Modelica Library for Batch Chemical Processes

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There has been a significant increase in the development and functioning of batch processing plants in the recent years. This is mainly because of new market environment which demands high value and low volume products.

Characteristics of Batch Processes:

- **Feature: Flexible, Low volume high quality products**
- **Applications: multiproduct industries like fine/ specialty chemicals and pharma industry.**
- **Optimzation of design and operating parameters is crucial for Batch processes.**
- **Requires the development of versatile modeling and simulation tool.**

Objective and Approach

- **Objective:**
  - **Development of general purpose simulator for batch processes in the form of a Modelica library.**
  - **This module will help small sized business to enhance the productivity and also equally important for the academics.**
- **Approach:**
  - **Extension of "Batch Distillation Library[1] to enable simulation for rigorous simulation of complex batch systems**
  - **Object-oriented modeling capabilities of OpenModelica is leveraged to build models of batch processes.**
  - **Various functions to calculate properties such as enthalpy, vapor pressure, viscosity and reaction kinetics are developed.**
  - **Thermodynamic Activity coeffient model(NRTL) is developed for vapor-liquid equilibrium calculations.**

[1] Nikhil Sharma, Kannan Moudgalya, and Sunil Shah. "Development of Modelica Library for Batch Distillation". In: *Linköping University*. 2021.

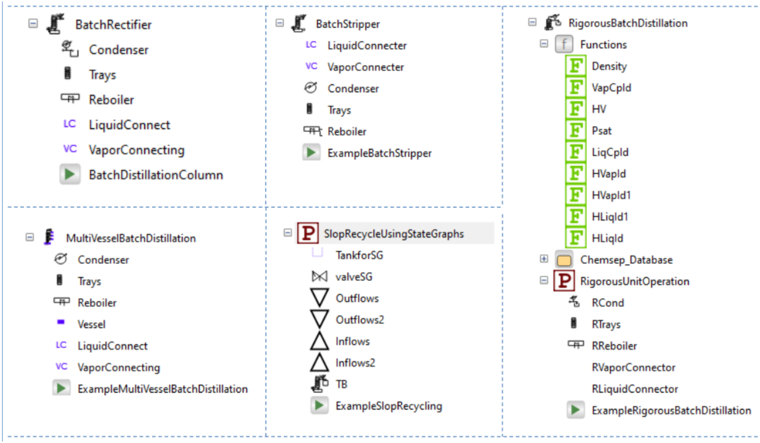
Overview of Batch Process Module

Following operations have been modeled which are also capable of handling multi-component systems:

- Simple Batch Distillation
- Rigorous Batch Distillation
  - Constand Molar Holdup
  - Constant Volume Hold up
- Reactive Batch Distillation
- Batch Reactor

Simple Batch Distillation

- **Batch Distillation Library**[2]**:**



Modelica library for Simple Batch Distillation

[2] Sharma, Moudgalya, and Shah, "Development of Modelica Library for Batch Distillation".

CMH	CVH

CMH

Accumulator Mass Balance:

$$\frac{dH_a}{dt} = D$$

Component Balance:

$$H_a \frac{X_{a,i}}{dt} = D(X_{D,i} - X_{a,i})$$

Condenser Hold Up:

$$H_c \frac{dX_{D,i}}{dt} = V_1(Y_{1,i} - X_{D,i})$$

CVH

Accumulator Mass Balance:

$$\frac{dH_a}{dt} = D$$

Component Balance:

$$\frac{d(H_a X_{a,i})}{dt} = D(X_{D,i} - X_{a,i})$$

Condenser Hold Up:

$$\frac{d(H_c X_{D,i})}{dt} = V_1(Y_{1,i} - X_{D,i})$$

CMH	CVH

CMH

Energy Balance:

$$0 = V_2(h_1^V - h_c^L) - Q_c$$

Related Equations:

$$L_R = R * V_1$$
$$D = V_1 * (1 - R)$$

CVH

Energy Balance:

$$\frac{d(H_c h_c^L)}{dt} = V_2(h_1^V - h_c^L) - Q_c$$

Related Equations:

$$L_R = R * V_1$$
$$D = V_1 * (1 - R)$$
$$H_c = V_c * \rho_c$$
$$\rho_c = \rho_c(X_D, T_c, P)$$

