stages in the column or by increasing the energy usage (the reflux). To quantify this trade-off, the two extreme cases are considered, Skogestad (1997) .(i) infinite reflux, which gives the minimum number of stages, N_{min} and (ii) infinite number of stages which gives minimum energy, ($Q_{min}=V_{min}\Delta H^{vap}$). The number of theoretical stages N in the column is selected to be $N=2.5*N_{min}$, which gives a corresponding boilup rate of $V=1.2V_{min}$.

For a binary separation we have the separation factor, S as calculated below:

$$S = \frac{\left(\frac{x_A^D}{x_B^D}\right)}{\left(\frac{x_A^B}{x_B^B}\right)}$$

$$= \frac{\left(\frac{0.99}{0.01}\right)}{\left(\frac{0.01}{0.99}\right)} \qquad (1)$$

$$= 98010$$

From Fenske minimum theortical number of stages, N_{min} is calculated below:

$$N_{min} = \frac{lnS}{ln\alpha} \qquad (2)$$

= ln(98010)/ln(2)=16.6

The Boilup V_{min} for binary liquid feed ($q_f=1$) with constant molar flows and constant relative volatility $\alpha=2$, is calculated below King (1971)

$$\frac{V_{min}}{F} = \frac{1}{(\alpha - 1)} + \frac{D}{F} \qquad (3)$$

$$\frac{1}{(2-1)} + 0.5 = 1.5$$

The actual number of stage N_t is calculated approximately 2.5*N_{min} which is 41 including total condenser.

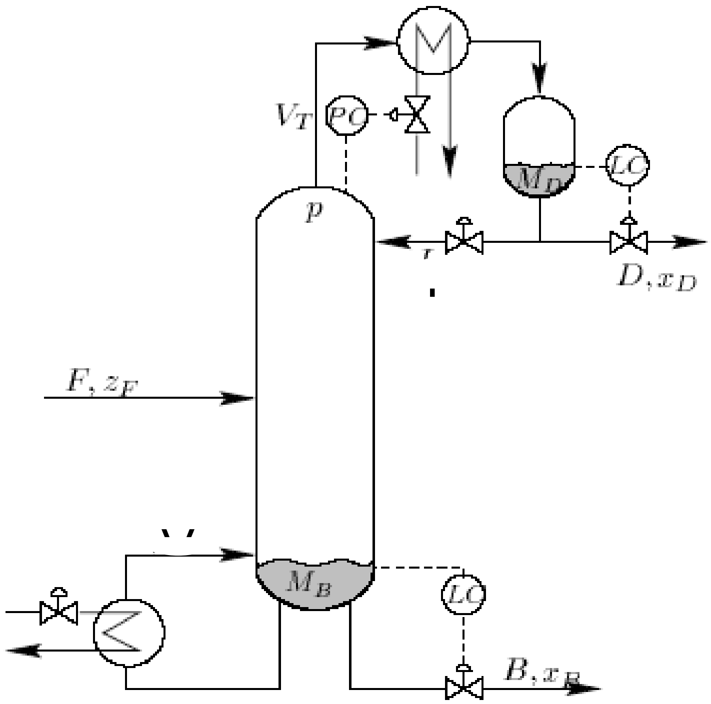


Figure1.**Typical Simple Distillation Column controlled with LV- configuration. (Skogestad & Postlethwaite, 1996)**

Table1. List of symbols and notations for Binary product distillation column (column A)

F	Feed rate, kmol/min
Z	Feed composition, mole fraction
q_f	Fraction of liquid in the Feed, (assumed to be 1 as the Feed is saturated liquid)
D	Distillate flow rate(top product), kmol/min
B	Bottom Product flow rate, kmol/min
x_A^D and x_B^B	Main component compositions of Top and Bottom product respectively.
$L=LT=$	Reflux flow, kmol/min
$V=V_B$	Boilup flow, kmol/min
N	Number of theoretical stages (including Reboiler)
N_T	Total number of stages (including total condenser)
α_{AB}	Relative volatility, 2 in this case

2 Optimization

2.1 Plant Economics and Objective Function

Optimal operation can be translated into simple control objectives. The control should be done for economics and stabilization. Before selecting controlled variables optimization problem is solved to find the optimal operating points with a defined objective function Skogestad (2000)

$$min\, J(u, x, d)$$

Subjected to:

Model equations: $f(u, x, d) = 0$

Operational constraints: $g(u, x, d) < 0$

$$y = f(x, u, d)$$

Where x is vector of all state variables, u is a vector of all input variables which are also manipulated variables and d is vector of all disturbances. f are the model equations and g are the inequality constraints. y is the vector of measurements.

There are mainly two types of cost associated with process plant: Capital Cost and Operational cost. Operational costs are costs of utilities, wages, maintenance, repair, feed, energy etc. The fixed capital cost has not been considered here because the project is specifically about the operation of Distillation Column and the timescale for optimal operation economics is in hours Skogestad (2012). To find optimal operation, we can measure the performance of the column according to our criteria or requirements. Generally the main criteria of optimal operation are to make profit subjected to some other constraints and specifications Alstad (2005). For process plant the objective function can be minimizing cost, J .It can further be modified to more specific objectives like maximizing the purity, minimizing the energy etc.

$$J = cost\ feed + cost\ energy - value\ products$$

The operational cost here is related to the amount and price of feed stream and energy required for heating and cooling. The objective function to be minimized can be written as follows, Jacobsen and Skogestad (2011).

$$J = \sum_{i=1}^{n_f} p_{f.i} F_{f,i} + \sum_{j=1}^{n_v} p_{v,j} F_{v,j} + \sum_{k=1}^{n_k} p_{p,k} F_{p,k} \tag{4}$$

Where n_f, n_v and n_p are the numbers of feed streams, utility streams and product streams respectively. p Stands for the respective prices of each stream in ($/kmol) and F (kmol/min) stands for corresponding flow rates in (kmol/min).

For a binary distillation column with one feed stream and two product streams the cost function can be written as follows:

$$J1 = p_F F + p_L L + p_v V - p_D D - p_B B \tag{5}$$

F, L, V, D and B are flow rates of feed, reflux, boilup, distillate and bottom product respectively. The objective function can further be simplified as given by Jakobsen and Skogestad (2011).

$$J_2 = p_F F + p_v V - p_D D - p_B B \tag{6}$$

When products' specifications are given the price of product is assumed to be constant irrespective of purity. Feed is given and *F=D+B (flow in = flow out)* is also constant Therefore J_2 can be further written as J_3 whose first term is constant and minimizing the objective function means minimizing *V*. For given product specifications the minimum optimal energy to run the column is given by.

$$\begin{aligned} J_3 &= (p_F F - p_D D - p_B B) + p_v V \\ &= k + p_v V \end{aligned} \tag{7}$$

When product's specifications are not given the price becomes a function of product purity fraction in product streams. The price dependent on purity can be written as

$$p = p_{i0} x_i \tag{8}$$

Where x_i is the mole fraction of the component one gets paid for and p_{i0} is the price of the pure component?

2.2 Optimal Operation for Minimum Energy

There are mainly five degree of freedom for binary product distillation column namely distillate flow rate D, reflux flow rate L, Vapor flow rate from the top V_T, bottom product flow rate B and boilup flow rate V. The notations are already given in table1.The pressure P, in the column is controlled by the manipulated variable V_T, the level of the bottom product is controlled by B and the level in the distillate tank is controlled by D. For a given pressure P and given feed F, the remaining degrees of freedom are 2 and they are the reflux flow rate L and boilup flow rate V. Equation (7) gives the objective function to minimize the energy for optimal operation and is re-written below:

$$min.(J) = \min.(-P)\text{ , Where }\begin{aligned} J &= (p_F F - p_D D - p_B B) + p_v V \\ &= k + p_v V \end{aligned}$$

Constraints

Purity$D$: $x_A^D \geq 0.99$ (Given)

Purity B: $x_B^B \geq 0.99$ (Given)

Flow constraints: $min \leq D, B, L\ etc. \leq max$

$0 \leq D, B \leq F = 1$

Column capacity (flooding): $V \leq Vmax, V \leq 4.008$

Pressure: P, given (d)

P given and is manipulated by L

Feed: F, given (d)

F is 1 Km/min

Table 2. Data for optimal operation at minimum energy

F	z_f	q	α	L	V_0	D	B	x_A^D	x_B^B	J
1	0.5	2	1	1.0017	1.5017	0.5	0.5	0.99	0.99	-0.99

On running the optimizer for objective function given by equation (7), the minimum value of energy for optimal operation comes out to be 1.5017 Kmol/min. This value is same as the one calculated by (King (1971), refer to equation (3).The above value of energy has been obtained when purity constraints on top and bottom products are active. The data for optimal operation with objective function to minimize the energy is given in Table 2.

2.3 Optimal Operation for minimizing the cost

The design of the column (number of stages, optimal feed location etc.) is fixed and the objective is to optimize the operation when the energy is fixed however products' specifications are not fixed and products are valued based on their purities. This situation is likely to happen in real plant when the available energy is less than the minimum energy required for optimal operation .In this sections the analysis has been done on how the column will behave when the available energy is less than minimum energy required to run the column at optimal. Four different tasks have been done. The first three tasks have same objective functions: minimizing the product loss, however each task varies because of given specifications. In task 4 the objective function is to minimize loss due to impurities. All four tasks are described below and for clarity and comparison results are given in tabulated form in next section.

