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# Control Structures for a Generic Two-Component Distillation Column

## Simulation Scenarios in Aspen Dynamics

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## Nomenclature

$Q_C$	Condenser duty [kW]
$Q_H$	Reboiler duty [kW]
$x_{B,i}$	Component purity in bottoms product stream(H: heavy component)
$x_{D,i}$	Component purity in distillate product stream (L: light component)
$B$	Bottoms product flow
$CV$	Control variable
$D$	Distillate product flow
$F$	Feed flow
$L$	Reflux flow
$MV$	Manipulated variable (valve)
$V$	Reboiler vapour flow



# 1 Introduction

The main purpose of a distillation column is to obtain as much pure product as possible (but not too pure!) and lose as little product as possible (within limits). For this project, the primary goal is to control  $x_{D, \text{methanol}}$  and  $x_{B, \text{water}}$  after a step change error in feed flow rate is induced on the system. The problem consists of two parts: 1. Establish an ideal steady-state model for the column, and 2. perform several scenarios with different control structures, and evaluate their performance.

A previous study by Luyben [1], followed up by a correction paper [2] investigate several control structures for a column. In the first paper, multiplicative versus additive feed-forward was investigated in tandem with a temperature controller. It was found that additive controllers usually yield superior results in terms of set point deviance.

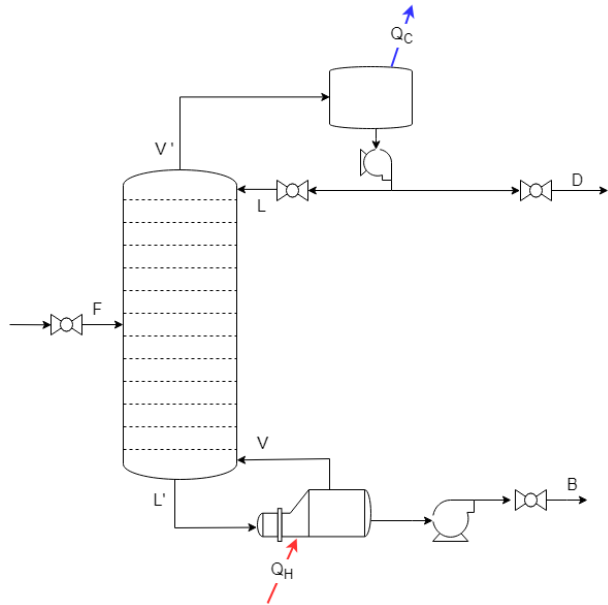
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## 1.1 Theoretical remarks about distillation

Distillation is a method of separating components with different volatility. In the design process, one must first establish what the goal of the system is. For example, "how pure should the distillate be?", "what are the flowrates?". Luyben states that a multi-stage distillation column has 5 degrees of freedom:  $x_{D,i}$  (distillate composition),  $x_{B,i}$  (bottoms composition),  $P$  (operating pressure of the column),  $N_T$  (number of trays) and  $N_F$  (feed inlet stage). All of these are assumed constant during steady-state [3, p.29].

In binary distillation, the *relative volatility*,  $\alpha$ , is a helpful factor determining how easy it is to separate the two components. Non-ideality in VLE (Vapour-Liquid Equilibrium) will likely exist.  $\alpha$  is often assumed constant, but will depend on the liquid activity or the fugacity of each component in the mixture [3, 4]. It is helpful to understand that the VLE of the

methanol-water system greatly affects designing and simulating. This is explored in section 2.



**Figure 1** – A pressurised column schematic with reflux and a reboiler.

For analysing binary systems, the McCabe-Thiele method is a graphical way of illustrating the relationship between the VLE, reflux ratio, and number of trays. The reflux ratio can be interpreted both as  $L/F$  (feed basis) and  $L/D$  (distillate basis). More often, the latter is the used, but for the purposes of this project,  $L/F$  is the standard. In any case, distillation columns are highly non-linear, so calculations are either semi-analytical or based on simulations.

Through some conclusions can be drawn [3]:

1. There is an inverse proportional relationship between  $N_T$  and  $L/D$  given that the product purities remain the same.
2. The more trays in the column, the less energy required ( $V \propto Q_H$ )
3. Increasing  $L/D$  increases light component purity in the distillate.
4. An infinite reflux ratio yields the minimum

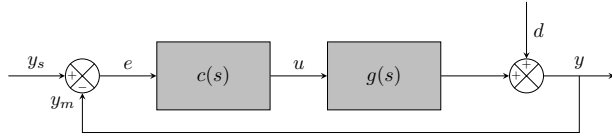
number of trays  $N_{T,min}$  required.

5. A lower relative volatility requires more stages for the same purity.

## 1.2 Control Theory

### 1.2.1 Control structures

The most common control structure to achieve the set point is the standard feedback control structure shown in figure 2. This method requires the controller to be tuned correctly according to the system  $g$ . In many cases,  $g$  is non-linear, while  $c$  is linear.

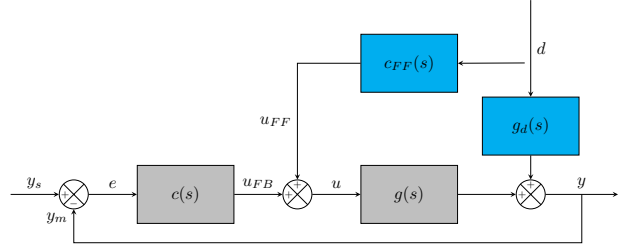


**Figure 2** – A feed-back controller block diagram.

To mitigate some of the initial error that occur to the controlled process variable, a feed-forward controller can be implemented, as shown in figure 3. The blue blocks represent the feed-forward structure. Unlike the feedback controller, the feed-forward has no input of the current states (only  $d$ ), which makes it a model-based controller.  $c_{FF}$  can be calculated on the form shown in Eq. (1a). Eq. (1b) shows the lead-lag form of  $c_{FF}$ , where  $\tau_1$  and  $\tau_2$  represent the lead and lag time constants, respectively. The lead-lag unit is ideal is assuming that  $g_d$  and  $g$  are first-order approximates. It is also possible to choose a pure gain feedforward controller where  $\tau_1 = \tau_2$  [5, p.270].

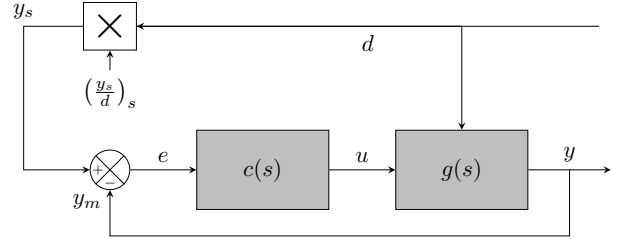
$$c_{FF} = \frac{-g_d}{g} \quad (1a)$$

$$= K_{FF} \frac{\tau_1 s - 1}{\tau_2 s - 1} \quad (1b)$$



**Figure 3** – Additive feedforward  $c_{FF}(s)$  with feedback  $c(s)$  controller block diagram

Figure 4 shows the ratio control structure where  $d$  directly influences the feedback loop. In this scenario, the multiplier block  $(\frac{y_s}{d})_s$  is a factor that remains constant. Here,  $d$  and  $y$  are usually flow rates (for example feed and reflux) and  $c(s)$  is a flow controller.

