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Ternary distillation column
Dynamical model
Model simulation results
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Conclusion and perspectives

Observer Design for a Ternary Distillation Column with Side Stream

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Problem statement

Goal

- Improving purity control in distillation columns.
- Optimizing installation costs and energy.

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- High cost of the measures.
- Nonlinear coupling between controlled physical quantities.

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 - Based on a simple model ⇒ Poor control performances.
 - High energy consumption.

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Solution

Need for and advanced controller using a model based state estimation.



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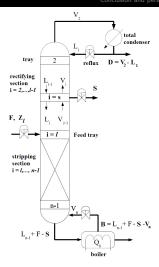


FIGURE: Ternary distillation column with side stream.

- n Number of trays (18 tray).
- *i* Tray index i=1,...,n.
- Feed Tray.
- s Extraction tray.
- Z Feed flow molar fraction.
- F Molar feed rate.
- 5 Extracted molar flow rate.
- L Reflux molar flow rate.
- V Vapour molar flow rate.

Modelling assumptions

Classical assumptions 1

- Constant column internal pressure.
- Constant molar retention.
- L_i 's are equal, V_i 's are equal, for all i = 1, ..., n.
- Trays walls are adiabatic.
- Liquid and outgoing vapour of each tray are in thermal equilibrium.
- Homogeneous mixture in each tray.
- Feed flow rate is continuous and in the liquid phase.
- We assume a theoretical boiler and total condenser.

Special assumption

- Assume a non-ideal mixture ².
- 1. Leads to solving an ODE system
- 2. Leads to solving an ADE system



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Material balance equations

Total condenser,
$$i = 1$$
:
$$N_1 \frac{dx_{j,1}}{dt} = V_f(y_{j,2} - x_{j,1})$$
 Upper rectifying section, $i = 2, ..., s$:
$$N_i \frac{dx_{j,i}}{dt} = L(x_{j,i-1} - x_{j,i}) + V_f(y_{j,i+1} - y_{j,i})$$
 Lower rectifying section, $i = s+1, ..., l-1$:
$$N_i \frac{dx_{j,i}}{dt} = (L-S)(x_{j,i-1} - x_{j,i}) + V_f(y_{j,i+1} - y_{j,i})$$
 Feed tray, $i = l$:
$$N_l \frac{dx_{j,l}}{dt} = (L-S)(x_{j,l-1} - x_{j,l}) + F(Z_{j,l} - x_{j,l}) + V_f(y_{j,l+1} - y_{j,l})$$
 Stripping section, $i = l+1, ..., n-1$:
$$N_i \frac{dx_{j,l}}{dt} = (F+L-S)(x_{j,l-1} - x_{j,l}) + V_f(y_{j,i+1} - y_{j,l})$$

- Component index, j=1 for Benzene, j=2 for Toluene, j=3 for o-Xylene.
- N Molar retention.
- x Liquid phase molar fraction.
- y Vapour phase molar fraction.

 $N_n \frac{dx_{j,n}}{dt} = (F + L - S)(x_{j,n-1} - x_{j,n}) + V_f(x_{j,n} - y_{j,n})$ Thermodynamic constraints, i = 1,...,n:

Vapour phase molar fractions

Remark

The correlation between physical quantities from

- Antoine formula.
- Vapour Liquid Equilibrium (VLE).
- Murphree efficiency.

allowed to get the vapour molar fractions $y_{j,i}$ functions of liquid molar fractions $x_{j,i}$.

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Liquid molar retention in each tray
Liquid and vapour Murphree efficiency
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Feed flow rate
Benzene composition in feed rate
Toluene composition in feed rate
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Steady state quality of Benzene in top product
Steady state quality of Benzene in bottom product
Steady state quality of Toluene in top product
Steady state quality of Toluene in bottom product

C. Afri et al., nadri@lagep.univ-lyon1.fr

$$n = 18,$$

 $s = 6, l = 9$
 $N_1 = 20 \text{ mol}$
 $N_{18} = 20 \text{ mol}$
 $N_i = 8 \text{ mol}$
 $e^l = 1, e^v = 1$
 $P_T = 760 \text{ mmHg}$
 $F = 1.67 \text{ mol/min}$
 $Z_{Ben,l} = 0.6$
 $Z_{Tol,l} = 0.3$
 $T_l = 379, 32 \text{ K}$
 $S = 0.167 \text{ mol/min}$
 $V_f = 7.0086 \text{ mol/min}$
 $V_f = 0.0017 \text{ mol/min}$
 $X_{1,1} = 0.95$
 $X_{1,18} = 8.87 \times 10^{-5}$
 $X_{2,1} = 0.05$
 $X_{2,18} = 0.67$

