Simulation of Multi Component Distillation Column Using Open-Source Simulator

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ABSTRACT

Process simulation is a successful tool for design, optimization and control of chemical processes. Chemical industry process simulations support the entire life cycle of a chemical process from development, design and construction to optimization of operation. Distillation is the most commonly used separation process in the chemistry and petrochemical industry, mostly employed in continuous processes but also used in discontinuous processes. Multicomponent distillation use for separation of more than two components. For such operation needs two columns for separation of components. Most of the distillation processes involve with more than two components. The multicomponent separations are carried out by using the same type of distillation columns, reboilers, condensers, heat exchangers. In multicomponent systems same degree of freedom is not achieved because of the presence of other components.

We simulating Rig-Distillation column which giving results as Condenser Duty and Reboiler Duty 27773.3 KW and -28958 KW resp. Also have Min. R. R. equal to 0.57136*1.5 = 0.85704. Simulated Rig-Distillation column also Flow Stream Data and Temperature Data At Various Stages. Min. number of feed stages are 12 excluding Reboiler. As per results simulation gives quick results for multicomponent distillation column that also getting from practically from piolet plants. Practical methods is time consuming and has costly.

We simulating Rig-Distillation column which giving results as Condenser Duty and Reboiler Duty 25838 KW and -31215.4 KW resp. Also have Min. R. R. equal to 0.57136*1.1 = 0.6284. Simulated Rig-Distillation column also Flow Stream Data and Temperature Data At Various Stages. Min. number of feed stages are 20 excluding Reboiler. Optimal feed condition is 9.

We simulating Rig-Distillation column which giving results as Condenser Duty and Reboiler Duty 26744.7 KW and -32121.5 KW resp. Also have Min. R. R. equal to 0.57136*1.2 = 0.6856. Simulated Rig-Distillation column also Flow Stream Data and Temperature Data At Various Stages. Min. number of feed stages are 17 excluding Reboiler. Optimal feed condition is 7.

We simulating Rig-Distillation column which giving results as Condenser Duty and Reboiler Duty 27651 KW and -33028.5 KW resp. Also have Min. R. R. equal to 0.57136*1.3 = 0.7427. Simulated Rig-Distillation column also Flow Stream Data and Temperature Data At Various Stages. Min. number of feed stages are 16 excluding Reboiler. Optimal feed condition is 7

We simulating Rig-Distillation column which giving results as Condenser Duty and Reboiler Duty 27651 KW and -33934.8 KW resp. Also have Min. R. R. equal to 0.57136*1.4 = 0.7999. Simulated Rig-Distillation column also Flow Stream Data and Temperature Data At Various Stages. Min. number of feed stages are 14 excluding Reboiler. Optimal feed condition is 7.

As per simulation date we simulating the rig. Column for different R. R. ration as taken Min. R. R. *1.1, Min. R. R. *1.2, Min. R. R. *1.3, Min. R. R. *1.4 and Min. R. R. *1.5. By simulation study value of min. reflux ration increase the decrease in the number of stages and but increase the reboiler duty and coolant load also increase for condenser. For R.R. 1.5*Min, R.R. is optimum value where optimum number of stages are requires and also min. heat load on reboiler and min. coolant supply to condenser. Hence, according to results, the best suitable value while selecting R. R. will be 1.5 times of Min. R. R.

Keywords *– Multi Component Distillation, Process Simulation, Modeling and Simulation, Rig. Distillation Column, DW SIM, Open Source Media.*

1. INTRODUCTION

Simulation is operation of a model of system. Model can reconfigured and experimented impossible too expensive or impractical to do in system it represents. Simulation is a tool to performance of a system, existing or proposed,

under different configurations of interest and over long periods of real time. A model should be a close approximation to the real system and incorporate most of its salient features. Model should not be so complex that it is impossible to understand and experiment with it. Multicomponent distillation use for separation of more than two components. Multicomponent operation needs two columns for separation of components. The distillation processes involve with more than two components. The multicomponent separations are carried out by using the same type of distillation columns, reboilers, condensers, heat exchangers.