3. Optimization Results

Task 1: Minimizing the Cost for Fixed D/F

The minimum optimal energy to run the column is found to be $V_0 = 1.5017$ Kmol/min. (Refer to section 2.2). Now optimization is done to minimize cost (economics). with fixed D/F (normalized with respect to F) and for various values of energy lower than V_0. It should be noted that each time optimization is done with fixed energy (in terms of percentage of minimum energy V_0 required for optimal operation) and D/F. Since products' specifications are not given the price of top and bottom product is directly proportional to mole fractions of valuable components in each stream. The objective function combining equation (7) and equation (8) becomes:

$$p_D = p_{A0} x_A^D,\ p_B = p_{B0} x_B^B \tag{9}$$

$$J = p_F F + p_v V - p_{A0} x_A^D D - p_{B0} x_B^B B \tag{10}$$

A special case is considered here such that

$$p_{A0} = 1,\ p_{B0} = 1$$

$$p_F = 0,\ p_V = 0$$

The optimization result for task 1 is given in Table 3.It should be noted that the notations x for mole fractions are used such that subscripts are for the component and superscripts are for streams.

The values marked in bold and underlined are fixed specifications.

Table 3. Task1: Minimizing cost for given energy and fixed D/F

F	z_f	*α*	*L*	*V*	%ofV_0	*D/F*	*B*	x_A^D	x_B^B	J_1
1	*0.5*	*2*	1.0017	**1.5017**	100%	**0.5**	0.5	0.99	0.99	-0.99
			0.9717	**1.4716**	98%	**0.5**	0.5	0.9843	0.9843	-0.9843
			0.9416	**1.4416**	96%	**0.5**	0.5	0.9768	0.9768	-0.9768
			0.9266	**1.4266**	95%	**0.5**	0.5	0.9726	0.9726	-0.9726
			0.8515	**1.3515**	90%	**0.5**	0.5	0.9495	0.9495	-0.9495
			0.776	**1.2764**	85%	**0.5**	0.5	0.9251	0.9251	-0.9251
			7014	**1.2014**	80%	**0.5**	0.5	0.9003	0.9003	-0.9003
			0.6263	**1.1263**	75%	**0.5**	0.5	0.8754	0.8754	-0.8753
			0.5512	**1.0512**	70%	**0.5**	0.5	0.8504	0.8504	-0.8504

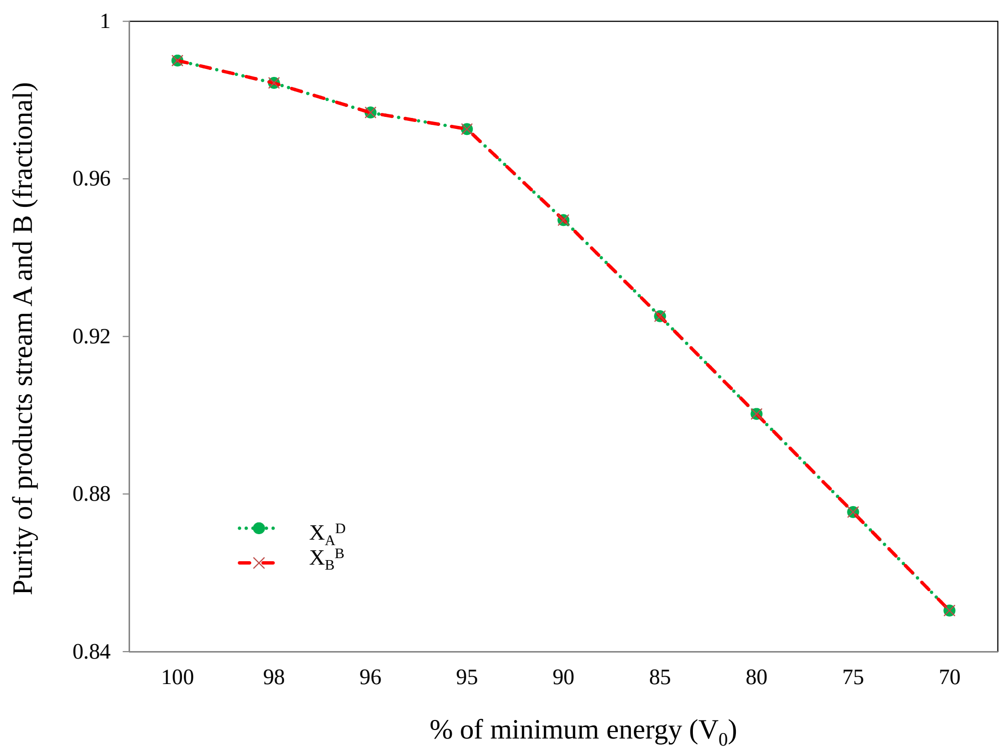


Figure 2. Task1: Products purities and cost versus energy for fixed D/F

Task 2: Minimizing the cost for Fixed x_A^D

In this task the top product D is only valuable product. The bottom product B has no value. The objective function for minimizing the cost is same as the one used for task 1 (equation 10). Following prices are used for calculating the cost. Prices of energy and feed are assumed zero for simplification.

$$p_{A0} = 1, p_{B0} = 0$$

$$p_F = 0, p_V = 0$$

The optimization result is given in table 4.

Table 4. Task 2: Minimizing cost for given energy and fixed top product purity

F	z_f	α	L	V	% of V_0	D	B	x_A^D	x_B^B	J_2
1	0.5	2	1.0017	**1.5017**	100%	0.499	0.500	**0.99**	0.989	-0.495
			0.9805	**1.4716**	98%	0.491	0.509	**0.99**	0.9729	-0.48625
			0.9603	**1.4416**	96%	0.481	0.519	**0.99**	0.9547	-0.47652
			0.9503	**1.4266**	95%	0.476	0.524	**0.99**	0.9457	-0.47158
			0.9003	**1.3515**	90%	0.451	0.549	**0.99**	0.9028	-0.4467
			0.8504	**1.2764**	85%	0.426	0.574	**0.99**	0.8636	-0.42174
			0.8006	**1.2014**	80%	0.400	0.599	**0.99**	0.8277	-0.39677
			0.7507	**1.1263**	75%	0.376	0.624	**0.99**	0.7947	-0.37182
			0.7008	**1.0512**	70%	0.350	0.649	**0.99**	0.7643	-0.34689

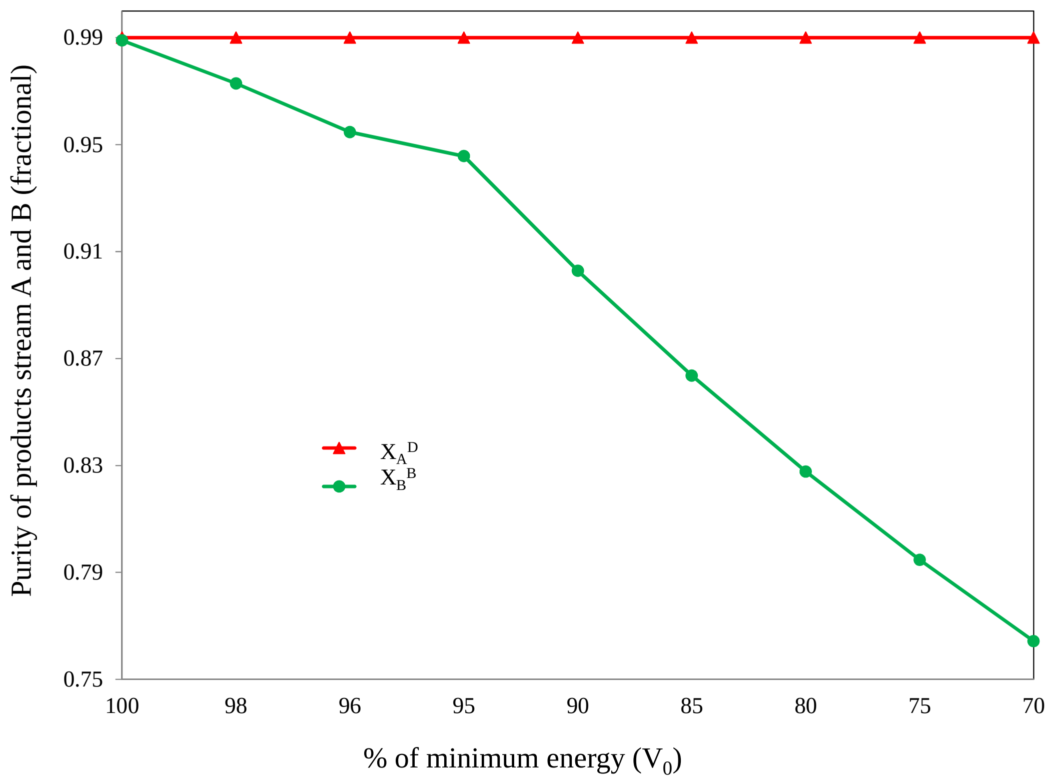


Figure 3. Task2: Bottom product purity versus energy for fixed top product purity

Task 3: Minimizing the Loss due to Impurities for Fixed $\mathbf{x_B^B}$

In this task the bottom B is only valuable product. The top product has no value. Equation (10) has been used for cost calculation. The objective function used for this task is similar to task 1 and task 2.

$$p_{A0} = 0, p_{B0} = 1$$

$$p_F = 0, p_V = 0$$

The optimized values are given in table 5.

