

An Industrial *i*-Butane/*n*-Butane Fractionator

Klemola and Ilme [*Ind. Eng. Chem.*, **35**, 4579 (1996)] and Ilme [Ph.D. Thesis, University of Lappeenranta, Finland (1997)] report data from an industrial *i*-butane/*n*-butane fractionator that is used here as the basis for this case study.

The column has 74 valve trays, the feed was introduced onto tray 37. The key design parameters for the valve trays are given in the table below.

Column Height	51.8m	Downcomer Area (center)	0.86 m ²
Column Diameter	2.9m	Tray Spacing	0.6m
Number of Trays	74	Hole Diameter	39mm
Weir Length (side)	1.859m	Total Hole Area	0.922 m ²
Weir Length (center)	2.885m	Outlet Weir Height	51mm
Liquid Flowpath Length	0.967m per pass	Tray Thickness	2mm
Active Area	4.9 m ²	Number of Valves per Tray	772
Downcomer Area (side)	0.86 m ²	Free Fractional Hole Area	18.82%

The measured compositions and flow rates of the feed and products for the C4 splitter are summarized in the table below.

Measured Feed and Product Flows and Compositions (mass %) for *i*-Butane/*n*-Butane Fractionator (Ilme, 1997)

Species	Feed	Top	Bottom
Propane	1.50	5.30	0.00
Isobutane	29.4	93.5	0.30
<i>n</i> -Butane	67.7	0.20	98.1
C4 olefins	0.50	1.00	0.20
Neopentane	0.10	0.00	0.20
Isopentane	0.80	0.00	1.10
<i>n</i> -Pentane	0.10	0.00	0.10
Total flow (kg/h)	26234	8011	17887

Other measured parameters are as follows:

Other details of the *i*-Butane/*n*-Butane Fractionator

Reflux Flow Rate	kg/h	92838
Reflux Temperature	°C	18.5
Column Top Pressure	kPa	658.6
Pressure drop per tray	kPa	0.47
Feed Pressure	kPa	892.67
Boiler Duty	MW	10.24

Rarely, and this is a case in point, are plant data in exact material balance and it will be necessary to reconcile errors in such measurements before continuing. The feed and product compositions as adjusted by Ilme so that they satisfy material balance constraints, are provided below. Note how the C4 olefins are assigned to isobutene and 1-butene.

Adjusted feed and product compositions (mass %) and flows
for *i*-Butane/*n*-Butane Fractionator (Ilme, 1997)

Species	Feed	Top	Bottom
Propane	1.54	4.94	0.00
Isobutane	29.5	94.2	0.3
<i>n</i> -Butane	67.7	0.20	98.1
Isobutene	0.13	0.23	0.08
1-butene	0.20	0.41	0.10
Neopentane	0.11	0.00	0.17
Isopentane	0.77	0.00	1.12
<i>n</i> -Pentane	0.08	0.00	0.11
Total flow (kg/h)	26122	8123	17999

To proceed with building a model of this column we specify the number of stages equal to the number of trays plus condenser and reboiler ($N = 76$). The common arrangement of locating the actual feed between stages may need modeling as two separate feeds; the liquid portion to the stage below and the vapor portion to the stage above. In this particular illustration the feed is (assumed to be) saturated liquid and we provide just a single feed to stage 38.

Upon computing the bubble point of the overhead product we will find that the measured reflux temperature is well below the estimated boiling point. Thus, we choose the subcooled condenser model. The steady-state concept of the so-called “sub-cooled” condenser often does not exist in practice. Instead, the condenser is in vapor-liquid equilibrium with the vapor augmented by a blanket of non-condensable gas (that has the effect of lowering the dew point of the overhead vapor). The sub-cooled condenser is a convenient work around for steady-state models (as is needed here), but not for dynamic models. We assume a partial reboiler.

The specifications made to model this column are summarized below:

Variable	Number	Value
Number of stages	1	$N = 76$
Feed stage location	1	39
Component flows in feed	$c = 8$	See other table
Feed pressure	1	120 psia
Feed vapor fraction	1	0
Pressure at the top of the column	1	658.6 kPa
Pressure drop per stage	$N - 1 = 75$	0.47 kPa
Heat duty on each stage except reboilers and condensers	$N - 2 = 74$	$Q_j = 0$
Reflux ratio (replaces heat duty of condenser)	1	$R = 11.588$

Bottoms flow rate (replaces heat duty of reboiler)	1	$B = 17999$ kg/h
Temperature of reflux	1	291.65 K
Total	165	

Finally, we must select appropriate methods of estimating thermodynamic properties. Ilme (1997) used the SRK equation of state to model this column, whereas Klemola and Ilme (1996) had earlier used the UNIFAC model for liquid phase activity coefficients, the Antoine equation for vapor pressures and the SRK equation for vapor phase fugacities only. For this exercise we used the Peng-Robinson equation of state. Computed product compositions and flow rates are shown in the table below.