Benefits of Simulation in Process Industry

1.Economic: cheaper to use simulation than to build numerous different-size pilot-plants

2.Operation: Easier to develop alternative operating approaches via a mathematical model than by experimental methods

3.Scale up: First-principles simulations can predict system performance in new and different operating conditions.

Application of MDC

1. In petrochemical and refining industry for recovery of aromatic hydrocarbons.

2. Separation of petroleum products from crude oil

3. Separation of naphtha, Kerosene, diesel and gasoline etc.

4. MDC use for separation of two or more component mixture having different volatilities

5. Petrochemical industry for separation of multi components

6. For Separation of more than two hydrocarbons mixtures.

Need of Modeling and Simulation of MDC

1. To optimize MDC by using optimum conditions obtained from simulation.

2. To develop alternative operating approaches for experimental methods.

3. Avoid to build different-size pilot-plants.

4. To predict system performance in new and different operating conditions.

5. Reduce cost of operation and increase economics

6. Saving of energy by reduce heat and heat loss.

7. Increase the recovery product by simulating various operating process.

Assumptions design and simulation models

1. The feed stream is composed of four components

2. The feed is introduced only at a point in column

3. Liquid and vapor flow rates constant for all trays.

4. Overhead product condensed in a total condenser

5. The heat losses are negligible and for an ideal system heat of mixing is zero.

6. For ideal systems of this kind, the molar heat of vaporization may be taken as constant and independent of the composition.

2. LITERATURE REVIEWS

Batch distillation operations the two-component separation more difficult because it has lowest relative volatility of 1.3 compared with 2.15 for three-component separation and 2.39 for four-component separation. Two-component separation had 25 as the minimum number of theoretical stages and is a kind of limiting factor. 10 and 20 theoretical stages applied for three and four component separations for last separation only batch distillation columns with 30, 40 and 50 theoretical stages to perform three separations needed. Total annual cost (TAC) always choses 30-stage column as one with lowest TAC but the annual profit always selects the combination with the highest annual profits. The highest annual profit is given by 50 stages followed by the 40 stages and last the 30 stages column. At constant reflux annual profit for 30-stage column higher than operating at variable reflux. Variable reflux operations using 40 and 50 stages columns 2.8 and 21.4% higher respect. makes them better choices in annual profit than counterparts operating at constant reflux. [3]

Simulation of the design models performed using Aspen Hysys to obtain optimum values of the most significant variables/parameters (column diameters 1.558 m, column height 17.048 m, cross section area 1.907 m^2, downcomer area 0.229 m^2, tray spacing 0.5m, weir length 1.200 m, hole area 0.191 m^2 and wet area 1.678 m^2). Steady state simulation shows that feed flow rate, temperature and pressure influence efficiency of distillation column. [7]

MESH equation represent the behavior of distillation column has been solved through MATLAB to study the effect of different parameter. MATLAB software we study the dynamic behavior of the product composition with the feed change with the timeThe effect of the feed condition and the feed composition on the steady state behavior. Developed code has been used to study the column and composition response to disturbance are close to the response of first order system. [12]

In Aspen Hysys multicomponent distillation process is stimulated under steady state condition. Calculations such as compositions, temperature, mass balance and energy balance can be done step by step. The composition, k values, temperature and flowrate will be further explained in discussion. The limitations of steady state techniques and the need for rigorous dynamic simulation for final selection of a workable and robust strategy is illustrated. [16]

Fenske-Underwood-Gilliland short-cut method to solve problem of four components (benzene, toluene, ethyl-benzene, and ortho-xylene) needed to be separated and purified to a mole fraction of 0.97 or better. Performance of system evaluated using distillation columns with 10, 20, 30, 40 and 50 theoretical stages with a boil-up vapor flow set at 100 kmol/h. The annual profit best quality index, while the best case for variable reflux was the column with 50 stages. The best case always required a reflux ratio close to the minimum.[17]

