International Journal of Scientific Engineering and Technology (ISSN : 2277-1581)
www.ijset.com, Volume No.1, Issue No.3, pg:-47-49 01 July 2012

A comparative study on predictions of vapour liquid equilibrium of Ethylene Oxide & Water Using Simulator

Rachana Devi, Prof.N.R.Vaghela, R.A.Soni
Department of Chemical Engineering,
Vishwakarma Government Engineering College, Ahmedabad-Gujarat
Tel : +91 9904828629, +91 9662064862
E-mail : rachana_1430@yahoo.com, nareshkumar.vaghela@gmail.com,
ronak.soni@zeppelin-india.com

Abstract
In process simulation, reliable and accurate property estimation methods play an important role in the solution of various simulation problems where convergence is often traced to failures in the reliable predictions of physical and thermodynamic properties. Convergence and reliability of the simulation is heavily dependent on the fluid package selected. Predictions of phase equilibrium using various thermodynamic models provide an idea about which model will be able to represent the entire process in better way. Paper presents a review on various simulation studies done for Ethylene oxide and Water system to highlight the fact that thermodynamic models were used with little knowledge or by intuitions. A comparative study is presented for the proper selection of fluid packages by determining vapour liquid equilibrium data for Eo-Water systems (Ethylene oxide and Water). The comparison was done with the help of making a model of experimental VLE data simulated VLE data (by various thermodynamic models).

Keyword: UNISIM, VLE, Ethylene oxide simulation

Introduction:
Ethylene Oxide was first reported in 1859 as being prepared from the reaction of potassium hydroxide on ethylene chlorohydrins. But nowadays it is mainly prepared by direct oxidation of ethylene with oxygen on silver based catalyst. In its final product stream along with ethylene oxide many other impurities like formaldehyde, acetaldehyde, unconverted ethylene, water and other inert gases are also present. So its purification consist of many stages which includes stripping zone, scrubbing zone, phase separator, an ethylene oxide purification zone and their interconnections. In its scrubbing step ethylene oxide is scrubbed from other impurities with help of excess of water which needs to be removed so it can be reused of ethylene oxide at atmospheric conditions is 10^{o}C. In process simulation, reliable and accurate property estimation methods play an important role in the solution of various simulation problems where convergence is often traced to failures in the reliable predictions of physical and thermodynamic properties.
Selection of Fluid Package

The appropriate selection of thermodynamic models has a strong influence on calculations. The appropriate selection of thermodynamic models has a strong influence on VLE and LLE calculations. This reason for scrubbing purpose as well as to get pure ethylene oxide. For commercial purpose like its use in epoxy paints, as surfactants demands highly pure ethylene oxide having purity of more than 99.5%. Ethylene Oxide is widely used petrochemical compound derived from ethylene. Ethylene Oxide can be manufactured mainly by two processes which include: 1) Direct oxidation of Ethylene with Oxygen and 2) Production from ethylene Chlorohydrins. But now it is produced mainly by direct oxidation process. Molecular Weight of Ethylene Oxide is 44.05 kg/kmole. The boiling point

The purpose of this study is to compare different thermodynamic models available for the simulation of process using UNISIM and select the best model for the simulation of Ethylene oxide & Water system. [5,6, 7].

makes this comparison of model using VLE, especially important. Fluid package selection can do mainly in two ways. One is in which it can be selected by using the selection chart or decision tree available from literature and second is it can done by cross verifying VLE data

obtained from simulator with that of the data available in literature which is very accurate method and gives surety of the results of process simulation with that particular property package. Various thermodynamic packages used for the simulation of EO-Water system. The presence of polar and non-electrolyte compounds makes necessary the use of the non-random two liquids (NRTL) model or Universal Quasi Chemical (UNIQUAC) model, WILSON which gives binary coefficients of our desired compound which in turn gives physical and chemical properties of our compound (Ethylene Oxide & water).

Next we collected VLE data of Ethylene Oxide and water from literature with different temperature & Pressure condition. After that we generated VLE data using UNISIM at the same temperature pressure condition as that collected from literature and calculated deviation of UNISIM from that of literature. The table shows the comparison of VLE data of UNISIM with that of literature and also shows the deviation of both the data [11].