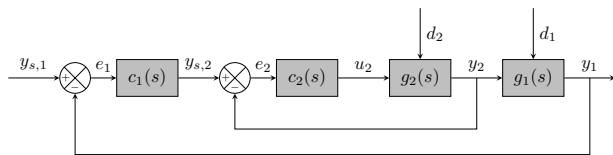


**Figure 4** – Ratio control block diagram with respect to a disturbance  $d$ .

Figure 5 shows a cascade controller block diagram. The fast inner loop and slow outer loop allow for more robust control. The controller time constants ( $\tau_c$ ) for  $c_1$  and  $c_2$  cannot have a small time-scale separation, which is defined as [6]:

$$\text{Time scale separation} = \tau_{c1}/\tau_{c2} \quad (2)$$

Generally, a larger time scale separation ( $\geq 5$ ) avoids the two controllers competing, resulting in resonance. This may introduce instability.



**Figure 5** – A two layer cascade controller block diagram.

### 1.2.2 Tuning

For the tuning of all controllers except level controllers, the SIMC method is used. Usually, the PI Eq. (3) method is used, but the derivative action is

## 2 Steady State Analysis

In Aspen Plus, the NRTL fluid package is chosen for the binary water-methanol system while the Rad-Frac model is used for the column. Figure 1 shows a scheme of a distillation column with a total condenser, reflux and reboiler. In reality, there is a pump before the reflux valve (L) to allow flow back into the column. There are 40 stages, of which the feed enters at stage 34 with 100 kmol/h and 50 mole% methanol. The feed temperature is set to 20 °C and 6 bar, with a pressure reduction valve before entering the column at 2.5 bar of pressure. The pressures at stage 1 (condenser) and 40 are respectively set to 2 and 2.3 bar. For the (total) condenser, the "Constant duty" heat transfer option was chosen to make the cooling measured in energy units directly. The same option is chosen for the reboiler. The vertical cylindrical reboiler and condenser drums both have an length/diameter ratio of 3, with a holdup time of 10 minutes when half full. The height and diameter for the two are 3.24 m and 1.08 m, respectively.

Figure 7 shows the McCabe-Thiele diagram adapted from the vapour-liquid equilibrium data. It is visible that the feed is undercooled ( $q > 1$ ). This illustrates that the feed enters the column at the ideal stage due to the non-ideal nature of the methanol-water mixture [3, p.11].

recommended when there is a dominant second-order process where  $\tau_2 \geq \theta$  [6].

$$K_c = \frac{1}{k'} \frac{1}{\tau_c + \theta} \quad (3a)$$

$$\tau_I = \min(\tau, 4(\tau_c + \theta)) \quad (3b)$$

$$\tau_D = \theta \quad (3c)$$

Where  $k' = k/\tau$  is the initial slope,  $k$  is the process gain,  $\tau$  is the process time constant,  $\theta$  is the process delay and  $\tau_c$  is the controller tuning parameter.

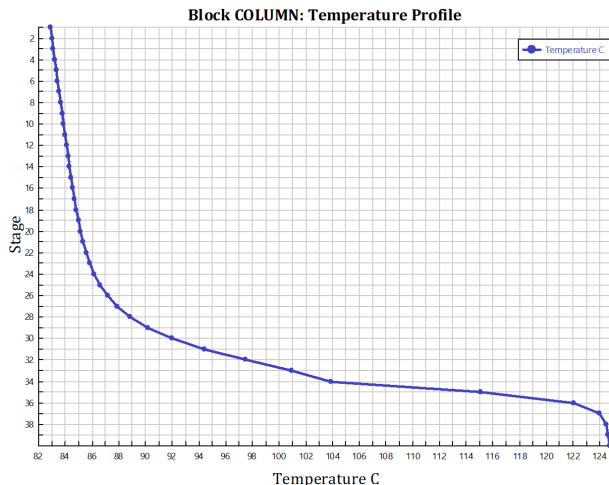
The design specifications of the column are to have a purity of methanol ( $x_{D,methanol}$ ) of 99.90 mole% in the distillate and 0.10 mole% in the bottoms. These specifications are achieved by varying the reflux ratio and distillate rate, respectively. Thus, both distillate and bottoms have a molar flow of 50 kmol/h. The solution yields a reflux rate (L) of 50.6 kmol/h ( $L/F = 0.506$ ) and a distillate rate (D) of 50.00 kmol/h, as shown in table 1. The table quantifies how much L and V must change in order to achieve a certain purity (which is assumed equal in distillate and bottoms).

**Table 1** – Required reflux (L/F) and reboil (V/F) ratios for different distillate light component ( $x_{DL}$ ) and bottoms heavy component ( $x_{BH}$ ) purity combinations.

$x_{DL} / x_{BH}$	L/F	V/F
0,9	0,222	0,854
0,99	0,424	1,016
0,999	0,506	1,103
0,9999	0,615	1,207
0,99999	0,794	1,373

Figure 6 shows a plot of temperatures by the stage after a steady-state calculation is performed. The vapour temperature is proportion proportional directly related to the mixture composition. In the upper stages (low number), the pressure becomes two bars and the temperature barely drops below 82 °C.

The water in the bottoms at 2.3 bar will boil at around 125 °C. During distillation, unless the column pressure changes, the temperature profile should always have this appearance. Small deviations close to the top or bottom will indicate significant changes in product compositions.

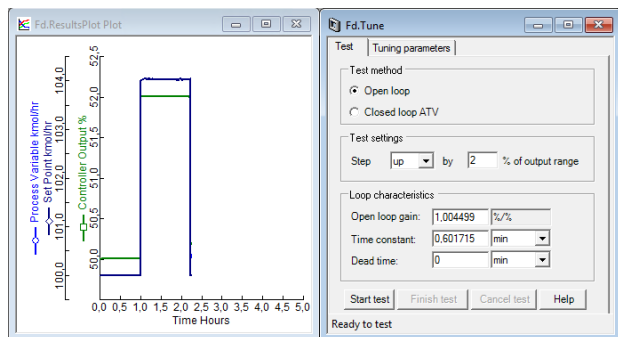


**Figure 6** – Column temperature plotted against the stage number

### 3 Dynamic simulation

#### 3.1 Open-loop experiments

The aspen integrated tuner shown in Figure 8 is used to obtain the gain, time constant, and delay of a single loop control MV-CV system. The example shows the feed disturbance valve being tuned (the valve is used to emulate a feed disturbance). The output range of all parameters are twice the value of the steady-state values calculated after initialisation.



