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"Process Simulation and Optimization of Binary Distillation Column Using Open Media Simulator (DWSIM)"

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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 used separation process in the chemistry and petrochemical industry mostly in continuous processes, but it is also used in discontinuous processes. Batch distillation is widely used for the separation of specialty and fine chemicals and for the recovery of small amounts of solvent to obtain products of high purity and added value.

Keywords – DWSIM, Open media simulator, Benzene-Toluene system, Ethanol-Water system, Short-cut Distillation and Rigorous Column.

INTRODUCTION

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. Simulation represents the application of modeling techniques to real systems which enabling information on plant characteristics to be gained without either constructing or operating the full-scale plant or the system under consideration[1] . A simulation of a system is the operation of a model of the system. The model can be reconfigured and experimented is impossible, too expensive or impractical to do in the system it represents. Simulation is a tool to evaluate the performance of a system, existing or proposed, under different configurations of interest and over long periods of real time. Simulation is used before an existing system is altered or a new system built to reduce the chances of failure to meet specifications, to eliminate unforeseen bottlenecks, to prevent under or over-utilization of resources and to optimize system performance[3].

Modeling is the process of producing a model which is a representation of the construction and working of some system of interest. A model is similar to a system but simpler than the system it represents. One purpose of a model is to enable the analyst to predict the effect of changes to the system. A model should be a close approximation to the real system and incorporate most of its salient features. The model should not be so complex that it is impossible to understand and experiment with it. A good model is a judicious tradeoff between realism and simplicity. Simulation practitioners recommend increasing the complexity of a model iteratively. An important issue in modeling is model validity. Model validation techniques include simulating the model under known input conditions and comparing model output with system output. A model intended for a simulation study is a mathematical model developed with the help of simulation software. Mathematical model classifications include deterministic or stochastic static (time is not taken into account) or dynamic (time-varying interactions among variables are taken into account). Simulation models are stochastic and dynamic[7].

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. Batch distillation is widely used for the separation of specialty and fine chemicals and for the recovery of small quantities of solvent during the production of high-purity and added-value products[6] . Batch processing is the main feature of the pharmaceutical, biochemical, and specialty chemical industries. In batch distillation columns 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 vapor in a crosscurrent pattern if the column contains plates[9].

Experimental Process

- 1. Start a new DWSIM Simulation. Click on “New steady-state Simulation” as a template for a new simulation.
- 2. The simulation configuration window will be opened. Add the two components required for simulation. Ensure that all the components are added from the same property package. Click the “Next” button.
- 3. Select and add the property package and click “Next”. Add the default flash algorithm for the simulation. Click “Next”.
- 4. The flow sheeting section of simulation window will be opened. Drag and drop the Material stream from the object palette. Rename it as “Feed”. This serves as input stream.
- 5. On clicking the “Feed” stream, general information about the block will be displayed on the left of the screen. Specify the feed compositions, flow rate, temperature and pressure for the inlet streams. Once composition and flow rate are specified for the inlet streams, the color of stream turns blue.
- 6. Add two more Material streams i.e., Drag and drop them into the flow sheet. Rename them as “Distillate” and “Bottoms”. These serves as output streams.
- 7. Add two energy streams, one is for condenser duty (C-Duty) and the other is for re-boiler duty (R-Duty).
- 8. Below the Unit Operation tab, locate the “Shortcut Column” block. Drag and drop into the flow sheet. Rename it as “DC”.
- 9. Click on “DC” block, the general information about the block is displayed on the left of the screen. Provide calculation parameters as shown in the screenshot given below.
- 10. Under Column configuration select “connections” tab. Click the dropdown button and give appropriate connections. If all the connections are given correctly, the blocks will turn blue.
- 11. Run the simulation by pressing “Solve flow sheet” button on the top corner of the screen.
- 12. To analyze/display the results, select on “Master property table” icon on the tool bar. A box will appear which is double clicked to modify it further. Select the streams which have to be shown in output and click “OK”. The property table will be opened showing all the results as shown in the figure below.

Problem Formulation

- Simulation of Benzene and Toluene Binary Components Mixture Problem Statement Mixture of components feed at rate of 100 kmol/hr. to the distillation column containing 40 % benzene and 60 % Toluene. Pressure at the condenser (T.P.) is 1 atm and the Reflux ratio is 1.4 times of min. R. R. Light Key component (LK) Benzene and heavy key (HK) component as toluene. Distillate contains 99% benzene and B.P. contains 99% of Toluene on a mole basis. Calculate
- 1. Min. R.R.
- 2. Min. number of stages.
- 3. Actual no. of stages.
- 4. Optimal feed stage location.
- 5. Condenser and Reboiler duty.