CMH	CVH
Total Mass Balance:	**Total Mass Balance:**
$0 = L_{j-1} + V_{j+1} - L_j - V_j$	$\frac{dH_j}{dt} = L_{j-1} + V_{j+1} - L_j - V_j$
Component Balance:	**Component Balance:**
$H_j \frac{dX_{j,i}}{dt} = L_{j-1}X_{j-1,i} + V_{j+1,i}Y_{j+1,i} - L_jX_{j,i} - V_{j,i}Y_{j,i}$	$\frac{d(H_j * X_{j,i})}{dt} = L_{j-1}X_{j-1,i} + V_{j+1,i} * Y_{j+1,i} - L_jX_{j,i} - V_{j,i} * Y_{j,i}$
Energy Balance:	**Energy Balance:**
$0 = L_{j-1} * h^L_{j-1} + V_{j+1} * h^V_{j+1} - L_j * h^L_j - V_j * h^V_j$	$\frac{d(H_j * h^L_j)}{dt} = L_{j-1} * h^L_{j-1} + V_{j+1} * h^V_{j+1} - L_j * h^L_j - V_j * h^V_j$

CMH	**CVH**
Overall Balance:	**Overall Balance:**
$\frac{dH_B}{dt} = L_N - VB$	$\frac{dH_B}{dt} = L_N - VB$
Component Balance:	**Component Balance:**
$H_B \frac{dX_{B,i}}{dt} = L_N(X_{N,i} - X_{B,i}) - V_B(Y_{B,i} - X_{B,i})$	$\frac{d(H_B X_{B,i})}{dt} = L_N(X_{N,i} - X_{B,i}) - V_B(Y_{B,i} - X_{B,i})$
Energy Balance:	**Energy Balance:**
$0 = L_N * h_N^L - V_B h_B^V + Q_R$	$\frac{d(H_B * h_B^L)}{dt} = L_N * h_N^L - V_B h_B^V + Q_R$

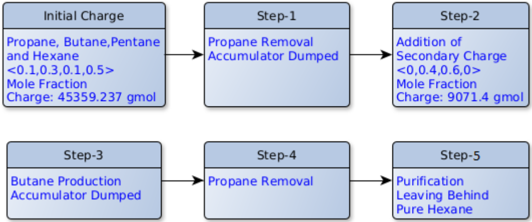
Equilibrium:

$\mathbf{Y}_{j,i} = K_{j,i} X_{j,i}$

Constraint:

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

Rigorous Batch Distillation: Example



No of Stages	**8**
Tray Hold Up,m^3	**2.24**
Condenser Hold Up,m^3	**22.4**
Pressure,Pa	**101325**

Mujtaba, Iqbal M. Batch distillation: Design and operation. Vol. 3. World Scientific Publishing Company, 2004.

