EXTENDED ABSTRACT

Complete Title of Paper

EFFECT OF FLOW DYNAMICS, ENERGY BALANCE AND PRESSURE DYNAMICS ON THE OVERALL RESPONSE OF DISTILLATION COLUMNS

Speaker and Authors

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Abstract

The fundamental equations describing distillation columns are well understood. The motivation for this work is to examine the effect of certain simplifications that are often made when studying distillation columns. Surprisingly, in spite of the fact that such assumptions are commonly used (e.g. to reduce computer time and the need for data) the understanding of their effect on the overall dynamic response seems to be poor (see review paper by Skogestad presented at DYCORD'92, Maryland, April 1992).

We study the following assumptions:

1. a) No liquid flow dynamics, that is, assume immediate responses for liquid.
   b) Alternatively, use simplified expressions for tray behavior.
2. Constant molar flows, that is, use a simplified energy balance.
3. Constant pressure and/or neglected vapor holdup.

Assumption 1a) above should not be used if the model is intended for control purposes, and examples that demonstrate this are presented.

Rigorous models of the actual tray hydraulics are very complicated (including downcomer dynamics etc.) and we propose to use simplified relationships, and discuss ways of estimating the key parameters, namely the effect of liquid and vapor flow on the liquid holdup on the tray (represented by hydraulic time constant, τ_L, and effect of vapor flow on liquid flow, K_2).

Assumption 2 holds for many relatively ideal mixtures, but it appears that for "nonideal" mixtures with even rather small deviations from the constant molar flows assumption, the static and dynamic behavior may be quite different. For example, it may cause the methanol-propanol mixture to yield multiple steady states. We study the deviation from constant molar flows caused by the components having different heats of vaporization as well as different heat capacities.

Assumption 3 of constant pressure often does not hold. In the paper open-loop pressure dynamics is studied, including the self-regulation caused by the heating of the column that may change the heat transferred in the reboiler and condenser. The possibility for open-loop inverse responses for the compositions to changes in condenser duty is also studied.

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1993 AIChE Annual Meeting St. Louis

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Motivation

Common distillation model assumptions:

- Neglected vapor holdup
- Neglected liquid flow dynamics
- Constant pressure on all trays

Purpose:

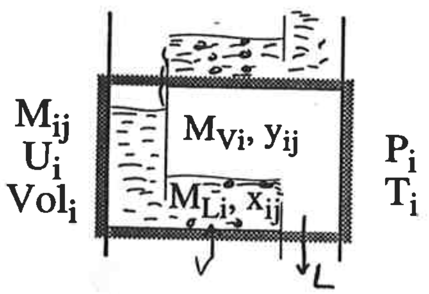
Study effects of modelling assumptions.

Derive 5 × 5 dynamic distillation model for control studies.

Model

- **Component balances:** $\frac{dM_{ij}}{dt} = .. \; ; \; j = 1,2$
- **Energy balance:** $\frac{dU_i}{dt} = ..$

$\Big\}$ 3×41 =123 states

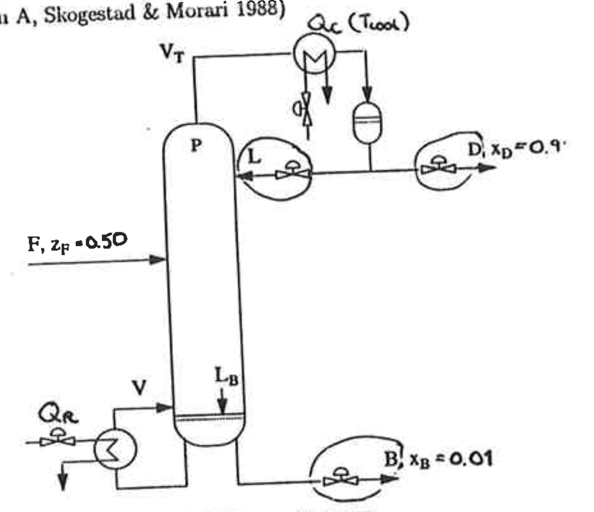


$$\left.\begin{array}{l} M_{ij}, U_i \text{ (states)} \\ \text{Fixed volume} \\ \text{VLE} \end{array}\right\} \Rightarrow \text{UV} - \text{flash}$$