**Figure 8** – Aspen Plus® open-loop experiment. In this example, the feed disturbance valve. The valve is opened by 2% (right) and response in feed is measured by the program (left). "Loop characteristics" are found to the right after pressing "Finish test".

The inaccuracy of the open loop tuner is prevalent

when performing the experiment. Firstly, the results may vary every time the experiment is run. Secondly, since the first-order plus dead-time model does not fit with non-linear cases.

**Table 2** – The open loop parameters for the most important control parameters. The control of F is not a part of any dynamics, but only to simulate a disturbance.

MV-CV	Gain	$\tau$ (min)	Delay (min)
$valve_{F-F}$	1	0.6	1.2
$valve_{L-L}$	1	0.6	1.2
$Q_{H-V}$	1.05	0.853	1.2
$valve_{L-x_D}$	0.00259	150.269	20.64
$Q_{H-x_B}$	0.02344	33.688	6.327

#### 3.2 AD0: No control

When stating "no control", it is assumed that no important state variables such as flow rates, temperatures, or composition are controlled. For a distillation column, it is necessary to regulate the levels in both the reboiler and reflux tanks. In this case, the level of each tank has a setpoint of 50% of the max height. Both tanks have a high gain P-controller ( $K_c = 1000$ ) with no integral action ( $\tau_I = 9999$  min). Therefore, the control structure in figure 9 becomes a basis for all the other simulation scenarios in this report. In

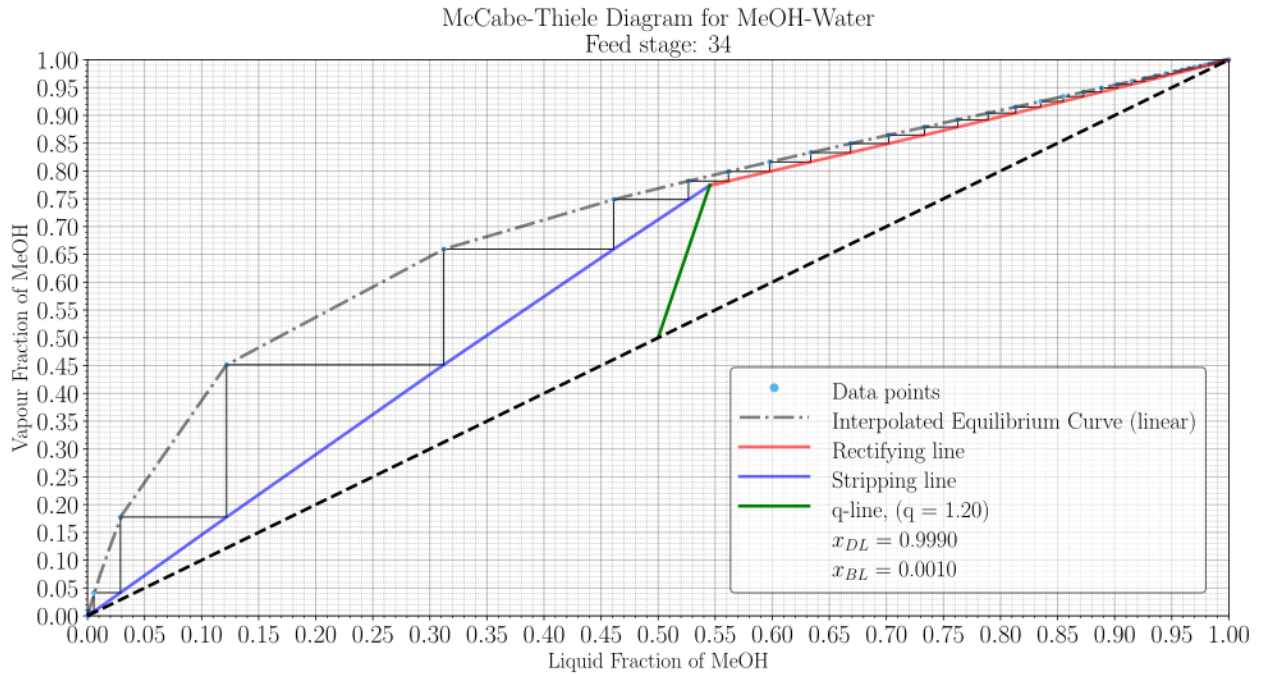


Figure 7 – McCabe-Thiele diagram adapted from Aspen calculations

addition to the level controllers, there is a pressure controller in the reflux drum that holds the pressure constant at 2 bar. This is not shown in the schematic, but is important for dynamics.

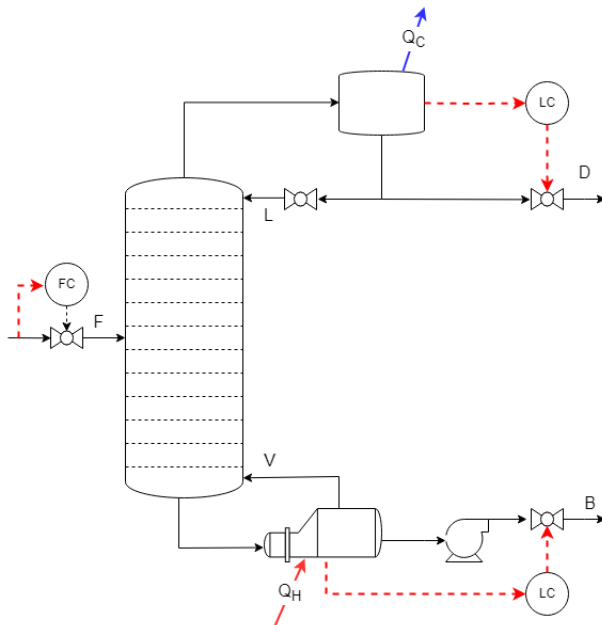


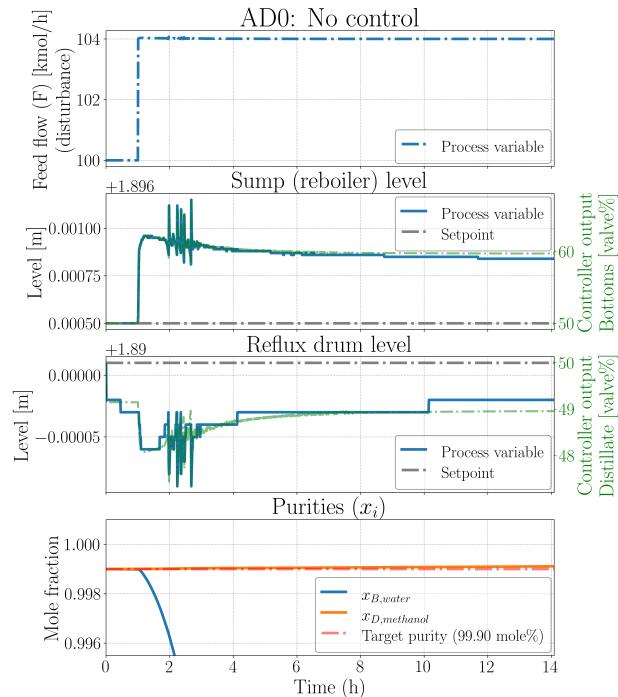
Figure 9 – AD0: Control scheme with P-controllers on reboiler and reflux tank levels. Otherwise, there are no state controllers

