Development of Modelica Library for Batch Distillation

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Agenda

- Introduction to Batch Distillation and Motivation
- Objective and Approach
- Overview of Batch Distillation Library
- Components of Batch Distillation Library in Detail:
  - Batch Rectifier
  - Batch Stripper
  - Multi-Vessel Batch Distillation
  - Slop Recycling using State-Graphs
  - Rigorous Batch Distillation
- Simulation Results and Validation
- Conclusions and Future Work
- Appendix

Introduction and Motivation

- Multi-product industries like fine/ specialty chemicals and pharma industry need to separate a large variety of solvents and in relatively small batch sizes and with stringent product quality requirements. Batch distillation systems are extensively used in these Industries .
- It separates a large variety of solvents.
- Provides flexibility and consistent operations.
- The batch distillation process is characterized by a large number of design and operating parameters to be optimized: the number of trays, the size of the initial charge to the still pot, and the reflux ratio as a function of time (during the product withdrawal periods and during the slop cut periods).
- This requires the development of a versatile modeling and simulation tool to optimize operations for both maximizing throughput and minimizing energy consumption

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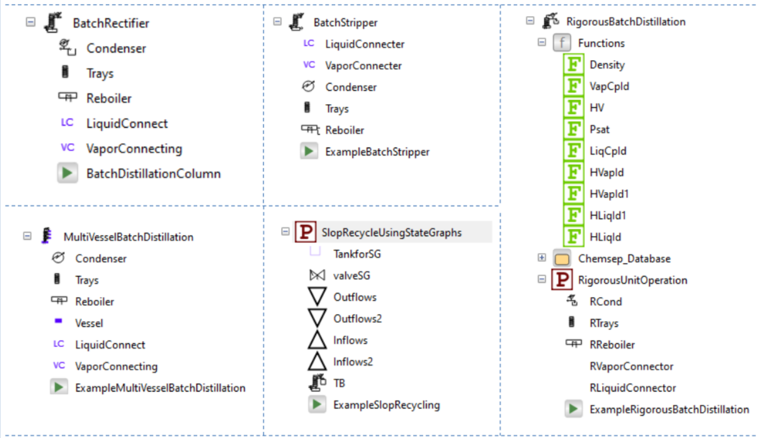
Objective and Approach

- This work primarily focuses on the development of Modelica Library for Batch Distillation.
- To help small sized business to enhance the productivity and also equally important for the academics.
- Object-oriented modeling languages like Modelica are support to the flexibility of developing different batch processes.
- ChemSep database of DWSIM is integrated to the library to enable property prediction and carry out rigorous batch distillation simulation.
- Discrete behavior is simulated using the State-graph package.

- The components present in the batch distillation library are:
  - Batch Rectifier
  - Batch Stripper
  - Multi Vessel Batch Distillation
  - Slop Recycling using State Graphs
  - Rigorous Batch Distillation Operation
- This can be used for binary as well as multi-component systems
- Examples of each operation is provided and validated with similar distillation systems available.

The library consists of the following components:



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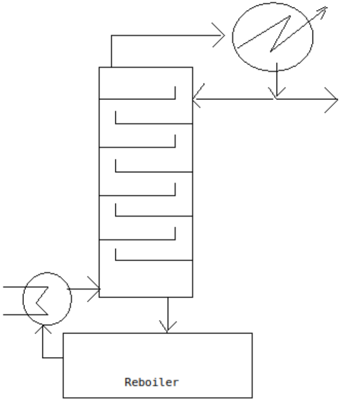
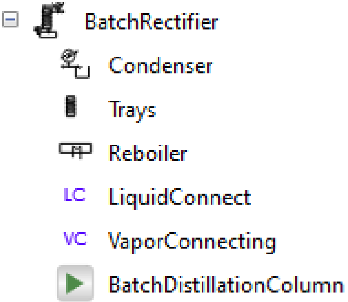
Batch Rectifier

