Solving Index-2 Separation Problems with APMonitor

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Differentiation Index

- Numerous definitions for index of differential-algebraic equation (tractability index, geometric index, kronecker index, strangeness index, etc.)
- Differentiation index of DAE is the number of times that all or part of the system must be differentiated with respect to time in order to reduce the system to its underlying ODE.
- Many chemical engineering problems can be written in the form

$$\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x}) + \boldsymbol{b}(\boldsymbol{x})\boldsymbol{y}$$

$$\boldsymbol{0} = \boldsymbol{g}(\boldsymbol{x})$$

Differentiation Index

- Differentiating the algebraic constraint:

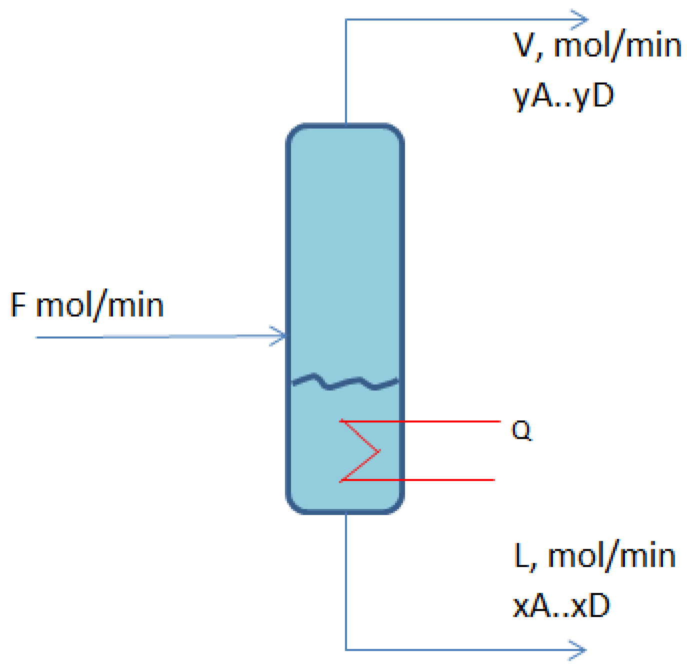
$$\mathbf{0} = \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{x}}(\boldsymbol{f}(\boldsymbol{x}) + \boldsymbol{b}(\boldsymbol{x})\boldsymbol{y})$$

- and a second time

$$\mathbf{0} = \left(\left(\frac{\partial \boldsymbol{g}}{\partial \boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x})\right)_{\boldsymbol{x}} + \left(\frac{\partial \boldsymbol{g}}{\partial \boldsymbol{x}}\boldsymbol{b}(\boldsymbol{x})\right)_{\boldsymbol{x}}\boldsymbol{y}\right)(\boldsymbol{f}(\boldsymbol{x}) + \boldsymbol{b}(\boldsymbol{x})\boldsymbol{y}) + \left(\frac{\partial \boldsymbol{g}}{\partial \boldsymbol{x}}\boldsymbol{b}(\boldsymbol{x})\right)\boldsymbol{y}'$$

- System has differentiation index-2.

Reactive Flash



$$EO + H_2O \overset{r_1}{\rightarrow} EG$$

$$EO + EG \overset{r_2}{\rightarrow} DEG$$

Dynamic representation of P-Q reactive flash

$$\tau \frac{dx_i}{dt} = z_i - x_i - \phi\,(K_i x_i - x_i) - \tau\left(x_i \sum_{j=1}^{r} \nu_{T,j} r_j - \sum_{j=1}^{r} \nu_{i,j} r_j \right),$$

$$i = 1..n-1$$

$$\tau C_p \frac{dT}{dt} = h_{feed} + q - h_{liq} - h_{liq}\tau \sum_{j=1}^{r} \nu_{T,j} r_j + \phi\left(h_{liq} - h_{vap}\right)$$

$$K_n\left(1 - \sum_{i=1}^{n-1} x_i\right) + \sum_{i=1}^{n-1} K_i x_i - 1 = 0$$

$$0 = 1 - l - \phi + \tau \sum_{j=1}^{r} \nu_{T,j} r_j$$

Ethylene Glycol System

$$C_2H_4O + H_2O \xrightarrow{r_1} C_2H_6O_2$$
$$C_2H_4O + C_2H_6O_2 \xrightarrow{r_2} C_4H_{10}O_3$$

$$r_1 = 3.2022\ x\ 10^9 \exp\left(-\frac{9360.845}{T}\right) x_A x_B$$

$$r_2 = 5.84\ x\ 10^9 \exp\left(-\frac{9360.845}{T}\right) x_A x_C$$

Stability of Steady States

Theorem (Maerz): $\boldsymbol{f}(\boldsymbol{x})$ ε C^2 on an open bounded region D, containing a stationary point $\boldsymbol{x}^*$, $\boldsymbol{f}(\boldsymbol{x}^*) = \mathbf{0}$. Let the matrix pencil (λA – B) be regular with index 2 and all its generalized eigenvalues have negative real parts. Additionally, let the DAE be in Hessenberg form of size 2. Then the DAE is Lyapunov stable at this stationary point.

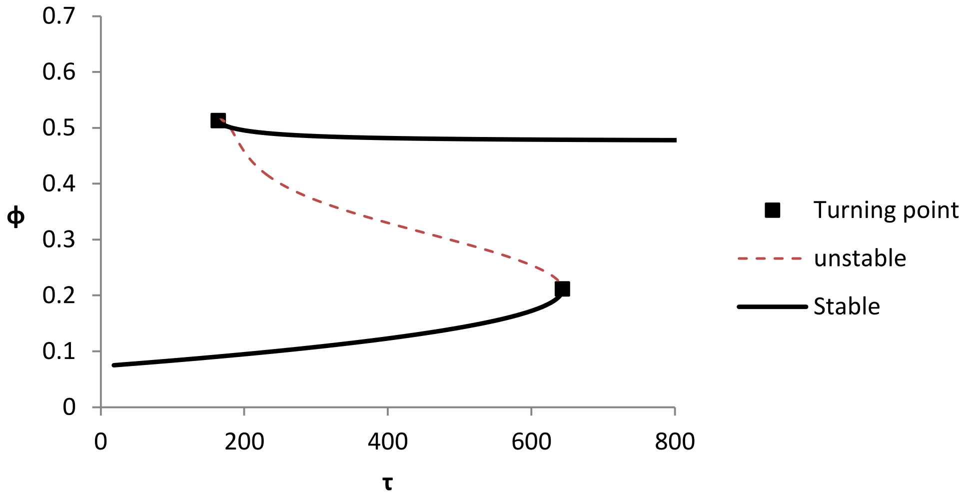
Hessenberg form of size 2:

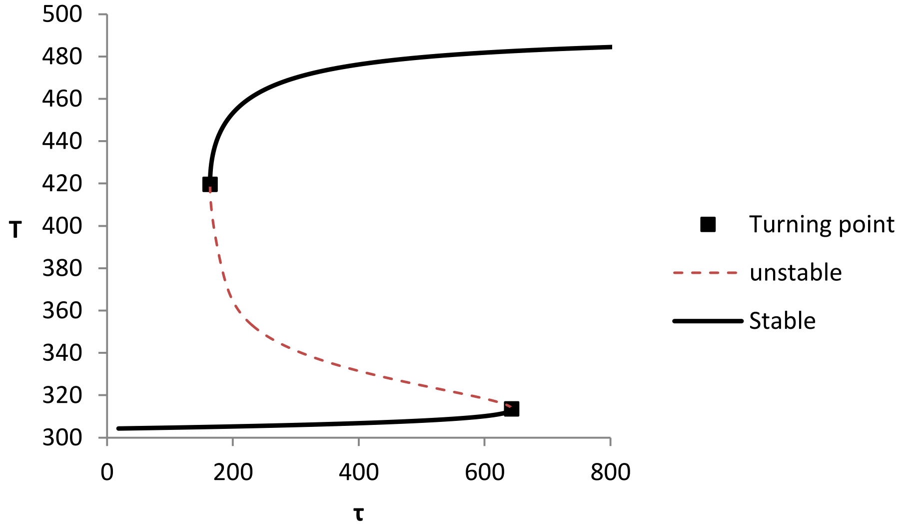
$$\boldsymbol{x}' = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y})$$

$$\mathbf{0} = \boldsymbol{g}(\boldsymbol{x})$$

$(\partial \boldsymbol{g} / \partial \boldsymbol{x})\ (\partial \boldsymbol{f} / \partial \boldsymbol{y})$ non-singular

Steady state solutions

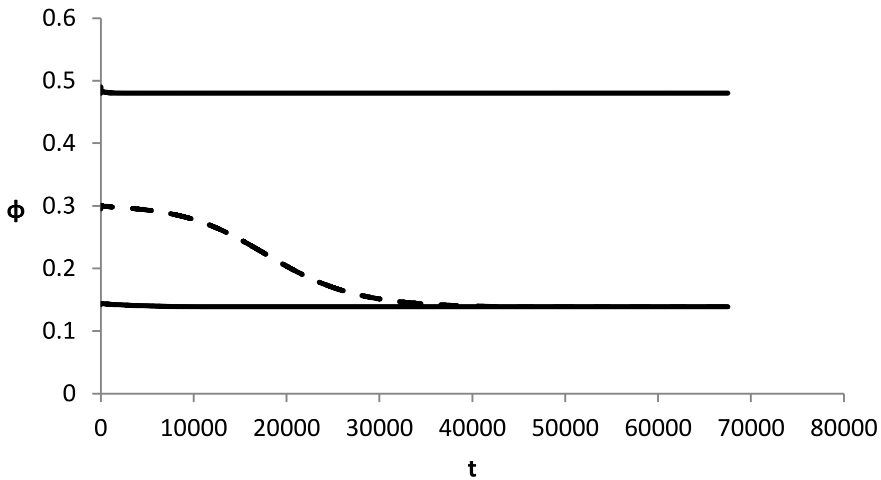


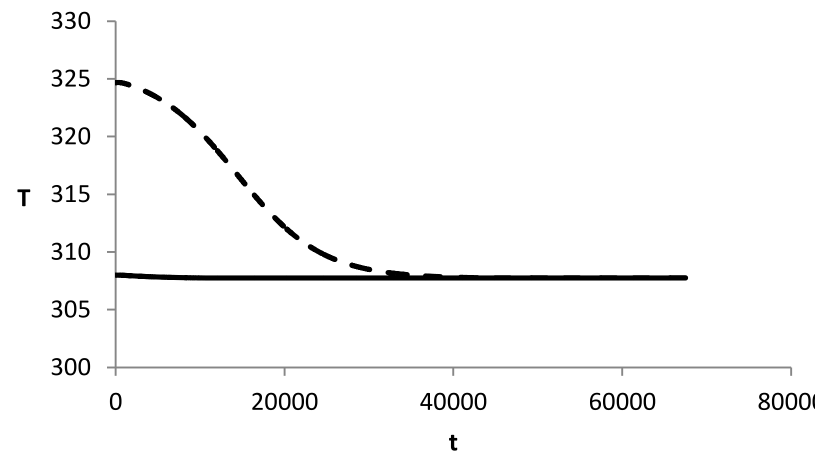


Simulation of perturbation from steady state with APMonitor

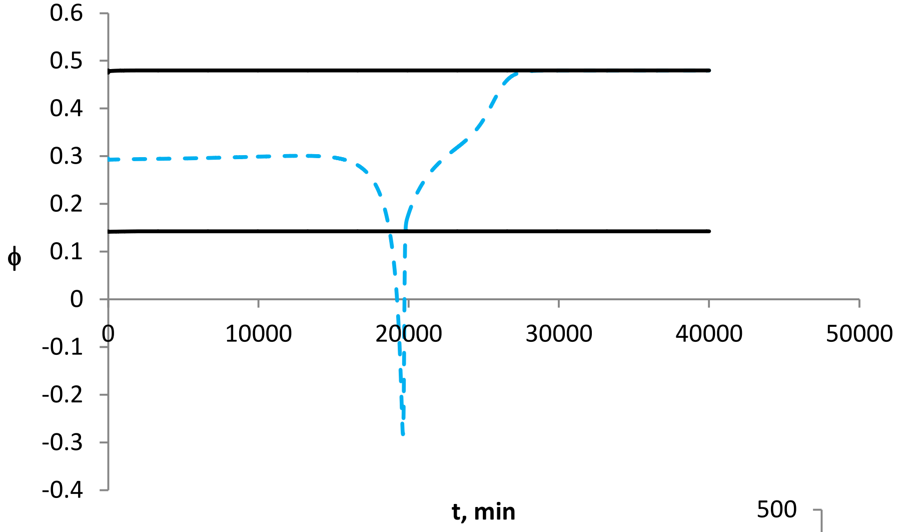
```
% option to read data from a CSV file
apm_option(server,app,'nlc.csv_read',1);

% imode = 4, switch to dynamic simulation
apm_option(server,app,'nlc.imode',4);

% nodes = 3, internal nodes in the collocation structure
apm_option(server,app,'nlc.nodes',3);

% time shift
apm_option(server,app,'nlc.time_shift',400);
```