Rigorous Batch Distillation: Results

	First						Second					
	CVH Boston	CMH Mujtaba	My CMH	My CVH	% Error CMH	Error in CVH	CVH Boston	CMH Mujtaba	My CMH	My CVH	Error in CMH	Error in CVH
Operation Step	1	1	1	1	-	-	2	2	2	2	-	-
Purpose	C3	C3	C3	C3	-	-	Removal	Removal	Removal	Removal	-	-
Reflux Ratio	5	5	5	5	-	-	20	20	20	20	-	-
Distillate Rate(mol/hr)	1.51	1.51	1.51	1.51	-	-	1.51	1.51	1.51	1.51	-	-
Time(s)	14652	14652	14652	14652	-	-	21168	21168	21168	21168	-	-
Distillate												
Propane	0.8	0.754	0.8	0.79503	0	0.62125	0.015	0.031	0.02014	0.01855	35.0322580645	23.6666666667
Butane	0.2	0.246	0.2	0.2049	0	2.45	0.985	0.969	0.979859	0.981446	1.12063983488	0.36081218274
Pentane	-	-	-	1.00E-07	-	-	-	-	0	1.00E-07	-	-
Hexane	-	-	-	-	-	-	-	-	0	-	-	-
Accumulated												
Propane	0.9888	0.981	0.991273	0.993446	0.2501011327	0.46986246	0.8497	0.85	0.850385	0.850088	0.04529411765	0.04566317524
Butane	0.0112	0.019	0.0081	0.00654	27.678571429	41.60714286	0.1503	0.15	0.149613	0.1499	0.258	0.26613439787
Pentane	-	-	0.000123	2.00E-06	-	-	-	-	8.00E-05	1.00E-06	-	-
Hexane	-	-	0.000528	2.00E-06	-	-	-	-	0.003	1.00E-06	-	-
(mol)	3691.9734	3695.106	3691.49	3691.49	0.0130932688	0.013093269	5339.04	5340.04	5333.16	5333.16	0.12883798623	0.11013215859
Still Pot												
Propane	0.0206	0.021	0.0206	0.020831	0	1.121359223	-	-	0.000106	0.000129	-	-
Butane	0.3254	0.325	0.3256	0.325675	0.061462815	0.084511371	0.3191	0.319	0.319418	0.319609	0.13103448276	0.15951112504
Pentane	0.109	0.109	0.10892	0.108911	0.0733944954	0.081651376	0.1135	0.113	0.113407	0.113375	0.36017699115	0.11013215859
Hexane	0.545	0.545	0.544728	0.544583	0.0499082569	0.076513761	0.5674	0.567	0.567069	0.5669	0.01216931217	0.08812125485
(mol)	41648.598	41704.44	41667.7	41664.1	0.0458646891	0.037220941	40008.296	40060.96	40026.1	40023.3	0.0870173855	0.03750222204

Figure: **Comparison Steps 1 & 2**

Rigorous Batch Distillation: Results

	Third				Fourth				Fifth			
	CVH Boston	CMH Mujtaba	My CMH	My CVH	CVH Boston	CMH Mujtaba	My CMH	My CVH	CVH Boston	CMH Mujtaba	My CMH	My CVH
Operation Step	3	3	3	3	4	4	4	4	5	5	5	5
Purpose	C4 Production	C4 Production	C4 Production	C4 Production	C5	C5	C5	C5	Removal	Removal	Removal	Removal
Reflux Ratio	25	25	25	25	15	15	15	15	25	25	25	25
Distillate Rate(mol/hr)	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51
Time(s)	86940	86940	86940	86940	102456	102456	102456	102456	108864	108864	108864	108864
Distillate												
Propane	-	-	2.00E-07	-	-	-	-	-	-	-	-	-
Butane	0.1644	0.254	0.259918	0.256163	-	-	-	-	-	-	-	-
Pentane	0.8356	0.745	0.739827	0.743583	0.8	0.613	0.6222	0.61978	0.0161	0.091	0.08701	0.085022
Hexane	-	-	0.00025	-	0.2	0.387	0.3777	0.380119	0.9839	0.909	0.912985	0.914978
Accumulated												
Propane	0.0002	-	0.00069	0.0008	-	-	-	0.00091	-	-	9.00E-08	-
Butane	0.99	0.988	0.828234	0.9873	0.0063	0.017	0.176	0.01717	0.0045	0.012	0.012	0.0121
Pentane	0.0098	0.012	0.0315	0.011825	0.9875	0.94	0.9425	0.943	0.7914	0.778	0.77931	0.779077
Hexane	-	-	0.139552	-	0.0061	0.043	0.0399	0.397	0.2041	0.21	0.208214	0.208742
(mol)	16590.522	16592.792	16570.9	16570.9	3910.2566	3913.026	3909.17	3909.17	5523.818	5529.72	5523.63	5523.63
Still Pot												
Propane	-	-	1.00E-10	-	-	-	-	-	-	-	-	-
Butane	0.0006	0.001	0.00192	0.00205	-	-	-	-	-	-	-	-
Pentane	0.1335	0.133	0.1329	0.1334	0.0173	0.023	0.0229	0.02322	0.0002	0.002	0.0018	0.00184
Hexane	0.8658	0.866	0.865168	0.864608	0.9827	0.977	0.977099	0.97678	0.9998	0.998	0.99818	0.99815
(mol)	32506.04	32542.72	32535.2	32532.9	28601.092	28629.694	28626	28625.9	26966.692	25958.52	27011.6	27066.6

Figure: **Comparison Steps 3,4,& 5**

Reactive Batch Distillation: Introduction

- **Characteristic:** Integration of reaction and distillation operation.
- **Advantage:** Shifting of Equilibrium
- **Economic Benefit:** Saving in equipment cost and reduction of heat load
- **Applications:** esterification, etherificatioon, nitration, transesterification, polycondensation, halogenation etc.