Table 5. Task 3: Minimizing cost for given energy and fixed bottom product purity

F	z_f	α	L	V	% of V_0	D	B	x_A^D	x_B^B	J_3
1	0.5	2	1.0017	**1.5017**	100%	0.500	0.499	0.989	**0.99**	-0.5
			0.9664	**1.4716**	98%	0.505	0.495	0.979	**0.99**	-0.49479
			0.9283	**1.4416**	96%	0.513	0.487	0.965	**0.99**	-0.48674
			0.9087	**1.4266**	95%	0.518	0.482	0.956	**0.99**	-0.48214
			0.8089	**1.3515**	90%	0.543	0.457	0.913	**0.99**	-0.45741
			0.7084	**1.2764**	85%	0.568	0.432	0.872	**0.99**	-0.43196
			0.6077	**1.2014**	80%	0.594	0.406	0.835	**0.99**	-0.40641
			0.5071	**1.1263**	75%	0.619	0.3808	0.801	**0.99**	-0.38086
			0.4065	**1.0512**	70%	0.644	0.355	0.770	**0.99**	-0.35533

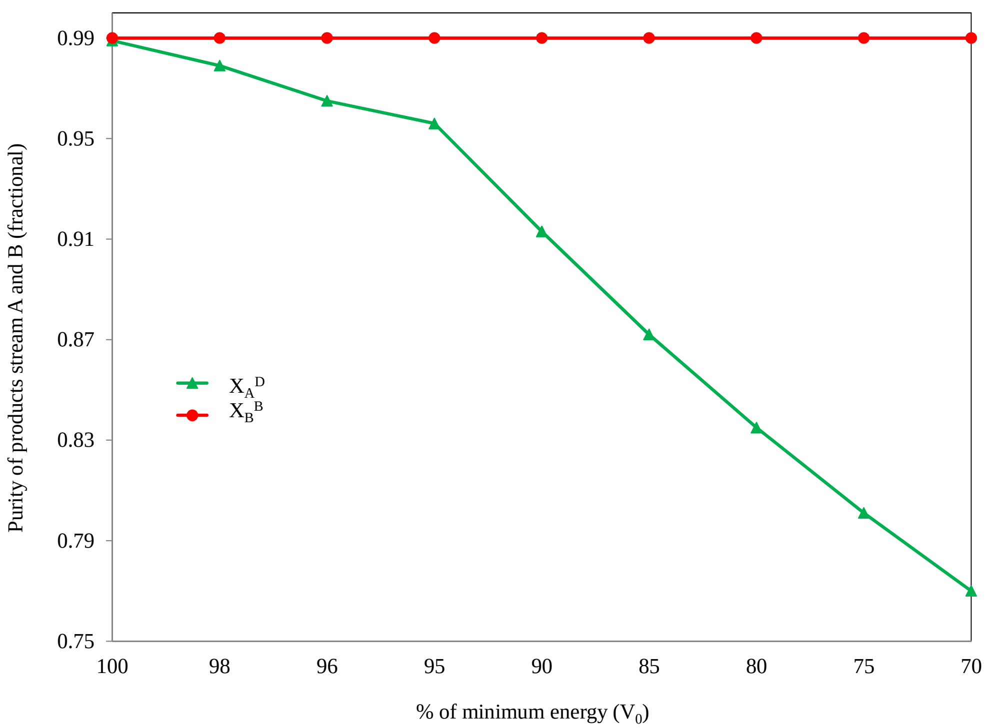


Figure 4. Task3: Top product purity versus energy for fixed bottom product purity

Task 4: Minimizing Loss due to Impurities with Fixed Energy

In this task the objective function is not same as other three tasks. The objective function is to minimize loss due to impurities costs. The objective function is written as follows:

$$J = p_{A0} * (1 - x_A^D) * D + p_{B0} * (1 - x_B^B) * B \qquad (11)$$

$p_{A0} = 1, p_{B0} = 1$

The optimized values are given in table 6 and 7.

$p_{A0} = 1.5, p_{B0} = 1$

Table 6. Task 4: Minimize Cost penalty due to impurities

F	z_f	*α*	*L*	*V*	*% of V*	*D*	*B*	x_A^D	x_B^B	J_4
1	0.5	2	0.9982	**1.5017**	100%	0.503	0.49	0.987	0.994	0.00935
			0.9661	**1.4716**	98%	0.505	0.494	0.979	0.990	0.01510
			0.9335	**1.4416**	96%	0.508	0.492	0.969	0.985	0.02272
			0.9172	**1.4266**	95%	0.509	0.490	0.964	0.982	0.02699
			0.8370	**1.3515**	90%	0.514	0.485	0.937	0.963	0.05032
			0.7608	**1.2764**	85%	0.515	0.484	0.912	0.938	0.07484
			0.6886	**1.2014**	80%	0.513	0.487	0.890	0.910	0.09967
			0.6199	**1.1263**	75%	0.506	0.494	0.870	0.880	0.12463
			0.5566	**1.0512**	70%	0.495	0.505	0.854	0.846	0.14962

Table 7. Task 4: Minimizing Cost penalty due to impurities

F	z_f	*A*	*L*	*V*	*%ofV*	*D*	*B*	x_A^D	x_B^B	J_5
1	0.5	2	1.0000	**1.5017**	100%	0.5017	0.4983	0.9888	0.992102	0.01235
			0.9715	**1.4716**	98%	0.5002	0.4998	0.9841	0.984496	0.01965
			0.9368	**1.4266**	95%	0.4898	0.5102	0.9810	0.961765	0.03345
			0.8863	**1.3515**	90%	0.4652	0.5348	0.9802	0.917688	0.05784
			0.8367	**1.2764**	85%	0.4397	0.5603	0.9798	0.876546	0.08244
			0.7874	**1.2014**	80%	0.414	0.586	0.9796	0.838863	0.10706
			0.7379	**1.1263**	75%	0.3883	0.6117	0.9794	0.804305	0.13169
			0.6885	**1.0512**	70%	0.3625	0.6375	0.9792	0.772538	0.15631

4. Discussion

When the Binary Product Distillation Column is run at lower energy than what is required for optimal operation then it is not possible to stick to specifications of products. The operation can be optimized for different objective functions for given specifications and constraints. In task 1 when D is fixed and normalized with F then the decrease in vapor flow rate increases the impurities in both top and bottom products equally. Which means D/F can be fixed when both products are equally valuable and the price of both products are dependent on their purities.

Similarly when one of the products is valuable and the other one has no value then the column can be operated at lower value of energy. and will still get one desired product at specifications

When the loss due to impurities is being minimized then the loss has increased as the price of one of the product has increased from 1 to 1.5. Also when top product is more valuable than the bottom product then the impurities in bottom product has increased more than when both top and bottom products were equally valuable.

5. Conclusion

When the available energy to run the column is less than the minimum energy required for optimal operation then products’ purity is degraded. In such case operation can still be optimal based on the objective function and the requirement. This case is more useful when the products’ specifications are not given and the price of the product is dependent on its purity

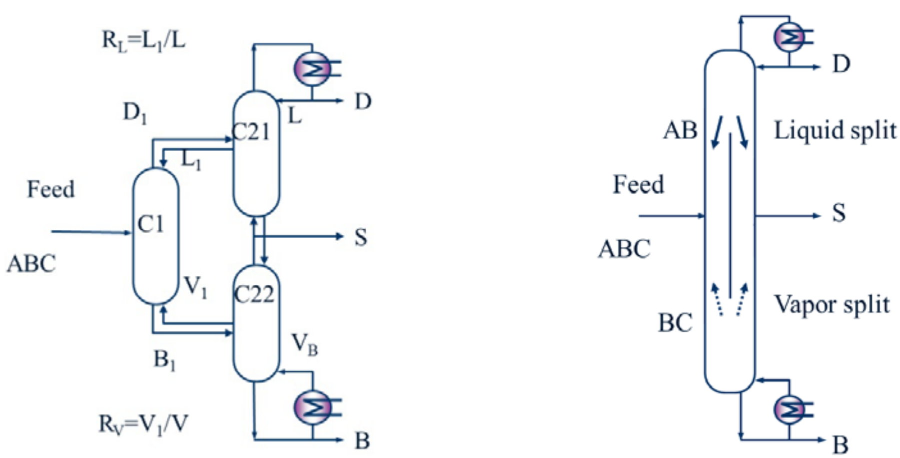
Chapter B

Divided Wall Column

6. Background

6.1 Brief Description of Divided Wall (Petlyuk) Column

The Petlyuk configuration represents an arrangement that can separate three or more components using a single reboiler and a single condenser. This configuration has even more thermal coupling than the pre-fractionator which increases efficiency; this also means that there are greater internal flows with no hold-ups due to not having an intermediate reboiler or condenser in the Petlyuk column. The exchange of vapor and liquid between the columns poses strict pressure and operability constraints. Figure 5. represents the thermodynamically equivalent implementation of three products divided wall column configuration. It is the most compact distillation column for the separation of these products that allows for both considerable energy and capital saving. There is a partition between the feed and side-draw sections of the column, which provides greater capacity and increased separation efficiency yet still externally resembles a normal side-draw column. This column is thermodynamically identical to the Petlyuk column provided that there is negligible heat transfer across the dividing wall section of the column.