It is visible from figure 10 that an increase in feed causes the water purity at the bottoms to decrease. Since the reboiler duty ( $Q_H$ ) is unregulated during the step change, the sump (reboiler drum) will have an influx of cold feed, which causes the vapour flow from the reboiler ( $V$ ) to decrease. A marginal decrease in reflux drum level is also observed, which is a consequence of a smaller  $V$ . It is hardly visible from the figure, but the distillate purity increases somewhat in this process due to less amount of water evaporating at lower temperatures.

It is also to be observed that the levels never really approach the set point line (marked in grey), since there is little-to-no integrating action on the level controller. However, in the scope of this project, this detail has little relevance due to the marginal deviations ( $< 1$  mm).

The noise in the levels occurring at  $t = 2$  h is not essential to the task and is not completely understood.

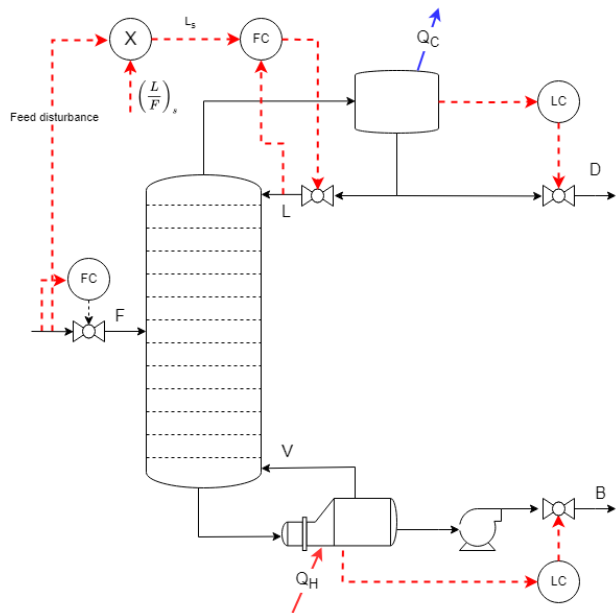
Despite this, they dissipate whenever both the reboil and reflux streams are regulated or set to regulate other states.



**Figure 10** – AD0: Sump (reboiler) level, reflux level and purity response to a 4% feed increase

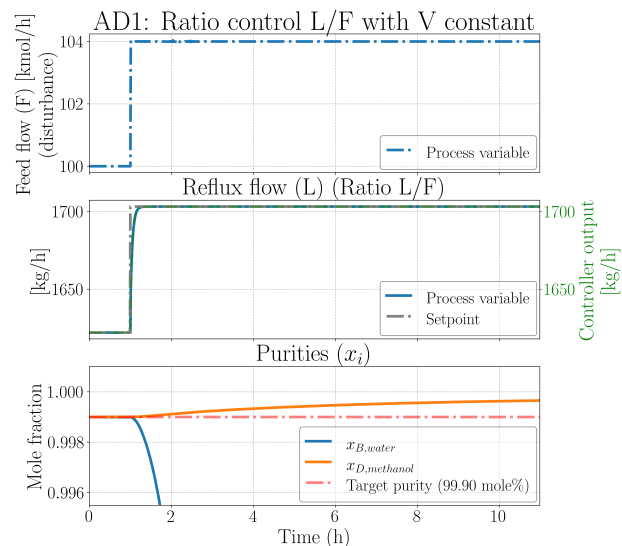
### 3.3 AD1: Control of the $L / F$ ratio with constant $Q_H$

The only difference between this scenario and AD0 is that the reflux increases proportionally to the feed. From figure 11, it is shown that the feed disturbance is measured and multiplied by the steady-state  $L/F$  ratio, and fed as a set point to the  $L$  flow controller. An important note is that the "flow controller" in Aspen is not a valve, but the  $L$  mass flow. This gives a measured controller gain of 1. From the values in table 2,  $\tau_c = 1.2$  min was calculated for  $L$ . It is also considered that there is an error in the flow reading of 25%. So, instead of increasing  $L$  with 4%, it is increased by 5%.



**Figure 11** – AD1: Control scheme with ratio control on reflux (reflux-to-feed).

In figure 12, it is visible that  $L$  (the blue line overlapped by the green line) increases due to the set point change. Since  $L$  is in the liquid phase (cold), the same effects take place as in AD0, except magnified. Methanol purity in distillate increases significantly, but a lot of cold methanol is dumped through the bottoms. For the sake of product purity, this case yields worse results than with no control whatsoever.

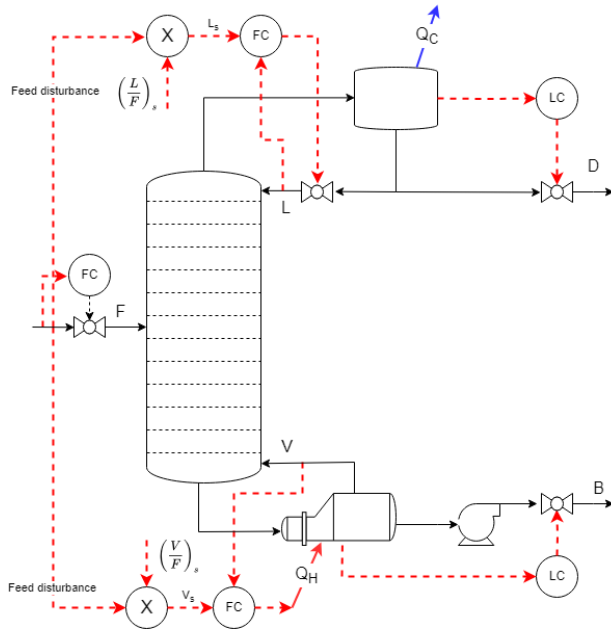




**Figure 12** – AD1: L/F ratio control with constant reboiler duty with 4% feed increase.

### 3.4 AD2: L/F & V/F ratio control

In this scenario, the reboiler vapour flow,  $V$ , is introduced as a control variable. The goal is to keep  $V/F$  constant, as illustrated in figure 13. In practice, measuring  $V$  is difficult, making this exact method somewhat infeasible. However,  $V$  will correspond to  $Q_H$  as long as the amount *and* composition of fluid in the reboiler drum remains constant. Aspen dynamics does not allow to take the reboiler duty as a process variable, which is the reason for choosing  $V$  as the process variable. Likewise to AD1, there is a 25% increase in feed mass flow measured, so both  $L$  and  $V$  have their set points increased by 5% instead of 4%.