Condenser and Accumulator

Accumulator Total Mass Balance:

$$\frac{dH_a}{dt} = D;$$

Component Balance:

$$\frac{H_a * X_{a,i}}{dt} = D * (X_{D,i} - X_{a,i})$$

Condenser Hold Up:

$$\frac{d(H_c * X_{D,i})}{dt} = V_1(Y_{1,i} - L_c X_{D,i} + r_{1,i} H_c)$$

Energy Balance:

$$\frac{H_c h_c^L}{dt} = V_2 h_1^V - L_c h_c^L - Q_c$$

Internal Plates: j = 1:NTrays

Total Mass Balance:

$$\frac{dH_j}{dt} = L_{j-1} + V_{j+1} - L_j - V_j + \Delta n_j H_j$$

Component Balance:

$$\frac{d(H_j * X_{j,i})}{dt} = L_{j-1}X_{j-1,i} + V_{j+1,i} * Y_{j+1,i} - L_j X_{j,i} - V_{j,i} * Y_{j,i} + r_{j,i}H_j$$

Energy Balance:

$$\frac{d(H_j * h_j^L)}{dt} = L_{j-1} * h_{j-1}^L + V_{j+1} * h_{j+1}^V - L_j * h_j^L - V_j * h_j^V$$

Equilibrium:

$$Y_{j,i} = K_{j,i}X_{j,i}$$

Constraint:

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

Reboiler

Overall Balance:

$$\frac{dH_B}{dt} = L_N - VB + \Delta n_B H_B$$

Component Balance:

$$\frac{d(H_B X_{B,i}}{dt} = L_N(X_{N,i} - X - B, i) - V_B(Y_{B,i} - X_{B,i}) + r_B H_B$$

Energy Balance:

$$\frac{d(H_B * h_B^L)}{dt} = L_N * h_N^L - V_B h_B^V + Q_R$$

Equilibrium:

$$Y_{j,i} = K_{j,i} X_{j,i}$$

Constraint:

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

Acetic Acid + Ethanol $\rightleftharpoons$ Ethyl Acetate + Water

No of stages	8
Inital charge	5
Compostion (MoleFraction)	<0.45,0.45,0,0.1>
Condenser Holdup	0.1 kmol
Tray Holdup	0.0125 kmol
Vapor load in condenser	2.5 kmol/hr
Pressure	1.01325 bar

Mujtaba, Iqbal M. Batch distillation: Design and operation. Vol. 3. World Scientific Publishing Company, 2004.

VLE:

$$K_1 = 2.25 * 10^{-2} T - 7.812, T > 347.6K$$

$$K_1 = 0.001 T <= 347.6$$

$$log(K_2) = -2.3 * 10^3 / T + 6.588$$

$$log(K_3) = -2.3 * 10^3 / T + 6.742$$

$$log(K_4) = -2.3 * 10^3 / T + 6.484$$

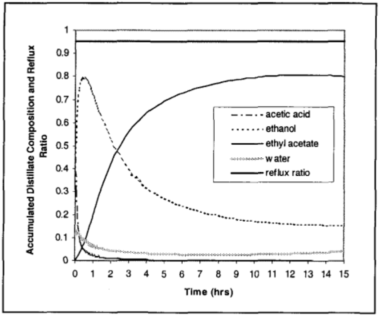
Kinetics:

$$r = k_1 C_1 C_2 - k_2 C_3 C_4$$

$$k_1 = 43.76 * 10^{-4}$$

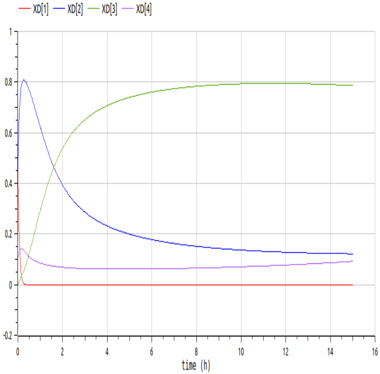
$$k_2 = 1.63 * 10^{-4}$$

Reactive Batch Distillation: Results



Distillate Profile

Mujtaba, Iqbal M. Batch distillation: Design and operation. Vol. 3. World Scientific Publishing Company, 2004.