Specified feed (Ilme, 1997) and computed product compositions (mass %) and flows for *i*-Butane/*n*-Butane Fractionator

Compound	Feed	Top	Bottom
Propane	1.54	4.95	0.00
Isobutane	29.49	93.67	0.53
<i>n</i> -Butane	67.68	0.73	97.89
Isobutene	0.13	0.29	0.06
1-butene	0.20	0.36	0.13
Neopentane	0.11	0.00	0.16
Isopentane	0.77	0.00	1.12
<i>n</i> -Pentane	0.08	0.00	0.12
Total flow (kg/h)	26122	8123.01	17999

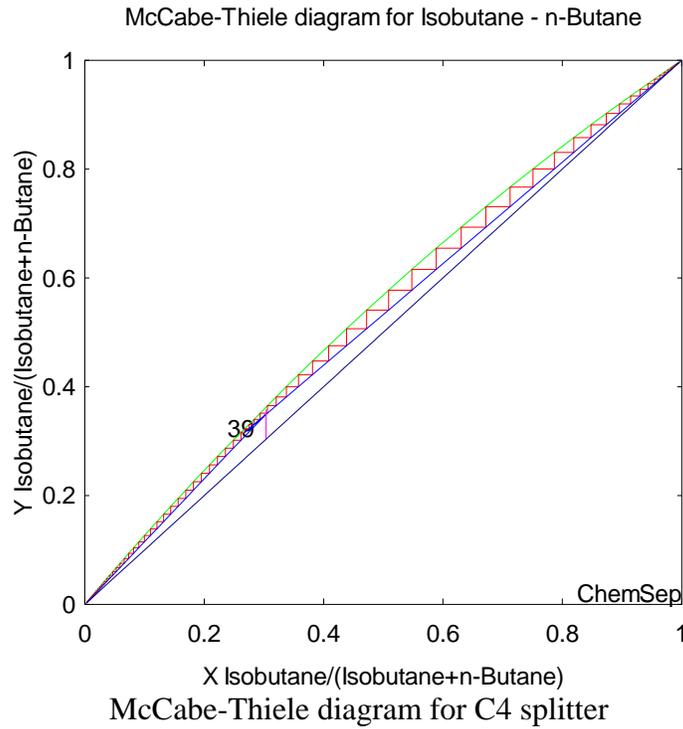
The agreement with the adjusted material balance (tabulated above) appears to be quite good and to a first approximation it seems that we have a good model of the column.

It must be noted that although this column is distilling a mixture containing at least 8 identifiable compounds, only two are present in significant amounts and, therefore, this is essentially a binary separation. It is usually relatively straightforward to match product compositions in processes involving only two different species simply by adjusting the number of equilibrium stages. We shall return to this point later.

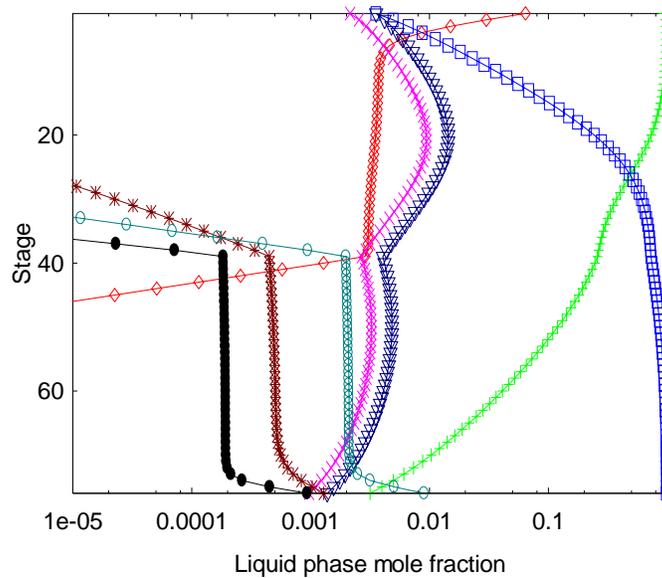
It is possible to estimate the overall efficiency for a column such as this one simply by adjusting the number of equilibrium stages in each section of the column that are needed to match the mass fractions of *i*-butane in the distillate and *n*-butane in the bottoms. Using the SRK equation of state for estimating thermodynamic properties Ilme (1997) found that 82 equilibrium stages (plus condenser and reboiler) and the feed to stage 38 were required. This corresponds to an overall column efficiency of $82/74 = 111\%$. Klemola & Ilme (1996) used the UNIFAC model for liquid phase activity coefficients, the Antoine equation for vapor pressures and the SRK equation for vapor phase fugacities only and found that 88 ideal stages were needed; this corresponding to an overall efficiency of 119%. With the Peng-Robinson equation of state for the estimation of thermodynamic properties we find that 84 stages are needed (while maintaining the feed to the center stage as is the case here); the overall column efficiency for this model being 114%. The differences between these efficiencies are not large in this case, but the important point here is

that efficiencies – all types – depend on the choice of model used to estimate thermodynamic properties. Caution must, therefore, be exercised when using efficiencies determined in this way to predict column performance.