**Figure 13** – AD2: Control scheme with ratio control on both reflux and reboil (feed basis).

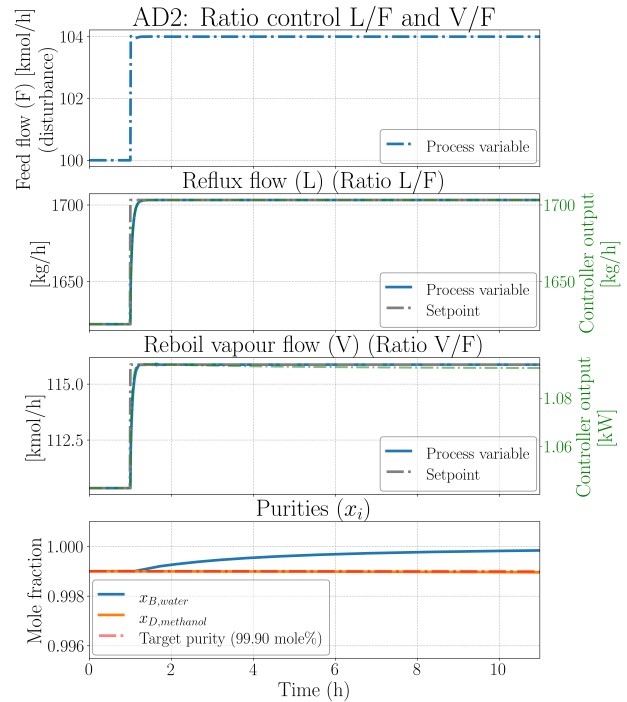
In figure 14, it is clear that the flow controllers reach the set point fairly fast (although  $V$  is not a valve-actuated flow controller). For  $V$ ,  $\tau_c = 1.2$  as well, since has quite fast dynamics as shown in table 2.

Despite this, the purities never approach the target of 99.90%. The distillate purity continues to drop after the graph over the course of 150 hours as a result of a gradual build-up in column temperature. It was found that a larger deviance in the mass reading only accelerates the dynamics of this process. The bottoms purity increases due to  $Q_{measured} \geq Q_{theoretical}$ . That is, increased boil-off of methanol yields better separation.

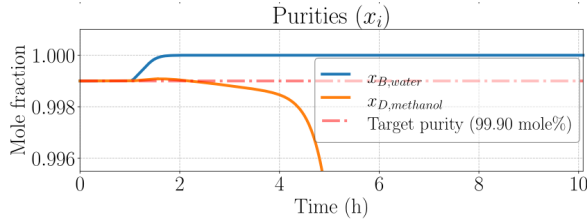
$$\begin{aligned} Q_{measured} &= Q_{theoretical} \frac{F_{measured}}{F_{theoretical}} \\ &= Q_{theoretical} \frac{1.05}{1.04} \end{aligned}$$

The accumulation of energy in the column will be proportional to how large  $F_{measured}$  is compared to  $F_{theoretical}$ . A scenario was assumed where

$\frac{F_{measured}}{F_{theoretical}} = \frac{1.25}{1.04}$  is shown in Figure 15. Only the purity plot is shown, since the rest is virtually the same as in Figure 14. Notice how the distillate purity drops around 2 hours in this exaggerated case.

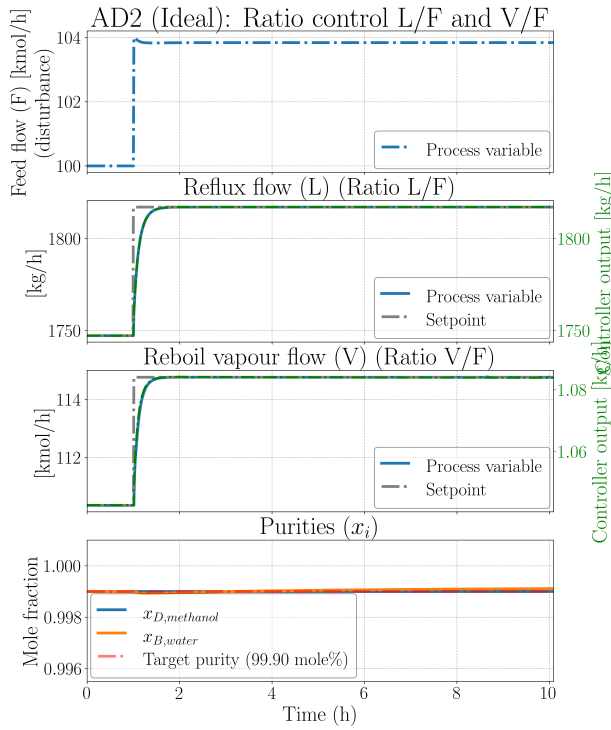


**Figure 14** – AD2: L and V response to a 4% feed increase. The L and V setpoints increase by 5% as a response (+25% error).



**Figure 15** – AD2: Purity response with an exaggerated error in flow measurement.

To illustrate how this is the "ideal" control structure, figure 16 shows how there is virtually no change in purity if there are no errors in flow measurements and with no delay.

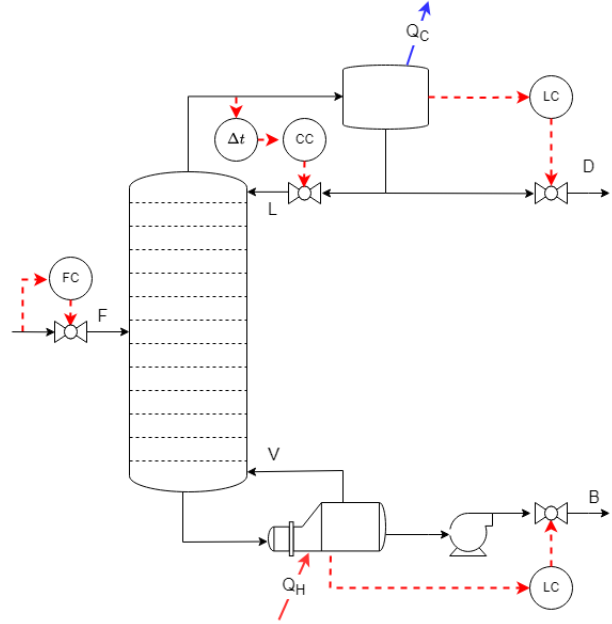


**Figure 16** – AD2 (Ideal): Reflux and reboil flow response to a 4% feed increase.

### 3.5 AD3: $x_D \leftrightarrow L$ control

In this scenario, the purity of the distillate is controlled directly with the reflux flow in a feedback loop

