

0.0.1 Distillation column model

The previously described column model is based on a steady state assumption. This means that all variables do not change with time. While a model like that offers valuable insight into the operation of a process many aspects remain unclear. In order to gain further insight into the process the dynamics have to be considered.

Due to that in this section a dynamic model of the ASU process will be developed.

First the balance equations have to be rewritten in dynamic form. To do so reservoir terms or holdups are introduced. Namely the component holdups n_{ij} and internal energy U_j for each stage. with that the component balance equations as presented in the previous section can now be rewritten as

$$\begin{aligned} \left(1 - \sum_{k=1}^{j-1} \zeta_k^R\right) \frac{dn_{ij}}{dt} = & (1 + s_j^V) \cdot V_j \cdot y_{ij} + (1 + s_j^L) \cdot L_j \cdot x_{ij} - V_{j+1} \cdot y_{ij+1} \\ & - L_{j-1} \cdot x_{i,j-1} - \sum_{l=1}^{n_F} \zeta_{lj} \cdot F_j \cdot z_{lj} - \zeta_j^R \cdot V_N \cdot y_{iN}, \\ & i = 1 \dots n_C - 1, \quad j = 1 \dots N, \quad k = 1 \dots n_F, \quad l = 1 \dots n_F. \end{aligned} \quad (0.1)$$

While the internal energy balances become

$$\begin{aligned} \left(1 - \sum_{k=1}^{j-1} \zeta_k^R\right) \frac{dU_j}{dt} = & (1 + s_j^V) \cdot V_j \cdot h_j^V + (1 + s_j^L) \cdot L_j \cdot h_j^L - V_{j+1} \cdot h_{j+1}^V \\ & - L_{j-1} \cdot h_{j-1}^L - \sum_{k=1}^{n_F} \zeta_{kj} \cdot F_k \cdot h_j^F - \zeta_j^R \cdot V_N \cdot h_N^V, \\ & i = 1 \dots n_C, \quad j = 1 \dots n_S, \quad k = 1 \dots n_F. \end{aligned} \quad (0.2)$$

In addition to the balance equations further constituent equations need to be introduced. From the steady state model we know the equilibrium equations

$$y_{ij} = K_{ij} \cdot x_{ij}, \quad i = 1 \dots n_C \quad j = 1 \dots n_S, \quad (0.3)$$

and the summation equations

$$1 = \sum_i^{n_C} y_{ij} \quad j = 1 \dots n_S, \quad (0.4)$$

$$1 = \sum_i^{n_C} x_{ij} \quad j = 1 \dots n_S. \quad (0.5)$$

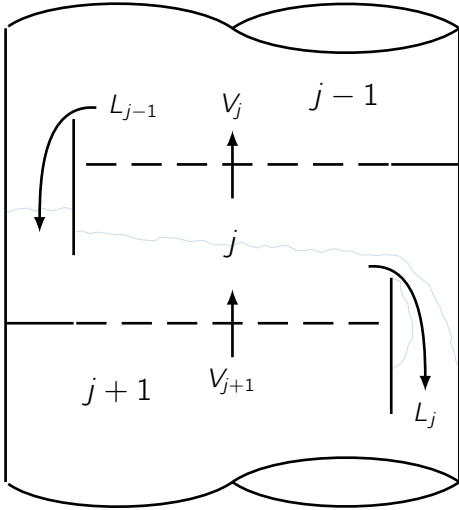


Figure 0.1: Column tray

Furthermore the accumulation of moles in each stage in vapour n_j^V and liquid n_j^L need to be considered with

$$n_{ij} = x_{ij}n_j^L + y_{ij}n_j^V \quad i = 1 \dots n_C \quad j = 1 \dots n_S, \quad (0.6)$$

$$(0.7)$$

These holdups are linked by the volume of a given stage V_{stage} . Thus the volume constraint can be written as

$$V_{stage} = \frac{n_j^V}{\rho_j^V} + \frac{n_j^L}{\rho_j^L} \quad j = 1 \dots n_S. \quad (0.8)$$

The internal energy in a stage corresponds to its enthalpy, reduced by pressure term

$$U_j = n_j^L \cdot h_j^L + n_j^V \cdot h_j^V - p_j \cdot V_{stage} \quad (0.9)$$

As we are no longer dealing in steady state hydraulic equations need to be introduced, which determine the liquid and vapour flow rates leaving a separation stage. As the mechanisms driving these flows might be very different depending on the type of internals used, it is not surprising that the corresponding equations are also very different. In the given model both trayed columns and columns with structured packing are employed.