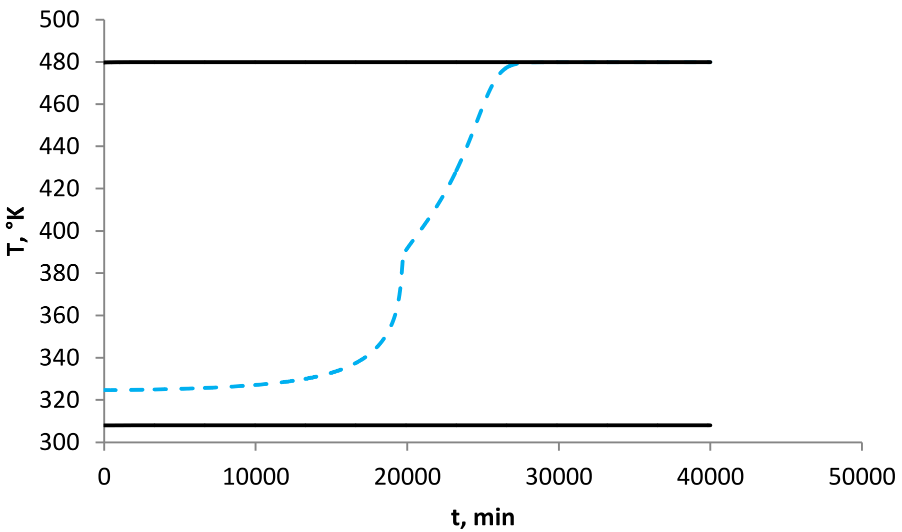
Simulation of perturbation from steady state with APMonitor τ suddenly switched from 500 to 480 by increasing feedrate.



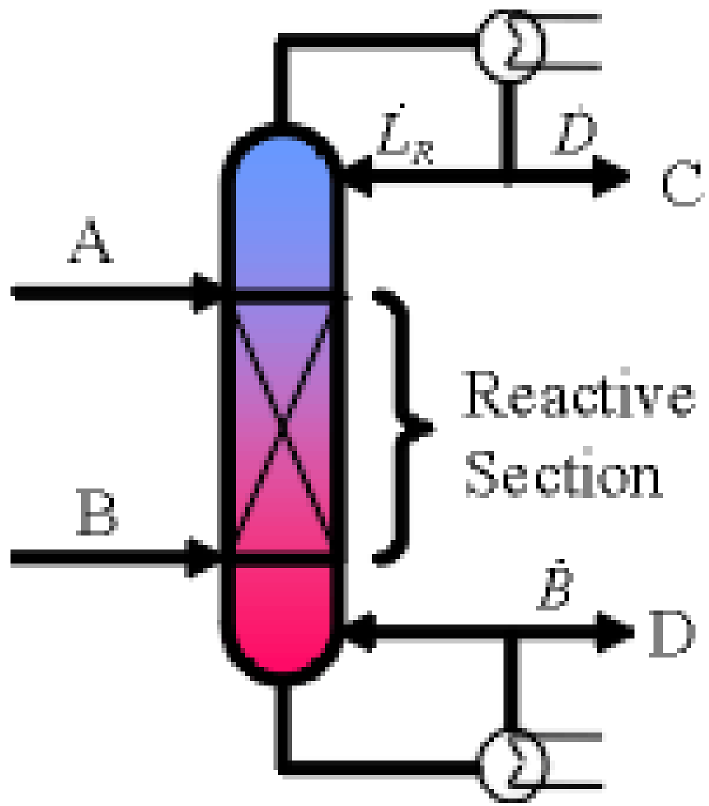


Simulation of perturbation from steady state with APMonitor
τ suddenly switched from 500 to 501 by decreasing feedrate.





Reactive Distillation

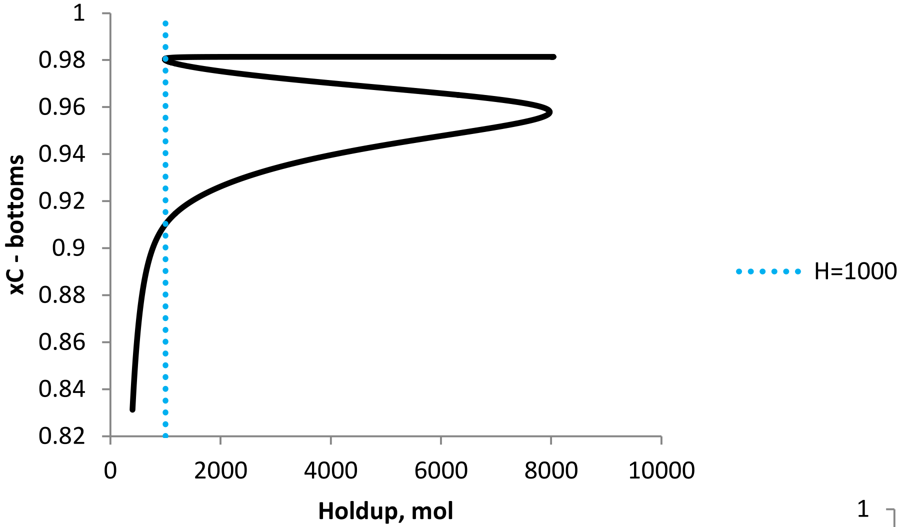


Luyben & Yu
Base Case : A+B → C

	A	B	C
Vapor pressure A_j	12.34	11.65	10.96
Vapor pressure B_j	3862	3862	3862
Heat of formation, kcal/mol	0	0	-10
Heat of vaporization, kcal/mol	6.944	6.944	6.944
Feed rate to column, mol/s	12.63	12.82	0
Feed stage location	10	2	---