(a) Implementation with three separate columns (b) DWC implementation with a side-product

Figure 5. Thermodynamically equivalent implementations of three-product Petlyuk column

6.2 The Column Model

The Divided Wall (Petlyuk) Column model for this study is same as Dwivedi et al. (2012). Compared to the product purities specifications given in Table 8, the number of stages is large in each sub-column. Therefore the required energy is close to the minimum energy using an infinite number of stages. The liquid flow dynamics are modeled by a simple linear relationship. The Divided Wall (Petlyuk) Column diagram is shown in fig.5. all the notations and nomenclatures are given in table 8 and matlab codes for the model and optimization are given in appendix. The column is divided into six sub-columns, each with twenty stages and forty states. The compositions are represented by x such that the subscripts are for the respective components A, B and C and superscripts are for respective streams D, S and B.

The simplified model assumptions are:

- Three components A (the lightest), B (medium) and C (the heaviest).
- constant relative volatility
- Equilibrium on all stages
- negligible vapor holdup
- one feed and three products (Top product D, Side product S and Bottom Product B)
- Constant internal molar flows (same vapor flow on all stages)
- total condenser

7. Optimal Operation of the column

Optimal operation is defined in terms of the objective function. The objective function basically depends on the given criteria as well as the operational requirements. The column can be optimally operated in two modes Ghadrdan et al. (2011)

- *Mode 1: Minimize the energy for given (fixed) product specifications.*
- *Mode 2: Minimize the products' impurities for given (fixed) energy.*

The simple derivation of objective functions for mode 1 and mode 2 is given in the following section.

7.1 Plant Economics and Objective Function

The basics of plant economics and objective function for binary product distillation column have already been discussed in Section 2.1 of Chapter A. In Divided Wall Column we also have side stream as one of the products, therefore the cost function for DWC (Petlyuk Column) is deduced in the following from using equation (4):

$$J_1 = p_F F + p_v V - p_D D - p_s S - p_B B \tag{12}$$

When products' specifications are given the price of product is assumed to be constant irrespective of purity. Feed is given and $F=D+B+S$ *(flow in = flow out)* is also constant Therefore J_1 can be further written as J_2 whose first term is constant and minimizing the objective function means minimizing V. For given product specifications the minimum energy to run the column at optimal conditions is given by.

Mode 1:→

$$\begin{aligned} J_2 &= p_F F + p_v V - p_D D - p_S S - p_B B \\ &= (p_F F - p_D D - p_S S - p_B B) + p_v V \\ &= k + p_v V \end{aligned} \tag{13}$$

The above form of equation can be used to get minimum energy for optimal operation. It is called mode 1 in order to make it specific in which mode of operation the column is running. In this paper, mode 1 has been used to get the minimum energy for optimal operation with fixed products' specifications.

When the products' specifications are not given then the price of each product (D, S, and B) depends on the purity of the main component present in it. Following cost function is written by combining equations (8) and (12):

$$J_2 = p_F F + p_v V - p_{A0} x_A^D D - p_{B0} x_B^S S - p_{C0} x_C^B B \qquad (14)$$

In order to take constant terms out from the equation (13) and make the equation even simpler following cost equation is deduced:

$$J_3 = p_F F + p_v V - p_{D0}(1 - x_B^D) D - p_{B0}(1 - x_A^S - x_C^S) S - p_{B0} x_B^B B \qquad (15)$$

For a given feed rate F and fixed boilup rate V equation (11) can be written as follows:

$$= k_1 + k_2 - k_3 - p_{A0} x_B^D D - p_{B0}(x_A^S + x_C^S) S - p_{C0} x_B^B B \qquad (16)$$

k_1, k_2 and k_3 are constant terms and thus can be removed. The objective function finally becomes a function of variable terms impurities in three product streams *D,S and B.*When prices of all three components are equal that is :

$$p_{A0} = p_{B0} = p_{C0} = 1 \qquad (17)$$

The objective function in equation (16) can be written as follows:

Mode 2:→ $$-J = x_B^D D + (x_A^S + x_C^S) S + x_B^B B \qquad (18)$$

The above form of equation has been used in Mode 2, where the objective function is to minimize impurities for given energy.

7.2 The Optimal Operation for Minimum Energy (Mode 1)

The operation is considered optimal for a given product specifications when the column is operated at energy as close to minimum energy. It should be noted that energy term referred here is only boilup V. In three products Petlyuk Column, there are seven degrees of freedom –L, V, S, D, B, R_L and R_V Out of these seven two of them (D and B) are used as manipulated variable to control the condenser and reboiler holdup and they have no steady state effects. L, V and S are used to control the impurity constraints in (19). R_L and R_V can be then used to minimize energy.as given by equation (13) and is rewritten below:

Mode 1:→ $$J = k + p_v V(energy)$$

In most of the cases in real plant R_V is fixed and cannot be used as a degree of freedom.because of which one of the components in the prefractionator is generally over purified Dwivedi et al. (2012) Following (19) constraints on product specifications are active at the optimal energy solution. The input data, parameters and product compositions for optimal operation are listed in Table 8. **The subscripts have been used for the components and superscripts for the product streams.**

Operational Constraints:

Impurity in distillate stream D : $x_B^D \le 0.5\%$ (19-a)

Light impurity in side stream S : $x_A^S \le 0.5\%$ (19-b)

Heavy impurity in side stream S: $x_C^S \le 0.5\%$ (19-c)

Impurity in bottom stream B : $x_B^B \le 0.5\%$ (19-d)

Table 8: Process parameters and optimal conditions for the Petlyuk column model

Relative volatilities [A, B, C]	[4.2 2.1 1]
Number of stages in C1, C21 and C22	20+20 (each sections)
Nominal feed flow rate (F)	1 kmol/min
Nominal feed composition [A, B, C]	[33.3 33.3 33.3](mol %)
Nominal liquid reflux (L)	0.9989 kmol/min
Nominal boilup (V)	1.3322 kmol/min
Nominal distillate flow rate (D)	0.3333 kmol/min
Nominal bottom flow rate (B)	0.3333 kmol/min
Nominal side-product (S)	0.3333 kmol/min
Nominal liquid split (R_L)	0.3189
Nominal vapor split (R_V)	0.57045
Nominal purity of distillate (x_A^D)	99.5 (mol %)
Nominal purity of side-product (x_B^S)	99.00 (mol %)
Nominal light impurity of side-product (x_A^S)	0.5 (mol %)
Nominal heavy impurity of side-product (x_C^S)	0.5 (mol %)
Nominal purity of bottom product (x_C^B)	99.5 (mol %)
Nominal heavy impurity of prefractionator top (x_C^{D1})	0.0055 (mol %)
Nominal light impurity of prefractionator bottoms (x_A^{B1})	0.00832 (mol %)

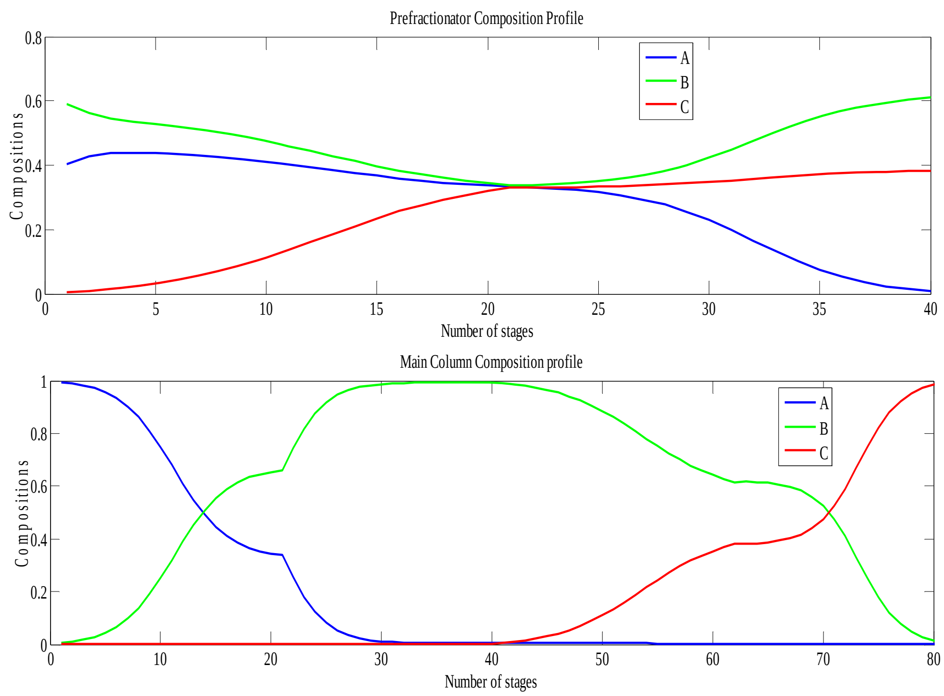


Figure 6. A, B and C compositions profiles in the Pre-fractionator and the Main Column

