

A Linear Time-Varying State-Space Model of Batch Distillation Columns for Control Applications

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Abstract

One of the first steps towards control is developing a mathematical model of the process of interest. A rigorous model is not always appropriated for on-line control tasks, especially for batch systems, which are characterised by frequent changes in process conditions. In this work, a linear time-varying state-space model for batch distillation columns was developed and tested. The model is suitable for on-line implementation and to predict the system behaviour from measurable and easily available information. Comparing the model predictions with the rigorous simulation results, the state-space model was able to predict the batch distillation column behaviour accurately, even for the nonideal mixture ethanol/water.

1. Introduction

Batch processing has become more and more important in the chemical industries and this trend is expected to continue as the interest in low-volume and high-value products is increasing.

Batch distillation, in particular, is the most frequent separation method in batch processes (Lucet *et al.*, 1996) and is widely used in the production of fine chemicals. Fine chemicals must be manufactured according to high and well-defined standards of purity, so the distillate composition control plays a significant role in the fulfilment of the market demands. However, due to the strongly nonlinear and time-varying behaviour of batch distillation columns, the composition control is not merely a task, but a real challenge.

One of the first steps towards control is developing a mathematical model of the process of interest. The model should predict how the system will behave in response to inputs and disturbances and may be used as a tool in control system analysis and design. When the process contains time delays due to transportation lags or measurement delays, the controller requires future values of the process state variables. In such cases, the control law cannot be implemented unless a model is employed to estimate the future state of the system.

The main advantage of batch distillation is its flexibility in purifying many kinds of products with different specifications. An increasing variety of products have been manufactured in batch plants and the deadline requirements have also become shorter. With frequent process changes, it is impractical to use rigorous models for control tasks because a rigorous dynamic model for batch distillation consists of a large number of nonlinear differential equations and demands much information about the system (compositions, vapour and liquid flow-rates, liquid hold-ups, in all stages every instant, tray hydraulics, energy balances, liquid-vapour equilibrium data). So, it is necessary to develop models which capture the essential elements of the dynamics.

In the classical control theory, the system is characterised by transfer functions using Laplace transformation. In the late 1950s and early 1960s, a time-domain approach using state variable system

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models began to emerge. This approach is commonly referred to as “modern” control theory.

The state-space methods are based on the description of the system by a set of coupled, first-order differential equations. One of the major advantages of the state-space approach is that it is very suitable to implementation by digital computers. Furthermore, it naturally and automatically handles the coordination of many variables and the time delay, which is relevant in many systems, can be modelled by introducing a delay element in the input vector.

A common approach in the state-space description of nonlinear systems is to linearize the model at an operating point. In the algorithm presented by Quintero-Marmol *et al.* (1991) to design an observer to predict compositions from temperature measurements in multicomponent batch distillations, the authors used a linearized state-space model of the system to calculate the open-loop eigenvalues. Average values of compositions were used in the linear model.

Sorensen and Skogestad (1996) developed a dynamic model of a combined batch reactor/distillation process and, based on a linearized version of the model, the controllability of the process depending on different reactor conditions and different times during a batch has been analysed. They concluded that the responses of the system changed considerably with the operating point.

In both works, the linearized models were used off-line as a tool for the design of an observer and for controllability analysis, respectively.

For continuous processes, only the operating point corresponding to the steady-state condition is normally considered. In the case of batch distillation, the system follows a trajectory along a wide range of operating conditions. Therefore, the linearized model must be time-varying.

In this work, for on-line control applications, a linear time-varying state-space model for batch distillation columns was developed and tested. The Taylor expansion was applied to linearize the system at the current operating point. The model was developed to be suitable for on-line implementation and to predict the system behaviour from measurable and easily available information.

Considering a 10s sampling period and using a rigorous simulator to represent a batch distillation column, the state-space model was tested with the ethanol/1-propanol and with the ethanol/water systems. Comparing the model predictions with the rigorous simulation results, the state-space model was able to predict the batch distillation column behaviour accurately, even for the nonideal mixture ethanol/water.

