Deliverable 1

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| To: | Prof. Rivera |
| From: | Jake Albin |
| Date Submitted: | November 18rd , 2019 |
| Subject: | **Final Project** |

# Summary:

This deliverable looks at the scope of work behind designing a column fit for producing styrene. As such, industrial uses and applications of the monomer are discussed. Other literature is reviewed as well, looking at the reaction mechanism and the associated safety data. To run this column, material and energy balances should to solved in addition to equations of state. All of this is investigated within the report. Research into common distillation methods, RADFRAC and DSTWU are reviewed and summarized as well, concluding a look into just the beginning of the project.

# Literature Review:

The main product of this mechanism is the styrene monomer, which has its wealth of industrial uses, markets, and customers. In its purest form, it is considered an important building block of the plastics industry. As such, it’s often used in a wide variety of packaging operations. A list of these uses is tabulated below. [1]

|  |  |
| --- | --- |
| Use | Description |
| Solid & Film Polystyrene | Used in food service containers, CD cases, appliance housings, etc. |
| Polystyrene foam | Found in food service products and building insulation. |
| Composites | Used in shower enclosures, boats, wind turbines, and more. |
| ABS Plastic | Used in medical devices, household appliances, and luggage. |
| SAN Plastic | Found in food containers and optical fibers. |
| SB Rubber (SBR) | Reduces dependence on natural rubbers, increases performance in tires and can improve efficiency. |
| SB Latex (SBL) | Used in paper coatings and carpeting. |

Some data was identified online highlighting the demand of styrene and to what percentage each use makes up the total use of styrene industrially. The co-polymers tab makes up the use for ABS, SAN, and other plastics. This is shown below. [3]

This monomer is so widely used because of its longevity and utility. It’s applications can reduce plant emissions, cushion gear used for military functions, and improve efficiency in other manufacturing processes. It’s this variability that keeps the demand for the product so high. [2]

It’s conventionally made by alkylating benzene with ethylene to producing ethylbenzene. Then, by dehydrating it, styrene is the resultant product. Styrene can be polymerized using standard plastic technology to produce a wide variety of polymers and copolymers. This can be done via batch or continuous processes, oftentimes by mass polymerization or emulsion. These reactions are as follows.

C7H8 + CH3OH 🡪 C8H8 + H2O + H2

C7H8 + CH3OH 🡪 C8H10 + H2O

Where C7H8 is toluene, CH3OH is methanol, C8H8 is styrene, and C8H!0 is ethylbenzene.

To distill crude styrene, a good sum of the attention is focused on keeping the product from polymerizing. Most polymerization inhibitors are only effective up to temperature limits of around 130 ºC, creating a dilemma when investigating process design. Thus, in order to keep the temperature low, several columns often utilize vacuum distillation to accomplish the feat.

Vacuum distillation is often called low temperature distillation because of the aforementioned reason. It works by keeping the pressure in the column below the vapor pressure of the liquid, allowing it to work effectively. There are several advantages of these types of designs in industry. This ideology increases the relative volatility of the components in the mixture. It also prevents the degradation of products because of its low temperature, keeping the purity at a desired level. [4]

There are four different components of this reaction mechanism which have their own safety and toxicity data. Each of these MSDS sheets are highlighted below.

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| --- | --- |
| **Toluene** | |
| Physical State | Liquid |
| Appearance | Colorless |
| Odor | aromatic |
| Odor Threshold | 1.74 ppm |
| pH | N/A |
| Melting Point/Range | -95ºC / -139 ºF |
| Boiling Point/Range | 111 ºC / 231.8 ºF |
| Flash Point | 4 ºC / 39.2º F |
| Evaporation Rate | 2.4 |
| Flammability (solid/gas) | N/A |
| UFL | 7.1 vol% |
| LFL | 1.1 vol% |
| Vapor Pressure | 29 mbar @ 20 ºC |
| Vapor Density | 3.1 |
| Specific Gravity | 0.866 |
| Solubility | Insoluble in water |
| Partition Coefficient | No data available |
| Autoignition Temperature | 535 ºC / 995 ºF |
| Decomposition Temperature | No data available |
| Viscosity | 0.6 mPa.s @ 20 ºC |
| Molecular Weight | 92.14 |

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| --- | --- |
| **Methanol** | |
| Physical State | Liquid |
| Appearance | Colorless |
| Odor | Mild, alcohol odor |
| Odor Threshold | No data available |
| pH | N/A |
| Melting Point/Range | -97.8ºC |
| Boiling Point/Range | 64.7 ºC |
| Flash Point | 9.7 ºC |
| Evaporation Rate | No data available |
| Flammability (solid/gas) | N/A |
| UFL | 35.6 vol% |
| LFL | 5.5 vol% |
| Vapor Pressure | 128 hPa @ 20 ºC |
| Critical Pressure | 79547 hPa |
| Solubility | Solubility in water, ethanol, ether, etc. |
| Autoignition Temperature | 455 ºC |
| Decomposition Temperature | No data available |
| Viscosity | 0.544 mPa.s @ 20 ºC |
| Molecular Weight | 32.04 g/mol |

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| --- | --- |
| **Styrene** | |
| Physical State | Liquid |
| Appearance | Colorless |
| Odor | pungent |
| Odor Threshold | No information available |
| pH | No information available |
| Melting Point/Range | -31 ºC |
| Boiling Point/Range | 145 ºC |
| Flash Point | 31 ºC |
| Evaporation Rate | No information available |
| Flammability (solid/gas) | No information available |
| UFL | 7.0 vol% |
| LFL | 1.1 vol% |
| Vapor Pressure | 7 mbar @ 20 ºC |
| Vapor Density | 1.22 |
| Specific Gravity | 0.906 |
| Solubility | Moderately soluble |
| Partition Coefficient | No data available |
| Autoignition Temperature | 490 ºC |
| Decomposition Temperature | No data available |
| Viscosity | 0.695 mPa.s @ 20 ºC |
| Molecular Weight | 104.15 |