- **Detailed tray hydraulics** $\longrightarrow L$
  (Francis weir for froth flow, Bennett et al. 1983)
- **Pressure drop correlation** $\rightarrow V$
  (Liebson et al. 1957)

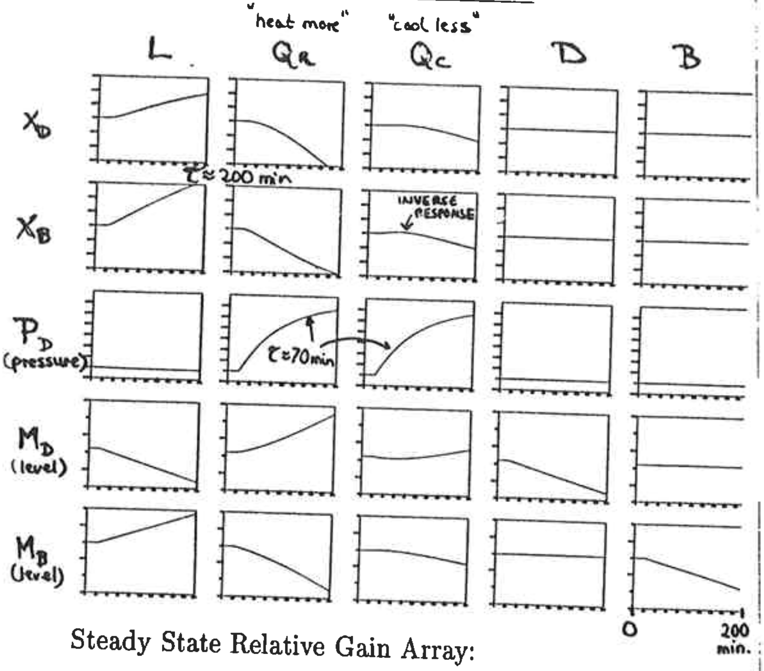
Column overview

Binary mixture, one feed, two products
(Column A, Skogestad & Morari 1988)



- 39 stages + reboiler + total condenser
- Relative volatility $\alpha = 1.5$
- $L/F = 2.73$

Open-loop responses overview



Steady State Relative Gain Array:

$$\begin{matrix} 36.76 & -64.65 & 28.88 & 0.0 & 0.0 \\ -35.72 & 63.49 & -26.76 & 0.0 & 0.0 \\ -0.04 & 2.16 & -1.12 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{matrix}$$

NEGATIVE!?

Will consider:

1. Including/neglecting vapor holdup (UV-flash)
2. Open loop pressure response : estimate
3. Understanding: Negative RGA/Inverse response
4. Tray hydraulics

1.)

Including vapor holdup (UV)

Assumptions applied to each control volume:

A1 Perfect mixing.

A2 Two phase system in thermal and vapor-liquid equilibrium.

$$\frac{dM_{i,j}}{dt} = V_{i-1}y_{i-1,j} + L_{i+1}x_{i+1,j} - V_i y_{i,j} - L_i x_{i,j} + F_i z_{i,j}$$

$$\frac{dU_i}{dt} = V_{i-1}h_{V,i-1} + L_{i+1}h_{L,i+1} - V_i h_{V,i} - L_i h_{L,i} + Q_i$$

$$\left.\begin{matrix} M_{i,j} \\ U_i \\ Vol_i \end{matrix}\right\} \underset{\text{(NOT REPORTED BEFORE)}}{\text{UV} - \text{flash}} \Rightarrow \left\{\begin{matrix} x_{i,j},\ y_{i,j} \\ h_{L,i},\ h_{V,i},\ T_i \\ M_{L,i},\ M_{V,i} \\ P_i \\ \text{etc} \end{matrix}\right.$$

NO problems numerically

Neglecting vapor holdup (hx)

A3 $M_V = 0,\ \ u_L = h_L$.

$$\left.\begin{matrix} M_{i,j} \\ U_i = H_i \end{matrix}\right\} \underset{h-\text{flash}}{\text{Bubble}} \Rightarrow \left\{\begin{matrix} y_{i,j} \\ h_{V,i},\ T_i \\ P_i \\ \text{etc} \end{matrix}\right.$$

Neglecting vapor holdup

- Does not affect the number of states.
- Does not imply constant pressure.
- Does not imply immediate vapor response.
- Does not reduce stiffness (opposite).