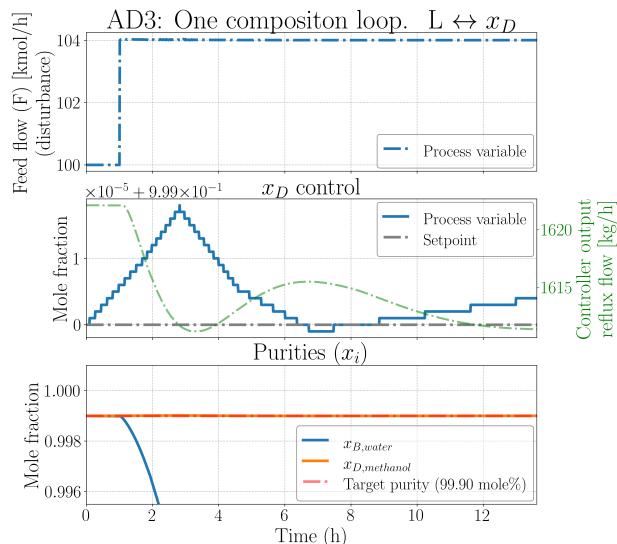
as shown in Figure 17. The tuning parameter,  $\tau_c$ , is 206.4 min for the  $L \leftrightarrow x_D$  controller. There is assumed a time delay,  $\Delta t$ , of 4 minutes to account for the delay in a gas chromatograph.



**Figure 17** – AD3: Control scheme with distillate composition control only.

It is shown in figure 18 that  $x_D$  varies marginally.  $Q_H$  remains constant throughout the process. The variations are so small that the signal becomes visually discontinuous. On the other hand,  $x_B$  decreases significantly even with less reflux flow.  $F$  must therefore be the sole factor for the dumping, and  $L$  is a counteracting force. This is illustrated by the green line (controller output) under " $x_D$  control".



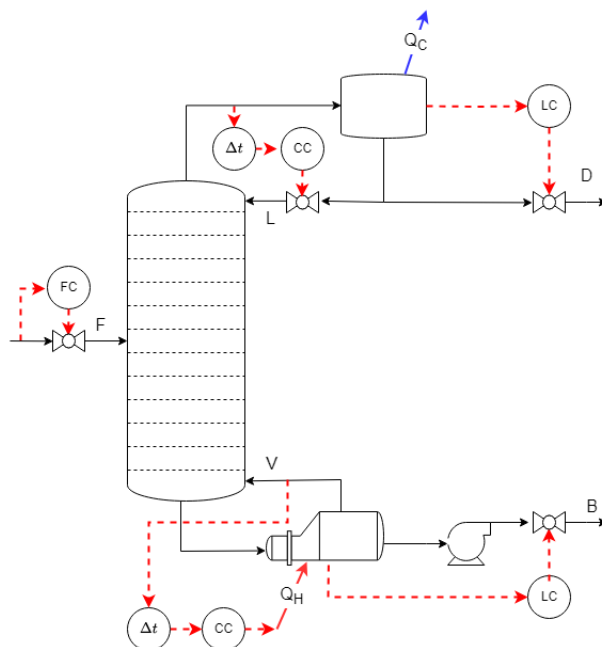


**Figure 18** – AD3: Distillate composition response to a 4% feed increase. The MV is L.

### 3.6 AD4: $x_D \leftrightarrow L$ & $x_B \leftrightarrow V$ control

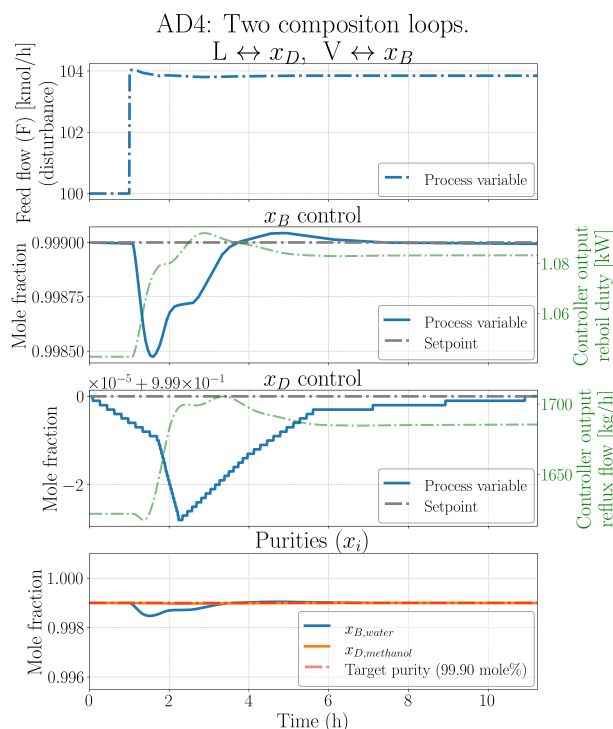
To solve the issue in AD3 with the excess reflux flow being dumped,  $x_B$  is regulated by  $Q_H$  with a simple feedback loop as illustrated in figure 19. Since both L and V are regulated, and they both greatly affect column dynamics, it is chosen to set the distillate composition controller (top) to fast and the bottoms composition controller to slow. The other way is also possible.

Additionally, the top controller has a  $\tau_c$  value of 20.6 min instead of 206.4 min, which is a factor of 10 in difference. For the bottom controller,  $\tau_c = 31.6$  min.



**Figure 19** – AD4: Control scheme with distillate and bottoms composition control.

It is shown in figure 20 that both controllers act similarly to the ratio controllers shown in AD2, but with more dynamics involved. According to plot 3, it would seem that a perfect steady-state was not achieved. Introducing the control loop on the bottoms composition prevented feed dumping to the bottoms. Weeping (low vapour flow) is indicated by a sharp increase in  $x_{DL}$ , which does not occur in this case. Unlike in AD3,  $x_{DL}$  decreased marginally since the reboiler prevented dumping. The initial (negative) slope of the  $x_D$  controller indicates that there is no initial interaction between the controllers. However, as the reboiler duty increases and the purity of the distillate decreases more rapidly, the reflux flow increases as a response.

