Ench446: Guide to using CHEMCAD’s kinetic reactor (for version 6.*, aka current version on vcl)

First open up chemcad, as you might have guessed. Like what you would normally do, add all the components you would ever need through the thermophysical tab at the top. Set all your units to the standard (K for temperature, Pa for pressure, s for time, and other SI units). For this guide I will model the “complete” combustion of methane for simplicity with the following (contrived) reaction rate.

\[
CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \quad r = 1 \times 10^5 \times \exp \left( -\frac{200000}{RT} \right) \times P_{CH_4}^{\frac{5}{2}} \quad [\text{moles/m}^3\text{s}] \quad (\text{this assumes the rate constant, } k, \text{ has units that balances everything. I know, very contrived example})
\]

When you first open chemcad, you will get a view like that to the left. To open VBA, where you will enter the rxns, click on the bottom left tab that says ‘Visual Basic’. Then expand the Reactions drop down and double click the RxnTemplate file.

This is the visual basic code for the default rxn rate you will find when you click help on the kinetic reactor (I know like me you are all so excited to see the code behind what seemed to be magic….. or not).
This is the reaction I wrote for the combustion of methane above. To do this I just copy/pasted the RxnTemplate function right below it in the same file. I changed the name at the two areas indicated and deleted most of the other code. Don’t change the parameter list that I circled in red or the name of pRateForm variable because chemcad reference’s this to perform its calculations. You do want to change what the pRateForm is equaled to and this is where your rate equation goes. After you are finished, exit out of the VBA window and refresh the VBA tab.

I just right clicked the reaction tab. After you refresh the reaction you just added should appear. Now add the kinetic reactor with your feed and product streams and your specified feed conditions.

Click on the reactor to get to the specifications window. Fill in your conditions making sure you tell Chemcad you are defining each reaction in the general specifications. In more specifications set the units of your properties and click ok.
Important things to watch out for

- Keep track of units and be consistent!!!!
- For multiple reactions you will need to write a reaction function for each of them
- The help window for the kinetic reactor will explain what is contained in each variable in the parameter list
- If the unit doesn’t converge it doesn’t necessarily mean your equations are wrong (although this could be the case), but maybe that for your specified conditions it couldn’t reach the specified conversion (if you choose this option). Try specifying volume instead, and then adjusting volume as needed until you get conversion you are seeking.
- The C variable contains the concentration/partial pressure of all your components. It is an array that is indexed starting at 0 not 1 like matlab. To be consistent in the kinetic data window, I would list all my components (even the ones that aren’t participating in th rxn) in the same order that I added them and give them the corresponding stoichiometric coeff( 0 when they aren’t participating). This is just so when you are writing your reactions you can be sure that C(0) corresponds to methane as is the case for my example.
- It will be frustrating at times but as engineers you will be expected to be able to learn how to use software to solve problems and this is a very good example. So keep on keeping on.
- Come to office hours/ email peeps if you need help (yea I said peeps).