Some thoughts after the DWC workshop in Trondheim 05-06 Oct. 2023

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Thank you all for coming!

I did not make a conclusion on Friday when we ended because it is a bit difficult when things are very fresh, at least for me.

However, I have been thinking a bit over the weekend and I have some thoughts and proposals for research based on what we discussed in the workshop.

1. **Implementation of active vapor split control**. I am sure that if we really want to, then we can implement active vapor split control in industrial columns. There are many ways of doing this and new ideas (and experimental implementations!) are welcome. The experimental Kaibel column in Trondheim (for example, see thesis of Dwivedi from 2013 and results presented by Halvorsen/Kloss at the workshop) demonstrates that even a crude vapor split works (even cycling on/off) if it is combined with temperature control of the prefractionator -- so I think it should not be so difficult if it is really needed.

2. **Need for active vapor split control**. Having said that vapor split control is possible, the question remains if it is necessary. How much losses are we getting by fixing the vapor split?

   2A. Some idea can be seen by looking at specific cases. Look at typical contour plots for V as a function in Rl and Rv (Appendix). We typically have a completely flat region (because of difference in the peaks in the Vmin-diagram) where V=Vmin. For example, Rv between 0.45 and 0.55 may be within the flat region, and Rv between 0.3 and 0.7 (or maybe 0.4 and 0.6 for a pure side stream) may keep V below 120% of Vmin. So if Rv goes outside this region, we are approaching to the point where we have no benefit of a DWC (Petlyuk) arrangement.

   2B. However, this assumes that Rl is adjusted online. In most cases, keeping Rl fixed is not acceptable if we want to achieve the expected benefits because V increases quite sharply outside the "bottom of the valley". (see also CS1 in the Table below). Fortunately, a simple temperature control of the prefractionator is all what is needed to adjust Rl if there are changes in Rv (see below).

   2C. As Ivar Halvorsen mentioned in his first talk, the "competitor", which is two two-product columns in series (direct or indirect split), does not have this problem of being nonoptimal as there are no extra degrees of freedom (like Rl, Rv) that need to be set to their optimal values. The reason is that a two-product column has two steady-state degrees of freedom (say, V and L) which both are fixed when we fix the two product compositions. So nothing can go wrong in normal two-product distillation if we control the product compositions. On the other hand, a three-product Petlyuk column has five steady-state degrees of freedom (say, V, L, S, Rl and Rv) and since we have "only" three product specifications (and controlling four is not a good idea as forces the column to make separations which it does not like and may give "holes" in the operating region; see the work og Wolff and Skogestad), there are two degrees of freedom left (say, Rl and Rv) for optimization (minimizing V), which means that we can easily set them wrong.

3. **Optimality of simple temperature control schemes.** The simulations of Xing (published 2016) demonstrate that very simple temperature control indirectly gives good composition control for all disturbances; see the table below for the deviation in product compositions from the nominal value of 99%. However, what is the penalty in terms of energy (V)?
   - New research idea (from discussion with Ivar): How much loss is there for each disturbance? (Compare V (which is fixed in the table) with Vopt. Here Vopt is found by adjusting Rl and Rv optimally to give the same product compositions as in the Table.

- Qian, Xing; Jia, Shengkun; Skogestad, Sigurd; Yuan, Xigang. Comparison of stabilizing control structures for dividing wall columns. DYCOPS Trondheim 2016, IFAC-PapersOnLine 2016 ;Volum 49.(7) s. 729-734 (2016)
- Qian, Xing; Jia, Shengkun; Skogestad, Sigurd; Yuan, Xigang. Control structure selection for four-product Kaibel column. Computers and Chemical Engineering 2016 ;Volume 93. s. 372-38
- S Jia, X Qian, X Yuan, S Skogestad. Control structure comparison for three-product Petlyuk column. Chinese Journal of Chemical Engineering 26 (8), 1621-1630

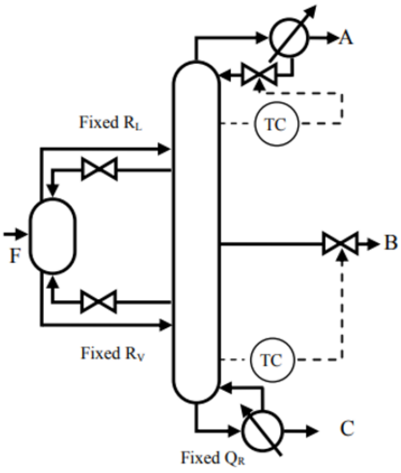


Fig. 5. Control structure with fixed split ratios (CS1)