One of most efficient biofuels as butanol for use as mixture with motor vehicle fuel. Butanol produced from acetone-butanol-ethanol fermentation process and separated in pure components via multicomponent distillation. Multicomponent distillation of ABE carried out using equilibrium-based model with modified Hang-Wanke method in MATLAB programming language and compared with simulation results using Aspen Plus V9. Feed stage number of trays, reflux ratio to butanol purity, butanol recovery and energy load of reboiler and condenser. Operating conditions in columns 1 and 2 recommended on butanol purity, recovery and reboiler load. Operating conditions for column 1 feed stage 4, reflux ratio 4, number of trays 20 trays, column efficiency 55.43%. Operating conditions for column 2 feed stage 2, reflux ratio 0.4, number of trays 10, column efficiency 54.94%. [20]

Simulation Software's for MCD

1. Aspen Plus

2. Pro FII

3. DW SIM

4. Pro Sim

5. CHEMCAD

6. Aspen HYSYS

7. ProMax

Process for simulation of Multicomponent Distillation Column using DWSIM

1. Create a New Simulation

2. Select compounds to the simulation.

3. Add an instance of the Inside-Out VLE Flash Algorithm too.

4. Check if the NRTL Interaction Parameters all set

5. Select it on the System of Units combo box.

6. Add the objects to the flowsheet (streams, pump, valve, recycle and distillation columns)

7. Setup the columns and their connections.

8. Enter initial estimates for the temperature profile of the Column and check the Override Temperature Estimates checkbox so DWSIM can use them.

9. After the columns are correctly configured and connected to their associated streams, setup the pump, valve and recycle connections using their Editor Panels.

11. Setup the pump and valve properties.

12. Calculate the flowsheet (press F5).

13. After flowsheet solves new Property Table .

14. Double-click on inserted table search for column energy streams.

15. Compare results obtained with duties specified in original problem.

Process for Batch multicomponent Distillation

The feed may be charged into the reboiler at the beginning of the operation and then heat is provided at the reboiler to evaporate part of the liquid to generate a vapor that rises through the column until it reaches the condenser where it is converted to liquid and collected at the reflux tank. From this reflux tank a part is returned to the column as liquid reflux that descends through the column contacting with the vapor counter-currently if the column is full of packing or contacting the vapor in a crosscurrent pattern if the column contains plates. The more volatile components concentrate at the top of the column and the less volatile or heavy compounds concentrate at the bottom. For multicomponent distillation cuts are used for separation of two or more components. Based on the volatility difference of components separation to be carried out. In this feed charged as batch for fix contact time. Then adjusting the temperature, pressure and heat the cuts of components to be separated. One heavy component are withdrawals from the bottom of column. The other light component to be separated from the top of column as cuts.

Examples of Multicomponent Distillation

1. Methanol, ethanol, benzene, toluene

2. Methanol, ethanol, 2-propanol, 1-propaonal, and toluene

3. Acetone, methanol, 2-propanol, 1-propanol, and toluene

4. Methanol, ethanol,2-propanol,1-propanol

5. Benzene, toluene, ethylbenzene, styrene

6. Benzene, toluene, aniline

7. Benzene, water, toluene

8. Benzene, water, toluene, aniline

9. Methanol, ethanol, benzene, water, toluene, aniline

Analysis of Parameters in Simulations

1. Effect of Feed Flow Rate

The higher the feed flow rate (increase in the feed rate) the greater the composition of the lighter ends in the bottom plate and the heavy components in the upper plate; the lower the feed rate (decrease in the feed rate) there is a reduction of the lighter ends in the bottom region and the heavier ends in the upper region. When the feed rate is increased, its velocity increases, its residence time (contact time of the vapor-liquid phases on each tray) in the column reduces, causing inefficient separation and a reduction in the percentage purity of each component, which might lead to weeping and decrease in the efficiency of the column performance.

