120d - A Dynamic Self-Optimizing PFR Embedded within a Steady-State Process Simulation

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Process simulation software packages often have a difficult time simulating chemical reactors or other unit operations that involve non-linear sets of differential equations, particularly if they are stiff. A solution to this problem is to solve the particular unit operation using a rigorous numerical software approach and then import the solution into the process simulation, usually using the extent of reaction based on the stoichiometry. Here we take a different approach. The process simulator, ChemCAD has an Excel module into which we embed MathCAD using Visual Basics as shown in Figure 1.

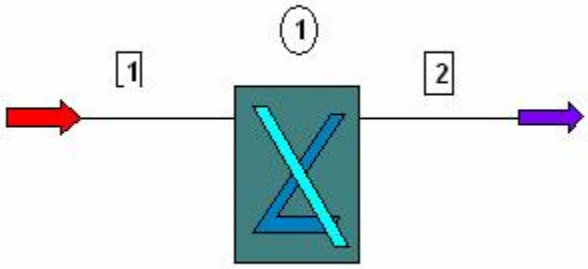

Figure 1. ChemCAD Excel Module Modified by Embedding MathCAD

The MathCAD software solves a system of non-linear differential equations using initial conditions taken from the Excel module of ChemCAD and operates on them. The MathCAD solution is exported to the Excel module and transferred to ChemCAD. The embedded object then acts as part of the system as the process simulator converges; continuously calculating the reactor conversion using MathCAD, each time ChemCAD calls the Excel module. Our ultimate goal is to demonstrate an interface between two fully functioning commercial codes to execute a reactor model that does exactly what we want.

In this presentation, a self-optimizing PFR solved in MathCAD is embedded into a ChemCAD flow sheet. For this simulation, the space-time is calculated to produce a maximum yield of m-Xylene, by the hydrodealkylation of mesitylene over a Houndry Detrol catalyst, and involves the two competing reactions as shown below.

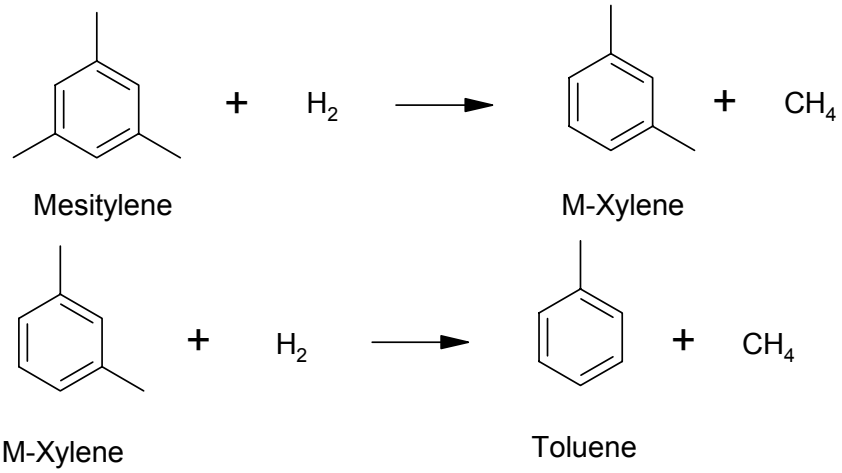

Figure 2. Reaction Network used in the Example, Fogler, 1999.

This example is based on a problem adapted from Fogler 1999, and is presented to show the interface and level of simulation that can be obtained using a well characterized non-linear kinetic model for this particular set of reactions. The purpose of this problem is to maximize the production of m-Xylene by determining the optimum space-time, such that it is fully dependent on the initial conditions in the inlet stream derived from the ChemCAD simulation. From our calculations the following concentrations can be plotted, which allow us to determine the optimum space-time for maximum m-Xylene yield.

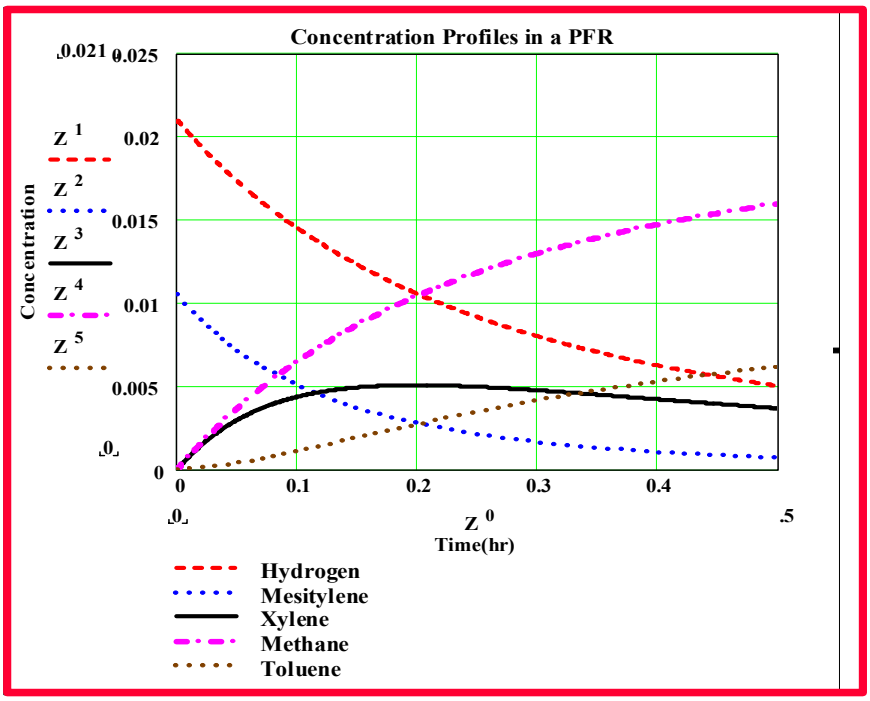

Figure 3. MathCAD Result Available from within the ChemCAD Simulation

Chemstation has recently introduced a new feature into their ChemCAD simulation program. This feature is called the Excel Data Map and permits users to export the stream properties. Some of the available stream data include the average total molecular weight, mass/mole fraction, entropy and many more. Our goal is to export the physical properties of each component from the input stream into the MathCAD program, operate on the equations and export the results to Excel for inclusion in the ChemCAD flowsheet.

This example demonstrates an important augmentation to ChemCAD in that it permits the rapid development of unit operation modules outside of the process simulator that are either not available or proprietary. Others may find this particular approach adaptable to other simulation packages. Using this approach, a system designer can draw on the vast thermodynamic and physical property libraries and existing modules to simulate a chemical system. Specific equipment simulations can now be inserted to decrease development cost for the final simulation.

Reference

Fogler, H. Scott; Elements of Chemical Reaction Engineering, Prentice Hall., Upper Saddle River, N.Y., N.Y, 1999.