Lab 1. Ethylene production by ethane steam cracking

Departamento de procesos y energía, Facultad de Minas, Universidad Nacional de Colombia - Sede Medellín

University of Cambridge

CMCL Innovations

**Objective:** To identify the impact of coke deposition during the thermal cracking of ethane and to develop strategies to counter it.

**Equipment:** kinetics™, Microsoft excel

**Prerequisites:** 🔥 Tutorial 1 and Tutorial 2 of kinetics shared with you on June 14.

**Activities:**

🔥 **Part A.** Addressing the effect of the presence of an inert species on conversion and yield

🔥 **Part B.** Use of temperature to compensate for the presence of deposits in the reactor.

**Report (Use web page: [Link](#))**

🔥 Decide what reactor model to use to represent the industrial production of ethylene

🔥 Plots of conversion and yield for different concentration of inerts species

🔥 Plots that describe the variation of conversion and yield with temperature and cross-sectional area

🔥 Temperature trajectory to counter the effect of deposits on a reactor

**Background**

Ethylene (C₂H₄) is one of the most important chemicals produced worldwide. It is used as a building block for a wide range of products such as plastics, solvents and cosmetics. Ethylene is mostly produced in the petrochemical industry in a process, known as steam cracking, that takes place in a long tubular reactor (around 80 m long) where a mixture of ethane and steam are heated up to temperatures of the order of 650°C. Through reaction
ethane decomposes to form ethylene and hydrogen. A typical Arrhenius expression for the reaction rate of (R1) includes a preexponential factor of $6.013 \times 10^{16} \text{ s}^{-1}$ and an activation energy of 343.088 kJ mol$^{-1}$.

Steam is added to the reactor with a ratio (dilution factor) that typically varies between 0.2 and 1 kg steam/kg hydrocarbons. The steam acts as an inert that slows secondary reactions and enables better control of the reactive flow temperature. The reactor, known to ethylene producers as a “coil”, is located in a furnace with multiple burners that provide the required energy for the highly endothermic cracking reaction.

$$C_2H_6 \rightarrow C_2H_4 + H_2$$

(R1)

An undesirable effect during the steam cracking of ethane is coke deposition on the walls of the tubular reactor. This coke layer, see Figure 1, increases up to a point in which the reduction in heat transfer across the reactor wall is so high that the external temperature of the coil, known as skin temperature, needs to be significantly increased to maintain the required heat flux to the reactor, another related possibility to maintain the required temperature of the process inside the reactor is to increase the initial gas temperature. Either of these two options decreases the thermal efficiency. The reduction in effective reactor volume and, therefore, in space time, as a result of coke deposition also affects ethylene yield and process selectivity. When the skin temperature is too high, above the specifications of the reactor wall, the furnace operation is interrupted and a decoking operation is conducted in which coke is burned off with a controlled air-steam mixture. The operation time before decoking is of the order of 20 to 90 days, depending on process conditions and load. In this laboratory experiment you will simulate a steam cracker and devise strategies to counteract the negative effects of coke deposition.

We will consider an ethane cracking process with a flow of 2025 kg h$^{-1}$ of ethane in a coil that has a length of 85 m and diameter of 0.108 m. Inlet conditions are 1100 K and 2.6 atm.
Note: This laboratory involves a chemical reaction not included in any of the mechanism available in your current version of kinetics™. Therefore, we ask you to follow the next instructions.

Download ethane mechanism file here

a. Open the new project where you expect to carry out the simulations
b. Go to the tab “Import & view Mechanisms” and select the option “import from XML format”, write the name you prefer for the mechanism to be created and then click in tab “select file”, explore in your computer and find the file that was sent to you called “mech_lab2”, click on “Import Mechanism”.
c. If kinetics™ display the message “mechanism imported successfully”, you can create any parent case and link it to the ethane mechanism that you have imported, you can find the new mechanism with the name you chose in step b. in the list of mechanism available.
d. Now you can go further with the rest of instructions.

Part A - Understanding the effect of steam as diluent

To understand the effect of coke deposition on the thermal cracking of ethane, your first assignment is to use kinetics™ to model the reactor before coke deposition takes place. This will be the base case in our analysis. While in a real industrial reactor temperature and pressure change along the coil, to understand the effect of coke deposition you can assume that the temperature and pressure remain constant along the reactor.

1. Select the type of reactor that best simulates the 85-m long coil;
2. Conduct a kinetics™ simulation and determine ethane conversion and ethylene yield at the exit of the reactor when the dilution factor is 0.
3. Repeat step 2 increasing the dilution factor (between 0.2 and 1 kg steam/kg hydrocarbons); you may use the Child Cases features of kinetics™. Notice there are two ways to modify the steam mass fraction at the inlet: either you keep the total mass inflow constant and modify the mass fraction or you can add or remove steam until you reach a desired mass fraction, modifying the total mass entering the reactor. The former maintains the space-time of the reactor approximately constant, but changes the amount of ethane that enters the reactor; the latter
means that the inlet mass flow of ethane will be constant. For this exercise you will use the former.

4. Prepare a plot of ethane conversion (X) and ethylene yield (Y) for different dilution factors;
5. Given the results from step 4, what dilution factor would you recommend to use in an ethane cracker?

Part B - Adjusting temperature to compensate for coke deposition

Coke deposition decreases ethane conversion. An ethane furnace operator has to maintain a constant ethane conversion, despite the formation of coke deposits. This is normally achieved by increasing the ethane input temperature. A rough estimate of coke deposition tell us that the cross-sectional area of the reactor decreases by 20% for every 380 h of operation.

1. Create four Child Cases in kinetics™ where the cross-sectional area decreases, due to coke deposition, to 20%, 40%, 60% and 80% of the clean-reactor value. Make a plot to compare ethane conversion (X) and ethylene yield (Y) at the exit of the reactor for the base and child cases. You may use the same base case used in Part A.
2. For a case without coke deposition, vary the inlet temperature from 900 K to 1300 K (the maximum temperature that the reactor wall can withstand). Plot X and Y vs. inlet temperature. You may use Child Cases here again.
3. From what you learned in points 1 and 2 above, identify a trajectory of inlet temperature that will guarantee the same values of X and Y at the exit of the reactor at 380 h, 760 h, 1140 h and 1250 h of operation.

Report
Complete the lab report [HERE](#)