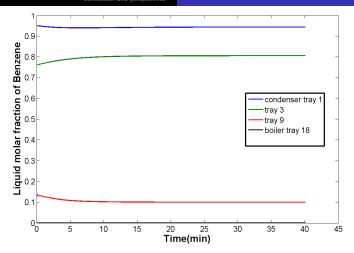


FIGURE: Response of the dynamic model starting from the experimental steady state, in 4 locations: liquid molar fractions of Benzene.

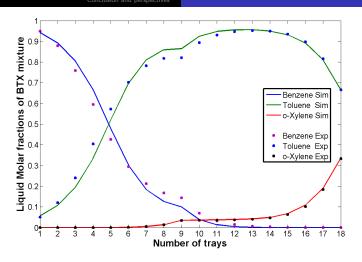


FIGURE: Final molar fraction profiles : simulation and experimental.



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Advanced controller problem

In addition to the output measures, advanced controllers require more informations about plan.

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- Column internal liquid molar fractions.
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Solution

Estimate them from the measurement of some.



State space representation

We consider the following new notations

$$\left\{ \begin{array}{ll} x_{i}^{1} = x_{1,i}; & 1 \leq i \leq l-1 \\ x_{i}^{2} = x_{1,n-i+1}; & 1 \leq i \leq n-l-1 \\ \overline{x}_{i}^{1} = x_{2,i}; & 1 \leq i \leq l-1 \\ \overline{x}_{i}^{2} = x_{2,n-i+1}; & 1 \leq i \leq n-l-1 \\ z_{i}^{1} = T_{i}; & 1 \leq i \leq l-1 \\ z_{i}^{2} = T_{n-i+1}; & 1 \leq i \leq n-l-1 \\ u^{T} = (L, V_{f}, F, S, Z_{1,l}, Z_{2,l})^{T} \\ y_{1} = (x_{1}^{1}, x_{1}^{2})^{T} = (x_{1,1}, x_{1,n})^{T}, \\ y_{2} = (\overline{x}_{1}^{1}, \overline{x}_{1}^{2})^{T} = (x_{2,1}, x_{2,n})^{T}, \end{array} \right.$$

where

- y_1 & y_2 Outputs system contains the top and bottom measures of light component (Benzene) and intermediate component (Toluene) respectively.
 - u Inputs system, S, F, $Z_{1,l}$ and $Z_{2,l}$ are uncontrolled inputs, V_f and L are manipulated inputs.
 - $\times \& \bar{x}$ State variables.

State space representation

The system belongs to the class of fully interconnected implicit systems written in the following compact format :

$$\begin{cases} \dot{x}(t) = f(x(t), \overline{x}(t), z(t), u(t)) & x \in \mathbb{R}^n, \quad u \in U \\ \dot{\overline{x}}(t) = \overline{f}(x(t), \overline{x}(t), z(t), u(t)) & \overline{x} \in \mathbb{R}^n \\ \varphi(x(t), \overline{x}(t), z(t)) = 0 & z \in \mathbb{R}^d \\ y(t) = [h(x(t)) \ \overline{h}(\overline{x}(t))]^T & y \in \mathbb{R}^p, \end{cases}$$

where,

$$h(x) = [x_1^1(t), x_1^2(t)]^T ; \bar{h}(\bar{x}) = [\bar{x}_1^1(t), \bar{x}_1^2(t)]^T$$

$$x = (x_1^1, ..., x_{l-1}^1, x_1^2, ..., x_{n-l+1}^2)^T ; \bar{x} = (\bar{x}_1^1, ..., \bar{x}_{l-1}^1, \bar{x}_1^2, ..., \bar{x}_{n-l+1}^2)^T$$

$$f = \begin{bmatrix} f^1(\bar{x}, x, z, u) \\ f^2(x, \bar{x}, z, u) \end{bmatrix} ; \bar{f} = \begin{bmatrix} \bar{f}^1(\bar{x}, x, z, u) \\ \bar{f}^2(x, \bar{x}, z, u) \end{bmatrix} ; \varphi = \begin{bmatrix} \varphi^1(x^1, \bar{x}^1, z^1) \\ \varphi^2(x^2, \bar{x}^2, z^2) \end{bmatrix}$$