- **Ans.** Process Flow Sheet of simulated distillation Column for the above problem

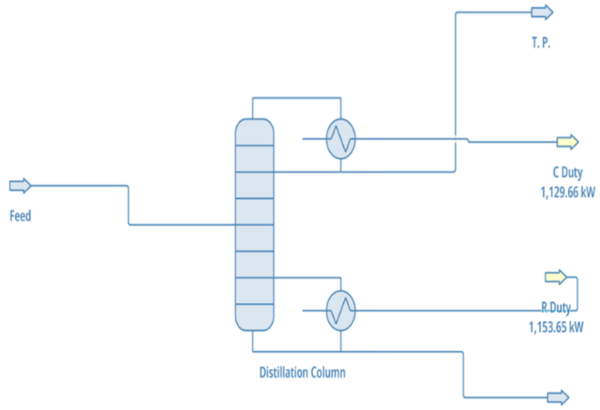

Fig1. Process Flow sheet for SC distillation Column for Benzene-Toluene System

1] Simulation Results for Benzene and Toluene Binary Mixture:

Heavy Key Molar Fraction	0.01
Light Key Molar Fraction	0.01
Condenser Pressure	1.01325 bar
Reboiler Pressure	1.01325
Reflux Ratio	2.317
Minimum Reflux Ratio	1.65509
Minimum Number of Stages	10.1614
Actual Number of Stages	19.2627
Optimal Feed Stage	8.78148
Stripping Liquid	192.207 kmol/hr.
Rectify Liquid	92.2071 kmol/hr.
Stripping Vapor	132.003 kmol/hr.
Rectify Vapor	132.003 kmol/hr.
Condenser Duty	1129.66 KW
Reboiler Duty	1153.65 KW

Table1: Results Obtained by Short Cut Column after Simulation.

- Table shows the actual feed condition for simulation of Rigorous distillation column. With help of above results, we simulating the Short Cut-Distillation column obtaining following results. Putting the data on Rigorous distillation obtained from the Shortcut distillation column, Optimal Feed Stage = 09
- Actual Feed Stage = 20 (Including Reboiler = 21)
- Reflux Ratio = 2.317 and Flow Rate = 100 kmol/hr.

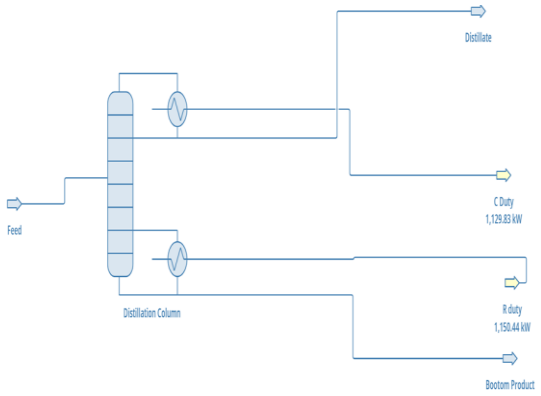

Fig 2. Process Flow Sheet for Simulated Rigorous Distillation Column for Benzene-Toluene System.

2] Results of Simulated Rigorous Distillation Column:

Condenser Duty	1129.83 KW
Reboiler Duty	-1150.44 KW
Condenser Specification Value	2.317
Condenser Specification Calculated Value	2.317
Reboiler Specification Value	60.204 kmol/h
Reboiler Specification Calculated Value	16.7233 kmol/h
Iterations Taken	62
Number of Stages	21
Condenser Pressure	1 atm
Reboiler Pressure	1 atm
Stream 'Feed' Stage Index	9

Table 2: Results of Simulated Rigorous Distillation Column

- Table shows the simulation results for of Rigorous distillation column. Results shows the Condenser Duty 1129 KW, Reboiler Duty -1150 KW, Iterations Taken 62, Number of Stages 21, Condenser Pressure 1atm and Stream 'Feed' Stage Index 9.

3] Temperature Data at Various Stages:

	T_0 (C)	T_F (C)
Condenser	95.2199	80.3865
Stage1	95.5328	80.7297
Stage2	95.8457	81.3337
Stage3	96.1586	82.341
Stage4	96.4715	83.8992
Stage5	96.7844	86.051
Stage6	97.0973	88.6122
Stage7	97.4102	91.1962
Stage8	97.7231	93.4091
Stage9	98.036	95.0672
Stage10	98.3489	96.0702
Stage_11	98.6618	97.4433
Stage_12	98.9747	99.1833
Stage_13	99.2876	101.185
Stage_14	99.6005	103.252
Stage_15	99.9134	105.165
Stage_16	100.226	106.769
Stage_17	100.539	108.005
Stage_18	100.852	108.896
Stage_19	101.165	109.511
Reboiler	101.478	109.921

Table 3 : Temperature Data at Various Stages for Benzene-Toluene System.

4] Temperature Data at Various Stages for Benzene-Toluene System:

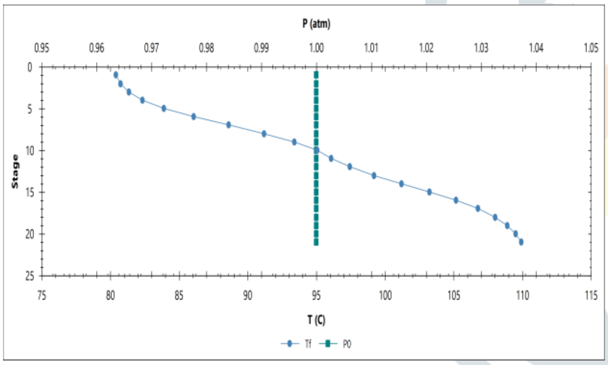

Fig 3. Temperature Data at Various Stages for Benzene-Toluene System.