2. Nonlinear Model

The assumptions made in the model of the batch distillation system are as follows:

- binary separation
- equimolal overflow ($L_j = L$, $0 \leq j \leq NP$; $V_j = V$, $1 \leq j \leq NP+1$)
- constant relative volatility. Therefore:

$$y_j = \frac{\alpha x_j}{1 + (\alpha - 1)x_j} \quad (1)$$

$$\frac{dy_j}{dx_j} = K v_j = \frac{\alpha}{[1 + (\alpha - 1)x_j]^2} \quad (2)$$

- theoretical stages
- negligible vapour hold-up

- constant liquid hold-up (S_j , $1 \leq j \leq NP$)
- constant pressure
- negligible reflux drum hold-up and total condenser:

$$x_o = y_1 \quad (3)$$

$$\dot{x}_o = \dot{y}_1 = \frac{dy_1}{dx_1} \dot{x}_1 = K_{v1} \dot{x}_1 \quad (4)$$

If the state variables are the liquid composition of the light component in every stage (still, trays and condenser), the state vector is given by:

$$\mathbf{x} = \begin{bmatrix} x_o \\ x_1 \\ \vdots \\ x_j \\ \vdots \\ x_{NP+1} \end{bmatrix} \quad (5)$$

And the input vector:

$$\mathbf{u} = \begin{bmatrix} L \\ V \end{bmatrix} \quad (6)$$

Then, under the above assumptions, the nonlinear model of the batch distillation column in the state-space representation is:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}) \quad (7)$$

$$\begin{bmatrix} \dot{x}_o \\ \dot{x}_1 \\ \vdots \\ \dot{x}_j \\ \vdots \\ \dot{x}_{NP+1} \end{bmatrix} = \begin{bmatrix} f_o(\mathbf{x}, \mathbf{u}) \\ f_1(\mathbf{x}, \mathbf{u}) \\ \vdots \\ f_j(\mathbf{x}, \mathbf{u}) \\ \vdots \\ f_{NP+1}(\mathbf{x}, \mathbf{u}) \end{bmatrix} = \begin{bmatrix} K_{v1}(Lx_o - Lx_1 + Vy_2 - Vy_1)/S_1 \\ (Lx_o - Lx_1 + Vy_2 - Vy_1)/S_1 \\ \vdots \\ (Lx_{j-1} - Lx_j + Vy_{j+1} - Vy_j)/S_j \\ \vdots \\ (Lx_{NP} - Lx_{NP+1} + Vx_{NP+1} - Vy_{NP+1})/S_{NP+1} \end{bmatrix} \quad (8)$$

3. Linearized Model

Linearization methods are often applied to nonlinear systems and are the mathematical formalization of the intuition that a nonlinear system should behave similarly to its linearized approximation for small changes. From the Lyapunov's Theory, it is possible to show that stable design by linear control guarantees the stability of the original physical system locally, what justify the use of linear control techniques in practice.

A point $(\mathbf{x}_e, \mathbf{u}_e)$ is an equilibrium point if:

$$\mathbf{f}(\mathbf{x}_e, \mathbf{u}_e) = \mathbf{0} \quad (9)$$

For the nonlinear systems represented by (7), the Taylor expansion at the equilibrium point $(\mathbf{x}_e, \mathbf{u}_e)$ is:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}_e, \mathbf{u}_e) + \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right)_{\mathbf{x}_e, \mathbf{u}_e} (\mathbf{x} - \mathbf{x}_e) + \left(\frac{\partial \mathbf{f}}{\partial \mathbf{u}} \right)_{\mathbf{x}_e, \mathbf{u}_e} (\mathbf{u} - \mathbf{u}_e) + \mathbf{f}_{h.o.t}(\mathbf{x}, \mathbf{u}) \quad (10)$$

where $\mathbf{f}_{h.o.t}$ stands for higher-order-terms in \mathbf{x} and \mathbf{u} . Considering (9) and neglecting any term of order higher than 1, the linearization (or linear approximation) of the nonlinear system (7) at the equilibrium point is given by:

$$\dot{\mathbf{x}} \cong \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right)_{\mathbf{x}_e, \mathbf{u}_e} (\mathbf{x} - \mathbf{x}_e) + \left(\frac{\partial \mathbf{f}}{\partial \mathbf{u}} \right)_{\mathbf{x}_e, \mathbf{u}_e} (\mathbf{u} - \mathbf{u}_e) \quad (11)$$