7.3 The Optimal Operation for Minimizing Impurities (Mode 2)

The minimum energy for running the column at optimal conditions so as to achieve given products' specifications ($x_A^D = 99.5, x_B^S = 99\%\ and\ x_C^B = 99.5\%$) has been calculated to be $V_0 = 1.3322$ in section 7.2 The need to change the mode (mode 1 to mode 2) of operation has emerged out for practical reasons like expensive energy or low supply of energy with respect to demand In this situation the objective function has changed from minimizing the energy to minimizing the sum of impurities in products. The optimal operation is minimizing impurities when the specifications on the products are not given. The cost function for this case has already been derived in section (7.1). The cost function is for minimizing impurities is (from equation 18)

Mode 2:→ $$-J = x_B^D D + (x_A^S + x_C^S)S + x_B^B B$$

The main idea is to see how the column would behave in case the given energy to run the column is minimum or lower than minimum in terms of optimal operation. It is quite obvious that by operating the column at below optimal energy one cannot stick to the given product specifications but the case study is useful for analysis purpose. In that case which product stream would be worst in terms of purity? and to what extent ? The case study has been done for following tasks. In each task the optimization has been done to minimize the sum of impurities in products for various percentage of optimal energy(V_0).The following table briefly describes how operations can be done to minimize impurities for different manipulated variables and specifications.

Table 9. Manipulated variables and fixed specifications for each task

	V	L	R_L	R_V	S	x_A^D	x_B^S	x_C^B
Task 1	Spec.	M.V.	M.V.	M.V.	M.V.			
Task 2	Spec.	M.V.	M.V.	M.V.	M.V	Spec.		Spec.
Task 3	Spec.	M.V.	M.V.	M.V.	M.V.	Spec.	Spec.	
Task 4	Spec.	M.V.	M.V.	M.V.	M.V.		Spec.	
Task 5	Spec.	M.V.	M.V.	Spec.	M.V.			
Task 6	Spec.	M.V.	M.V.	Spec.	M.V.		Spec.	

8. Optimization Results

Task 1: Minimizing sum of product impurities by decreasing energy for variable R_V, R_L, L and S

Table 10. Change in product impurities with change in the minimum energy (V_0) for the variable R_V

,% of V_0	L E-01	RL E-01	RV E-01	S E-01	X_B^D E-03	X_A^S E-03	X_C^S E-03	X_B^B E-03	J E-03
100%	9.985	3.107	5.704	3.351	3.56	2.40	7.32	0.81	4.71
98%	9.716	3.173	5.807	3.359	4.54	2.62	11.62	1.86	6.92
96%	9.452	3.078	5.835	3.404	4.25	3.13	23.94	1.99	11.28
95%	9.320	3.096	5.866	3.429	5.59	4.33	30.97	2.22	14.69
94%	9.172	3.099	5.907	3.447	9.72	4.50	39.84	1.99	19.18
92%	8.904	3.428	6.155	3.521	9.54	3.57	60.63	1.93	26.41
90%	8.632	3.453	6.260	3.585	10.8	3.33	78.17	1.43	33.28
85%	7.973	3.241	6.404	3.758	10.54	4.59	11.89	1.30	50.34
82%	7.622	4.323	7.142	3.928	3.19	10.56	145.99	3.27	63.47
80%	7.302	4.196	6.963	3.947	23.70	14.44	162.16	1.46	78.05

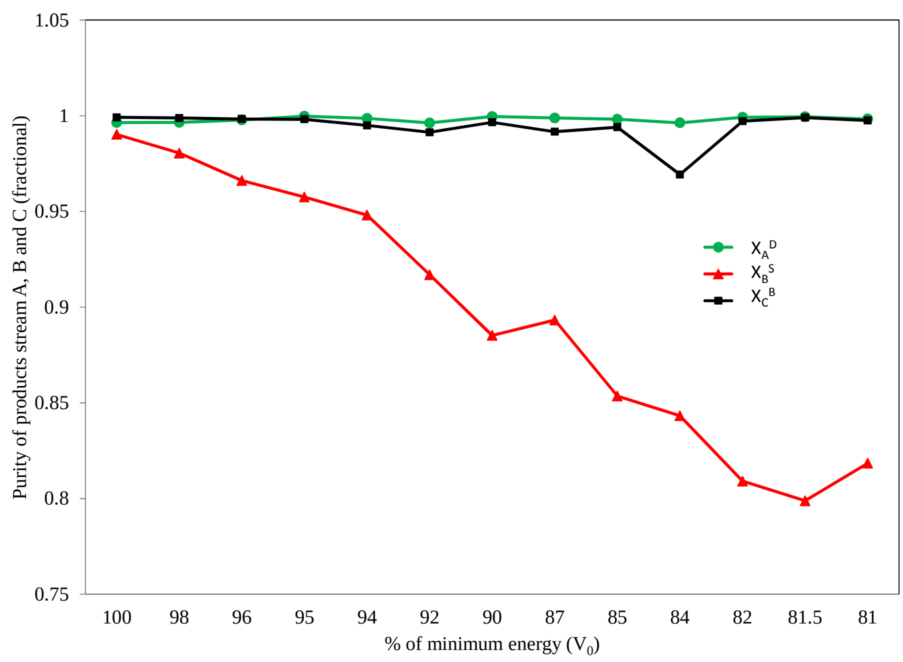


Figure 7. Variation in product purities with change in the minimum energy (V_0) for the variable R_V

Task 2: Minimizing sum of product impurities by decreasing energy for fixed top and bottom product specifications and variable R_V, R_L, L and S

Table 11. Change in product impurities with change in the minimum energy (V_0) for fixed top and bottom product purity and the variable R_V

% of V_0	L E-01	RL E-01	RV E-01	S E-01	X_B^D *E-03*	X_A^S *E-03*	X_C^S *E-03*	X_B^B *E-03*	*J* *E-03*
100%	9.988	3.185	5.707	3.332	**5.00**	4.674	5.01	**5.00**	6.56
98%	9.707	3.363	6.020	3.336	**5.00**	0.523	10.26	**5.00**	6.93
96%	9.444	3.185	5.937	3.377	**5.00**	1.287	21.65	**5.00**	11.06
95%	9.35	3.236	5.836	3.453	**5.00**	2.554	31.70	**5.00**	18.55
94%	9.185	3.222	5.982	3.442	**5.00**	3.355	37.61	**5.00**	17.378
92%	8.909	3.416	6.247	3.500	**5.00**	0.900	55.94	**5.00**	23.14
90%	8.642	3.780	6.560	3.581	**5.00**	0.605	077.61	**5.00**	31.22
85%	7.994	3.608	6.552	3.755	**5.00**	5.213	115.40	**5.00**	48.416
80%	7.355	3.477	6.766	3.951	**5.00**	11.824	152.28	**5.00**	67.871

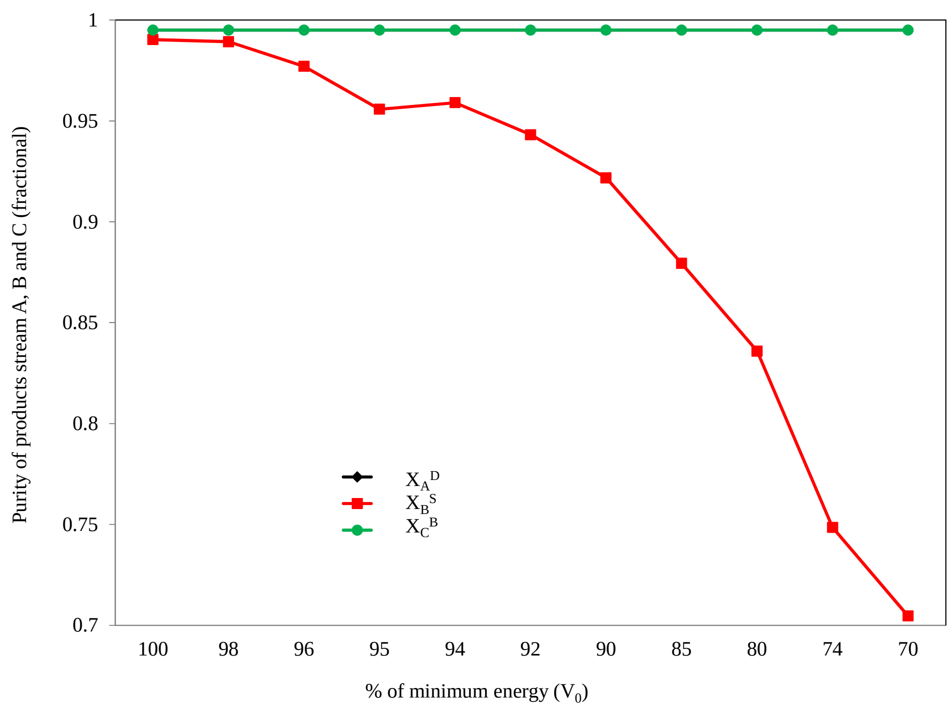


Figure 8. Variation in product impurities with change in the minimum energy (V_0) for fixed top and bottom purities and the variable R_V

