

Exercise 3: Rectification

Task 1 – The DSTWU model

100 kmol/h of a 50% mixture of 2-butanol ($C_4H_{10}O$) and methyl ethyl ketone (MEK, C_4H_8O) (Properties: NRTL) is to be separated in a rectification column at atmospheric pressure. The vaporous overhead product must leave the column with a purity of 95% MEK.

1. Estimate the minimum number of stages required for the separation task using the x,y-diagram.
2. Model the rectification using the DSWTU model. The feed is to be supplied as a saturated liquid, and the reflux is to be completely condensed.
 - What is the minimum reflux ratio? Which number of stages and which feed stage correspond to v_{min} ?
 - What happens when the reflux ratio is increased?
 - What happens if the product purity of MEK at the top is increased to 99%?

Task 2 – The RadFrac model and Design Specs

1. Based on the data from the DSTWU model, model the separation task using the rigorous RadFrac model.
 - Which data from the DSTWU model is required?
 - Which results do you obtain.
2. Design an internal column design spec to achieve a product of 99% MEK.
3. Create a second design spec to obtain a purity of 90% 2-butanol von 90 % in the bottoms.
 - Which parameters can be varied and within which limits?
 - What values do the parameters take?
 - What changes can you make to the column to decrease these values.

Task 3 – Sensitivity analysis

1. The total energy requirement of the column is to be minimized. Perform a sensitivity analysis to determine the influence of changes in the total number of stages and the feed stage location on the column's energy demand.
 - Within which limits should the total number of stages and the feed location reasonably be varied.
 - Display the results of your analysis graphically (e.g. energy requirement vs. number of stages). Also use the composition and temperature profiles from the block to evaluate your results.
 - For which combination of total number of stages and feed stage location is the energy requirement minimized.

Task 4 – Optimization of product yield

1. Delete the sensitivity analysis and the two internal column design specs.
2. Create an optimization to maximize the yield of MEK in the column. Vary the distillate-to-feed ratio and the reflux ratio within the same limits as in the internal column design specs. Create a constraint to ensure that the MEK purity at the top is at least 99% and integrate this constraint into the optimization.
 - What is the reflux ration?
 - How does this result differ from the on in Task 2?
 - What changes to the column can be identified from the results?