If the point $(\mathbf{0}, \mathbf{0})$ belongs to the neighbourhood of $(\mathbf{x}_e, \mathbf{u}_e)$ where the linear approximation is valid, and if the point $(\mathbf{0}, \mathbf{0})$ is also an equilibrium point, then:

$$\mathbf{0} \cong \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right)_{\mathbf{x}_e, \mathbf{u}_e} (\mathbf{0} - \mathbf{x}_e) + \left(\frac{\partial \mathbf{f}}{\partial \mathbf{u}} \right)_{\mathbf{x}_e, \mathbf{u}_e} (\mathbf{0} - \mathbf{u}_e) \quad (12)$$

From (12): $\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right)_{\mathbf{x}_e, \mathbf{u}_e} \mathbf{x}_e + \left(\frac{\partial \mathbf{f}}{\partial \mathbf{u}} \right)_{\mathbf{x}_e, \mathbf{u}_e} \mathbf{u}_e \cong \mathbf{0} \quad (13)$

Expanding (11) and substituting (13), equation (11) results in:

$$\dot{\mathbf{x}} \cong \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right)_{\mathbf{x}_e, \mathbf{u}_e} \mathbf{x} + \left(\frac{\partial \mathbf{f}}{\partial \mathbf{u}} \right)_{\mathbf{x}_e, \mathbf{u}_e} \mathbf{u} \quad (14)$$

If $\mathbf{A}_e = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right)_{\mathbf{x}_e, \mathbf{u}_e}$ and $\mathbf{B}_e = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{u}} \right)_{\mathbf{x}_e, \mathbf{u}_e}$, then:

$$\dot{\mathbf{x}} \cong \mathbf{A}_e \mathbf{x} + \mathbf{B}_e \mathbf{u} \quad (15)$$

For the batch distillation system, the point $(\mathbf{0}, \mathbf{0})$ is an equilibrium point, i. e., $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{0}, \mathbf{0}) = \mathbf{0}$. If the batch distillation column is assumed to be at steady-state at all times (which is true if the hold-up on the trays and in the reflux drum are negligible), every operating point may be considered an equilibrium point. So, at each sampling period, the \mathbf{A}_e and \mathbf{B}_e matrices are updated from the current data:

$$\mathbf{A}_e = \mathbf{A}_k = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right)_{\mathbf{x}_k, \mathbf{u}_k} \text{ and } \mathbf{B}_e = \mathbf{B}_k = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{u}} \right)_{\mathbf{x}_k, \mathbf{u}_k} \quad (16)$$

And, $\dot{\mathbf{x}}_k = \mathbf{A}_k \mathbf{x}_k + \mathbf{B}_k \mathbf{u}_k \quad (17)$

system	ethanol/ 1-propanol	ethanol/ water
Pressure (mmHg)	760	760
S_o (mol)	50.0	180.0
x_{So}	0.3300	0.1250
P (W)	1250	1250
R	0.5; 3.0	0.8
NP	10	20
I.D. (mm)	40	40
weir length (mm)	12	12
weir height (mm)	7	7
$\alpha_{average}$	2.07	3.95
Estimate of S_j (mol)	0.2	0.2