- **Object oriented model of each section of rectifier is developed as shown:**





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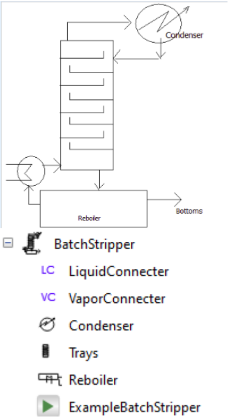
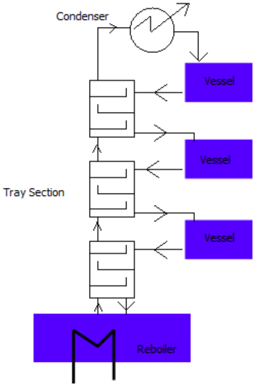
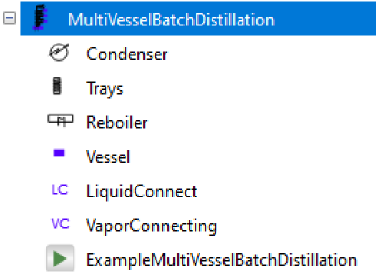
Batch Stripper

- It consists of same parts as that of batch rectifier.
- Feed (Binary/Multicomponent mixture) is charged in the condenser and product stream is taken from the reboiler.
- Batch stripper is used when the feed is low in light component and products are required in high purity.



- **Object oriented model of each section of Multi Vessel Column is developed as shown**

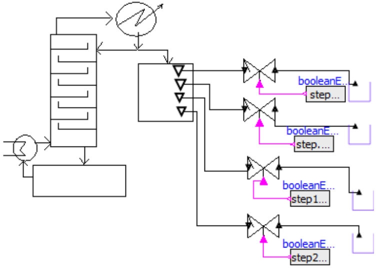


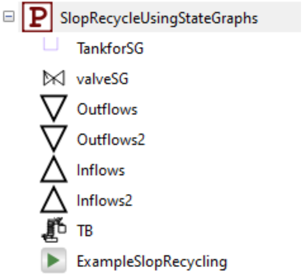


Multi Vessel Contd...

- The multi vessel batch distillation consists of:
  - Condenser
  - Several trays
  - Several intermediate vessel
  - Reboiler
- Strategy for operation used:total reflux
- No products changeovers are required during the operation which makes it simple.
- Possibility of lower energy requirement due to multieffect nature of operation

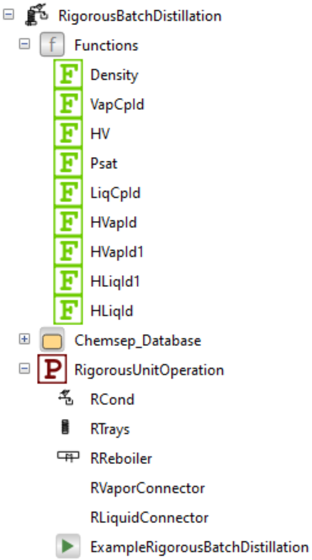
- **Diagram view and components of state graphs are shown:**





Rigorous Batch Distillation

- **Material balance, Energy balance and Thermodynamic functions are required to calculate density, saturation pressure, enthalpy of liquid and vapor, specific heat.**
- **ChemSep database of DWSIM is integrated to the library to enable property prediction.**



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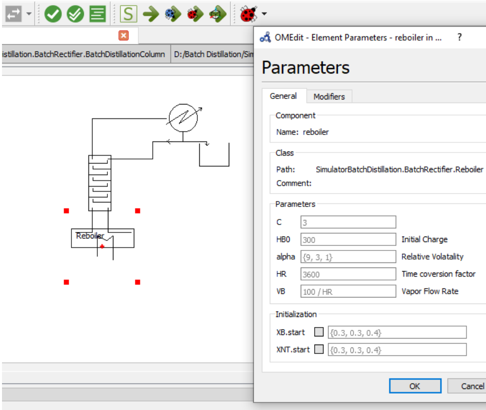
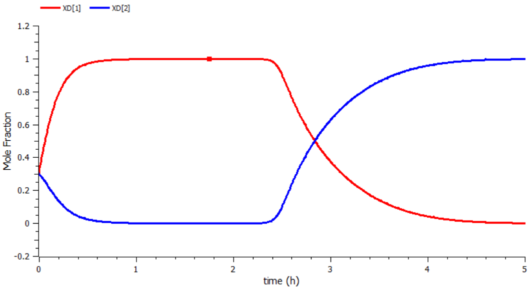
Input Specifications:

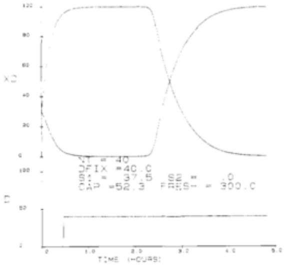
- No of components: 3
- Feed charge: 300 moles
- Initial mole fractions: 0.3,0.3,0.4
- No of trays : 40
- Tray holdup: 1 mole
- Condenser holdup:10 moles
- Vapor flow rate: 100 moles/hr
- Distillate rate: 40 moles/hr



Results and Discussions: Batch Rectifier Contd...