Distillate Profile using OpenModelica

Batch Reactor

A generalized chemical reaction for batch reactor:

$$aA + bB \rightarrow cC + dD$$

Reaction Rate:

$$r = kC_AC_B$$

$$k = k_0e^{-E_a/RT}$$

Overall Mass Balance:

$$\frac{dV}{dt} = 0$$

Component Balance

$$V\frac{dC_A}{dt} = -V_akC_AC_B$$

Energy Balance

$$\frac{dT}{dt} = \frac{-\Delta H_rkC_AC_B}{\rho C_p} - \frac{Q_M}{V\rho C_p}$$

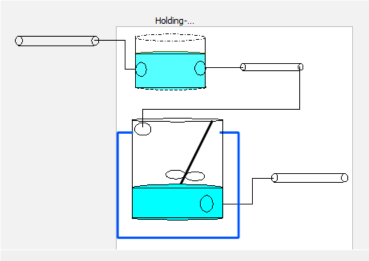


Diagram view of Batch reactor in OpenModelica

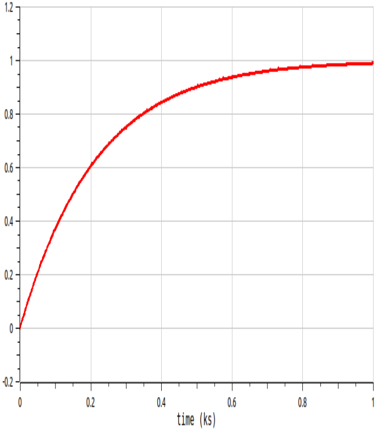
Reaction Involved:

$$(\mathbf{CH_3CO})_2 O + H_2\mathbf{O} \rightarrow 2CH_3\mathbf{COOH}$$

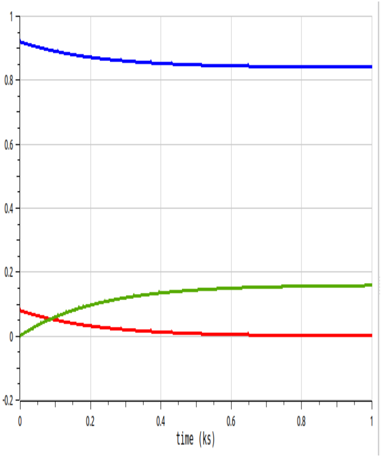
Input Parameters

k_0,Frequency Factor	153891.6
E_a, Activation Energy	44355.19
Total Inlet Flow	10000 mol/s
Temperature	308 K
Pressure	101325 Pa
Inlet Mole Fractions	0.08,0.92,0
Volume	4.25 m^3

Batch Reactor: Results



Conversion of Acetic Anhydride



Composition profile

Conclusions Future Work

1. **Progress has been for the development of general purpose simulator for Batch Processes with rigorous calculations.**
2. **This will help small-sized industry to use technology and important for academia to train students and make them industry ready.**
3. **Results of rigorous unit operations are validated against that available in the literature.**
4. **Library will enable solving flowsheets of batch processes. A large no of flowsheets to be outsourced from chemical engineering students**

Thank You...

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Appendix: Comparison of Software Packages

Features	CHEMCAD	BATCHFRAC	MultiBatchBS
Databank	CHEMCAD	ASPEN PLUS	CRANIUM
Operations			
Constant Reflux	Yes	Yes	Yes
Variable Reflux	No	Yes	Yes
Optimal Reflux	No	No	Yes
Fixed Equation	No	Yes	Yes
Models			
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.