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| --- | --- |
| **Ethylbenzene** | |
| Physical State | Liquid |
| Appearance | Colorless |
| Odor | aromatic |
| Odor Threshold | No information available |
| pH | No information available |
| Melting Point/Range | -95 ºC |
| Boiling Point/Range | 136 ºC |
| Flash Point | 22 ºC |
| Evaporation Rate | No information available |
| Flammability (solid/gas) | No information available |
| UFL | 6.8 vol% |
| LFL | 1.2 vol% |
| Vapor Pressure | No information available |
| Vapor Density | No information available |
| Specific Gravity | 0.860 |
| Solubility | Slightly soluble in water |
| Partition Coefficient | No data available |
| Autoignition Temperature | 432 ºC |
| Decomposition Temperature | No data available |
| Viscosity | No data available |
| Molecular Weight | 106.17 |

# Mathematical Models:

The property method that’s being used for the columns is the Redlich Kwong-Soave equation of state, which is used to accurately describe the liquid and vapor phase. As one might imagine, this is immensely helpful for determining details for both the distillate and bottoms product. The equation looks something like this:

where, and 0.42748))2

also, where Tc is the critical temperature of the component. This can be done for both styrene and methanol in the system.

This equation is a cubic equation because it represents a mathematical, third order polynomial. It suggests that a, an acentric constant, is a function of temperature.

For this system, there are going to be two degrees of freedom, because there are two phases and two components. This assumption is contingent on Gibb’s Phase Rule, which goes as follows:

Furthermore, from the columns, the overall balance is:

F = B + D

From this, a material balance is easily derived:

F\*Xstyrene = D\*Xstyrene,D + B\*Xstyrene,B

The exact same thing can be said for methanol, which is the other component within the system.

The overall energy balance for the column would just be the following:

Where Qr represents the heat from the reboiler and QC represents that from the condenser. All of this is easily computable through aspen and related software.

# DSTWU and RADFRAC:

Each of these concepts are simulative options within aspen plus that can be used for creating a distillation column. Each do things differently and are sufficient for different scenarios.

DSTWU is designed for a single feed, two product process with either a total or partial condenser. For calculations, it uses the Winn, Underwood, and Gilliland shortcut methods to determine stages and reflux ratios. The Winn calculations clarifies the quantity of stages, while the other two investigate the other parameter. Two crucial assumptions are made for the simulation style:

1. Constant molar overflow
2. Constant relative volatilities

From these assumptions and the prior entered data, aspen is able to estimate both the minimum reflux ratio and the minimum number of stages. In addition, it is also able to investigate the proper feed location and to quantify the responsibilities of the reboiler and condenser.

This simulation is very fast in nature, so I may be helpful to run this first to get a quick idea about the behavior of a column before running the idea through a more rigorous model.

As for RADFRAC, is it substantially more complex but can simulate all types of multi-stage column operations. For solids, liquids and gases, it can simulate distillation, absorption, stripping and azeotropic distillation. This makes it very useful for three-phase profiles and systems that exhibit non-ideal behavior. [5]

There are countless other things RADFRAC simulations than investigate as well. It can model systems where chemical reactions are occurring, including equilibrium and rate-controlled mechanisms. It can also factor in the packing of a given column, adding to the complexity of the calculations.

There are two modes for which RADFRAC can utilize. The first, the rating mode, uses specified column parameters to calculate the temperature and flow rate. This indicates that it uses data like heat duties and reflux ratio to calculate the aforementioned data.

The other mode from which this can work is the design option, which allows you to specify the temperature, flow rates, purities, and more to find out the rest of the column information. Obviously, this column is substantially more rigorous in nature.

# Project Management Report:

This project was done large in part on my own, given that I didn’t have a group upon submission.

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| Task | Led by | Total time | Progress |
| Research Material | Jake Albin | 2 hrs | Completed. |
| APEA Simulation | Jake Albin | 2hr | Completed. |
| MSDS Sheets | Jake Albin | 1 hr | Completed. |
| RADFRAC/DSTWU Review | Jake Albin | 2 hr | Completed. |
| Mathematical Models | Jake Albin | 1 hr | Completed. |
| Report Compilation | Jake Albin | 4hr | Completed. |
| Submitting on Canvas | Jake Albin | N/A | Completed. |

# References:

[1] Chevron Phillips Chemical Company, Styrene Monomer, Aromatics. (n.d.). http://www.cpchem.com/bl/aromatics/en-us/pages/styrenemonomer.aspx (accessed November 25, 2019).

[2] Styrene / Polystyrene Uses and Benefits - You Know Styrene, Uses and Benefits Comments. (n.d.). https://youknowstyrene.org/the-styrene-you-know/uses-and-benefits/ (accessed November 25, 2019).

[3] World Styrene Supply/Demand Balance, data provided by IHS, Inc. 14 Jul 2014, see

[http://www.ihs.com](http://www.ihs.com/)

[4] Hazal Öztan Follow, PROCESS DESCRIPTION OF STYRENE PROCESS, LinkedIn SlideShare. (2017). https://www.slideshare.net/Hazalztan/process-description-of-styrene-process (accessed November 25, 2019).

[5] <file:///Users/jalbin/Downloads/Homework%206%20RadFrac.pdf>