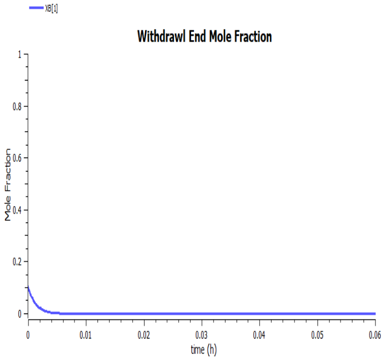
Distillate composition trajectories



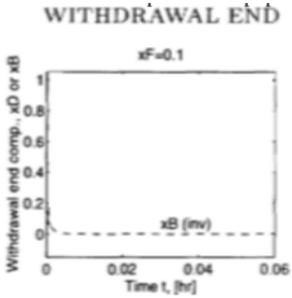
Reference: Luyben, William L. "Multicomponent batch distillation. 1. Ternary systems with slop recycle." *Industrial & engineering chemistry research* 27.4 (1988): 642-647.

Input Specifications:

Initial mole fraction: 0.1, 0,9; No of components: 2; Relative Volatility: 2,1; No of trays: 20; Initial feed: 10 kmol; Vapor flow rate: 10 kmol/hr; Trays holdup: 0.001 kmol; Reboiler holdup: 0.01 kmol



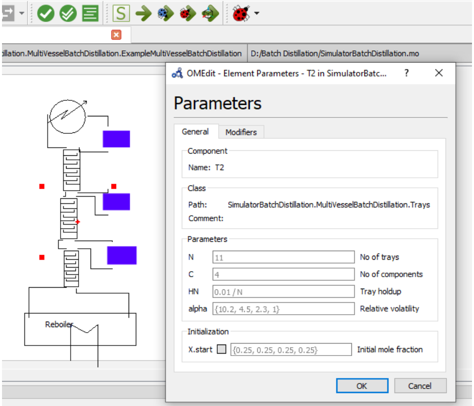
Time response of composition under total reflux



Reference: Sørensen, Eva, and Sigurd Skogestad. "Comparison of regular and inverted batch distillation." Chemical engineering science 22.51 (1996): 4949-4962.

Input Specifications:

- No of sections:3
- No of vessel: 3
- No of components: 4
- No of trays in each section:11
- Reboiler, trays and vessels hold up: 2.5 kmol each
- Vapor and Reflux flow rate: 10 kmol/hr each
- Relative Volatality: 10.2,4.5,2.3,1
- Initial mole fraction: 0.25, 0.25, 0.25, 0.25



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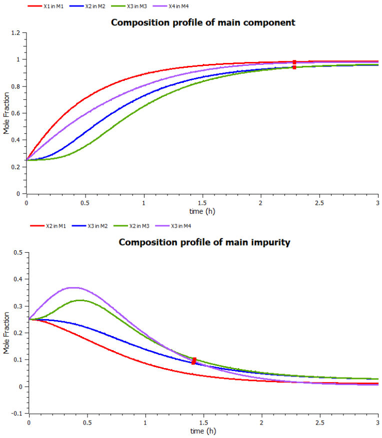
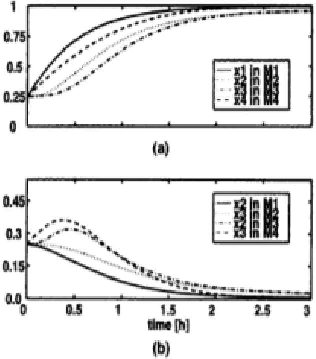
Results and Discussions: Multi Vessel Batch Distillation Contd...