2. Effect of Temperature

The effect of bottom heat could have contributed to the high temperature profile in the stripping section. The column temperature is influenced by the heat of reactions and the fresh feed rates. As the product (residue) leaves the column at the bottom, there is temperature drop, but as part of the bottom product (residue) are returned back into the column.

3. Effect of Pressure

Pressure is controlled by refluxing in the column. As the residue leaves the column, there is pressure drop, which later rises as a result of the presence of the reboiler which aid refluxing.

4. Effect of Column Properties and Molar Flow

The models were used to predict the column properties (density and molecular weight) and net molar flow of the five components of the crude oil mixture separated in a multicomponent distillation column. The effect of column properties and net molar flow of the five components.

Problem Statement

Mixture of components feed at rate 5000 kg/hr. to the distillation column containing 5 % Propane , 10 % i-Butane, 30 % i-Pentane, 46 % n-Hexane and 9 % n Heptane. Pressure at condenser (T.P.) is 1.8 bar and at reboiler (B. P.) is 2 bar. Distillate containing 1 % of n-Hexane and B.P. contains 1% of i-Pentane. Here, i-Pentane and n-Hexane are the light key and heavy key components.

Calculate

1. Min. R.R.

2. Min. number of stages

3. Actual no. of stages

4. Feed stage location.

5. Reboiler and condenser Duty.

We Simulating SC by Change Min. R. R. = 0.57136*1.5 = 0.85704 by using the SC column simulation with help of Problem statement and find the optimum feed conditions for the Rig. Distillation column.

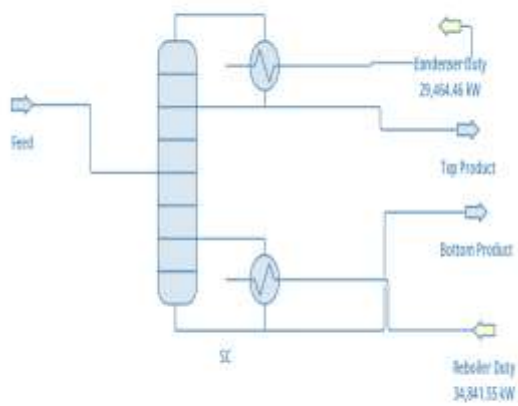

Fig. Simulated SC in DWSIM

Then Results Obtained as,

Minimum Reflux Ratio	0.57136
Minimum Number of Stages	6.66622
Actual Number of Stages	14.0439
Optimal Feed Stage	6.51283
Stripping Liquid	6923.97
Rectify Liquid	1923.97 kmol/h
Stripping Vapor	4168.97 kmol/h
Rectify Vapor	4168.87 kmol/h
Condenser Duty	29464.5 kW
Reboiler Duty	34841.5 kW

Table Feed Data For Rigorous Distillation Column

The actual feed condition for simulation of Rigorous distillation column. With help of above results we simulating the Rig-Distillation column obtaining following results.

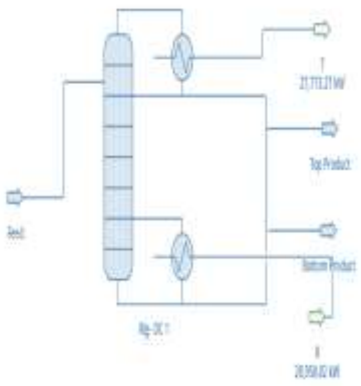

Fig. Simulated Rigorous Distillation Column

Reboiler and Condenser Duty For Rigorous Column

Condenser Duty	27773.3 KW
Reboiler Duty	-28958 KW
Condenser Specification Value	0.857 (R.R.)
Condenser Specification Calculated Value	0.857 (R.R.)
Reboiler Specification Value	2755 kmol/h
Reboiler Specification Calculated Value	2755 kmol/h
Iterations Taken	27

Table No. Reboiler and Condenser Duty For Rigorous Column

Similarly we simulating the Rig. Column for R. R. 1.1 – 1.4 times of Min R. R. and calculating various results. We get conclusion after simulation optimum value for R. R. will be 1.5* min. R. R.