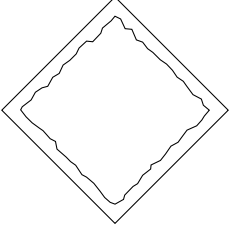
Trayed hydraulics

Trayed column hydraulics can be approximated by the following system of equations. All equations presented here were taken from [?].

The liquid flow rates are calculated from the well established Francis formula, derived from the law of Bernoulli and taking effects like bubbling into account

$$L_j = \frac{2}{3} \sqrt{2g\rho_j^L} \ell_{weir} \Phi h_{ow}^{\frac{2}{3}} \quad j = 1 \dots n_S. \quad (0.10)$$

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Where h_{ow} denotes the height of the liquid over the weir, which can be calculated from the froth height h_f and the weir height h_w

$$h_{ow} = h_f - h_w. \quad (0.11)$$

While the weir height is a tray design parameter the froth height is computed from the clear liquid height and the relative froth density

$$h_f = \frac{n^L MW^L}{A_{active} \varrho^L \Phi}. \quad (0.12)$$

Lastly in terms of liquid flow rates, the relative froth density is dependent on the degree of aeration within the liquid, expressed by the aeration factor β from an empirical equation

$$\beta_j = 1 - 0.3593 \left(\frac{V_{j-1} MW_{j-1}^V}{A_{active} \sqrt{\varrho_{j-1}}} \right)^{0.177709} \quad j = 1 \dots n_S, \quad (0.13)$$

$$\Phi_j = 2\beta_j - 1. \quad (0.14)$$

The pressure difference between stages is the driving force for the vapour streams. The pressure drop is modeled as having two contributions, the dry and wet pressure drop. While dry pressure drop stems from the vapour flowing through the holes with in tray, the wet pressure drop is caused by the liquid holdup on the stage.

$$p_j - p_{j+1} = h_j^{liq} \varrho_j^L g + 0.5 \xi \varrho_{j+1}^V \left(\frac{q_{j+1}^V}{A_h} \right)^2 \quad (0.15)$$

Structured packing hydraulics

write somewhere that stage indices will be omitted for convenience.

Structured packings and their hydraulic behaviour are currently still under investigation. The number of available correlations for calculation of internal flow-rates is much more limited than for trays or even dumped packings. Among the most established models is the one developed by Bravo et al. [?] at the University of Texas. This model has been extended to be valid in the loading region and account for different types of packing material [?]. As main linking factor between vapour and

liquid flow-rates as well as the pressure drop, the liquid holdup has been identified by the authors. It is expressed in dimensionless form h_t in terms of the corrugation side S , and the film thickness δ

$$h_L = \frac{4}{S} \delta. \quad (0.16)$$

One very important factor while estimating the hydraulic behaviour is the dry pressure drop per meter packing δp_{dry} . Within in the presented model it is estimated by

$$\delta p_{dry} = \left(\frac{\rho^G}{\rho_{air,1bar}} \right)^{0.4} \left(\frac{C_1 \rho^G v_G^2}{S \epsilon^2 (\sin \Theta)^2} + \frac{C_2 \mu_G v_G}{S^2 \epsilon \sin \Theta} \right) \quad (0.17)$$

Another prerequisite for calculating the holdup is the knowledge of the amount of wetted area of the available surface area within the packing. It seems reasonable to assume that this will be dependent on the characteristic of the liquid flow through the packing. To characterize the current, well known dimensionless numbers are used. Namely *Weber* (We), *Froude* (Fr) and *Reynolds* (Re) numbers

$$We = \frac{v_L^2 \rho_L S}{\sigma}, \quad (0.18)$$

$$Fr = \frac{v_L^2}{Sg}, \quad (0.19)$$

$$Re = \frac{v_L S \rho_L}{\mu_L} \quad (0.20)$$

With that an approximation for the holdup correction factor F_t due to partial wetting can be expressed as

$$F_t = \frac{A_1 (We Fr)^{0.15} S^{A_2}}{Re^{0.2} \epsilon^{0.6} (1 - 0.93 \cos \gamma) (\sin \Theta)^{0.3}} \quad (0.21)$$

$$h_L = \left(\frac{4F_t}{S} \right)^{\frac{2}{3}} \left\{ \frac{3\mu_L v_L}{\rho_L \epsilon \sin \Theta g \left[\left(\frac{\rho_L - \rho_G}{\rho_L} \right) \left(1 - \frac{\delta p}{\delta p_{flood}} \right) \right]} \right\}^{\frac{1}{3}} \quad (0.22)$$

0.0.2 Integrated condenser / reboiler unit

As it has been stated on several occasions the condenser reboiler unit is essential in the cryogenic air separation process. When it comes to dynamics the pressure profile deserves much attention, as it is crucial for feasible operations of the entire process. The pressure difference between the low and high pressure column enables the heat exchange in this unit.

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