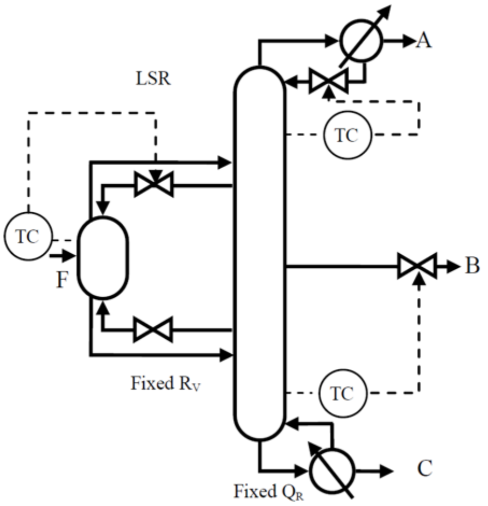
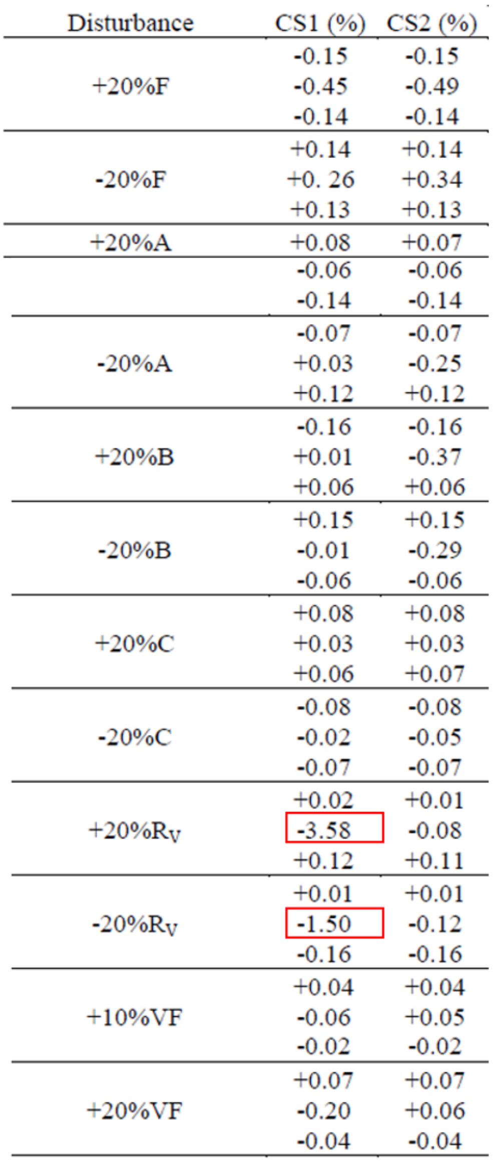
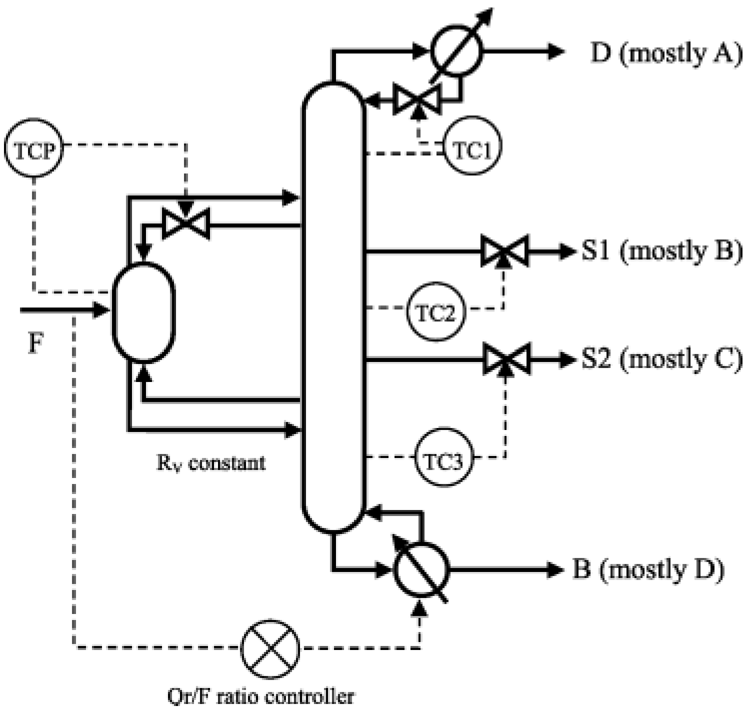


Fig. 10. Control structure with an active liquid split (CS2)



Disturbance	CS1 (%)	CS2 (%)
+20%F	-0.15	-0.15
	-0.45	-0.49
	-0.14	-0.14
-20%F	+0.14	+0.14
	+0. 26	+0.34
	+0.13	+0.13
+20%A	+0.08	+0.07
	-0.06	-0.06
	-0.14	-0.14
-20%A	-0.07	-0.07
	+0.03	-0.25
	+0.12	+0.12
+20%B	-0.16	-0.16
	+0.01	-0.37
	+0.06	+0.06
-20%B	+0.15	+0.15
	-0.01	-0.29
	-0.06	-0.06
+20%C	+0.08	+0.08
	+0.03	+0.03
	+0.06	+0.07
-20%C	-0.08	-0.08
	-0.02	-0.05
	-0.07	-0.07
+20%R_V	+0.02	+0.01
	-3.58	-0.08
	+0.12	+0.11
-20%R_V	+0.01	+0.01
	-1.50	-0.12
	-0.16	-0.16
+10%VF	+0.04	+0.04
	-0.06	+0.05
	-0.02	-0.02
+20%VF	+0.07	+0.07
	-0.20	+0.06
	-0.04	-0.04