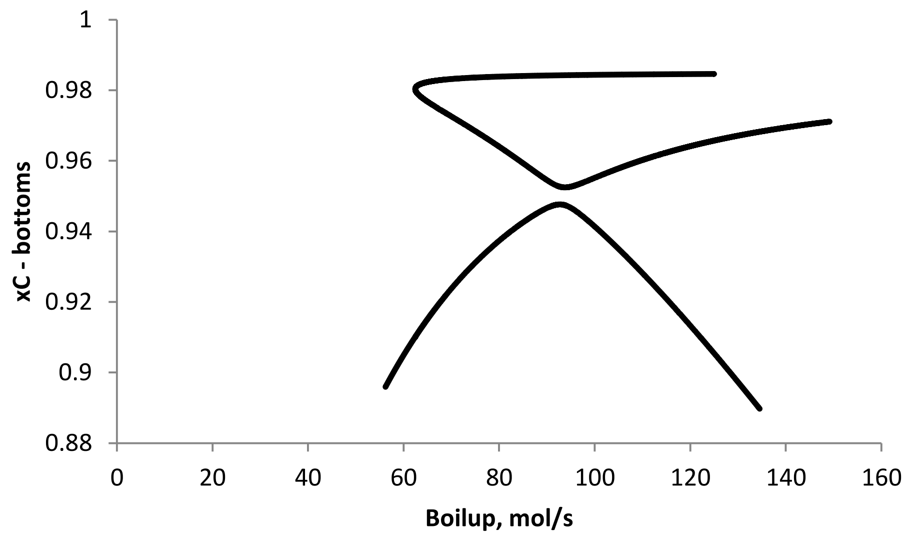
- Infinite reflux ratio (product C is the heavier than reactants)
- Total reboiler with no sub-cooling
- Liquid sensible heat effects neglected
- Feed rate of A and B :12.63 and 12.82 mol/s
- 16 stages with reactive stages (holdup = 1000 mol) from stage 2 to 10.
- Target 98 mole% of component C in bottoms stream