BUT:
- Simplifies the algebraic equation set (flash)
  (Bubble-h rather than UV)

- Why has not UV-flash been used before?
- Probably because it is not needed in static simulation where pressure is specified

Estimation of Pressure dynamics

) Fixed Q_R & Q_C (No self-regulation in reboiler/condenser)

$$\frac{dU}{dt} = Fh_F - Dh_D - Bh_B + \overbrace{Q_R + Q_C}^{\text{const.}}$$

Assume:

- "One component mixture" (T function of pressure only)
- $\Delta\bar{T} \approx \Delta T_D \approx \Delta T_B$

Neglected vapor holdup (hx)

$$U = \Sigma(M_{L,i}h_{L,i}) = M_{L,tot}c_{PL}\Delta\bar{T}$$

$$\frac{d\Delta U}{dt} = -D\Delta h_D - B\Delta h_B + \cdots$$

$$M_{L,tot}\cancel{c_{PL}}\frac{d\Delta\bar{T}}{dt} \approx -D\cancel{c_{PL}}\Delta T_D - B\cancel{c_{PL}}\Delta T_B + \cdots$$

$$\boxed{\tau_P \approx \frac{M_{L,tot}}{F}}$$!!

SIMULATION: $\tau_P \approx 74$ min

ESTIMATE M_L/F = 71 min

Pressure dynamics

Including vapor holdup (UV)

$$\tau_P \approx \frac{M^*_{L,tot}}{F}$$

$$M_L^* = M_L(\underbrace{1}_{\text{heat liquid}} + \overbrace{\frac{M_V c_{PV}}{M_L c_{PL}}}^{\text{heat vapor}} + \overbrace{\frac{M_V}{M_L}\frac{R}{c_{PL}}(K^2-K)}^{\text{Evaporization}} - \overbrace{(\frac{M_V}{M_L}+\frac{v_L}{v_V})\frac{R}{c_{P}}}^{\text{pV-work}}$$

Typical values:

$\frac{c_{PV}}{c_{PL}} \approx 0.5$; $K \approx \frac{h_{vap}}{RT} \approx 9$; $\frac{R}{c_{PL}} \approx 0.05$; $\frac{v_L}{v_V} \approx 0.0$

which gives

$$\frac{M_L^*}{M_L} = \frac{\tau_P(UV)}{\tau_P(hx)} \approx 1 + 4\frac{M_V}{M_L} -$$

$$\begin{cases} = 1.04 \text{ for our example} \\ \approx 5 \text{ for } M_V \approx M_L \text{ (>10 bar)} \end{cases}$$

Pressure dynamics

B) With 'self-regulation' in condenser

$$Q_C = (UA)_C(\underset{\text{spec}}{T_{cool}} - \underset{\text{column temp.}}{T_D})$$ (Qc depends on column temp.)

$$\tau_P \approx \frac{M^*_{L,tot}}{F + \underbrace{\left(\frac{\delta Q_C}{\delta T_D}\right)_{T_{cool}}}_{UA}/c_{PL}} << \frac{M^*_{L,tot}}{F}$$

BUT: Effect of neglecting M_V as above.

