1. Batch Distillation Column Operating Conditions

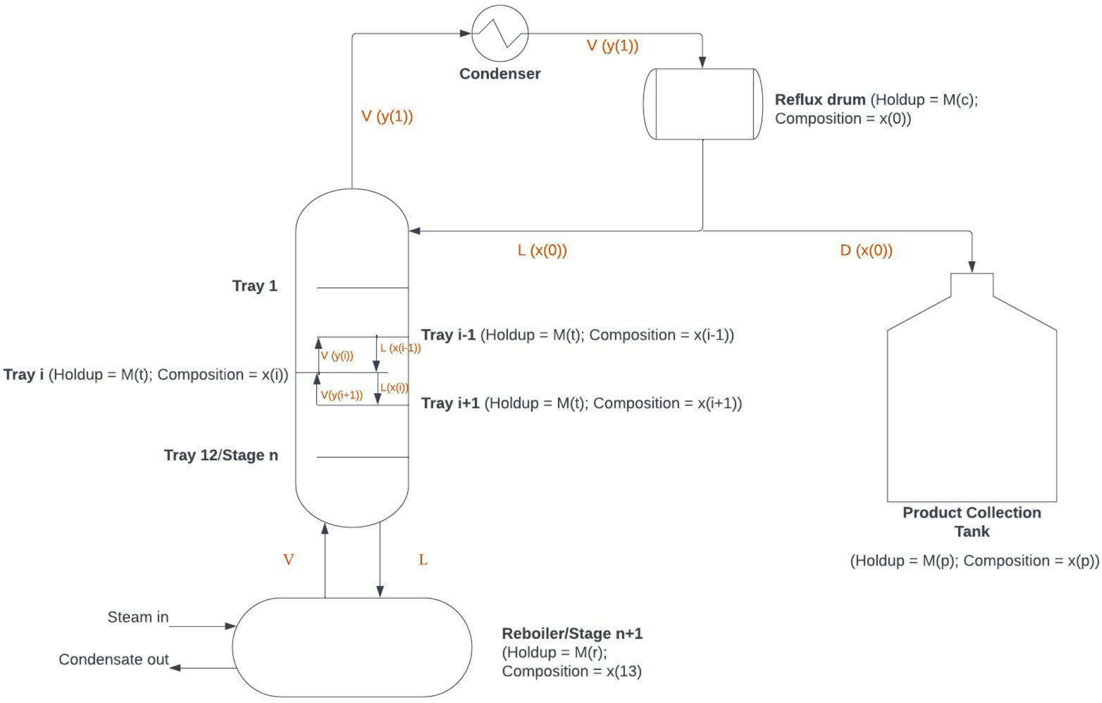

Figure 1- Batch Distillation

The batch distillation column studied is used to separate Methanol from a Methanol-Water mixture. The column is also equipped with a partial reboiler and a total condenser + reflux drum system.

The column will be operating under the following conditions.

• Column pressure (kPa)	97.99
• No. of ideal trays in the column	12
• Vapor boil-up rate (mol/min)	0.25
• Feed charge to the column (mol)	50
• Tray holdup (mol)	0.2
• Reflux drum holdup (mol)	0.2
• Feed composition (Methanol molar fraction)	0.3
• Relative volatility for Methanol – Water mixture	1.6

2. Dynamic Mathematical Model for the Ideal Batch Distillation Column under Constant Reflux Ratio

Nomenclature:

$M_R = Molar\ holdup\ in\ the\ reboiler$

$M_T = Molar\ holdup\ in\ each\ tray$

$Mc = Molar\ holdup\ in\ the\ condenser - reflux\ drum$

$M_p = Molar\ holdup\ in\ the\ product\ tank$

$a = Relative\ volatility\ of\ methanol\ to\ water$

$L = Liquid\ flowrate\ in\ the\ column$

$V = Vapor\ flowrate\ of\ the\ column$

$D = Distillate\ flowrate\ from\ the\ column$

$R = Reflux\ Ratio$

$x_i = Methanol\ mole\ fraction\ of\ the\ liquid\ of\ the\ i^{th}\ plate$

for i = 1, 2…,12

$y_i = Methanol\ mole\ fraction\ of\ the\ vapor\ leaving\ the\ i^{th}\ plate$

for i = 1, 2…,12

The following assumptions were used to develop the model for binary batch distillation:

- Molar holdup of all trays (M_T) is constant.
- Molar holdup in the reflux drum (M_R) is constant.
- Boil-up rate (V) is constant.
- Initially a feed of 50 mol with a Methanol mole fraction of 0.3 is charged to the column (50 mol = reboiler holdup + holdups in trays + reflux drum holdup).
- The Methanol-Water mixture forms an ideal binary mixture.
- Where α is the relative volatility of the binary system, the relationship between the liquid (x) and vapor (y) Methanol compositions of an ideal equilibrium stage can be given by the equation below,

$$y = \frac{\propto x}{1 + (\propto - 1)x}$$

Dynamic model:

A. General Equations

$R = \frac{L}{D}$;   (by definition)

L does not vary spatially because the molar holdups in the trays and the reflux drum are constant.