Steady state solutions as function of reactive stage holdup and boilup rate

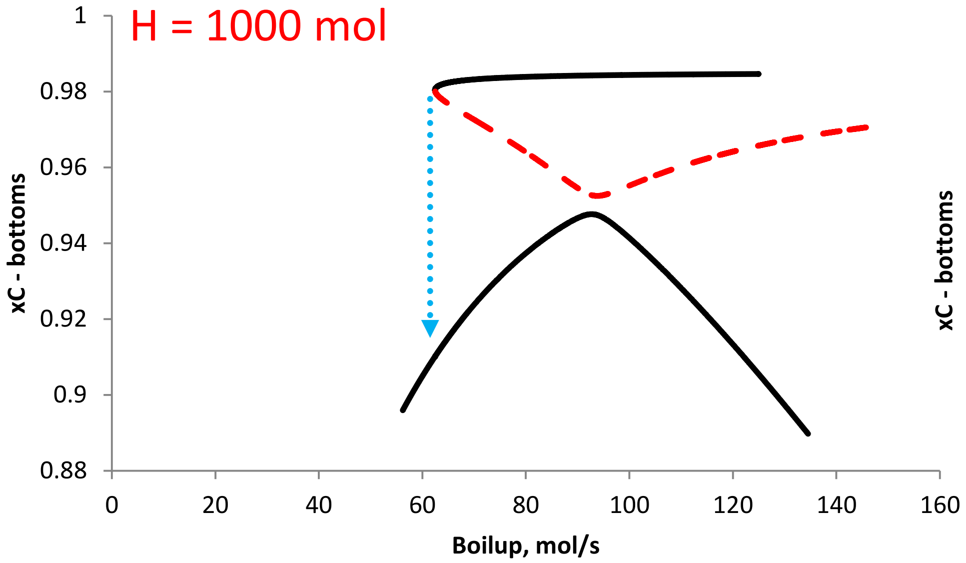


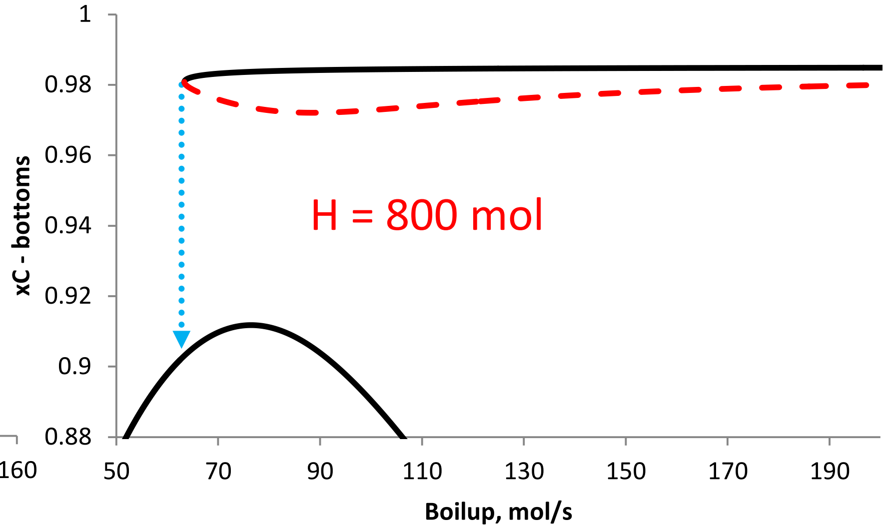
H = 1000 mol

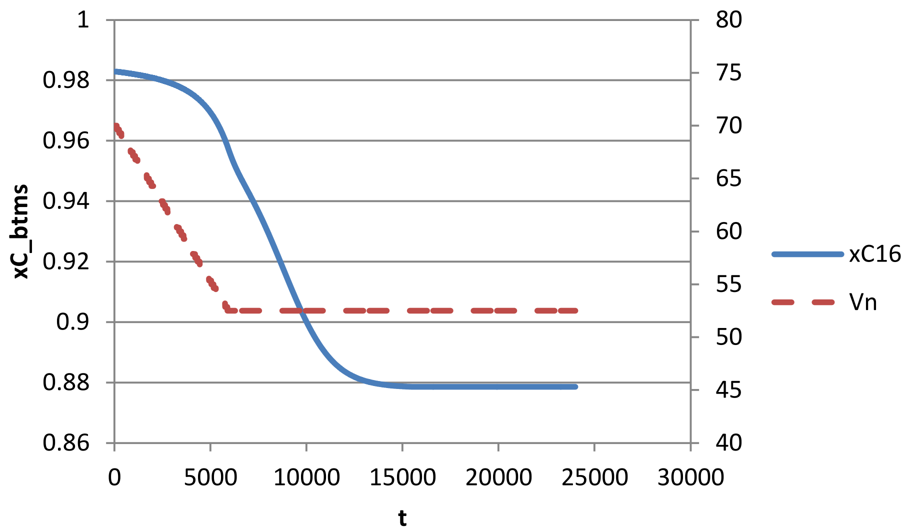
Vn = 62.47 mol/s



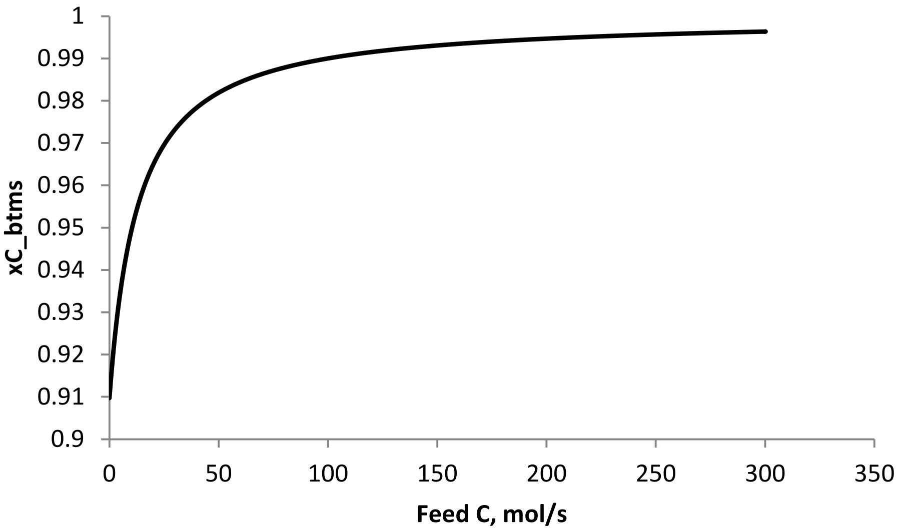
Stability of Reactive Distillation Column Steady States (evaluated directly from index-2 system)