SIMULATION (Fixed T_{cool} & Q_D): τ_p = 2.3 min

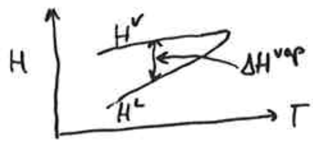
ESTIMATE : 2.3 min

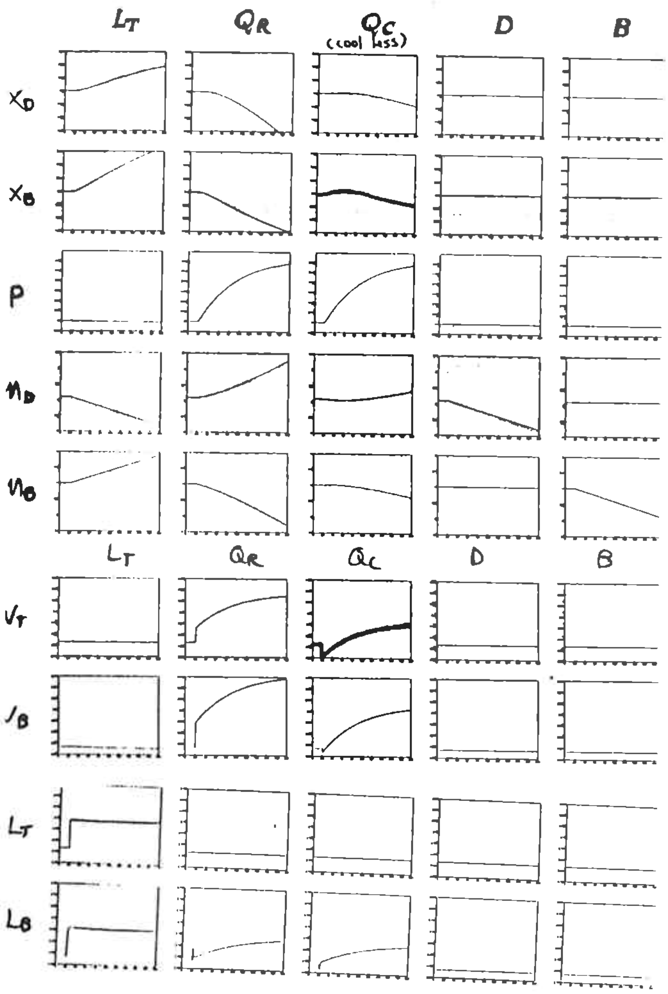
3. Understanding:

- INVERSE RESPONSE
- NEGATIVE RGA-ELEMENT

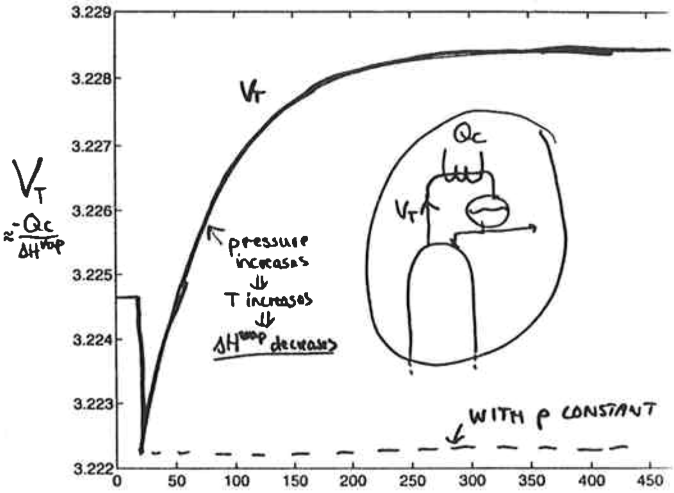
key

- ΔH^{vap} decreases as T increases





INCREASE Q_C ("COOL LESS



Relative Gain Array Analysis

RGA($\omega = 0$):

	L_T	Q_R	Q_C	D	B
x_D	36.76	−64.65	28.88	0.00	0.00
x_B	−35.72	63.49	−26.76	0.00	0.00
P_D	−0.04	2.16	−1.12	0.00	0.00
M_D	0.00	0.00	0.00	1.00	0.00
M_B	0.00	0.00	0.00	0.00	1.00

LICATION OF NEGATIVE RGA :

Pairing $Q_C \rightarrow P_D$ (negative RGA):

1: Overall system unstable, or

2: Pressure loop unstable, or

3: Remaining system unstable if pressure loop fails. (BAD!)