CONCLUSION

We select the problem for simulation multicomponent mixture of components feed distillation column containing 5 % Propane , 10 % i-Butane, 30 % i-Pentane, 46 % n-Hexane and 9 % n Heptane. Pressure at condenser (T.P.) is 1.8 bar and at reboiler (B. P.) is 2 bar. Distillate containing 1 % of n-Hexane and B.P. contains 1% of i-Pentane. Here, i-Pentane and n-Hexane are the light key and heavy key components. In this we have to calculated Min. R.R., Min. number of stages, Actual no. of stages and Feed stage location.

First we simulate the short Cut Distillation column in DWSIM for generating data for rigorous column with help of problem statement. By putting resulting values in again SC distillation column to get minimum values for R. R. and stages. From second SC distillation column obtained values we optimize the SC column to get optimum feed values from third SC distillation column which is useful for rigorous distillation column. With help of results obtained from third SC distillation column we simulating the Rig-Distillation column.

We simulating Rig-Distillation column which giving results as Condenser Duty and Reboiler Duty 27773.3 KW and -28958 KW resp. Also have Min. R. R. equal to 0.57136*1.5 = 0.85704. Simulated Rig-Distillation column also Flow Stream Data and Temperature Data At Various Stages. Min. number of feed stages are 12 excluding Reboiler. As per results simulation gives quick results for multicomponent distillation column that also getting from practically from piolet plants. Practical methods is time consuming and has costly.

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REFERENCES

1. Allen C. Paul's, Edward M. Rosent and Computer Aided Chemical Process Design: The Flow Tran System, Computers and Chemical Engineering, Vol. I. pp. 11-21. Pergamon Press, 1977.

2. Anu Maria, Introduction to Modelling and Simulation, proceeding the winter simulation conference, U.S.A, NY 13902-6000, 1997.

3. A. Narvaes Garcia, L. E. Vilchis-Bravo and J. C. Zavala-Loria, Performance indices to design A Multicomponent Batch Distillation Column Using A Shortcut Method, Journal of Chemical Engineering, ISSN 0104-6632, Vol. 32, No. 02, pp. 595 - 608, April - June, 2015.

4. B.S Thirumalesh and Ramesh. V, Case Study On Multicomponent Distillation and Distillation Column Sequencing, International Journal Of Engineering Sciences & Research Technology, Thirumal's, 4(8), ISSN: 2277-9655, August, 2015.

5. Chan Hong and James R. Fair, Prediction of Point Efficiencies on Sieve Trays Multicomponent Systems, American Chemical Society, Ind. Eng. Chem. Process Des. Dev., Vol. 23, No. 4, 1984.

6. Dr. Pradeep and Jagat Kumar, System Models and System Simulation, Website or URL- http:,//www.ddegjust.ac.in.

7. Dagde, Kenneth Kekpugile Kpalap and Emmanuel Kilsibari, Computer Aided Design Of A Multi-Component Distillation Column For Processing Of Nigerian Bonny Light Crude Oil, International Journal of Chemical and Process Engineering Research, ISSN(e): 2313-0776, Vol. 3, No. 1, pp. 10-22 , 2016.

8. Dr. B. Krishna, Modelling and Simulation in chemical engineering, website or URL- http:,//www.nitsri.ac.in.

9. Jackson Gunorubon and Omonigho Diepriye, Simulation of a Multi-component Crude Distillation Column, American Journal of Scientific and Industrial Research, Vol-013, 4(4): 366-377, 2013.

10. J. C. Zavala-Loria , L. E. Vilchiz-Bravo and J. A. Rocha-Uribe, Performance Indices to Design A Multi Component Batch Distillation Column Using A Shortcut Method, Journal of Chemical Engineering, ISSN 0104-6632, Vol. 32 (02), pp. 595 - 608, June, 2015

11. Saeid Asadi, Simulation of The Multicomponent Distillation of Spearmint Essential Oil By A Predictive Soave-Redlich Kwong Equation of State and Comparison With Experiments, Chem. Ind. Chem. Eng. Q. 20 (3) 417−423 (2014).