Task 3: Minimizing sum of product impurities by decreasing energy for fixed top and side product specifications and variable R_V, R_L, L and S

Table 12. Variation in product impurities with change in the minimum energy (V_0) for fixed top and side product purity and the variable R_V

% of V	L E-01	RL E-01	RV E-01	S E-01	X_B^D *E-03*	X_A^S *E-03*	X_C^S *E-03*	X_B^B *E-03*	*J* *E-03*
100%	9.985	6.837	4.295	3.3473	**5.00**	3.947	6.053	0.852	5.298
98%	9.711	6.739	4.127	3.303	**5.00**	1.752	8.248	13.801	9.602
96%	9.441	6.576	3.821	3.107	**5.00**	0.384	9.616	67.727	28.781
95%	9.309	6.573	3.857	3.142	**5.00**	0.726	9.274	58.549	25.365
94%	9.176	6.593	3.8647	3.049	**5.00**	1.171	8.829	82.565	34.479

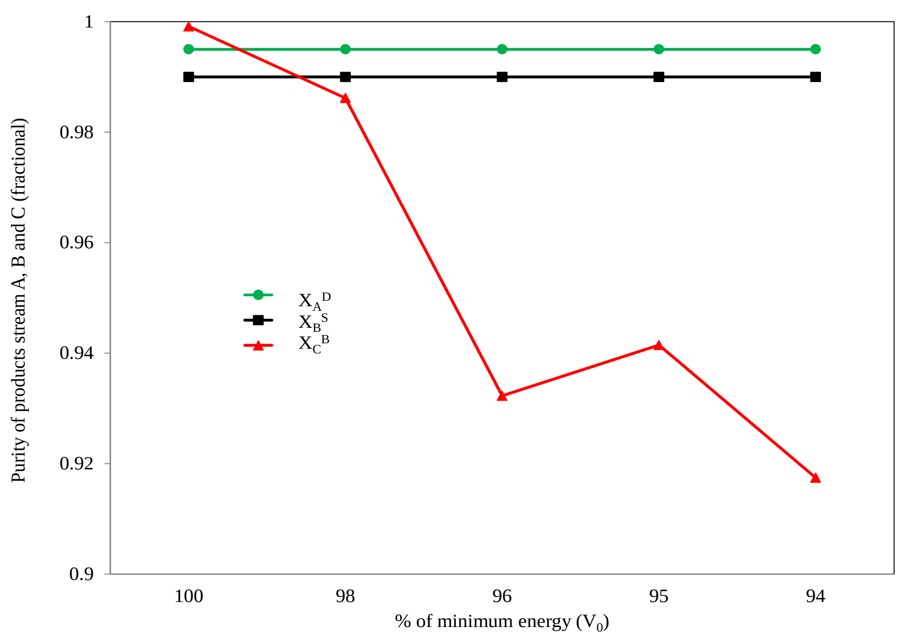


Figure 9. Variation in product purities with change in the minimum energy (V_0) for fixed top and side product purities and the variable R_V

Task 4: Minimizing sum of product impurities by decreasing energy for fixed side stream specifications and variable R_V, R_L, L and S

Table 13. Product impurities with change in the minimum energy (V_0) for fixed side stream purity and the variable R_V

% of V	L E-01	RL E-01	RV E-01	S E-01	X_B^D E-03	X_A^S E-03	X_C^S E-03	X_B^B E-03	-J E-03
100%	9.991	3.141	5.715	3.3589	2.04	2.758	7.24	0.373	4.161
98%	9.722	3.188	5.828	3.275	2.17	2.113	7.89	24.73	12.38
96%	9.454	3.333	6.068	3.124	1.28	0.668	9.33	66.67	27.19
95%	9.276	3.474	6.188	3.111	14.27	0.548	9.45	58.46	28.45
94%	9.126	3.394	6.062	2.954	21.18	2.94	7.06	92.21	43.80
92%	8.922	3.469	6.237	0.630	0.752	2.15	7.85	44.86	271.6
90%	8.388	3.871	6.550	2.611	74.81	0.57	9.42	12.64	77.45
85%	7.986	3.898	6.733	1.9057	3.26	3.23	6.77	30.19	146.6
82%	7.497	4.264	7.121	1.9638	28.42	1.92	8.07	28.59	144.5
81%	7.396	4.802	7.297	1.464	22.13	9.62	0.38	35.17	189.8

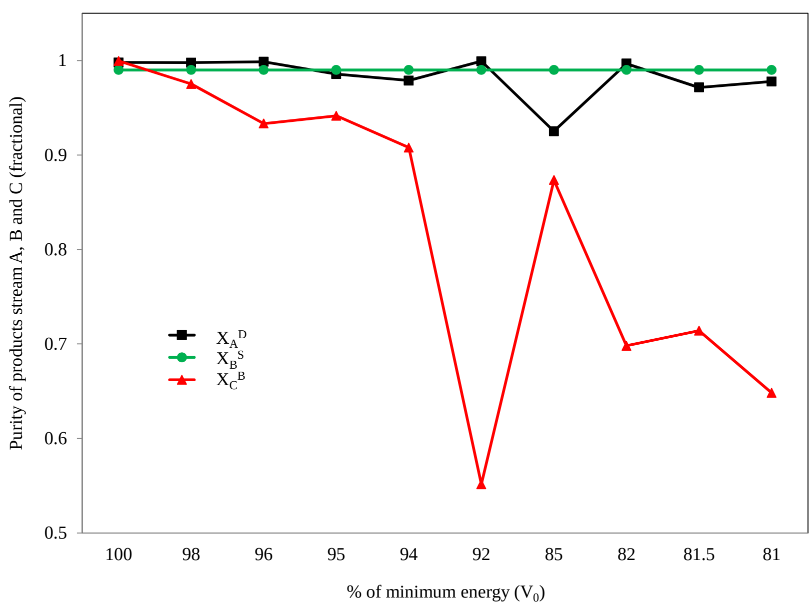


Figure 10. Variation in product purities with change in the minimum energy (V_0) for fixed side stream purity and the variable R_V

Task 5: Minimizing sum of product impurities by decreasing energy for fixed R_V, and variable R_L, L and S

Table 14. Variation in product impurities with change in the minimum energy (V_0) for the fixed R_V

% of V_0	L E-01	RL E-01	RV E-01	S E-01	X_B^D E-03	X_A^S E-03	X_C^S E-03	X_B^B E-03	-J E-03
100%	9.985	3.107	**5.705**	3.351	3.56	2.40	7.32	0.81	4.713
98%	9.736	3.097	**5.705**	3.384	3.46	7.27	12.25	1.19	8.147
96%	9.479	2.944	**5.705**	3.437	2.20	8.66	25.18	1.67	12.906
95%	9.355	2.860	**5.705**	3.474	0.221	9.46	32.99	1.85	15.418
94%	9.237	2.900	**5.705**	3.494	1.37	14.80	37.09	5.04	20.206
92%	9.021	3.084	**5.705**	3.592	3.75	30.43	52.65	8.62	33.79
90%	8.810	3.148	**5.705**	3.752	0.41	41.16	73.60	3.40	44.235
85%	8.126	2.436	**5.705**	3.878	1.78	36.24	110.20	5.95	59.099
82%	7.833	2.714	**5.705**	4.107	0.79	59.44	131.44	2.83	79.427
81%	7.615	1.9871	**5.705**	4.058	1.68	40.07	141.50	2.44	74.893

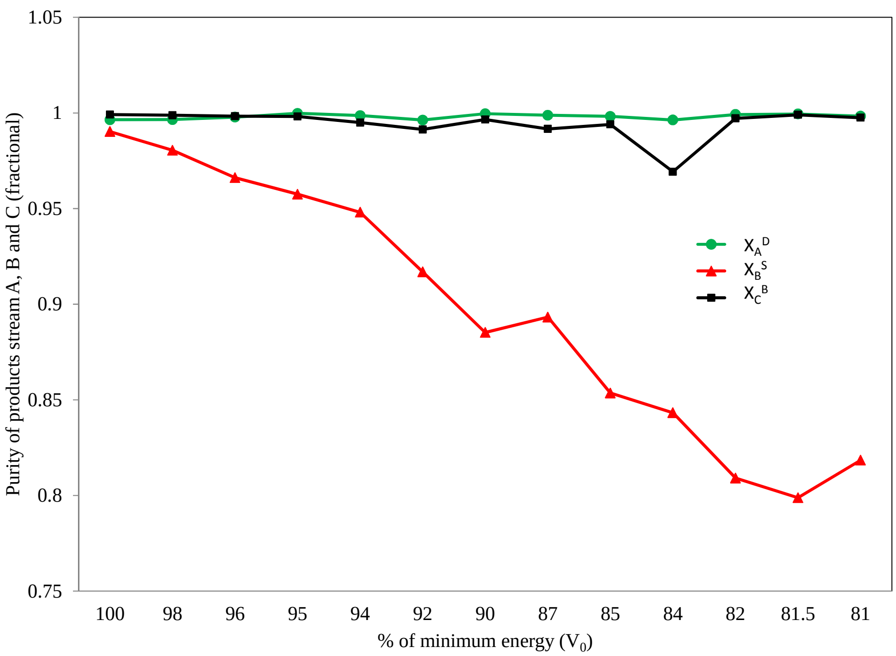


Figure 11. Variation in product purities with change in the minimum energy (V_0) for fixed R_V

9. Discussion

Mode 1: For a given feed, the steady state optimization gives minimum energy, V_0 =1.3322 Kmol/min to run the column at optimal conditions while fulfilling the products' specifications at the same time. For simplification it is called mode 1 in this report. In this mode of operation the objective function was to minimize the energy usage. The basic parameters, input variables, product compositions in the prefractionator and the main column are given in table 2. The total sum of impurities in this case was 6.67E-3 Kmol/min.