$\lambda_{P_D,Q_C}(0)$ and $\lambda_{P_D,Q_C}(j\infty)$ have different signs:

1: Overall system has a RHP transmission zero, or

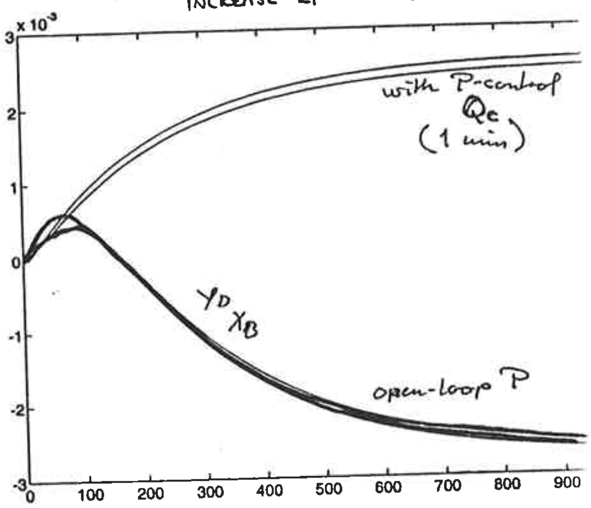
2: $g_{P_D,Q_C}(s)$ has a RHP zero, or

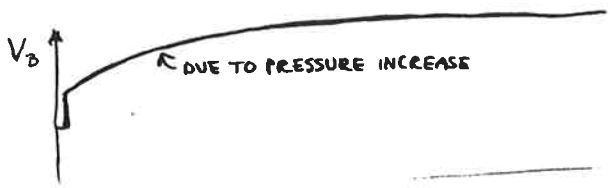
3: Remaining system has a RHP transmission zero.

"REMAINING SYSTEM (WITH Q_C CONST.) HAS A RHP ZERO"

$$\begin{pmatrix} x_D \\ x_B \end{pmatrix} = G' \begin{pmatrix} L \\ Q_R \end{pmatrix}$$

INCREASE L_T AND Q_R AT T=20 MIN





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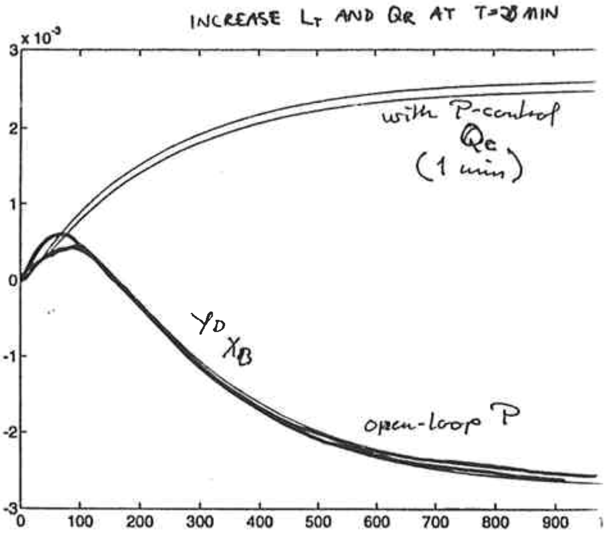
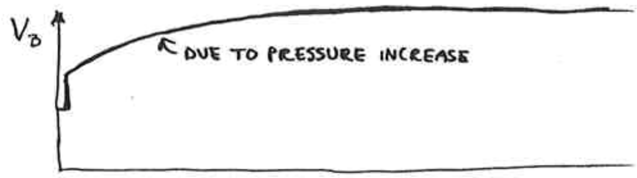
INCREASE L_T AND Q_R AT T=20 MIN





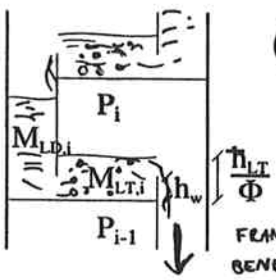
IMPLICATION:

- WITH Q_R AND Q_C AS INDEPENDENT VARIABLES
  NEED PRESSURE CONTROL!