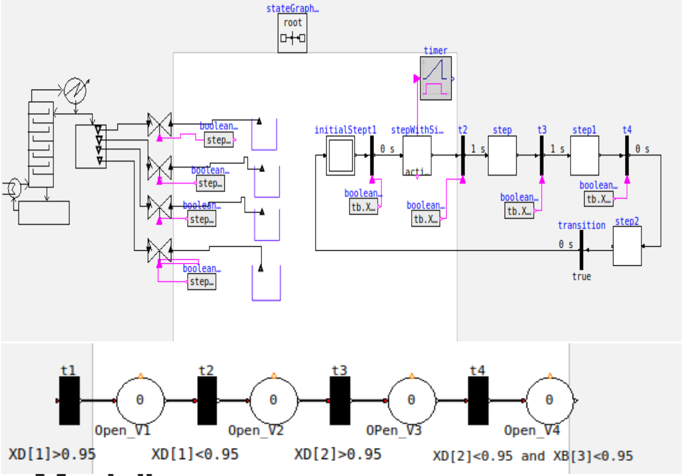




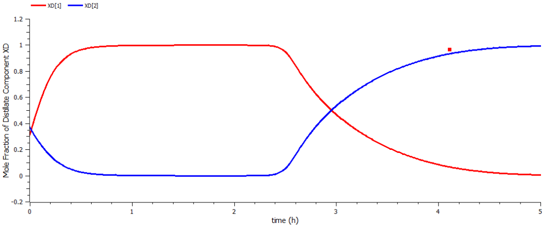
Composition profile:
(a) Main component
(b) Main impurity

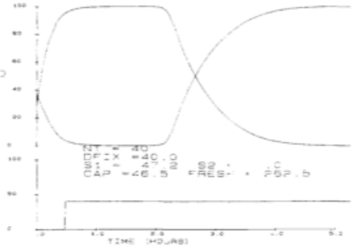
Reference: Skogestad, Sigurd, et al. "Multivessel batch distillation." AIChE Journal 43.4 (1997): 971-978.

- **Diagram view of slop recycling using state graphs.**



Results and Discusions: Slop Control using State Graphs Contd...



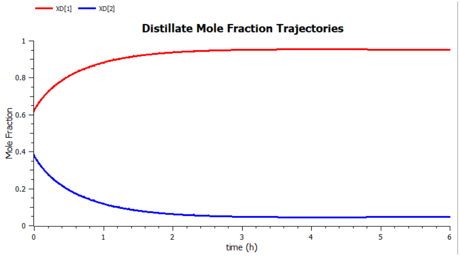


Validation with published paper

Reference: Luyben, William L. "Multicomponent batch distillation. 1. Ternary systems with slop recycle." Industrial & engineering chemistry research 27.4 (1988): 642-647.

Input Specifications:

Binary mixture of Cyclohexane and Toluene; Composition: 0.62,0.38; Operating Pressure: 1 atm; Initial charge: 200 mol; Liquid holdup in each tray and condenser: 2.5 mol; Reboiler heat duty: 3KW; Stage efficiency: 75 %; VLE calculation: Raoult's law; Enthalpy data: calculated by importing DWSIM enthalpy functions in OpenModelica



Conclusions and Future Work

- A general purpose batch distillation simulator in the form of a Modelica library is developed consisting of rectification, stripping, multi vessel column, slop recycle and rigorous batch distillation which is suitable for binary as well multi-component.
- It caters to low volume and high quality products
- The simulation results are in agreement with the already available tools.
- Releasing it as an open source tool will help small scale industries to enhance the productivity. It will be equally important for the academics as well.
- Future work aims towards developing a general purpose batch process simulator which will include various operations of batch process. For example reactive batch distillation, batch reactor etc.

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Thank You...

Appendix: Comparison of Software Packages

Features	CHEMCAD	BATCHFRAC	MultiBatchBS
Databank	CHEMCAD	ASPEN PLUS	CRANIUM
<u>Operations</u>			
Constant Reflux	Yes	Yes	Yes
Variable Reflux	No	Yes	Yes
Optimal Reflux	No	No	Yes
Fixed Equation	No	Yes	Yes
<u>Models</u>			
Shortcut	No	No	Yes
SemiRigorous	Yes	No	Yes
Reduced Order	No	No	Yes
Rigorous	Yes	Yes	Yes

Reference: Diwekar, Urmila. Batch distillation: simulation, optimal design, and control. CRC press, 2011.

Appendix: Comparison of Software Packages Contd...