Table 1: VLE Data comparison for EO-Water at 1 atm Pressure for NRTL

Mole Fraction	A(^{0}C)	B	C(^{0}C)	D(^{0}C)	% Deviation
0.951	11.5	1	11.52	10.42	9.548611
0.953	11.7	0.9	10.37069	11.99	15.61425
0.91	11.8	0.8	12.26858	12.71	3.598005
0.89	11.9	0.7	12.94321	12.85	0.720115
0.875	12	0.6	12.97478	12.85	0.961742
0.615	13.2	0.5	13.51375	12.85	4.911664
0.56	13.7	0.4	14.42966	12.85	10.94734
0.432	14.3	0.3	14.88937	13.61	8.592481
0.274	15	0.2	16.36442	16.4	0.217447
0.232	15.1	0.1	28.06781	26.72	4.801991

Table 2 : VLE Data Comparison for EO-Water at 1 atm Pressure for Wilson

Mole Fraction	A(^{0}C)	B	C(^{0}C)	D(^{0}C)	% Deviation
0.951	11.5	1	11.52	10.42	9.548611
0.953	11.7	0.9	10.37069	11.52	11.08225
0.91	11.8	0.8	12.26858	12.01	2.107628
0.89	11.9	0.7	12.94321	12.34	4.660406
0.875	12	0.6	12.97478	12.68	2.271976
0.615	13.2	0.5	13.51375	13.16	2.617704
0.56	13.7	0.4	14.42966	13.95	3.324152
0.432	14.3	0.3	14.88937	15.43	3.631008
0.274	15	0.2	16.36442	18.66	14.0279
0.232	15.1	0.1	28.06781	27.8	0.954168

Table 3: VLE Data Comparison for EO-Water at 1 atm Pressure for UNIQUAC

Mole Fraction	A(^{0}C)	B	C(^{0}C)	D(^{0}C)	% Deviation
0.951	11.5	1	11.52	10.42	9.548611
0.953	11.7	0.9	10.37069	11.78	13.58931
0.91	11.8	0.8	12.26858	12.35	0.663679
0.89	11.9	0.7	12.94321	12.578	2.821604
0.875	12	0.6	12.97478	12.69	2.194904
0.615	13.2	0.5	13.51375	12.87	4.763667
0.56	13.7	0.4	14.42966	13.33	7.620857
0.432	14.3	0.3	14.88937	14.55	2.279251
0.274	15	0.2	16.36442	17.72	8.28373
0.232	15.1	0.1	28.06781	27.3	2.735568

Table **Error! No text of specified style in document.**-4: Comparison of Average Deviation at 1 atm Pressure

	NRTL	WILSON	UNIQUAC
TOTAL DEVIATION	59.91364466	54.22580201	54.50118156
AVG DEVIATION	4.992803721	4.171215539	4.192398582

Table 5: VLE Data Comparison for EO-Water at 5^{0}C Temperature for NRTL

MOLE FRACTION	A(mm Hg)	B(mm Hg)	DEVIATION
0.0253	111.1	144.2368616	29.82615804
0.0408	171.1	216.8428325	26.73456018
0.0562	215.7	246.9203059	14.47394805
0.0727	266	317.2010856	19.24852843
0.1231	405.4	428.6602517	5.737605246
0.154	544.5	472.1638293	13.28487984
0.2299	584.9	533.9689119	8.707657392

Table 6: VLE Data Comparison for EO-Water at 5^{0}C Temperature for WILSON

MOLE FRACTION	A(mm Hg)	B(mm Hg)	DEVIATION
0.0253	111.1	122.7850975	10.51763948
0.0408	171.1	179.189736	4.728074809
0.0562	215.7	209.1171971	3.051832574
0.0727	266	269.9471996	1.483909626
0.1231	405.4	366.1801135	9.674367663
0.154	544.5	406.9084629	25.26933648
0.2299	584.9	472.0888231	19.28725883

Table 7: VLE Data Comparison for EO-Water at 5^{0}C Temperature for UNIQUAC

MOLE FRACTION	A(mm Hg)	B(mm Hg)	DEVIATION
0.0253	111.1	115.434493	3.901433815
0.0408	171.1	171.0140637	0.0502258
0.0562	215.7	201.2415495	6.703036871
0.0727	266	264.4717493	0.57453033
0.1231	405.4	368.655317	9.063809312
0.154	544.5	413.7340242	24.01578987
0.2299	584.9	485.5149272	16.99180591