Mode 2: Starting with the minimum energy for optimal operation as obtained in mode 1, optimization has been conducted to minimize the sum of impurities of all three product streams. Starting with the base value for the optimal energy V_0=1.3322 (V_0=V_{min}),simulations were done to minimize the impurities for various lower values of V_0 in terms of percentage like 98%, 96%, 95% until the optimization was converging. and results were consistent.. Two different cases were considered here:

Case I: *Given energy and remaining degree of freedoms L, S, R_L and R_v varying*

The above case was further divided into four tasks (task1, task 2, task 3 and task 4) by fixing different product specification in each task .The results for all four tasks are given in tables (Table10-14) in previous section. For all four tasks for minimizing impurities the total sum of impurities have decreased when compared to running the column for minimizing the energy. Sum of impurities in mode 1 at V_0 =1.3322 was 6.67E-3 and for tasks 1, 2, 3 and 4 the sum of impurities are 4.71E-03, 6.56E-03, 5.28E-06 and 4.16 respectively.

It is clear from graphs for task1 that the decrease in the amount of boilup below optimal value V_0, has mainly increased the impurities in side product S and there was not much effect on distillate and bottom product. The impurities of heavy component C mainly increased in the side product S and it could be due to the insufficient number of stages in that section of column. In task 2 as the top product and side stream purity have been fixed therefore the effect was seen in the increase in the impurities in the bottom product. Similarly when top product and side product purity are fixed in task 3 then the impurities in the side stream has increased .The interesting result is from task 4 where on fixing the side stream purity the effect on product purity degradation has been mainly seen on bottom product with not much impact on top product' purity.

Case II: Given energy and remaining degree of freedoms L, S and R_L (R_V fixed)

In this case the total impurities for optimal boilup V_0=1.3322 decreased from 6.7E-03 to 4.7E-03. On decreasing the boilup further, it is observed that the sum of total impurities in the product is more in *case II*. To investigate it further we kept on decreasing the boilup and resulting total impurities went on increasing. In this case also the main impact was clearly visible in the side product S where impurities have increased.

10. Conclusion

The study has been conducted for the sensitivity analysis of given energy on products' compositions. When the vapor flow rate (energy) is decreased, one can no longer stick to the desired product specifications. The optimal in terms of minimizing the impurities sum of all three products tends to increase the impurity in the side stream. In particular this applies when R_V is also a degree of freedom. The top and bottom products purities did not drift much from the optimal values. The results obtained are useful when product specifications are not given and one gets paid for the purity in all three products. The other case could be that the side stream has no value and one get paid for the purity in both top product and bottom product.

11. Further Work

The further work should aim at developing the simple and robust control structure for the Energy-Efficient Divided Wall (Petlyuk). Lower value of energy means that the energy should be lower than the minimum energy required for running the column at optimal conditions.

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Appendices

Divided Wall (Petlyuk) Column steady state optimization data

1.

Table 1 Minimizing impurities for given energy and varying R_V,R_L,L and S

%of V	S	D	B	X_A^{B1}	X_C^{D1}	X_A^D	X_B^S	X_C^B
100	0.335132	0.333718	0.33115	0.003999	0.013495	0.996441	0.990285	0.999186
98	0.335988	0.333971	0.330041	0.004332	0.015173	0.995457	0.985757	0.998141
96	0.340485	0.333685	0.32583	0.005185	0.03615	0.995753	0.972934	0.998015
95	0.342852	0.333715	0.323433	0.00718	0.037367	0.994407	0.964699	0.997781
94	0.344726	0.335038	0.320237	0.007473	0.043649	0.990285	0.95566	0.998008
92	0.352143	0.335273	0.312584	0.005886	0.017554	0.990465	0.935796	0.998072
90	0.358485	0.335767	0.305748	0.005474	0.027632	0.989203	0.918506	0.998571
85	0.375853	0.335141	0.289005	0.007533	0.086808	0.989454	0.876467	0.998699
82	0.392882	0.330237	0.276882	0.001791	0.006325	0.996813	0.843446	0.996727
80	0.394686	0.335588	0.269726	0.023316	0.009984	0.976296	0.823401	0.998541

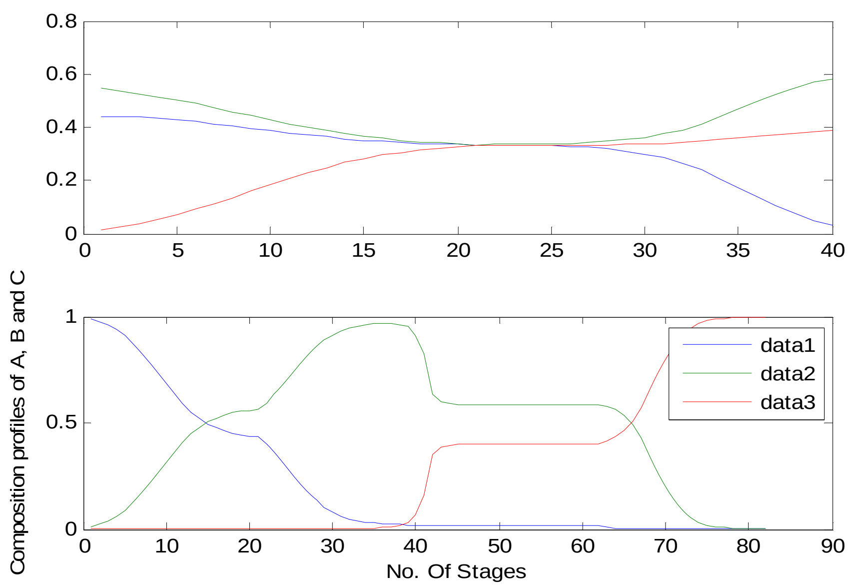

Figure 1 : The composition profiles of A, B and C at 81% V_0 for the variable R_V.

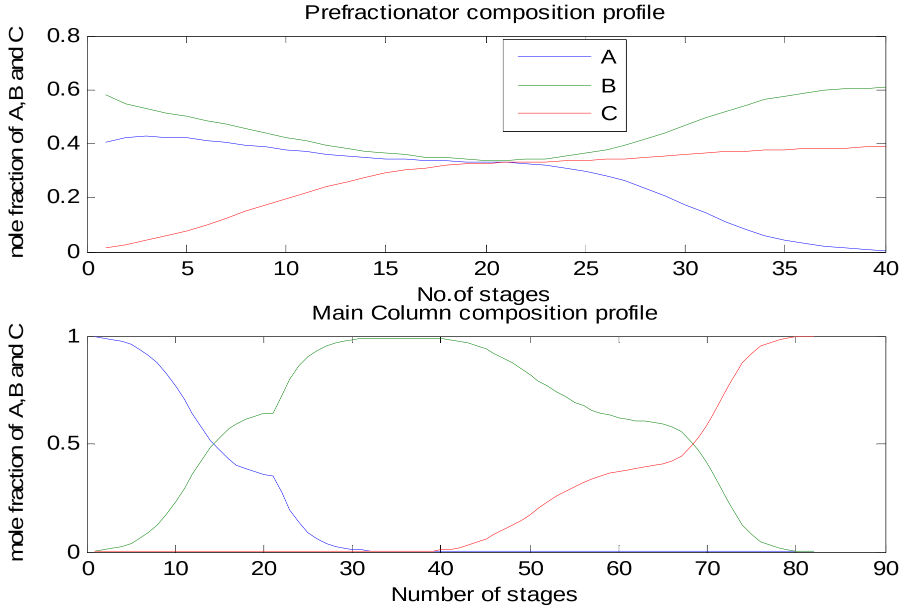

Figure 2: The composition profiles of A, B and C at 98% V_0 for the variable R_V.