State space representation

f , \bar{f} and ϕ are \mathscr{C}^1 functions with respect to their arguments and satisfy the following triangular structure :

$$f^i = \left[\begin{array}{c} f_1^i(x_1^i, x_2^i, \bar{x}^i, z_2^i, u) \\ \vdots \\ f_k^i(x_{k-1}^i, x_k^i, x_{k+1}^i, \bar{x}^i, z_k^i, z_{k+1}^i, u) \\ \vdots \\ f_{n_i-1}^i(x_{n_i-2}^i, x_{n_i-1}^i, x_{n_i}^i, \bar{x}^i, z_{n_{i-1}}^i, z_{n_i}^i, u) \\ f_{n_i}^i(x, \bar{x}, z, u) \end{array} \right]$$

$$\vec{f}^i = \left[\begin{array}{c} \vec{f}^i_1(\vec{x}^i_1, \vec{x}^i_2, x^i, z^i_2, u) \\ \vdots \\ \vec{f}^i_k(\vec{x}^i_{k-1}, \vec{x}^i_k, \vec{x}^i_{k+1}, x^i, z^i_k, z^i_{k+1}, u) \\ \vdots \\ \vec{f}^i_{n_i-1}(\vec{x}^i_{n_i-2}, \vec{x}^i_{n_i-1}, \vec{x}^i_{n_i}, \vec{x}^i, z^i_{n_{i-1}}, z^i_{n_i}, u) \\ \vdots \\ \vec{f}^i_{n_i}(\vec{x}^i_{n_i-2}, \vec{x}^i_{n_i-1}, \vec{x}^i_{n_i}, x^i, z^i_{n_{i-1}}, z^i_{n_i}, u) \end{array} \right]$$

$$\phi^{i} = \left[\begin{array}{c} \phi^{i}_{1}(x^{i}_{1}, \bar{x}^{i}_{1}, z^{i}_{1}) \\ \vdots \\ \phi^{i}_{k}(x^{i}_{k-1}, x^{i}_{k}, x^{i}_{k+1}, \bar{x}^{i}_{k-1}, \bar{x}^{i}_{k}, \bar{x}^{i}_{k+1}, z^{i}_{k}) \\ \vdots \\ \phi^{i}_{1}(x^{i}_{n_{i}}, \bar{x}^{i}_{n_{i}}, z^{i}_{n_{i}}) \end{array} \right]$$

where $n_1 = l - 1$, and $n_2 = n - l + 1$.

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State Estimation

Estimation problem

By knowing the outputs y(t) and inputs u(t), how we can estimate the unknowns (x(t), z(t))?

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By knowing the outputs y(t) and inputs u(t), how we can estimate the unknowns (x(t), z(t))?

Solution

State space observer design.

Estimation problem

Two approaches are possible

1. An implicit observer

$$\begin{cases} & \dot{\hat{x}}(t) = f(\hat{x}(t), \dot{\hat{x}}(t), \hat{z}(t), u(t)) - K_{\theta}(\hat{y}_{1}(t) - y_{1}(t)) \\ & \dot{\hat{x}}(t) = \bar{f}(\hat{x}(t), \dot{\hat{x}}(t), \hat{z}(t), u(t)) - \bar{K}_{\theta}(\hat{y}_{2}(t) - y_{2}(t)) \\ & \varphi(\hat{x}(t), \dot{\hat{x}}(t), \hat{z}(t)) = 0 \\ & \hat{y}(t) = [h(\hat{x}(t)) \ \bar{h}(\dot{\hat{x}}(t))]^{T} \end{cases}$$

Principle : Resolution of algebro-differential equations \Rightarrow use of iterative optimisation techniques for algebraic equations resolution

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Principle : Resolution of algebro-differential equations \Rightarrow use of iterative optimisation techniques for algebraic equations resolution

Disadvantages

- Optimization can increase the computing time.
- The algorithm may become difficult to implement on-line for complex systems and/or fast dynamic systems.