Fig. shows the pressure in atm and temperatures in oC of various stages of distillation column including condenser and reboiler.

5] Flow Stream Data:

	[V] Benzene (-)	[V] Toluene (-)	[L] Benzene (-)	[L] Toluene (-)
Condenser	0.995882	0.00411761	0.989264	0.0107356
Stage1	0.989264	0.0107356	0.972344	0.0276557
Stage2	0.977458	0.0225424	0.943136	0.0568637
Stage3	0.957132	0.0428682	0.895575	0.104425
Stage4	0.924174	0.0758262	0.824928	0.175072
Stage5	0.875506	0.124494	0.732835	0.267165
Stage6	0.812507	0.187493	0.630733	0.369267
Stage7	0.743124	0.256876	0.535372	0.464628
Stage8	0.678642	0.321358	0.459064	0.540936
Stage9	0.627178	0.372822	0.404946	0.595054
Stage10	0.594616	0.405384	0.373328	0.626672
Stage_11	0.548305	0.451695	0.331414	0.668586
Stage_12	0.486675	0.513325	0.280478	0.719522
Stage_13	0.411481	0.588519	0.224641	0.775359
Stage_14	0.328764	0.671236	0.169839	0.830161
Stage_15	0.247375	0.752625	0.121499	0.878501
Stage_16	0.175495	0.824505	0.0826614	0.917339
Stage_17	0.117736	0.882264	0.0537117	0.946288
Stage_18	0.0747081	0.925292	0.0333093	0.966691
Stage_19	0.0444057	0.955594	0.0194898	0.98051
Reboiler	0.0238945	0.976105	0.0103783	0.989622
Condenser	0.995882	0.00411761	0.989264	

Table 4 : Flow Stream Data Table

- Table shows the fractions of vapor and liquid streams for both the components benzene and toluene for various stages of distillation column. For condenser stream shows the maximum fraction of benzene for liquid and vapor state. For reboiler stream shows the maximum fraction of toluene for liquid and vapor state.

6] Graphical Representation of Flow Stream Data:

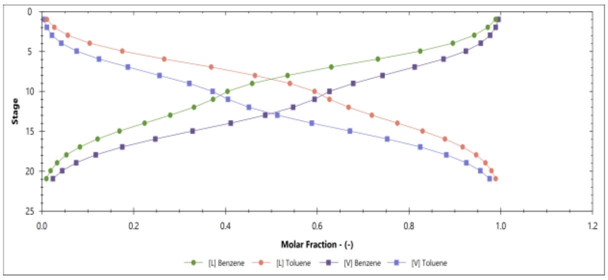

Fig 4. Graphical Representation of Flow Stream Data

CONCLUSION

First case we select the problem for simulation using DWSIM open media simulator mixture of components feed at rate 100 kmol/hr. to the distillation column containing 40 % benzene and 60 % Toluene. Pressure at condenser (T.P.) is 1 atm and Reflux ratio 1.4 times of min. R. R.

By simulating the Short Cut-Distillation column shows the results. Optimal Feed Stage = 09, Actual Feed Stage = 20 (Including Reboiler = 21) and Reflux Ratio = 2.317 and Flow Rate = 100 kmol/hr. These results are used again for feed conditions for rigorous column for optimization.

The simulation results for of Rigorous distillation column.

Results shows the Condenser Duty 1129 KW, Reboiler Duty -1150 KW, Iterations Taken 62, Number of Stages 21, Condenser Pressure 1atm and Stream 'Feed' Stage Index 9. This is clear that the with the help of DWSIM we can optimized the process by simulating using Short-Cut and Rigorous distillation column. Second case we select the problem for simulation using DWSIM open media simulator mixture of components feed at rate 100 kmol/hr. to the distillation column containing 50 % ethanol and 50 % water. Pressure at condenser (T.P.) is 1 atm and Reflux ratio 1.4 times of min. R. R.

By simulating the Short Cut-Distillation column shows the results. Optimal Feed Stage = 09, Actual Feed Stage = 19 (Including Reboiler = 20), Reflux Ratio = 3.9 and Flow Rate = 100 kmol/hr. These results are used again for feed conditions for rigorous column for optimization.

The simulation results for of Rigorous distillation column. Results shows the Condenser Duty 2114 KW, Reboiler Duty -2111 KW, Iterations Taken 17, Number of Stages 19, Condenser Pressure 1 atm and Stream 'Feed' Stage Index 9. This is clear that the with the help of DWSIM we can optimized the process by simulating using Short-Cut and Rigorous distillation column

Applications

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

2. Separation of petroleum products from crude oil 3. Separation of naphtha, Kerosene, diesel, and gasoline etc.

4. For separation of two or more component mixture having different volatilities.

5. Petrochemical industry for separation of multi-components.

6. For the Separation of more than two hydrocarbon mixtures.

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