Table 1. Dimensions and operating conditions of the batch distillation column

t (s)	x_{NP+1} (sim.)	x_{NP+1} (lin. mod.)	rd (%)	x_o (sim.)	x_o (lin. mod.)	rd (%)
20	0.3083	0.3088	-0.2	0.9991	0.9993	-0.02
60	0.3058	0.3059	-0.03	0.9979	0.9983	-0.04
110	0.3019	0.3018	0.03	0.9948	0.9955	-0.1
170	0.2967	0.2965	0.1	0.9899	0.9907	-0.1
200	0.2939	0.2937	0.1	0.9871	0.9880	-0.1
400	0.2743	0.2739	0.1	0.9640	0.9654	-0.1
801	0.2322	0.2317	0.2	0.8799	0.8828	-0.3
1201	0.1900	0.1894	0.3	0.7560	0.7591	-0.4
1602	0.1499	0.1493	0.4	0.6318	0.6349	-0.5
2003	0.1135	0.1128	0.6	0.5070	0.5101	-0.6
2404	0.0819	0.0813	0.7	0.3858	0.3887	-0.8
2805	0.0559	0.0554	0.9	0.2757	0.2783	-0.9
3206	0.0358	0.0354	1.1	0.1834	0.1854	-1.1
3606	0.0212	0.0210	1.3	0.1122	0.1137	-1.4
4007	0.0115	0.0113	1.5	0.0621	0.0631	-1.6
4077	0.0102	0.0100	1.6	0.0553	0.0563	-1.7

Table 2. Ethanol/1-Propanol (R = 3.0)

Future values are then predicted by the Euler method:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \dot{\mathbf{x}}_k T_a \quad (18)$$

The Euler method, which usually works well at high sampling rates, provided good results in this study.

4. Algorithm

In the following algorithm, the linear time-varying model is used to predict the future state of the batch distillation column from the current state. It was developed to be appropriated for on-line implementation and to predict the system behaviour from measurable and easily available information.

- (1) Define T_a , S_o , x_{So} , P, R and α
- (2) Estimate S_j , $1 \leq j \leq NP$ (e.g., by simulation)
- (3) At each sampling period:

(3.1) Obtain $\mathbf{x}_k = (x_o, x_1, \dots, x_j, \dots, x_{NP+1})^T_k$.

The full state may be estimated from temperature measurements using techniques such as observers or Kalman filter.

t (s)	x_{NP+1} (sim.)	x_{NP+1} (lin. mod.)	rd (%)	x_o (sim.)	x_o (lin. mod.)	rd (%)
20	0.3078	0.3078	0.0	0.9982	0.9990	-0.1
60	0.3036	0.3033	0.1	0.9760	0.9877	-1.2
110	0.2981	0.2977	0.1	0.7332	0.8033	-9.6
170	0.2914	0.2910	0.1	0.5551	0.5620	-1.2
200	0.2880	0.2875	0.1	0.5453	0.5477	-0.4
400	0.2644	0.2639	0.2	0.5128	0.5145	-0.3
801	0.2131	0.2123	0.4	0.4377	0.4398	-0.5
1201	0.1563	0.1552	0.7	0.3436	0.3462	-0.8
1602	0.0957	0.0943	1.4	0.2284	0.2315	-1.4
2003	0.0374	0.0360	3.8	0.1000	0.1032	-3.2
2203	0.0137	0.0125	9.2	0.0414	0.0440	-6.4
2233	0.0108	0.0096	11.2	0.0337	0.0362	-7.4

Table 3. Ethanol/1-Propanol (R = 0.5)

(3.2) Obtain $\mathbf{u}_k = (\mathbf{L} \mathbf{V})_k^T$.

From the still composition, estimate the latent heat of vaporisation of the still content and, as the heating power is known, the vapour flow rate is: $V_k = P / \Delta H^{\text{vap}}$. And L_k is given by:

$$L_k = \frac{R_k}{R_k + 1} V_k.$$

(3.3) Obtain S_{NP+1} : $(S_{NP+1})_k = S_o - \sum_{j=1}^{NP} S_j - \sum_{p=1}^k (V - L)_p \tau_a$

(3.4) Calculate \mathbf{A}_k and \mathbf{B}_k

(3.5) Calculate $\dot{\mathbf{x}}_k = \mathbf{A}_k \mathbf{x}_k + \mathbf{B}_k \mathbf{u}_k$

(3.6) Predict the future state of the system: $\mathbf{x}_{k+1} = \mathbf{x}_k + \dot{\mathbf{x}}_k \tau_a$

5. Results and Discussion

In order to simulate the column behaviour, a rigorous batch distillation simulator was used. At each sampling period, \mathbf{x}_k and R_k values were read from the simulator and the future state of the system was then predicted by the linear time-varying state-space model.

