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University of Bahrain
College of Engineering
Department of Chemical Engineering

THERMAL CRACKING OF ACETONE: REACTOR SIMULATION AND ANALYSIS USING ASPEN PLUS

Abstract

The purpose of the project is to simulate a cracking reaction using Aspen-plus. Utilizing the plug flow reactor (PFR) system to convert acetone into ketene and methane. Simulations were based under numerous operating parameters. There are seven various cases described in this project. To enhance the productivity of the reactor, all of these systems are discussed in order to derive the best operating case. Based on analysis, the reactor will operate best in the third case, which is surrounded by a heat exchanger with a constant heating medium temperature.

Objective and Motivation

Most students are not exposed to Aspen Plus software which is a very powerful tool to simulate and model the reactions we deal with casually. It can also be used to do sensitivity analysis among many other functions. This skill is required in most chemical engineering practices especially post-graduate applications and during the undergraduate studies. The aim of this project is to simulate and analyze the acetic anhydride reaction in a plug flow reactor (PFR) to identify the most efficient heat transfer scheme for maximizing the conversion, to apply the knowledge of chemical reactions engineering on simulation software and to analyze the reactions and choose the most appropriate operating scheme among different possible cases

Design and Implementation

The simulation consists of 3 main procedures:

1- Setting up the Properties:

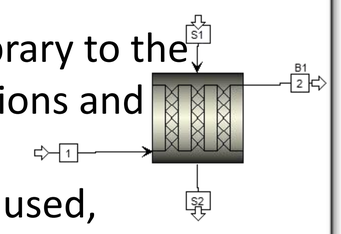
Starting by defining the components and the method to be used such as Equation of States or Activity Coefficient models.

2- Starting the Simulation:

Begin by defining the reactions along with the stoichiometry and entering the kinetic data.

3- Modeling the Flowsheet:

Firstly, add the RPLUG model from the model library to the flowsheet, then enter it and input the specifications and configuration depending on the operating case.

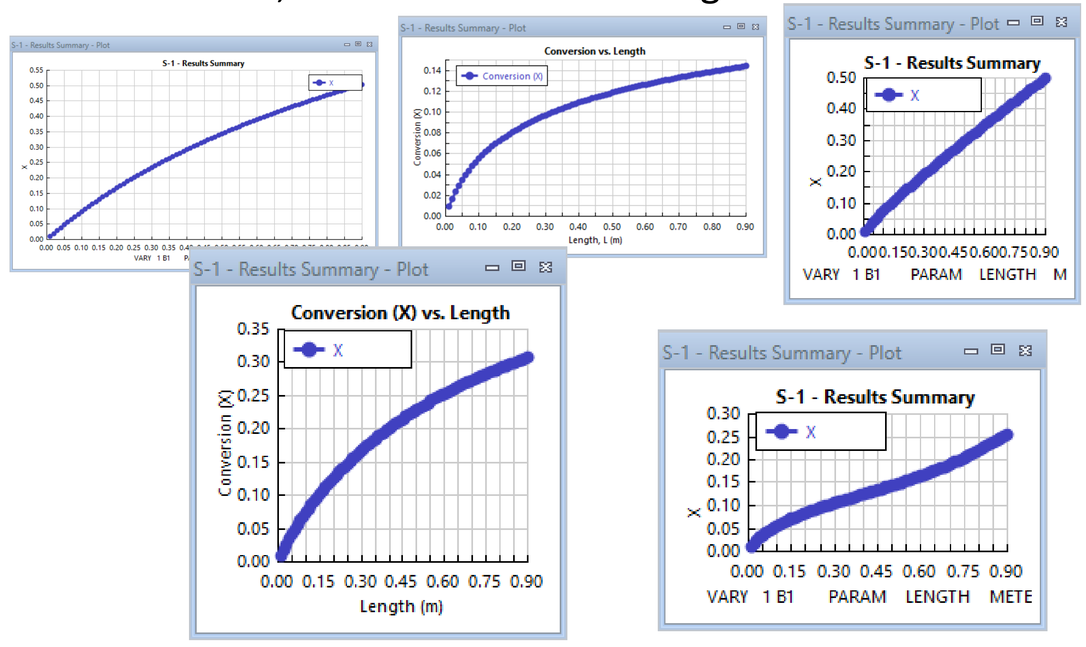


For the analysis, a set of various tools has been used, such as the Sensitivity Analysis toolset, Fortran coding language, Properties Analyzer, and other tools in the software.

Results

For each operating case, different variables where tested and analysed, including conversion, rate of reaction, concentration, temperature profiles along with Localized Heat Absorbed/Transferred and the Duty to name a few.

Plots of conversions to determine the best operating scheme, in order of appearance left to right: (Isothermal, adiabatic, constant thermal fluid, co-current thermal fluid, counter-current thermal fluid. As noticed, the first and third case give the best conversion.



Conclusion

It is possible to operate the reactor under numerous conditions that are based on temperature, thus enhancing efficiency of the reactor. Furthermore, since ketene is noncorrosive, carbon steel is chosen as the material to construct the reactor's piping system. Among the cases, observing all operating conditions for reactor case 3 is the most preferred since in this case, increasing the residence time temp of the reactor increases the conversion obtained.

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