B. Condenser – Reflux Drum

Overall material balance,

$$In + Generation = Out + Accumulation$$

$$V = L + D + \frac{dM_c}{dt}$$

Since M_C is constant (0.2),

$V = L + D$ ---------------------------------- Equation 1

Material balance for Methanol,

$$Vy_1 = Lx_0 + Dx_0 + \frac{dM_c x_0}{dt}$$

$\frac{dx_0}{dt} = (y_1 - x_0) \times \frac{V}{M_C}$ ----------------------------- ODE 0

C. Trays

Material balance for Methanol,

$for\ i = 1,2 \ldots, 12$

$$Vy_{i+1} + Lx_{i-1} = Vy_i + Lx_i + \frac{dM_T x_i}{dt}$$

$\frac{dx_i}{dt} = [L(x_{i-1} - x_i) + V(y_{i+1} - y_i)] \times \frac{1}{M_T}$ -------------------------- ODE 1 – 12

D. Reboiler

Overall material balance for reboiler,

$$L = V + \frac{dM_R}{dt}$$

$\frac{dM_R}{dt} = L - V = -D$ --------------------------- ODE 15

Material balance for Methanol,

$$Lx_{12} = Vy_{13} + \frac{dM_R x_{13}}{dt}$$

$$M_R \frac{dx_{13}}{dt} + x_{13} \frac{dM_R}{dt} = Lx_{12} - Vy_{13}$$

$\frac{dx_{13}}{dt} = [Lx_{12} + Dx_{13} - Vy_{13}] \times \frac{1}{M_R}$ -------------------------------- ODE 13

E. Product Collection Tank

Overall material balance for product collection tank,

$D = \frac{dM_P}{dt}$ --------------------------- ODE 16

Material balance for Methanol,

$$Dx_0 = \frac{dM_p x_p}{dt}$$

$$Dx_0 = M_p \frac{dx_p}{dt} + x_p \frac{dM_p}{dt}$$

$$Dx_0 = M_p \frac{dx_p}{dt} + Dx_p$$

$\frac{dx_p}{dt} = \left(x_0 - x_p\right) \times \frac{D}{M_p}$ ----------------------------------ODE 14

3. Determining the Steady State Liquid Molar Fractions of Trays, Reboiler and Reflux Drum under Total Reflux Conditions

3.1 Dynamic Mathematical Model for the Ideal Batch Distillation Column under Total Reflux

The above mathematical model will be slightly simplified under the total reflux conditions where $D = 0$.

$$D = 0$$

$$\therefore V = L$$

$$\therefore R \rightarrow \infty$$

Since D = 0, ODE 14,15, and 16 will be not relevant for this model. In total, there would be 14 ordinary differential equations in this model.

$$\frac{dx_0}{dt} = (y_1 - x_0) \times \frac{V}{M_C} \quad \text{------------------------------ ODE } 0'$$

$$\frac{dx_i}{dt} = [L(x_{i-1} - x_i) + V(y_{i+1} - y_i)] \times \frac{1}{M_T} \quad \text{------------------------------ ODE } 1' - 12'$$

$$\frac{dx_{13}}{dt} = [Lx_{12} + Dx_{13} - Vy_{13}] \times \frac{1}{M_R} \quad \text{------------------------------ ODE } 13'$$

3.2 Obtaining Steady State Liquid Compositions under Total Reflux

The column is operated under total reflux until steady state is achieved in order to increase the reflux drum liquid composition (from 0.3 to a higher value closer to 1) before distillate product removal from the column is begun. The steady state liquid compositions so achieved are depicted in Figure 2 below (Python code is attached at the end of this document).