Table 2 Minimizing impurities for given energy fix R_V varying R_L, L and S

% of V	*S*	*D*	*B*	X_A^{B1}	X_C^{D1}	X_A^D	X_B^S	X_C^B
100	0.335132	0.333718	0.33115	0.003999	0.013495	0.996441	0.990285	0.999186
98	0.338396	0.332022	0.329582	0.012058	0.016499	0.996538	0.980482	0.998808
96	0.343695	0.331082	0.325223	0.014432	0.04452	0.997802	0.966152	0.998326
95	0.347414	0.330121	0.322465	0.015512	0.062454	0.999779	0.957545	0.998153
94	0.34939	0.328614	0.321996	0.024515	0.055006	0.998623	0.948106	0.994962
92	0.35923	0.323614	0.317156	0.049332	0.023438	0.996254	0.916924	0.991379
90	0.375217	0.318021	0.306762	0.066153	0.015008	0.999587	0.885241	0.996596
87.5	0.374607	0.325136	0.300257	0.041111	0.138581	0.997062	0.883462	0.995249
85	0.387811	0.31985	0.292339	0.06014	0.139736	0.998218	0.853567	0.994046
83	0.391633	0.314171	0.294196	0.082068	0.121655	0.997618	0.831539	0.976455
82	0.41069	0.309167	0.280143	0.095141	0.101076	0.999211	0.809122	0.997175
81.5	0.416732	0.307027	0.276242	0.100504	0.093928	0.999467	0.798842	0.999033
81	0.40581	0.317605	0.276585	0.06655	0.197677	0.998318	0.818426	0.997562

Table 3 Minimizing impurities for given energy for fixed top and bottom purity and varying R_V, R_L, L and S

% of V_0	*S*	*D*	*B*	X_A^{B1}	X_C^{D1}	X_A^D	X_B^S	X_C^B
100%	0.333226	0.333443	0.333331	0.007782	0.005849	0.995	0.990316	0.995
98%	0.3336	0.334833	0.331567	0.000819	0.011784	0.995	0.989213	0.995
96%	0.33777	0.334571	0.327659	0.002096	0.030217	0.995	0.977062	0.995
95%	0.345341	0.330651	0.324008	0.020615	0.011216	0.995	0.955751	0.995
94%	0.344153	0.333848	0.321999	0.005527	0.029248	0.995	0.959033	0.995
92%	0.349974	0.334692	0.315334	0.001399	0.031265	0.995	0.943165	0.995
90%	0.358137	0.334791	0.307072	0.000812	0.012921	0.995	0.921781	0.995
85%	0.375504	0.333041	0.291455	0.008407	0.040475	0.995	0.87938	0.995
80%	0.395156	0.330313	0.274532	0.010811	0.092118	0.995	0.835896	0.995
74%	0.441604	0.304453	0.253943	0.005247	0.182471	0.995	0.748502	0.995
70%	0.469275	0.290664	0.240061	0.116857	0.075525	0.995	0.704661	0.995

Matlab Codes for Binary Product Distillation Column

- Colamod.m is column A model based on Skogestad and Postlethwaite which has been used in this report for operational analysis.
- aOptimizationscript.m file is a script file to run optimization. Here constraints and parameters can be changed according to the requirement

```
% Output
xprime=[dxdt';dMdt'];


clc
clear all
close all

F=1;                                % Feed flow rate
zF=0.5;                             % Feed composition
qF=1.0;                             % Feed liquid fraction
pV=0.01;                            % Steam price
pF=1;                               % Feed price
pB0=1;                              % Bottom product price
pA0=2;                              % Top product price

%Parameters vector
Par=[F zF qF pF pV pA0 pB0]';

%Number of decision variables
NV=86;

%Define the constraint limits
Vmax=1.50170*0.75;
%Xdmin=0.99;
%Xbmax=0.01;
```

```
%Define the lower and upper bounds
lb=zeros(NV,1);
ub=ones(NV,1);

%Define constraints through lower and upper bounds
%ub(1)=Xbmax;
%lb(1)=ub(1);
%lb(41)=Xdmin;
%ub(41)=lb(41);
ub(84)=Vmax;
lb(84)=ub(84);

%Change upper bounds for x(83:86) since they can be higher than one !
ub(86)=F;
ub(85)=0.5*F;
lb(85)=ub(85);
ub(83)=Vmax;
 %Initial Values
x0=ones(NV,1)*0.5;
 %fmincon options
options = optimset('TolFun',10e-8,'TolCon',10e-8,'MaxFunEvals',1e4,...
    'Display','none','Algorithm','interior-point','Diagnostics','off'...
    );
%run fmincon
[x,fval,exitflag]=fmincon(@(X)ObjFun(X,Par),x0,...
     [],[],[],[],lb,ub,@(X)nonlcon(X,Par),options);

%Print selected values
[exitflag F pV fval x(1) x(41) x(83) x(84) x(85) x(86)]
```

- Objfun is a function file with objective function.

```
function [ J ] = ObjFun(X,par)
%OBJECTIVE Summary of this function goes here
%   Detailed explanation goes here

J=par(1)*par(4)+par(5)*X(84)-par(6)*X(85)*X(41)-par(7)*X(86)*(1-X(1));
%J=1;
End
```

- Nonlcon.m

```
function [ c, ceq ] = nonlcon(X,par)

U=zeros(7,1);

U(1:4)=X(83:86);

U(5:7)=par(1:3);

s=X(1:82);

ceq=[colamod(0,s,U)];
c=[];

end
```

Matlab Codes for Divided Wall (Petlyuk) Column

Note : The codes for the model and optimizer have been taken from Deeptanshu Dwivedi (a doctoral candidate at Sigurd's process control group). Some of the files related to optimization have been modified for use.

Following are the files which have been modified for use during optimization of the column. The unused parts of codes or comments have been deleted from the original.

- Specs.m

```
global dyndata

indmat_Yes_S1


[Nz,n] = size([dyndata.x_nom;dyndata.u_nom]);% all decision variables
including inputs U and compositions and holdup on stages

%Feed rate, composition & quality
Ns=10;
As=zeros(Ns,Nz);bs=zeros(Ns,1); %linearity constraints where Ns are
product/feed specifications
% Ain=-eye(4,Nz);bin=zeros(4,1);

% These are the values of only As which contributes in specifications and
% thus=1 and not 0.
As(1,6)=1;
As(2,7)=1;
As(3,8)=1;
As(4,9)=1;

bs(1:4)=dyndata.u_nom([6:9]);% corresponding values of equality
constraints.
%bs(11:12)=dyndata.u_nom([3:4]);

% Levels, totally unnecessary constraints

As(5,11+im_mt)=1;bs(5)=x_nom(im_mt);% im_mt=368+11=379 position in x_nom
means condenser hold up
As(6,11+im_mr)=1;bs(6)=x_nom(im_mr);%im_mr=367+11=378(As)...367 is w.r.t.
only x_nom but
As(7,11+im_xt(2))=1;bs(7)=0.005;
As(8,11+im_xS1(1))=1;bs(8)=0.005;
As(9,11+im_xr(2))=1;bs(9)=0.005;
As(10,11+im_xS1(2))=1;bs(10)=0.99;
%%%%%%%%%%the following commands can be used when finding nominal or
%%%%%%%%%%optimal points. These are inequality constraints for all states
%%%%%%%%%%and input vectors.
Ain=-eye(Nz+4,Nz);bin=zeros(Nz+4,1); %Non-negativity of state, helps
optimizer
%inequality constraints, setting lower and upper bounds, - signs -eye sets
%bound on all input and state vectors should be greater than 0.used for
```

```
%defining greater than so -1 value of As
```

- Optimizer.m file for running the optimizer.

```
% Main Optimization file
% optimization done to find optimal energy and optimal operational points.
clear all; close all; clc;

global coldata dyndata hydraulic termodata UU alfa
% COLUMN DATA %%

% Number of stages
coldata.Nt = [20 20 20 20 20 20];
% Initial holdup in reboiler and condenser
coldata.M0 = [1 1 1 1 1 1 1 1 1 1 1 1];

hydraulic.k1 = 1/0.063;

% THERMODYNAMIC DATA %%

load Nominal.mat
x_nom=1.03*x_nom % optimization done with diffrent intial values for same
initial values vmin=1.3362
%at 1.03*x_nom we get imin boilup=1.332244.
dyndata.x_nom = x_nom;
dyndata.u_nom = u_nom;
options = optimset('fmincon');
options = optimset(options,'TolFun',1e-10,'TolCon',1e-
13,'MaxFunEvals',500000,'Display','iter');
% ,'Algorithm','interior-point'

Specs

alfa=[4.215374389 2.102194688 1]

%
[x_nom1,fval,exitflag,output,lambda,grad,hessian] = fmincon(@(x)
Objective(x),[u_nom;x_nom],Ain,bin,As,bs,[],[],@(x)
Petlyuk_dist(x),options);

x_nom=x_nom1(12:end);u_nom=x_nom1(1:11);

dxdt = norm(Petlyuk_dxdt(0,[u_nom; x_nom]))


[[x_nom([im_xt()]); 1-sum(x_nom([im_xt()]))] [x_nom([im_xS1()]); 1-
sum(x_nom([im_xS1()]))] [x_nom([im_xr()]); 1-sum(x_nom([im_xr()]))]]
% the first term is x_nom([im_xt()] is fraction of A in top and fraction of
% B in top and 1-sum(x_nom([im_xt()]))] is remaining fraction and is
% fraction of C in top and similarly the other terms follow. also
% onprinting the results of A B and c fraction are top to bottom in matrix.
xf=x_nom;
```

```
Plot_Profiles
% print selected variables
fval
%V L Rl Rv S D B
[u_nom(2) u_nom(1) u_nom(3) u_nom(4) u_nom(5) u_nom(10) u_nom(11)
x_nom([im_xt(2)]) x_nom([im_xS1(1)]) 1-sum(x_nom([im_xS1()]))
x_nom([im_xr(2)]) x_nom([im_x2(20)]) 1-
(x_nom([im_x1(1)])+x_nom([im_x1(21)])) x_nom([im_xt(1)]) x_nom([im_xS1(2)])
1-sum(x_nom([im_xr()]))]
```