The geometric features of the column adopted in the runs (Table 1) were the same as the dimensions of the pilot-scale batch distillation in our laboratory. Based on the work of Oisiovici *et al.* (1998), the sampling period was chosen to be 10 s. It corresponds to 278 times the step size used to integrate the differential equation of the simulator (1×10^{-5} h).

The runs were carried out with the ideal binary mixture ethanol/1-propanol and with the ethanol/water system, which presents nonideal behaviour. For the results presented here, the operating conditions and the values of S_j and α used in the linear model are shown in Table 1.

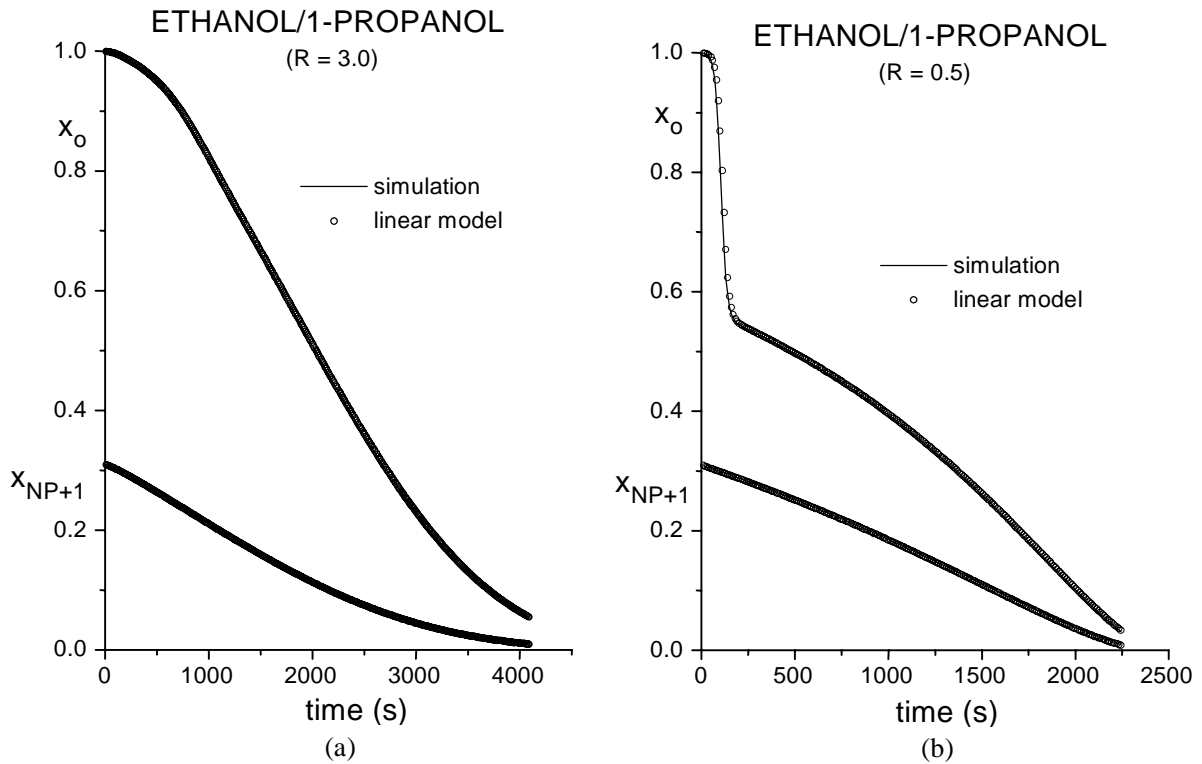


Figure 1. Comparison between the simulation and the linear model predictions for the ethanol/1-propanol system