BUT:

- WITH T_{cool} AS INDEPENDENT VARIABLE:
  - NO INVERSE RESPONSE (P SELF-REGULATED)
  - NOT REQUIRED TO CONTROL PRESSURE

4 Tray hydraulics



$M_L, \Delta P \to L, V$

FRANCIS: $L = f_1(M_{Li}, \varphi_i)$

BENETT: $\varphi_i = f_2(V_i)$

LIEBSON: $V = f_3(\Delta P_{dry})$ ΔP

$$\Delta P_i = \Delta P_{wet,i} + \Delta P_{dry,i} = (\hbar_{LT,i} + \hbar_{dry,i})\rho_{L,i} g$$
$$M_{L,i} = \frac{\hbar_{LT,i} A_T}{v_{L,i}} + \frac{\hbar_{LD,i} A_D}{v_{L,i}}$$
$$\hbar_{LD,i} = 2\hbar_{LT,i} + \hbar_{dry,i}$$

$$\Delta P_i \ \& \ M_{L,i} \implies \Delta P_{dry,i} \ \& \ \hbar_{LT,i}$$

V_{i-1} : (Liebson et al. 1957)

$$\Delta P_{dry,i} = \frac{1}{2}\rho_{V,i}\xi_{dry}\left(\frac{V_{i-1} v_{V,i}}{A_H}\right)^2$$

L_i : (Francis weir for froth flow, Bennett et al.1983)

$$\hbar_{LT,i} = \hbar_{uw,i} + \hbar_{ow,i} = \Phi_i h_w + \Phi_i c_f \left(\frac{L_i v_{L,i}}{l_w \Phi_i}\right)^{(2/3)}$$

$$\Phi_i = exp(c_1 \left(\frac{V_{i-1} v_{V,i}}{A_T}\sqrt{\frac{\rho_{V,i}}{\rho_{L,i} - \rho_{V,i}}}\right)^{c_2})$$

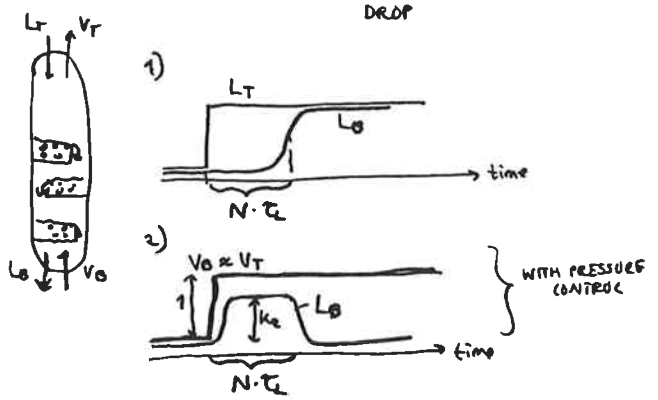
Rijnsdorp (1961):

$$dL_i = \frac{1}{\tau_L} dM_i + K_2 dV_{i-1}$$

DESIRED

$$\tau_L \approx \frac{2}{3}\frac{M_{ow}}{L} \qquad \text{LARGE}$$

$$K_2 \approx \left(\frac{1}{2} + \underbrace{\frac{3\,\hbar_{uw}}{2\,\hbar_{ow}}} - 3\underbrace{\underbrace{\frac{A_D}{(A_T + 2A_D)}}_{\approx 0.1}\frac{\hbar_{dry}}{\hbar_{ow}}}_{\text{MAKE LARGE BY INCREASING PRESSURE DROP}}\right) \qquad \leq 0$$



Calculated hydraulic data

$$\tau_L \approx 2.4 \text{ sec.}$$
$$\Sigma\tau_L \approx 93 \text{ sec.}$$
$$K_{2(Top)} \approx 0.5$$
$$K_{2(Bot)} \approx 0.8$$

Conclusions

- Simulation with rigorous energy balance (UV-flash) is feasible.
- Control with condenser and reboiler duty as manipulated inputs is sensitive to pressure control failure, due to $\Delta h_{vap} = f(T(P))$.
- The effect on pressure dynamics (τ_P) of neglected vapor holdup may be estimated from M_L^*/M_L.
- Large downcomer and high tray pressure drop prohibits inverse responses for boilup changes