12. Shukla Gaurav, Study the Dynamic Behavior of Distillation Column with Fundamental Modelling and Simulation by MATLAB, International Journal of Engineering Research & Technology (IJERT), ISSN: 2278-0181 IJERTV6IS040665, Vol. 6 Issue 04, April-2017.

13. Vishal Parmar, Nirali Tharwala, Ronak Prajapati and Parth Patel, Modeling And Simulation Of Distillation Column, Assistant Professor and students, IJARIIE-ISSN(O)-2395-4396, Vol-3 Issue-3, 2017.

14. Zakia Nasri and Housam Binous, Rigorous Distillation Dynamics Simulations Using a Computer Algebra, Wiley Periodicals Inc., August 2009.

15. Samia Latreche and Mabrouk Khemliche, Modeling And Simulation of The Distillation Column Plates, Advances in Engineering: an International Journal (ADEIJ), Vol.2, No.2, 2011.

16. Ivy Wong Fui Ann, Modeling And Simulation of Distillation Column, JAN 2014.

17. Zavala-Loria , L. E. Vilchiz-Bravo and J. A. Rocha-Uribe, Performance Indices to Design A Multi Component Batch Distillation Column Using A Shortcut Method, Brazilian Journal of Chemical Engineering, ISSN 0104-6632, Vol. 32, No. 02, pp. 595 - 608, April - June, 2015.

18. Bruce Earl Baugher, Computer Simulation of A Multicomponent, Multistage Batch Distillation Process, 1985.

19. Saeid Asadi, Simulation of Multicomponent Distillation of Spearmint Essential Oil By Predictive Soave-Redlich Kwong Equation of State and Comparison With Experiments, Chemical Industry & Chemical Engineering Quarterly, 20 (3) 417−423 (2014).

20. Tri Widjaja , Kornelius Kevin Iskandar, Fikran Sahid , Siti Nurkhamidah , Ali Altway and Atha Pahlevi Putra, Modelling and simulation of multicomponent acetone-butanol-ethanol distillation process in a sieve tray column, Heliyon, 7 2021.

21. Rahul Anandi Sai, Rahul Jain, Kannan M. Moudgalya, P. R. Naren, Peter Fritzson and Daniel Wagner, Chemical Process Simulation Using Open Modelica, American Chemical Society, January 7, 2019.

22. Shukla Gaurav, Study the Dynamic Behavior of Distillation Column with Fundamental Modelling and Simulation by MATLAB, International Journal of Engineering Research & Technology (IJERT, ISSN: 2278-0181 IJERTV6IS040665, Vol. 6 Issue 04, April-2017.

23. Suresh Kumar and Mohammed Wajid Ali, Modeling and Control of a Multi-Component Continuous Crude Distillation Column Using Lab View, International Journal of Advanced Research in Electrical, Electronics and Instrumentation Engineering, ISSN (Print) : 2320 – 3765, ISSN (Online): 2278 – 8875, Vol. 3, Issue 11, November 2014.

24. Jackson Gunorubon and Umuze Omonigho Diepriye, Simulation of a Multi-component Crude Distillation Column, American Journal Of Scientific And Industrial Research, 2013.

25. Ulrich Preißinger and Thomas Grützner, Robust Initialization of Rigorous Process Simulations of Multiple Dividing Wall Columns via V_{min} Diagrams, Chem Engineering 2018.

26. Gustavo León, Modeling Multicomponent Distillation With Open Source And CAPE-OPEN, CAPE OPEN Annual Meeting Lyon, 2013.

27.Tobias Seidel, Lena-Marie R¨anger, Thomas Grutzner and Michael Bortz, Simultaneous simulation and optimization of multiple dividing wall columns, Fraunhofer Institute for Industrial Mathematics, 2018.