Table 8: Comparison of Average Deviation at 5^{0}C Temperature

	NRTL	WILSON	UNIQUAC
TOTAL	118.0133372	74.01241946	61.30063191

DEVIATION			
AVG DEVIATION	16.85904817	10.57320278	8.75723313

Table 9: VLE Data comparison for EO-Water at 20^0C Temperature for NRTL

MOLE FRACTION	A(mm Hg)	B(mm Hg)	DEVIATION
0.0253	190.4	231.3190229	21.49108
0.0408	291.8	337.6777696	15.72233
0.0562	371.1	394.6824574	6.354745
0.0727	471.7	511.3920553	8.414682
0.1231	670.2	696.6572909	3.947671

Table 10: VLE Data comparison for EO- Water at 20^0C Temperature for WILSON

MOLE FRACTION	A(mm Hg)	B(mm Hg)	DEVIATION
0.0253	190.4	220.0680977	15.58198
0.0408	291.8	318.7762151	9.244762
0.0562	371.1	371.1305206	0.008224
0.0727	471.7	473.0639033	0.289146
0.1231	670.2	647.228226	3.4276

Table 11: VLE Data comparison for EO- Water at 20^0C Temperature for UNIQUAC

MOLE FRACTION	A(mm Hg)	B(mm Hg)	DEVIATION
0.0253	190.4	211.0673575	10.8547
0.0408	291.8	309.9254873	6.211613
0.0562	371.1	363.6299038	2.01296
0.0727	471.7	475.6891192	0.84569
0.1231	670.2	660.2792993	1.48026

Table 12: Comparison of Average Deviation at 20^0C Temperature

	NRTL	WILSON	UNIQUAC
TOTAL DEVIATION	55.93051	28.55172	21.40523
AVG DEVIATION	11.1861	5.710343	4.281046

Note: Where, A=Literature value
B= HYSYS value

Table shows individual deviation and overall deviation of NRTL, WILSON & UNIQUAC. Similarly VLE data were compared at other temperature and pressure condition and was found that average deviation of all three fluid packages were nearly same.

Conclusion:

activity model have better accuracy for the EO-Water system. So conclusion was we can select any fluid package for predicting binary coefficients of our compounds (Ethylene Oxide & water). So we had chosen UNIQUAC as a fluid package to simulate our distillation column.

Vapour liquid equilibrium prediction for the EO-Water system were investigated using different property packages like NRTL, WILSON, UNIQUAC. Among those property packages, activity models have strong predictability. But from the present study, UNIQUAC

Acknowledgement:

I would like to acknowledge all the faculty members of Chemical department, Vishwakarma government engineering college Chandkheda and for their invaluable guidance and assistance throughout the work. I would like to express my deep sense of gratitude to my external guide Mr. R. A. Soni for guidance and for giving me the opportunity to work in the Zeppelin System India Pvt. Ltd.

References:

1. K.F.Coles and Felix Popper, "Vapor-Liquid Equilibria Ethylene Oxide-Acetaldehyde and Ethylene Oxide-water System", Industrial and engineering Chemistry, vol-42(1950), 1434-1438.
2. K.E.MacCormack, J.H.B.Chenier, "Vapor-Liquid Equilibria in Dilute Aqueous Solutions of Ethylene Oxide", Industrial and engineering Chemistry, vol-47(1955), 1454-1457.
3. Rahmat Sadegi and Yasaman Shahebraihimi,"Vapor Pressure Osmometry Determination of Solvent Activities of Different Aqueous and Non aqueous Polymer Solutions at 318.15 k", Journal of Chemical Engineering", vol-56,2946-2954.
4. P.P. McClellan, "manufacture and Uses of Ethylene Oxide and Ethylene Glycol", Industrial and Engineering Chemistry, 42(1950), 2402-2404.
5. www.che.cemr.wvu.edu/publications/projects/ethylene/eo-a.
6. en.wikipedia.org/wiki ethylene-ox.
7. www.sbioinformatics.com/design_thesis/ethylene-oxide/ethylene/ethylene252oxide_properties&uses.
8. www.scribd.com/doc/51221759/project-ethylene-oxide-reparired.
9. www.atsdr.cdc.gov/toxprofiles/tp137-c4.
10. Joe McGonigle, Michelle Darjean, Tammy Lai, EO Report, 1-10.
11. www.et.byu.edu/groups/uolab/files/aspentech/A_short_primer_for_using_AspenPlus.d
12. S.B.Thakor, B.I.Bhatt, Introduction to Process Engineering and Design, Tata McGraw-Hill Publishing Company Limited,(2009), 441-475