The above is from DYCOPS-2016. In the Table there is a loss for disturbances in F. This would be 0 with a ratio controller as shown below for Kaibel:



4. **Importance of vapor split for Kaibel.**
   In the workshop it was repeatedly claimed that vapor split control is more important for Kaibel columns (see the last figure), but I did not really see any convincing proof presented. Actually, Xing showed in 2016 (CCE paper) that the above simple control structure works well in terms of composition control. However, in the paper she did not include Rv-disturbances and again it is unclear how much the energy loss is (what is V compared to Vopt?). (Xing says that this is something she will look into.)

5. **What is really happening with the vapor split in a dividing wall column?** (without active vapor split control). In the simulations (e.g., see table above), it is usually assumed that Rv is constant during operation. However, this is obviously not true, and adding a model for the hydraulics is recommended to get more realistic results. Experimental results will also be useful to study this.

   In particular, Rv depends on Rl. If we increase Rl, then we send more liquid into the prefractionator, which will mean that more vapor goes to the main column, that is, Rv will decrease. However, according to the contour plots below this is the opposite of what we should do. Similarly, when the feed rate increases, Rv will decrease (and may go outside the optimal region). This means that the constant Rv- assumption may be too optimistic, in particular for trayed columns where the pressure drops depend more strongly on the liquid load.

6. **What should the operators do to keep operation optimal?** If we assume that one uses the simple temperature control scheme shown above, then the operators need to set the setpoints correctly. Looking at Figure 10 the operators must set the following (which should NOT be changed frequently):
   - For reflux L: **Temperature setpoint in top of main column** (based on purity of D and possibly S)
   - For liquid split Rl: **Temperature setpoint in top of prefractionator**
   - For side stream S (or split Rs): **Temperature setpoint in bottom of main column** (based on purity of S and possiblky B)

- **Heat input / boilup V**: can be set in feedforward to F, but we still must set Q/F (it can be set based on the purity of B; or rather it should be set so that all purity specs (D,S,B) are met). We must avoid setting V too high, because then we may have no benefit of DWC.

Of these, the most difficult to set is probably the temperature setpoint in the prefractionator, which depends on the feed composition (which may vary). In particular, it is not clear (for example, if we cannot achieve the desired purity in the side stream) whether we should increase or decrease the setpoint to improve operation. To help the operators, more insight into desired temperature profiles will be useful (since this is the most likely data to be available).

Lena Ranger presented some results on this on Friday. Another approach may be to estimate compositions in the prefractionator because we know that if we avoid A over the top and C in the bottom then we are at the preferred split which is always optimal.

7. **Startup of DWC columns.**
For "later" startups, one just needs to drain the column, including condenser holdup and any side stream holdup, into the reboiler. Ther column is then ready for a relatively fast startup. It can be noted here that packed columns are faster to start up then trayed columns because of less liquid holdup.
Research idea: For the first startup, the similarity to multivessel distillation shows that one may want to have condenser and side stream holdups corresponding to the feed composition. In this way startup is faster and one may avoid off-spec products.

8. **Estimation of compositions** (including in the prefractionator) from column temperature. If you look at the PhD thesis of Dwivedi, then all his simulations assume that we can measure compositions. It is an obvious research idea to look into estimation (and also look at the sensitivity to errors etc.).

APPENDIX. Typical Contour/Valley diagrams for V as a function of Rl and Rv

(From the Thesis of Ivar Halvorsen from 2001)

Left: Products 97% , finite stafes
(but note that feed is 50% liquid)

Right: Pure products with infinite stages

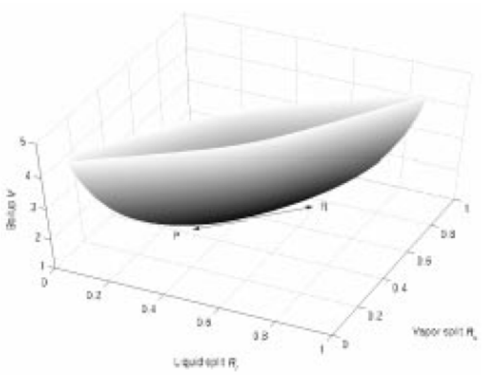


Figure 7.6: Optimal solution surface. $V(R_l,R_v)$ (base case)

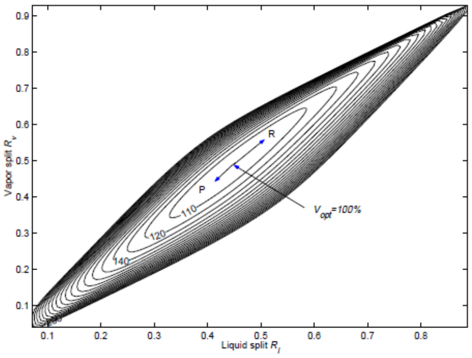


Figure 7.7: Contour plot of V corresponding to Figure 7.6:.