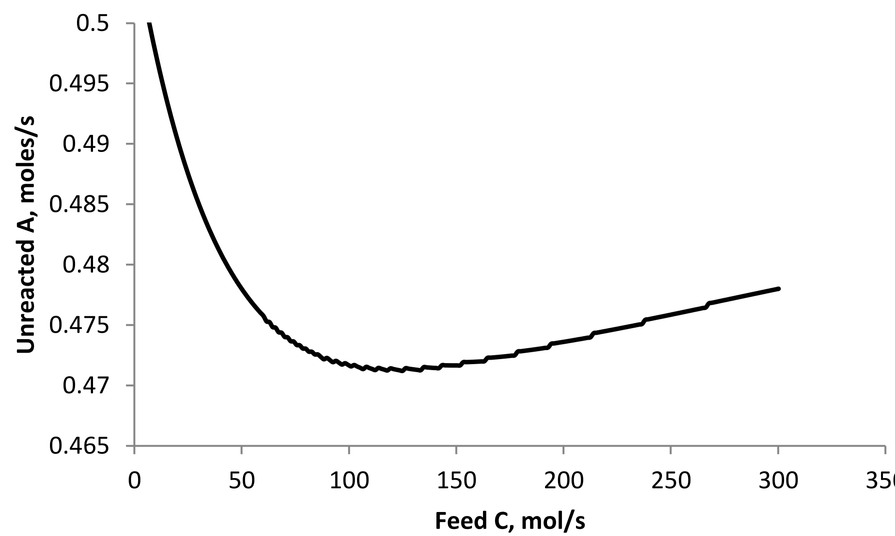




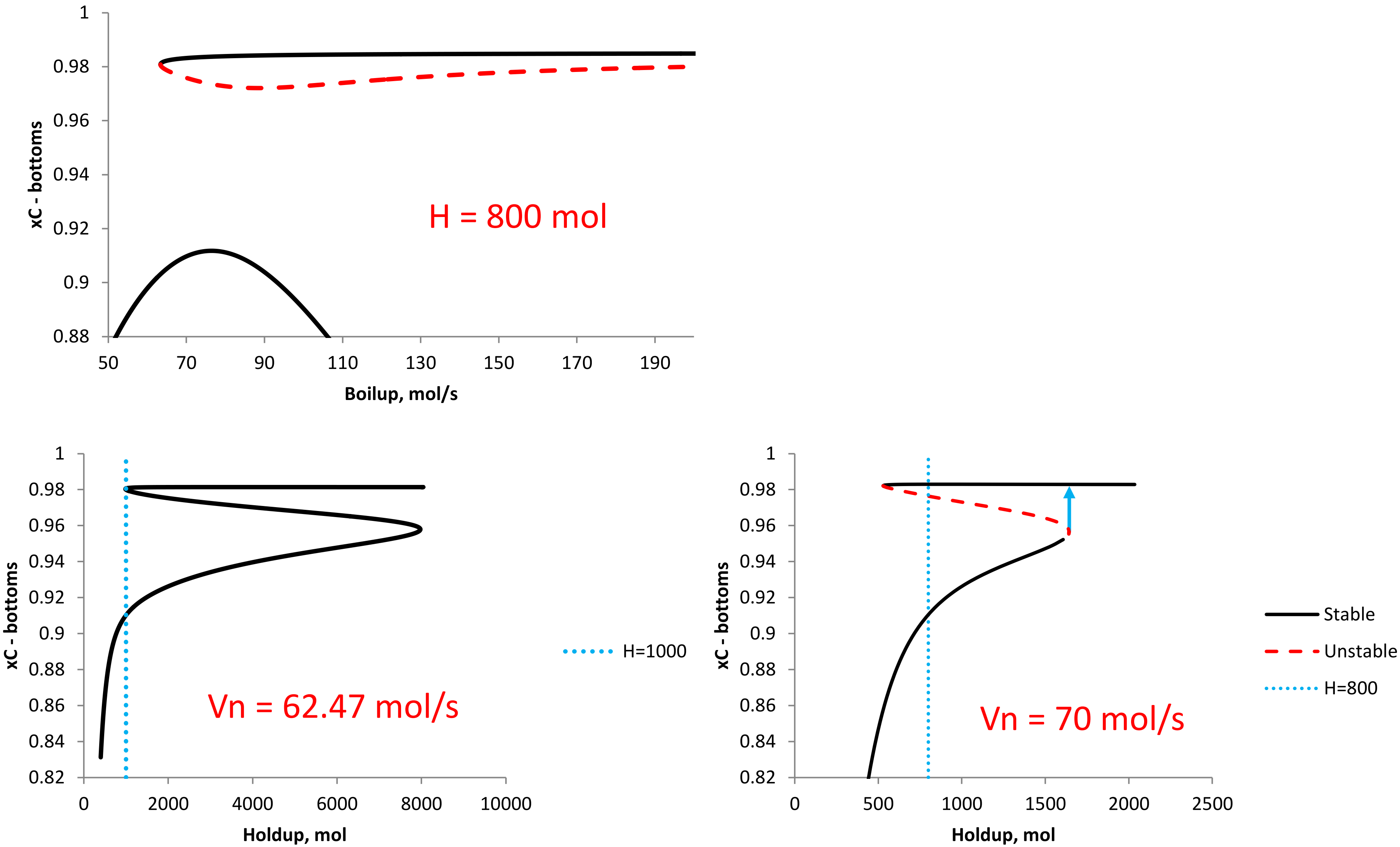


Steady State Transitions (add pure ‘C’ to column bottoms. H = 800 mol, Vn = 70 mol/s)





How to transition from low purity steady state at H=800 mol and Vn = 62.47 mol/s



Dynamic Simulation (using APMonitor)
Constant liquid holdup

$$H_j \frac{dx_{A,j}}{dt} = f_{A,j} - V_j y_{A,j} - L_j x_{A,j} + L_{j-1} x_{A,j-1} + V_{j+1} y_{A,j+1} - H_j r_j, \qquad j = 2..15$$

$$H_j \frac{dx_{B,j}}{dt} = f_{B,j} - V_j y_{B,j} - L_j x_{B,j} + L_{j-1} x_{B,j-1} + V_{j+1} y_{B,j+1} - H_j r_j, \qquad j = 2..15$$

$$H_j C_{p,avg,j} \frac{dT_j}{dt} = f_{T,j} h_{f,j} - h_{l,j} L_j - h_{v,j} V_j + h_{l,j-1} L_{j-1} + h_{v,j+1} V_{j+1}, \qquad j = 2..15$$

$$f_{T,j} - V_j - L_j + \nu_T H_j r_j + L_{j-1} + V_{j+1} = 0, \qquad j = 2..15$$