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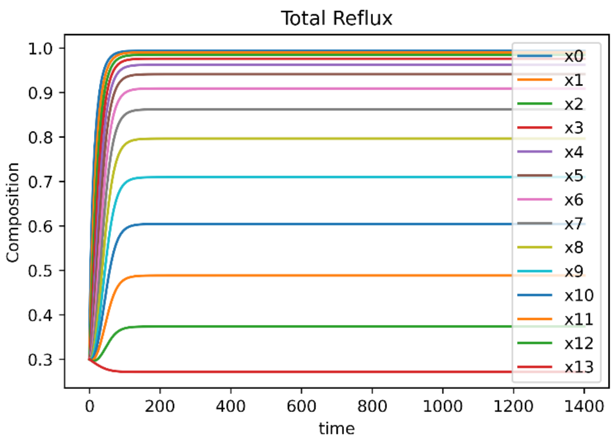


Figure 2- Liquid Compositions at Each Point under Total Reflux

Steady state was evaluated for the reboiler liquid composition as it takes the longest to achieve the steady state (steady state time calculation is explained in the code).

Therefore,

$$Time\ taken\ to\ achieve\ steady\ state = 79.5\ min$$

Steady state Methanol mole fractions of each equilibrium stage were obtained as follows.

$$x\_steady = [0.98949073, \quad 0.98362642, \quad 0.97489337, \quad 0.96197404, \quad 0.94303537, \quad 0.91565157, \quad 0.87687632, \quad 0.82364912, \quad 0.75373713, \quad 0.66719487, \quad 0.56774415, \quad 0.46289115, \quad 0.36198576, \quad 0.27306857]$$

4. Obtaining Liquid Compositions and Molar Holdups at Each Point under a Constant Reflux of 6

Next, the reflux ratio of the column was changed to 6 (the initial conditions of the column before the reflux ratio change is made will be maintained at the steady state liquid compositions obtained under total reflux).

The liquid compositions achieved in the column's reflux drum, trays, reboiler and collection tank, as well as the molar holdups in the reboiler and collection tank, vary with time as shown in Figures 3 and 4 (Python code is attached at the end of this document).

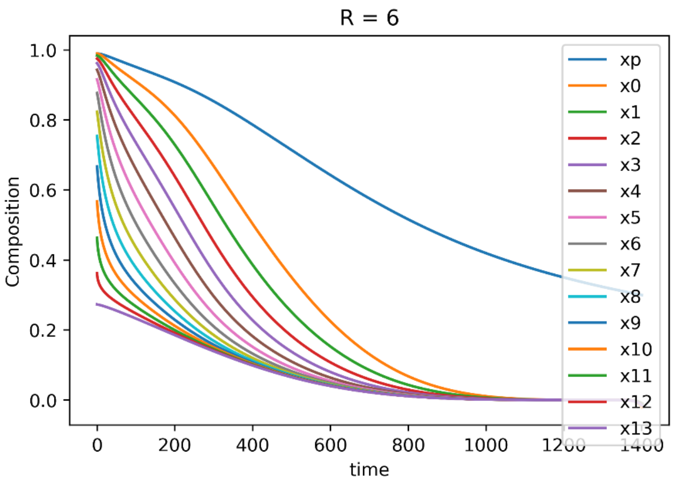


Figure 3 - Liquid Compositions at Each Point under Constant Reflux (R=6)

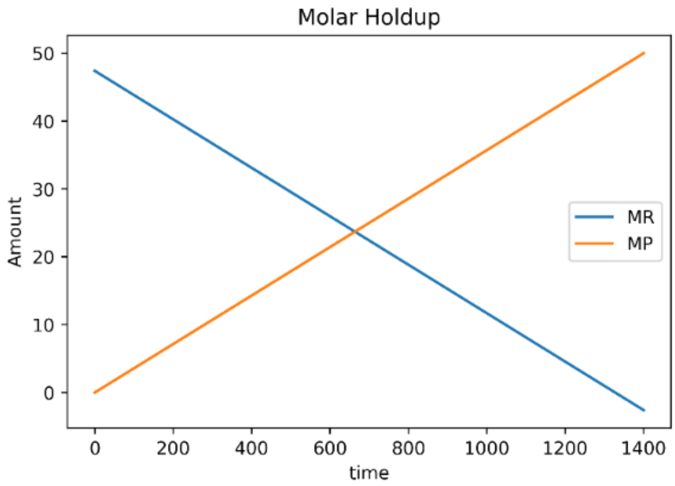


Figure 4 - Molar Holdup at Reboiler and Product Tank Under Constant Reflux

The purity required in the product collected in the collection tank (x_p) was decided to be **0.9**. Due to the limited number of trays available, it is reasonable to assume a distillate purity of 90%. This will ensure a higher yield of the desired compound. However, if a higher level of purity is required, additional purification methods, such as utilizing additional trays or passing the distillate through a second fractionation column, can be implemented.