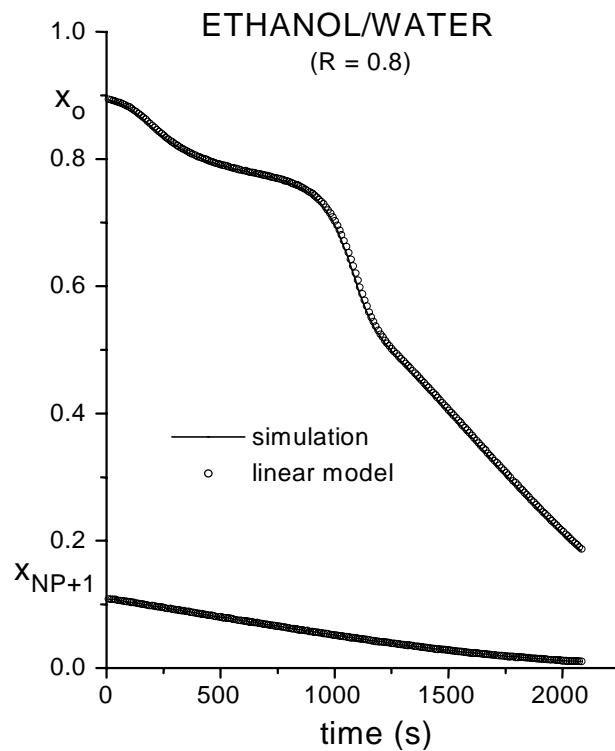


Figure 2. Comparison between the simulation and the linear model predictions for the ethanol/water system

t (s)	x_{NP+1} (sim.)	x_{NP+1} (lin. mod.)	rd (%)	x_o (sim.)	x_o (lin. mod.)	rd (%)
20	0.1080	0.1081	-0.1	0.8919	0.8928	-0.1
60	0.1060	0.1062	-0.1	0.8869	0.8883	-0.2
100	0.1038	0.1038	0.0	0.8793	0.8815	-0.2
200	0.0979	0.0979	0.0	0.8496	0.8529	-0.4
400	0.0860	0.0860	0.0	0.8027	0.8042	-0.2
600	0.0742	0.0743	-0.1	0.7813	0.7821	-0.1
801	0.0627	0.0628	-0.1	0.7625	0.7638	-0.2
1001	0.0516	0.0517	-0.2	0.6956	0.7024	-1.0
1402	0.0319	0.0320	-0.4	0.4404	0.4442	-0.9
1803	0.0170	0.0171	-0.6	0.2832	0.2871	-1.4
2003	0.0117	0.0118	-0.8	0.2103	0.2137	-1.6
2083	0.0100	0.0101	-0.8	0.1839	0.1871	-1.7

Table 4. Ethanol/Water (R = 0.8)

Figures 1 (a) and (b) compare the distillate and still compositions obtained in simulation with the values predicted by the linear state-space model. In Tables 2 and 3, some instantaneous composition values were quantitatively compared.

The linear model provides good estimates of the distillate and still compositions, as it is shown in Figures 1 (a) and (b). However, comparing Tables 2 and 3, those estimates are more accurate for R = 3.0 than for R = 0.5. The smaller the reflux ratio, the greater are the changes in composition with time. Between the sampling instants, the linear model does not get any new information about the system. This fact is more critical when R is small because the compositions change more significantly at each sampling period (as it is shown in Figures 1 (a) and (b), especially at the beginning of the distillate withdrawal).

The results for the ethanol/water system are presented in Figure 2 and Table 3. In this case, the linear time-varying state-space model also provided good estimates of the distillate and still compositions.

6. Conclusions

A linear time-varying state-space model for batch distillation columns has been developed and tested. Some runs were carried out with the system ethanol/1-propanol and ethanol/water. Comparing the model predictions with the rigorous simulation results, the state-space model was able to predict the batch distillation column behaviour accurately.

The results have shown that, for the same sampling period, the predictions are better for higher reflux ratios.

The algorithm of the linear model was developed to be suitable for on-line implementation. The main disadvantage of the linear state-space model is that it demands the knowledge of the full state of the system. This problem may be solved if an observer or the Kalman filter is employed.