As an alternative to varying the number of stages we may prefer to maintain a one-to-one correspondence between the number of stages and the number of actual trays, 74 in this case (plus condenser and reboiler), with the feed to tray 38. Using the Peng-Robinson equation of state and a Murphree stage efficiency of 116% we find the product mass fractions that are in excellent agreement with the plant data. The McCabe-Thiele diagram for this case, assembled from the results of the simulation, is shown below



Composition profiles computed from this model are shown below. Note that the mole fractions are shown on a logarithmic axis so that all of the composition profiles can easily be seen.



X Propane ◆ X Isobutene ✕ X Isopentane ○
 X Isobutane + X 1-butene ▽ X n-Pentane ●
 X n-Butane □ X Neopentane ✱

Liquid phase mole fraction profiles for
i-Butane/*n*-Butane Fractionator

It must be remembered that this is essentially a binary separation and that it is usually relatively straightforward to match product compositions in processes involving only two different species. In other cases involving a greater number of species with significant concentrations it will likely be necessary to vary both the number of stages and the component efficiencies to match plant data. We do not recommend adjusting thermodynamic model parameters in order to fit plant data since this can have unfortunate consequences on the prediction of product distributions, process temperatures and/or pressures.

When we create a nonequilibrium model of this – or any – column we do not need to guess how many stages to use in each section of the column. The real column had 74 valve trays; the model column includes 74 model trays with the feed to tray 38 (plus a (subcooled) condenser and a reboiler, both of which are modeled as equilibrium stages as described above). All operating specifications are the same as for the corresponding equilibrium stage model. It is necessary to choose models that allow for the estimation of the rates of interphase mass transfer; that means selecting vapor and liquid flow models and correlations to estimate the mass transfer coefficients in each phase as discussed above. In this case the AIChE correlations were used. It is known that this method is more conservative than others (i.e. the predicted efficiencies are lower). The importance of the flow model is clear from the simulation results tabulated below. The predicted component Murphree efficiencies vary more widely from stage to stage and from component to component than might be expected for a system like this. The Baur efficiency, on the other hand,

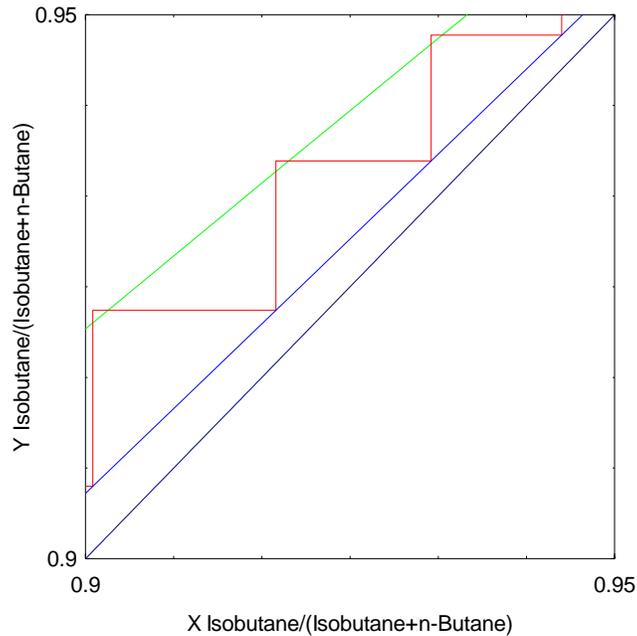
does not change by more than a few percentage points over the height of the column; the value in the table below is an average of that computed for each tray from the simulation.

Vapor flow model	Liquid flow model	iC4 in Distillate (%)	nC4 in Bottoms(%)	Efficiency(%)
Mixed	Mixed	90.2	96.3	63
Plug	Mixed	92.2	97.2	78
Plug	Dispersion	93.9	98.0	106

Internal vapor and/or liquid composition data rarely is available, but such data is the best possible for model discrimination and validation. It is often relatively easy to match even a simple model only to product compositions. In the absence of composition profiles, the internal temperature profile can often be as useful provided that it is known to which phase a measured temperature pertains. The table below compares the few available measured tray temperatures with those computed during the simulation. The agreement is quite good.

Tray	Temperature (°C)	
	Measured	Predicted
9	47.5	48.6
65	62.2	62.5
74	63.2	63.1

A portion of the McCabe-Thiele diagram for the simulation involving plug flow of vapor and dispersion flow of the liquid is shown below. For a nonequilibrium column these diagrams can only be constructed from the results of a computer simulation. Note that the triangles that represent the stages extend beyond the curve that represents the equilibrium line; this is because the efficiencies are greater than 100%.



Expanded view of upper right corner of McCabe-Thiele diagram for C4 splitter.

In this particular case the converged composition and temperature profiles have the same shape as those obtained with the equilibrium stage model (with specified efficiency) and, therefore, are not shown. The reason for the similarity is that, as noted above, this is basically a binary separation of very similar compounds. The important point here is that, unlike the equilibrium stage model simulations, the nonequilibrium model predicted how the column would perform; *no parameters were adjusted to provide a better fit to the plant data*. That is not to say, of course, that NEQ models cannot be used to fit plant data. In principle, the mass transfer coefficients and interfacial area (or parameters in the equations used to estimate them) can be tuned to help the model better fit plant data.