After changing the column reflux ratio to 6, the time period for which the distillate from the batch distillation column must be collected so that the liquid composition of the collection tank reaches 0.9 was calculated (calculation is explained in the code). The Methanol yield achieved at the end of this time period was also calculated as follows.

$$Yield = \frac{x_p \times M_p}{0.3 \times 50}$$

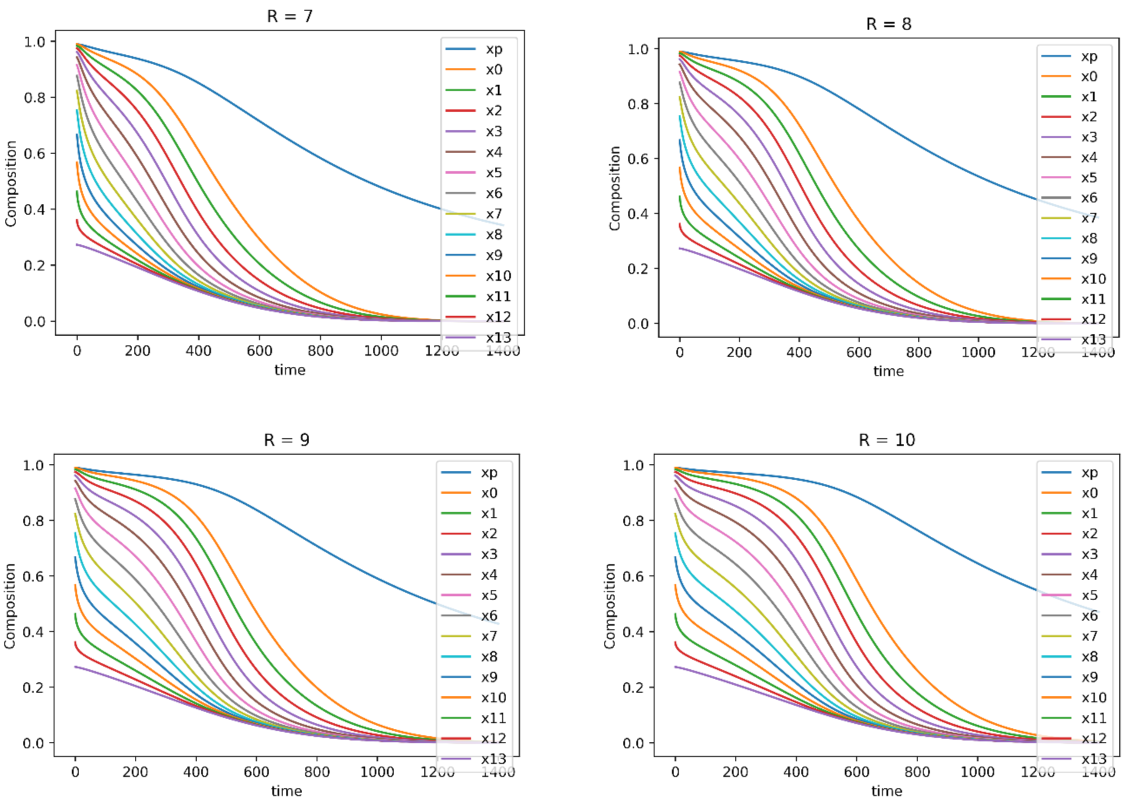
Therefore, when operating the column under constant reflux of 6,

- Time taken for x_p to reach 0.9 = 216 min
- Yield of Methanol = 46.3%

5. Calculating Time Taken for X_p to Reach 0.9 and the Consequent Yield under Different Reflux Ratios

Then, the same code from the above section was run to calculate the liquid compositions of equilibrium stages under constant reflux ratios of 7, 8, 9, and 10. The product collection for each reflux ratio was begun at the steady state liquid compostitions obtained under total reflux.

The Figures 5-8 depict how the liquid compositions achieved in the column's reflux drum, trays, reboiler and collection tank vary with time under different reflux ratios.



Figures 5,6,7,8 - Liquid Compositions at Each Point under Constant Reflux (R=7,8,9,10)

The product collection times and Methanol yields obtained for a required product purity of 0.9 under different reflux ratios are summarized in Table 1 below.

Table 1 – Time Taken for X_p to Reach 0.9 and the Consequent Yield

Reflux Ratio	**Time taken for x_p to reach 0.9 (min)**	**Yield**
6	216	46.3%
7	307	57.5%
8	398	66.3%
9	484	72.7%
10	567	77.3%

Thus, it can be concluded that with increasing reflux ratio, **the distillation time required to achieve a given product purity increases**, while **the amount of Methanol recovered in the product also increases**.