Features	CHEMCAD	BATCHFRAC	MultiBatchBS
Configurations			
Rectifier	Yes	Yes	Yes
Semi-Batch	No	Yes	Yes
Recycle Waste Cut	No	Yes	Yes
Stripper	No	No	Yes
Middle Vessel	No	No	Yes
Options			
Design Feasibility	No	No	Yes
Optimzation	No	Yes	Yes
Reactive Distillation	No	Yes	Yes
3 Phase Distillation	Yes	Yes	Yes
Uncertainity Analysis	No	No	Yes

Reference: Diwekar, Urmila. Batch distillation: simulation, optimal design, and control. CRC press, 2011.

Appendix: Model for Batch Rectifier

Still Pot

$$\frac{dH_{Bj}}{dt} = -D$$

$$\frac{d[H_B x_{Bj}]}{dt} = Lx_{1j} - Vy_{Bj}$$

$$y_{Bj} = \frac{\alpha_j x_{Bj}}{\sum \alpha_k x_{Bk}}$$

Internal Trays

$$H_n \frac{dx_n}{dt} = L[x_{n+1} - x_{nj}] + V[y_{n-1} - y_{nj}]$$

$$y_{Bj} = \frac{\alpha_j x_{Bj}}{\sum_{k=1}^{3} \alpha_k x_{Bk}}$$

Bottom Trays

$$H_N \frac{dx_N}{dt} = L[x_{N+1} - x_{Nj}] + V[y_{N-1,j} - y_{N,j}]$$

$$y_{Nj} = \frac{\alpha_j x_{Nj}}{\sum_{k=1}^{3} \alpha_k x_{Nk}}$$

Reflux Drum

$$H_D \frac{dx_D}{dt} = Vy_{Nj} - [L + D]x_{Dj}$$

$$L = V - D$$

Reboiler

$$0 = L_N - V_B - B$$
$$\frac{d[H_B x_{Bj}]}{dt} = L_N X_N - V_{y_B} - Bx_B$$
$$R_B = \frac{V_B}{L_N}$$

Trays

$$0 = L_{j-1} + V_{j+1} - L_j - V_j$$
$$H_j \frac{dx_j}{dt} = L_{j-1}x_{j-1} + V_{j+1}y_{j+1} - L_j x_j - V_j y_j$$
$$V_j = V_{j+1}$$

Condenser

$$\frac{dH_c}{dt} = V_1 - L$$
$$\frac{dH_c x_D}{dt} = V_1 y_1 - Lx_D$$

Equilibrium

$$y_j = \frac{\alpha_j x_j}{\sum_{j=1}^{n} \alpha_j x_j}$$

Reboiler

$$\frac{dH_N}{dt} = L_{N-1} - V_N$$

$$\frac{dx_{N,i}}{dt} = L_{N-1}(x_{N-1,i} - x_{N,i}) - V_N(y_{N,i} - x_{N,i})$$

$$0 = L_{N-1}h^L_{N-1} - V_N h^V_N + Q_R$$

$$y_{j,i} = K_{j,i}x_{j,i}$$

$$\sum y_{j,i} = 1$$

$$K_{j,i} = K_{j,i}(y_j, x_j, T_j, P)$$

$$h^L_j = h^L_j(x_j, T_j, P)$$

$$h^V_j = h^V_j(y_j, T_j, P)$$

Trays

$$0 = L_{j-1} - V_j - L_j + V_{j+1}$$

$$H_j \frac{dx_{j,i}}{dt} = L_{j-1} x_{j-1,i} - V_{j+1} y_{j+1,i} - L_j x_{j,i} - V_j y_{j,i}$$

$$0 = L_{j-1} h^L_{j-1} - V_j h^V_j - L_j h^L_j + V_{j+1} h^V_{j+1}$$

$$y_{j,i} = K_{j,i} x_{j,i}$$

$$\sum y_{j,i} = 1$$

$$K_{j,i} = K_{j,i}(y_j, x_j, T_j, P)$$

$$h^L_j = h^L_j(x_j, T_j, P)$$

$$h^V_j = h^V_j(y_j, T_j, P)$$

Appendix: Rigorous Model Continued...

Condenser

$$\frac{dH_N}{dt} = L_{N-1} - V_N$$

$$H_c \frac{dx_{D,i}}{dt} = V_2(y_{2,i} - x_{D,i})$$

$$0 = V_2(h_2^L - h_1^L)Q_c$$

$$L_1 = rV_2$$

$$L_D = V_2(1 - r)$$

$$T_1 = T_1(x_{D,j}, P)$$

$$h_1^L = h_1^L(x_j, T_j, P)$$