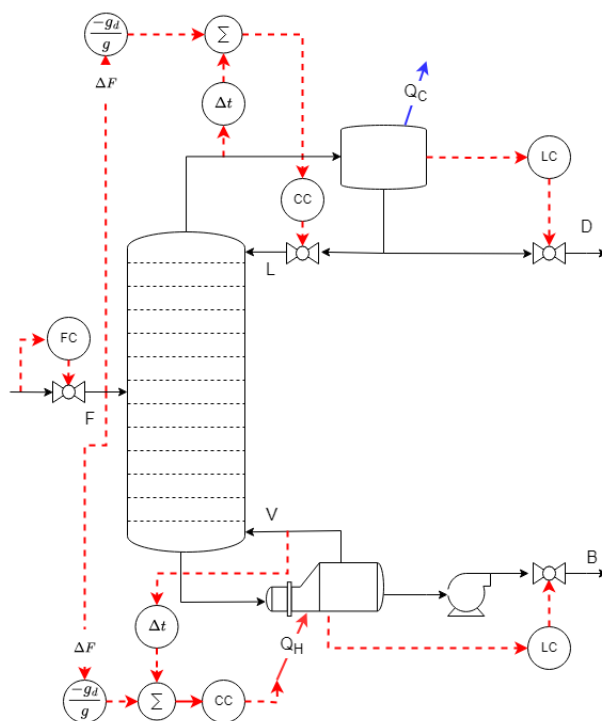


**Figure 20** – AD4: Distillate and bottoms composition response to a 4% feed increase. None of the compositions are controlled directly, but indirectly through flow ratio controllers L/F and V/F.

### 3.7 AD5: Feedback & Feedforward control

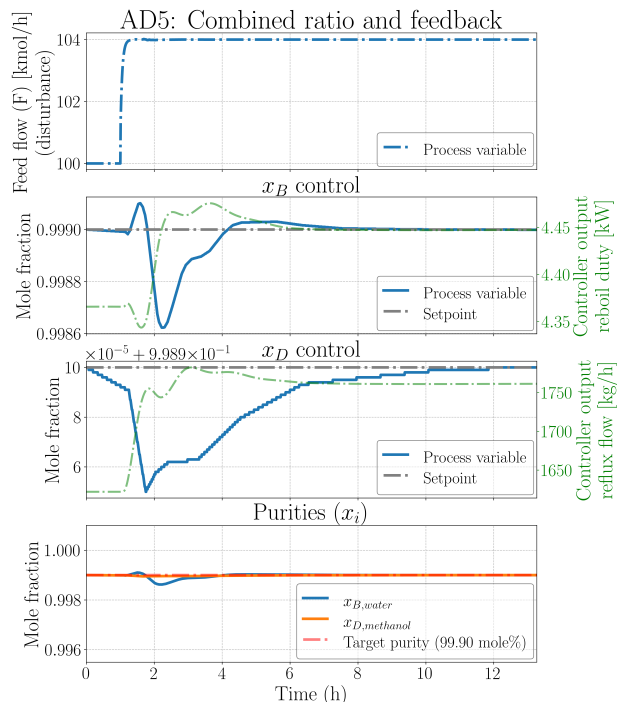
By combining the single-loop composition feedback from AD4 with additive feed-forward, some of the initial error in both compositions should be mitigated. A detail of importance in the figure is  $\Delta F$ , which equals  $d = F_{measured} - F_s$ .

The same feedback tuning parameters apply to this control structure as in AD4. For the feed-forward gains,  $K_{FF,reflux} = 0.731$  and  $K_{FF,reboil} = 0.0238$  were used.



**Figure 21** – AD5: AD4 feedback & pure gain feed forward control scheme.  $-g_d/g$  is the gain multiplier block.

Figure 22 shows the feedback + feed-forward response of both compositions to a feed disturbance. The initial increase in  $x_BH$  is caused by the feed forward controller, but is quickly reverted by the sudden downpour of incoming feed. Minor fluctuations in  $x_{DL}$  did occur, but were nearly nullified due to the fast controller response. The feed-forward response might have quelled the initial loss for both composition controllers. They both reach set-point, but quite slowly after 6 hours from the initial step change. A big uncertainty with this method of control is the feed-forward controller, since it is a model based tuning method. When the model is nonlinear, it becomes difficult to create a linear model working in all both directions. This was the main reason for choosing a pure gain controller feed-forward control.



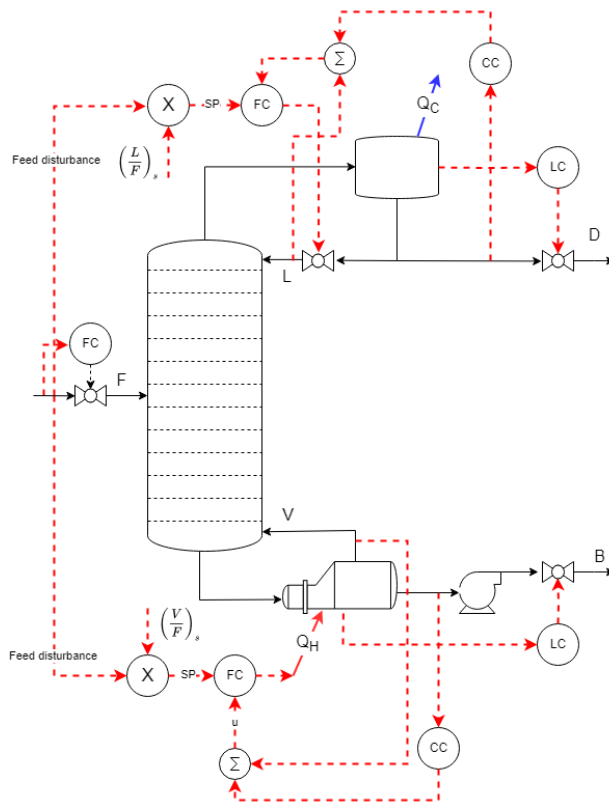
**Figure 22** – AD5: Distillate and bottoms purity response to a 4% feed increase. The MVs are L and V.

### 3.8 AD6: Ratio and composition cascade

Assuming the same case as in AD2 with an error in reading and flow controllers. The only difference with this controller is the introduction of a compensating intensive variable feedback (composition). This gives two separate fast ratio controllers, both with slow composition controlled paired closely. A deviation in composition is sent as a summation block to the flow controller, changing the setpoint live.