Observer algorithm

2. An explicit observer:

$$\left\{ \begin{array}{l} \dot{\hat{x}} = f(\hat{x}, \hat{\bar{x}}, \hat{z}, u) + \mathcal{K}_{\theta}(\hat{y}_{1} - y_{1}) \\ \dot{\hat{\bar{x}}} = \bar{f}(\hat{x}, \hat{\bar{x}}, \hat{z}, u) + \overline{\mathcal{K}}_{\theta}(\hat{y}_{2} - y_{2}) \\ \dot{\hat{z}}(t) = -\left(\frac{\partial \varphi}{\partial z} \mid_{(\hat{x}, \hat{z}, \hat{\bar{x}})}\right)^{-1} \left(\left[\frac{\partial \varphi}{\partial x} \mid_{(\hat{x}, \hat{z})}, \frac{\partial \varphi}{\partial \bar{\bar{x}}} \mid_{(\hat{\bar{x}}, \hat{z})}\right] \left[\dot{\hat{x}}, \dot{\hat{\bar{x}}}\right]^{T} + \Lambda \varphi(\hat{x}, \hat{\bar{x}}, \hat{z}) \right), \end{array} \right.$$

where.

$$K_{\theta} = \textit{diag} \big(-\textit{r}_{1} \boldsymbol{\Delta}_{\theta} \boldsymbol{\delta}_{1} \ \boldsymbol{S}_{1}^{-1} \ \boldsymbol{C}_{1}^{T}, \ -\textit{r}_{2} \boldsymbol{\Delta}_{\theta} \boldsymbol{\delta}_{2} \ \boldsymbol{S}_{2}^{-1} \ \boldsymbol{C}_{2}^{T} \big) \ ; \\ \overline{K}_{\theta} = \textit{diag} \big(-\overline{\textit{r}}_{1} \bar{\boldsymbol{\Delta}}_{\theta} \boldsymbol{\delta}_{1} \ \bar{\boldsymbol{S}}_{1}^{-1} \ \bar{\boldsymbol{C}}_{1}^{T}, \ -\overline{\textit{r}}_{2} \bar{\boldsymbol{\Delta}}_{\theta} \boldsymbol{\delta}_{2} \ \bar{\boldsymbol{S}}_{2}^{-1} \ \bar{\boldsymbol{C}}_{2}^{T} \big), \\ \boldsymbol{K}_{\theta} = \textit{diag} \big(-\overline{\textit{r}}_{1} \bar{\boldsymbol{\Delta}}_{\theta} \boldsymbol{\delta}_{1} \ \bar{\boldsymbol{S}}_{1}^{-1} \ \bar{\boldsymbol{C}}_{1}^{T}, \ -\overline{\textit{r}}_{2} \bar{\boldsymbol{\Delta}}_{\theta} \boldsymbol{\delta}_{2} \ \bar{\boldsymbol{S}}_{2}^{-1} \ \bar{\boldsymbol{C}}_{2}^{T} \big), \\ \boldsymbol{K}_{\theta} = \textit{diag} \big(-\overline{\textit{r}}_{1} \bar{\boldsymbol{\Delta}}_{\theta} \boldsymbol{\delta}_{1} \ \bar{\boldsymbol{S}}_{1}^{-1} \ \bar{\boldsymbol{C}}_{1}^{T}, \ -\overline{\textit{r}}_{2} \bar{\boldsymbol{\Delta}}_{\theta} \boldsymbol{\delta}_{2} \ \bar{\boldsymbol{S}}_{2}^{-1} \ \bar{\boldsymbol{C}}_{2}^{T} \big), \\ \boldsymbol{K}_{\theta} = \textit{diag} \big(-\overline{\textit{r}}_{1} \bar{\boldsymbol{\Delta}}_{\theta} \boldsymbol{\delta}_{1} \ \bar{\boldsymbol{S}}_{1}^{-1} \ \bar{\boldsymbol{C}}_{1}^{T}, \ -\overline{\textit{r}}_{2} \bar{\boldsymbol{\Delta}}_{\theta} \boldsymbol{\delta}_{2} \ \bar{\boldsymbol{S}}_{2}^{-1} \ \bar{\boldsymbol{C}}_{2}^{T} \big), \\ \boldsymbol{K}_{\theta} = \textit{diag} \big(-\overline{\textit{r}}_{1} \bar{\boldsymbol{\Delta}}_{\theta} \boldsymbol{\delta}_{1} \ \bar{\boldsymbol{S}}_{1}^{-1} \ \bar{\boldsymbol{C}}_{1}^{T}, \ -\overline{\textit{r}}_{2} \bar{\boldsymbol{\Delta}}_{\theta} \boldsymbol{\delta}_{2} \ \bar{\boldsymbol{S}}_{2}^{-1} \ \bar{\boldsymbol{C}}_{2}^{T} \big), \\ \boldsymbol{K}_{\theta} = \textit{diag} \big(-\overline{\textit{r}}_{1} \bar{\boldsymbol{\Delta}}_{\theta} \boldsymbol{\delta}_{1} \ \bar{\boldsymbol{\Delta}}_{1} \ \bar{\boldsymbol{A}}_{1}^{T} \ \bar{\boldsymbol{A}}_{2}^{T} \ \bar{\boldsymbol{$$

