SIMULATION OF TAME PROCESS IN DWSIM

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About Flowsheet:

Here, TAME (tert-amyl methyl ether) process simulated in DWSIM as described by W.L. Luyben to get closer results as suggested by author. TAME process contains reactive distillation and also recovery column to separate C5 stream (mainly for methanol recovery).

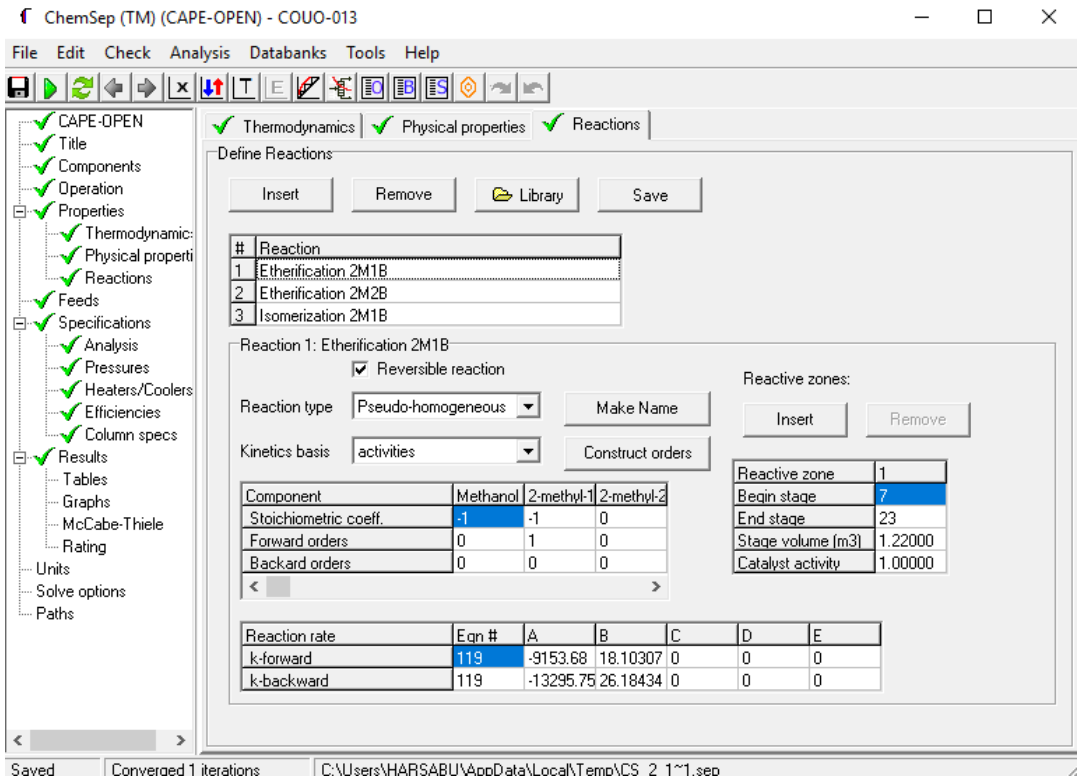
- Here, conversion reactor used for conversion type process to form methyl tert-pentyl ether (TAME). Two reaction used named as Etherification 2M1B and Etherification 2M2B as defined 50% conversion of base component also reaction phase is in liquid.
- For reactor feeds two streams used named as fees and methanol have molar flowrate 1040 kmol/h and 313 kmol/h.
- Outlet stream of reactor has molar rate of 1227 kmol/h and fed to the reactive column for the separation of TAME and other components. In reactive distillation three reaction carried out which added in chemsep column with the help of given kinetics data. (Note that here kinetics data are adjusted according to unit system/ Equation in chemsep column also screenshot of that added in abstract)

Reaction	A_F (kmol/(s /kg))	E_F (kJ/mol)	A_R (kmol/(s kg))	E_R (kJ/mol)	ΔH_{RX} (kJ/mol)
R1	1.3263×10^{8}	76.103737	2.3535×10^{11}	110.540899	−34.44
R2	1.3718×10^{11}	98.2302176	1.5414×10^{14}	124.993965	−26.76
R3	2.7187×10^{10}	96.5226384	4.2933×10^{10}	104.196053	−7.67

(Figure 1: kinetics data for reactive column) [1]

Here, Reactive distillation column contains 35 total stages and feed location at 23 and 28 stage. Reaction begin and end stages also defined in chemsep column as begin stage 7 and end stage 23 and also stage volume defined as 1.22 m^3. Reactive column operates at 4 bar pressure. Column output contains 94.7% pure TAME which found in bottom product due to high boiling point of TAME and from top of the column mix methanol and isopentane stream with other components found, from which methanol and water are separated with the help of two additional column which operated at different pressure due to azeotropic condition of methanol.