$$K_{i,j} x_{i,j} - y_{i,j} = 0, \qquad i = A, B, C, \qquad j = 1..16$$

$$\sum_{i=1}^{3} x_{i,j} = \sum_{i=1}^{3} y_{i,j} = 1, \qquad j = 1..16$$

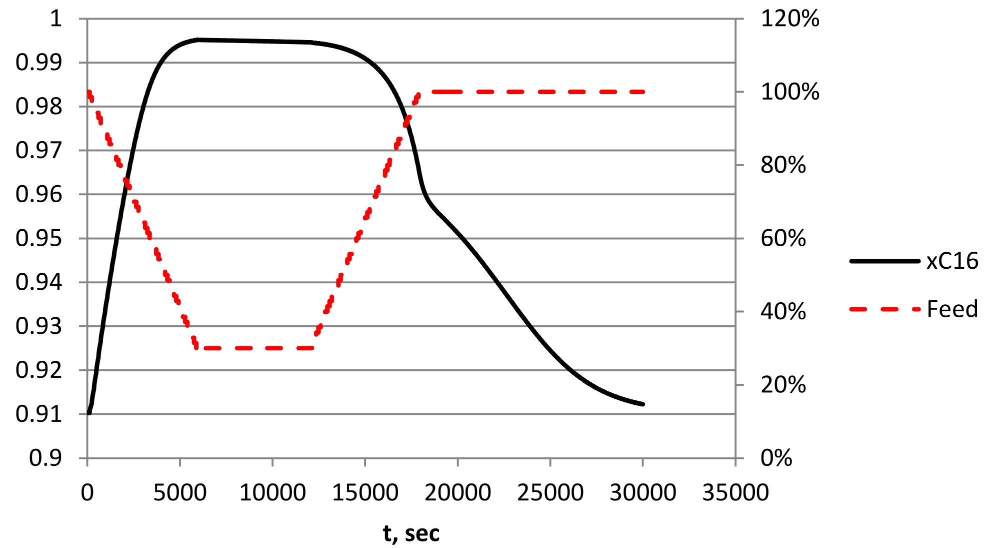
$$-L_1 + V_2 = 0$$

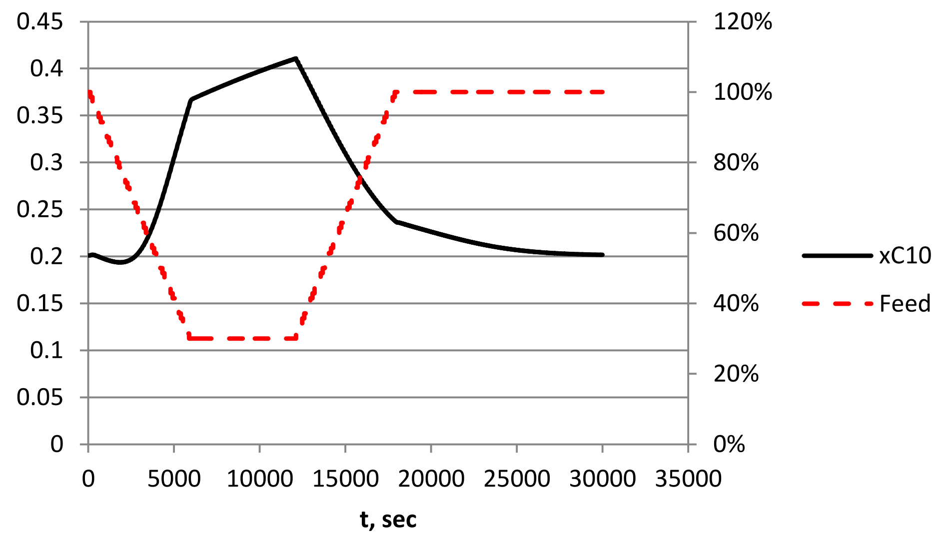
$$-V_{16} - L_{16} + L_{15} = 0$$

$$-L_1 x_{i,1} + V_2 y_{i,2} = 0, \qquad i = A, B$$

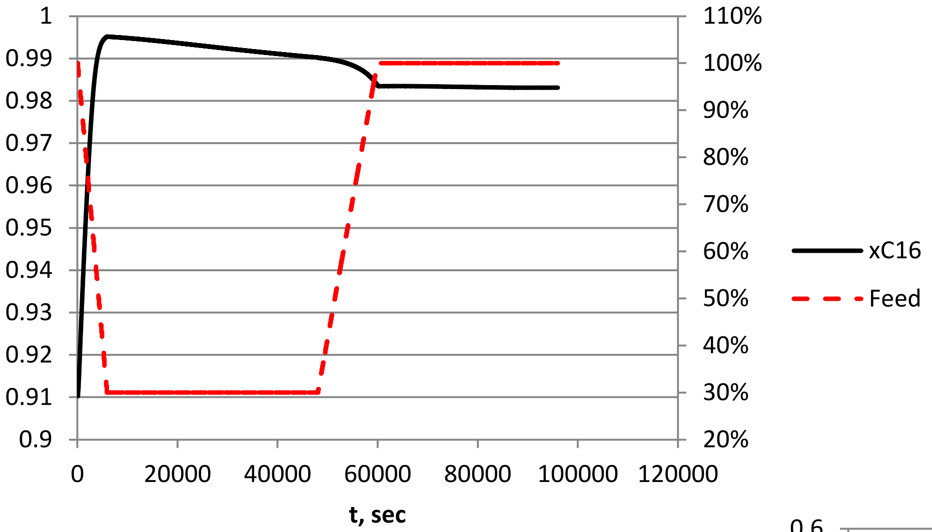
$$-L_{16} x_{i,16} - V_{16} y_{i,16} + L_{15} x_{i,15} = 0, \qquad i = A, B$$

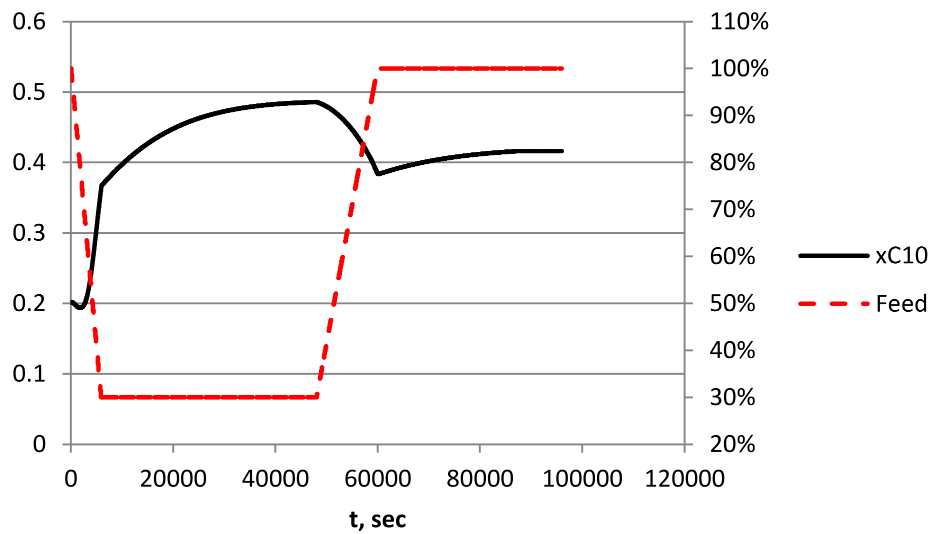
Dynamic Simulation (using APMonitor)
Starting from steady state at H=800 mol, Vn=70 mol/s



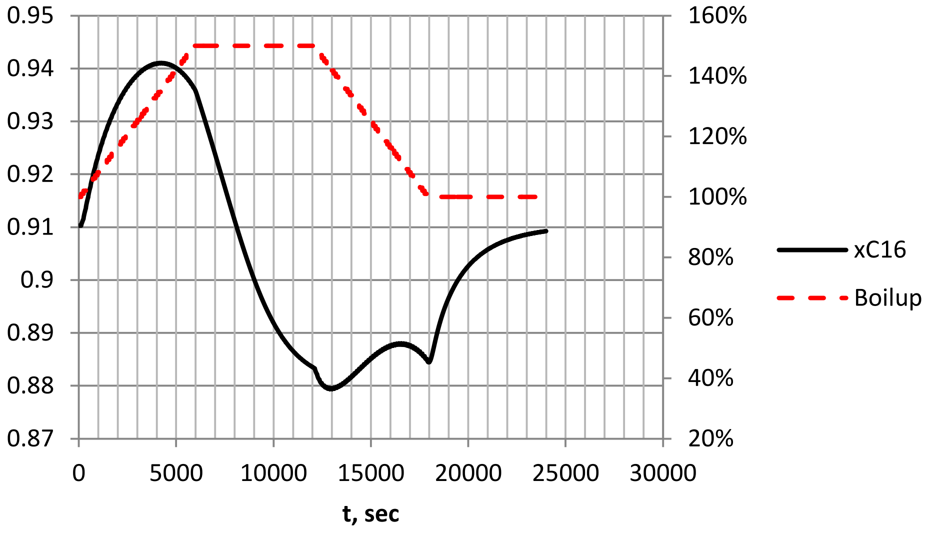


Dynamic Simulation (using APMonitor)
Increase time at low feed rate. Slow down feed ramps.