Principle: Ordinary differential equations (ODE) resolution.

Advantage

Compared to the implicit observer, the time of calculus = time of ODE integration.

Observer algorithm

$$S_n = \begin{bmatrix} s_{11} & s_{12} & 0 & \cdots & 0 \\ s_{12} & s_{22} & s_{23} & \cdots & 0 \\ 0 & s_{23} & \ddots & \ddots & \vdots \\ \vdots & \cdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & s_{n-1n} & s_{nn} \end{bmatrix}, A_n(t) = \begin{bmatrix} 0 & a_1(t) & 0 & \cdots & 0 \\ 0 & 0 & a_2(t) & \cdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 & a_{n-1}(t) \\ 0 & \cdots & \cdots & 0 & 0 \end{bmatrix}$$

S satisfies the inequality

$$\forall t \leq 0, A_n^T(t)S_n + S_nA_n(t) - \rho C_n^T C_n \leq -\eta I_n$$

The a_i 's are unknowns and satisfy : $\forall t \geq 0, \alpha_1 \leq a_i(t) \leq \alpha_2$ where, $\alpha_1, \alpha_2 > 0$.

- $r_1\&r_2$ positive constants tuning parameters of the observer greater than 1 \triangle_{θ} is a diagonal matrix of $(\theta, \theta^2, ..., \theta^{n_i})$
 - θ tuning positive constant observer parameter.
- $\rho \& \eta$ are positive constants.

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	Liquid molar retention in boiler
	Liquid molar retention in each tray
	Liquid and vapour Murphree efficiency
	Internal pressure
	Feed flow rate
	Benzene composition in feed rate
	Toluene composition in feed rate
	Feed temperature
	Side stream liquid flow rate
	Steady state vapour flow rate
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-	

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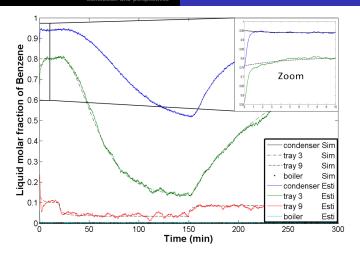


FIGURE: True and observed trays temperature in the presence of initial estimations errors and output added noises.

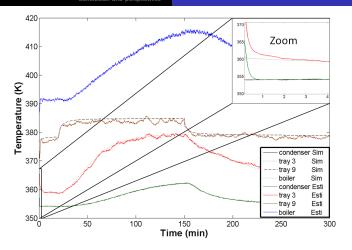


FIGURE: True and observed Benzene molar fractions in the presence of initial estimations errors and output added noises.

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Conclusion:

- Mathematical model validation describing the dynamic of ternary mixture fractions in a distillation column with 18 trays.
- High gain explicit observer performances validation.

Perspectives:

- Synthesis of an observer based on trays temperature measurements.
- Synthesis of a suitable control law.

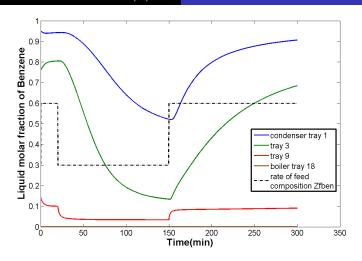
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Thanks for your attention

About our research team "Nonlinear systems and Processes (SNLEP)" : sites.google.com/site/snlepteam



 $\ensuremath{\mathrm{Figure}}$: Open loop response to the feed disturbances .