(Chemsep User interface/ Reaction addition and control windows)



- For separation of C5 product from top of the reactive column additional column used which operated at 2.5 atm pressure. In this column total 11 stages used with no condenser having feed location at 1, 5 stages. Here, as input recovered water from the methanol recovery column used with makeup of water. For the column simulation boilup ratio of 1.11 taken. From the simulation here as top product which almost contains C5 product found and fed to the compound separator where C5 product stream separated and second stream from the separator recycle back to column. Here, for compound separator data are taken from the W.L. Luyben's work having in kmol/h data which converted in mol/s for the simulation. (compound separator used because of small amount of water in top of the column found and due to quite solubility in pentanes there will be two organic layer formed which must separated to form C5 product stream and water stream recycled back to column)
- Also bottom stream of the column fed to another column which separate methanol and water having total stages 32 and feed location at stage 16 also column operated at 1 atm pressure. From the top of the column 99.9% pure methanol found and from bottom 99.9% water found. Both of the streams recycled back in process for continuous operation.
- Here, simulated flowsheet and stream data are attached as below;

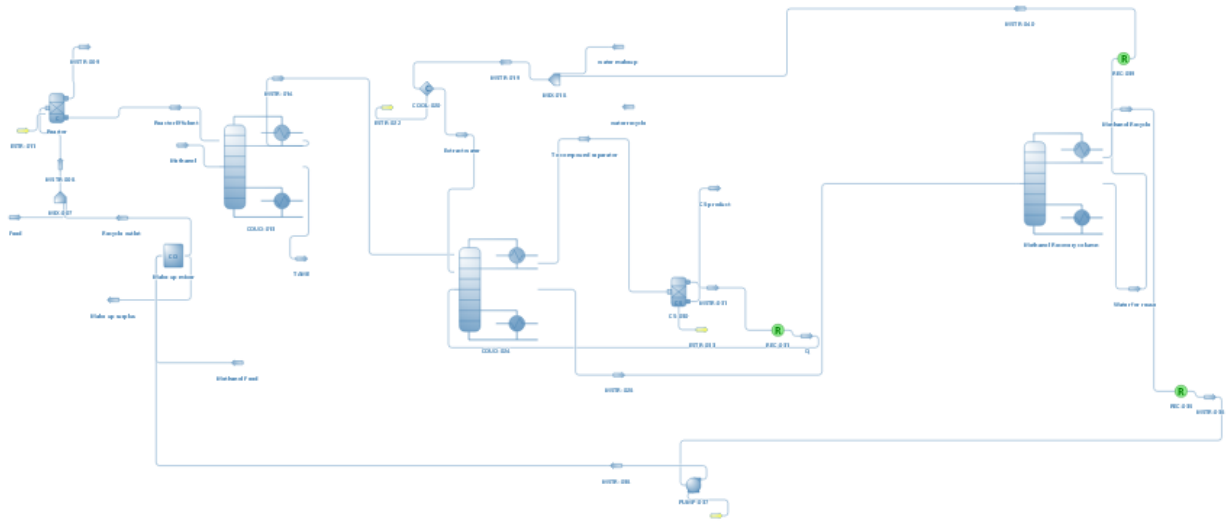


Figure 2: Simulated flowsheet

Stream Data							
Object	water recycle	TAME	Methanol Recycle	Methanol	Feed	C5-product	
Temperature	374.03452	407.14403	337.78042	300	343	357.09682	K
Pressure	101325	400000	101325	405300	1013250	250000	Pa
Molar Flow	1026	234.04556	264.08034	235	1040	894.60378	kmol/h
Molar Fraction (Mixture) / Methanol	0.0001	0.05159556	0.9998173	1	0	0.05618187	
Molar Fraction (Mixture) / 2-methyl-1-butene	0	1.6263542E-05	0	0	0.082318457	1.7175158E-17	
Molar Fraction (Mixture) / 2-methyl-2-butene	7.44208E-19	0.00044298894	1.8611131E-16	0	0.15848226	0.032127888	
Molar Fraction (Mixture) / Methyl tert-pentyl ether	1.1911909E-15	0.94719914	4.882985E-25	0	0.000100013	2.3933759E-08	
Molar Fraction (Mixture) / N-pentane	1.585493E-19	0.00012941436	8.3389368E-17	0	0.085011117	0.098793854	
Molar Fraction (Mixture) / Isopentane	0	7.1933714E-05	1.1332619E-16	0	0.48198611	0.56030301	
Molar Fraction (Mixture) / 1-pentene	6.4985071E-22	1.4382213E-05	6.3763783E-17	0	0.03660094	0.042545815	
Molar Fraction (Mixture) / Trans-2-pentene	1.2693892E-20	0.00042294424	7.6093602E-16	0	0.1555011	0.18066356	
Molar Fraction (Mixture) / Water	0.9999	0.00010737367	0.0001827011	0	0	0.029383978	

Figure 3: Stream Data

During simulation it's observed that reactive column set up is key element for process control because minor change in input data gives wide difference in results in terms of purity and molar flow. And also chemsep interface for DWSIM needs improve for future aspects during simulation it's observed that numbers of time it gives fluctuation in results and response for simulation.

References:

[1] Luyben, W. L. (2013). *Distillation design and control using Aspen simulation*. John Wiley & Sons.