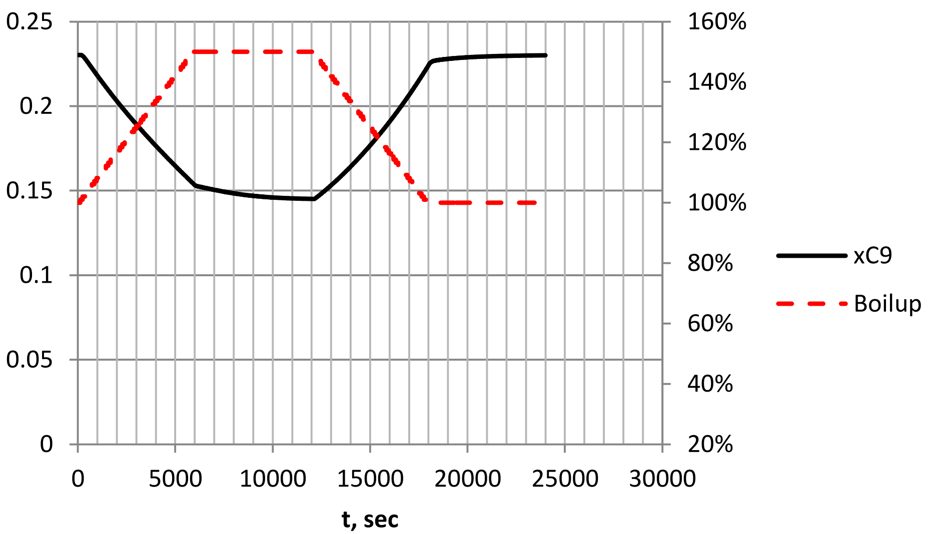




Dynamic Simulation (using APMonitor) – Adjust boilup rate
Steady state transition not possible.



H = 800 mol
100% = 70 mol/s boilup



Dynamic Simulation – Introduce Holdup as dynamic variable

$$\frac{d\left(H_j x_{A,j}\right)}{dt} = f_{A,j} - V_j y_{A,j} - L_j x_{A,j} + L_{j-1} x_{A,j-1} + V_{j+1} y_{A,j+1} - H_j r_j, \qquad j = 2..15$$

$$\frac{d\left(H_j x_{B,j}\right)}{dt} = f_{B,j} - V_j y_{B,j} - L_j x_{B,j} + L_{j-1} x_{B,j-1} + V_{j+1} y_{B,j+1} - H_j r_j, \qquad j = 2..15$$

$$C_{p,avg,j} \frac{d\left(H_j \left(T_j - T_0\right)\right)}{dt} = f_{T,j} h_{f,j} - h_{l,j} L_j - h_{v,j} V_j + h_{l,j-1} L_{j-1} + h_{v,j+1} V_{j+1}, \qquad j = 2..15$$

$$\frac{dH_j}{dt} = f_{T,j} - V_j - L_j + \nu_T H_j r_j + L_{j-1} + V_{j+1}, \qquad j = 2..15$$

$$K_{i,j} x_{i,j} - y_{i,j} = 0, \qquad i = A, B, C, \qquad j = 1..16$$

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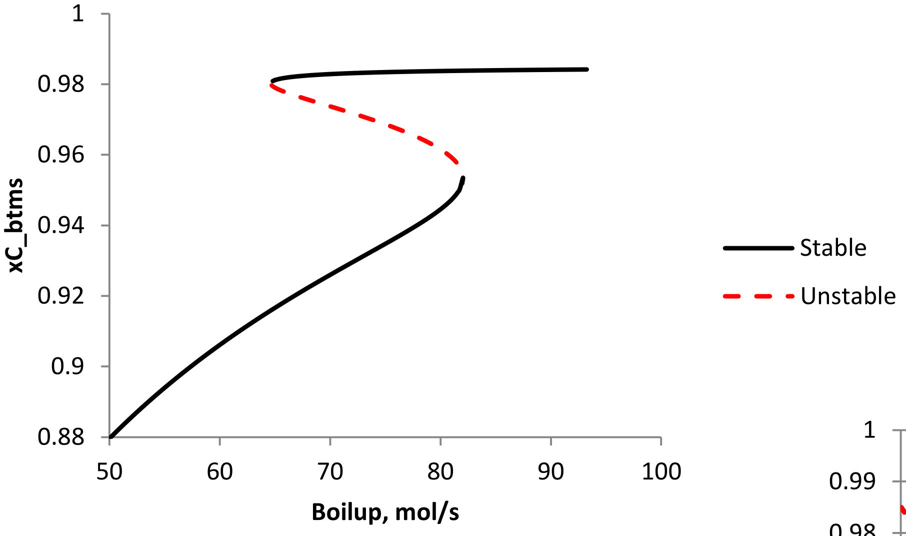
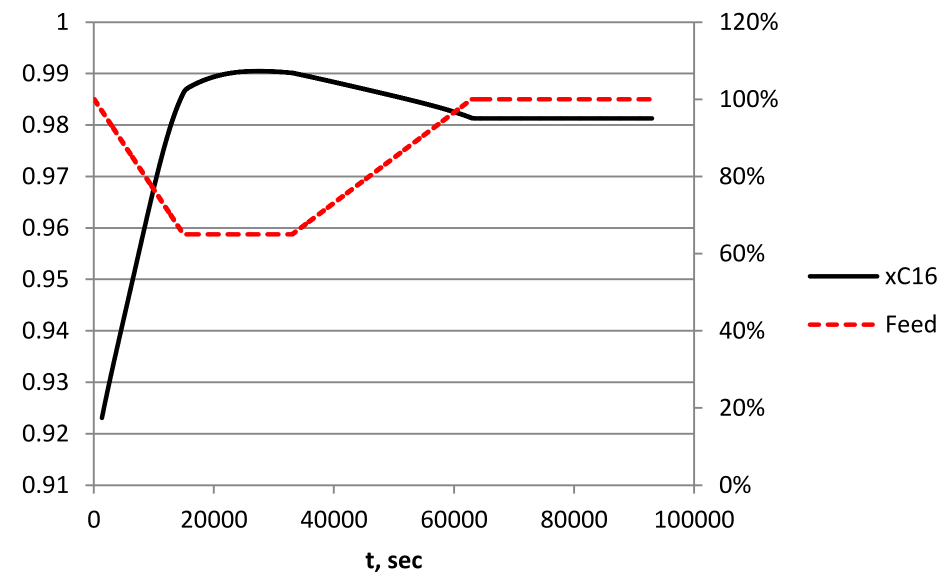
$$-L_{16} x_{i,16} - V_{16} y_{i,16} + L_{15} x_{i,15} = 0, \qquad i = A, B$$

Dynamic Simulation – Introduce Holdup as dynamic variable





Conclusions

- Differential algebraic systems defining reactive flash and reactive distillation systems were in Hessenberg form of size 2.
- Stability of steady states can be calculated at each point on the bifurcation path.
- APMonitor can reliably traverse the orbit of these index-2 DAE IVP.
- Index reductions such as that proposed by Kumar et al. (2009) (*Comput. Chem. Engng*., 33, p. 1336) to solve for intermediate vapor flows not required.
- Theses dynamic simulations are a powerful tool for checking viability of various steady state transitions.