The model is simple and its format is appropriated for studying the controllability and observability properties of the system and for the design and implementation of an on-line control law.

7. Nomenclature

A, **B** = Jacobian matrices

ΔH^{vap} = latent heat of vaporisation

L = liquid flow rate, mol/time

NP = number of trays

P = heating power

R = reflux ratio

rd = relative deviation = $\left(\frac{x_{\text{sim.}} - x_{\text{lin. mod.}}}{x_{\text{sim.}}} \right) \times 100$

S = liquid hold-up, mol

S_o = initial charge, mol

Ta = sampling period

t = time

u = input vector

V = vapour flow rate, mol/time

x = state vector

x = liquid composition of the light component, mole fraction

x_{so} = composition of the light component in the initial charge, mole fraction

y = vapour composition of the light component, mole fraction

α = relative volatility

subscripts:

o = condenser

NP+1 = still

j = tray

k = current values

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Appendix. Elements of the A and B matrices

Condenser:

$$\begin{aligned} a_{o0} &= \left(\frac{\partial f_o}{\partial x_o} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \frac{(LKv_1)_k}{S_1} & b_{o1} &= \left(\frac{\partial f_o}{\partial u_1} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \left(\frac{\partial f_o}{\partial L} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \frac{[Kv_1(x_o - x_1)]_k}{S_1} \\ a_{o1} &= \left(\frac{\partial f_o}{\partial x_1} \right)_{\mathbf{x}_k, \mathbf{u}_k} = -\frac{[Kv_1(L + VKv_1)]_k}{S_1} & b_{o2} &= \left(\frac{\partial f_o}{\partial u_2} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \left(\frac{\partial f_o}{\partial V} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \frac{[Kv_1(y_2 - y_1)]_k}{S_1} \\ a_{o2} &= \left(\frac{\partial f_o}{\partial x_2} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \frac{(Kv_1VKv_2)_k}{S_1} \end{aligned}$$

Tray j ($1 \leq j \leq NP$):

$$\begin{aligned} a_{j,j-1} &= \left(\frac{\partial f_j}{\partial x_{j-1}} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \frac{L_k}{S_j} & b_{j1} &= \left(\frac{\partial f_j}{\partial u_1} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \left(\frac{\partial f_j}{\partial L} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \frac{(x_{j-1} - x_j)_k}{S_j} \\ a_{j,j} &= \left(\frac{\partial f_j}{\partial x_j} \right)_{\mathbf{x}_k, \mathbf{u}_k} = -\frac{(L + VKv_j)_k}{S_j} & b_{j2} &= \left(\frac{\partial f_j}{\partial u_2} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \left(\frac{\partial f_j}{\partial V} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \frac{(y_{j+1} - y_j)_k}{S_j} \\ a_{j,j+1} &= \left(\frac{\partial f_j}{\partial x_{j+1}} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \frac{(VKv_{j+1})_k}{S_j} \end{aligned}$$

Still:

$$\begin{aligned} a_{NP+1,NP} &= \left(\frac{\partial f_{NP+1}}{\partial x_{NP}} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \left(\frac{L}{S_{NP+1}} \right)_k \\ a_{NP+1,NP+1} &= \left(\frac{\partial f_{NP+1}}{\partial x_{NP+1}} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \left(\frac{V - L - VKv_{NP+1}}{S_{NP+1}} \right)_k \\ b_{NP+1,1} &= \left(\frac{\partial f_{NP+1}}{\partial u_1} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \left(\frac{\partial f_{NP+1}}{\partial L} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \left(\frac{x_{NP} - x_{NP+1}}{S_{NP+1}} \right)_k \\ b_{NP+1,2} &= \left(\frac{\partial f_{NP+1}}{\partial u_2} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \left(\frac{\partial f_{NP+1}}{\partial V} \right)_{\mathbf{x}_k, \mathbf{u}_k} = \left(\frac{x_{NP+1} - y_{NP+1}}{S_{NP+1}} \right)_k \end{aligned}$$