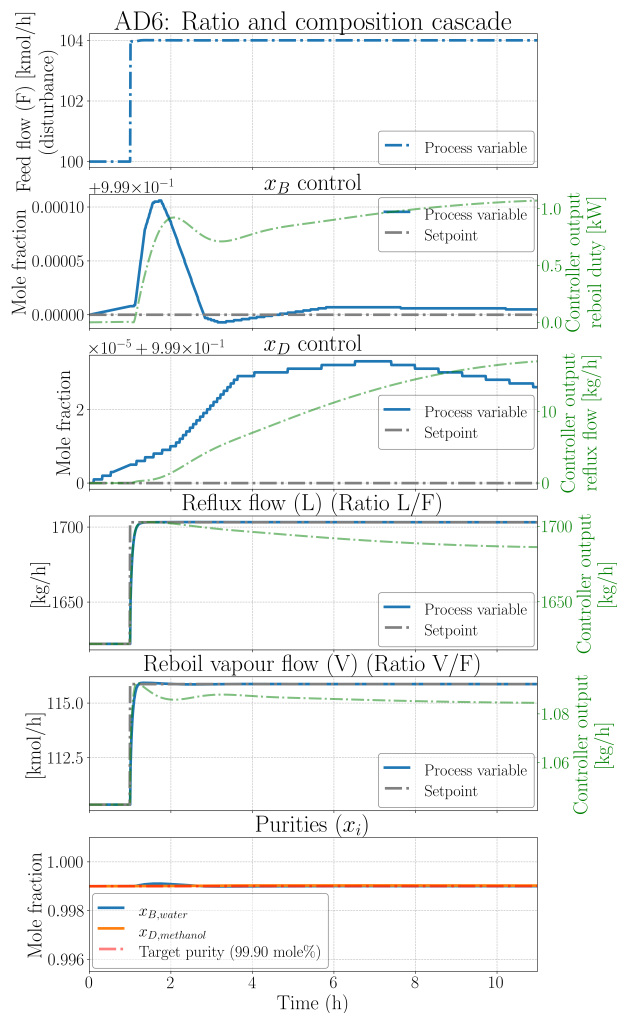
$\tau_c$  for both flow controllers are set to 1.2 min while being respectively 20.6 and 31.6 for  $L \leftrightarrow x_{DL}$  and  $V \leftrightarrow x_{BH}$ . This gives a time scale separation 17 and 26 for the controllers. It is arguably possible to introduce a third cascade loop for both controllers, controlling the temperature in the column. The CC sends a setpoint. However, for the distillate controller ( $x_{DL}$ ),  $\tau_c$  would have to increase to  $1.2min \cdot 25 = 30min$  so the time scale separation becomes the square of 5.

This structure is also proposed by Skogestad in his paper [6].



**Figure 23** – AD6: Ratio control on inner loop with outer composition loop cascade. The composition is read and sent to each respective controller. An input change to the L or V flow controller is imposed by the composition controller if there is an offset from the composition setpoint.

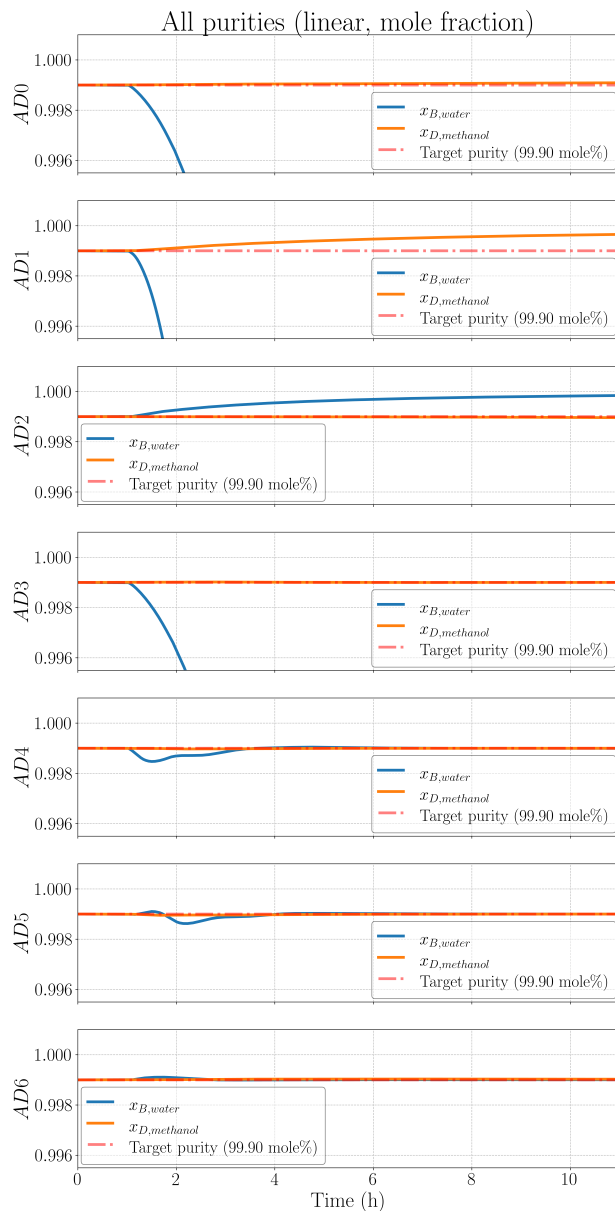
There is very little deviance in the composition from its' setpoint. A good reason for this is that both L and V were adjusted close to their setpoint before minor adjustments were made to accommodate for the mass reading errors. The approach to setpoint is also quite fast, at under 2 hours from the step on F.



**Figure 24** – AD6: Distillate and bottoms purity response to a 4% feed increase. L and V are increased by 5% instead of 4%.

### 3.9 Comparison

Figure 25 shows how the compositions of all the different scenarios compare.



**Figure 25** – Summary of the purity responses from all experiments (AD0-5)

Visually, it is clear that all scenarios AD0-AD3 are quite infeasible in terms of composition control. A common trait among the controllers is that they fail to accommodate for column dynamics. Either they cause dumping of liquid through the bottoms or lack self-regulation through intensive variables, which leads to a gradual accumulation/loss of system energy. AD3 shows a less steep control, where column weeping increases  $x_{DL}$  and consequently forces the

$L \leftrightarrow x_D$  controller to reduce L. This is why a less steep gradient is observed.

The main difference between controlling the compositions with (AD4) and without feed-forward (AD5) is the initial response. The highest peak of error for  $x_B$  is counteracted, and even overshoot. Arguably, the setpoint is reached faster with feed-forward too.

The experiments show that systems where no control of intensive variables, is inconsistent. In practice, this could be for several reasons. intensive variables is often slow, but will always reach setpoint if tuned correctly. In this study, errors were emulated

by adding extra flow to the ratio flow controllers. In reality, there are more sources of disturbance that a column can experience (feed composition, temperature). Controlling extensive variables are faster and in cases less accurate. Knowing that the ratio of one stream should change approximately to another stream is a powerful tool in column control. Controlling both streams and temperatures/compositions in tandem, either in cascade or in feed-forward creates a fast and robust control structure. Cascade control will always end up at setpoint, while feed-forward may not unless compositions are controlled.

## 4 Conclusion

In a distillation column with feed disturbances, it has been shown in this study that only adjusting extensive variables such as flows is a poor method to achieving a desired and consistent product stream, as they rarely are the objective themselves. Only adjusting intensive variables can obtain these objectives reliably, but the column dynamics for product compositions have proven to be slow. Through combining the two methods, either through cascade or feed-forward, it is possible to improve on the methods. The methods for feed-forward (AD5) and cascade (AD6) seem superior of all the methods presented, with the cascade being more robust.

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