Cover Letter:

Non-linear Optimization and Control of a Plug Flow Reactor (With a Complex Reaction)

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The modeling of reactors has always been a significant and important skill for chemical engineers Depending on the reaction and demands set, this can be a simple or complex task. There are many complex and non-linear equations that are tied together in a reactor model that demand very vine-tuned parameters in order to converge. This project goes through this demanding process of modeling a plug flow reactor with a complex reaction. There are not numerous sources or examples that cover this topic so this paper should be a good source. The complex reaction is the decomposition of acetone into ketene and methane. The unstable ketene also decomposes into carbon monoxide and ethylene. This reaction brings a complex nature since ketene is a desired reactant in many other reactions. Obtaining a maximum amount of ketene from this reactor is what the optimizer will attempt to achieve.

Main Contributions and Takeaways:

- Model built in both scipy and gekko of a PFR with a complex reaction
- Analysis shown on what key parameters affect a PFR with a similar reaction
- Analysis of techniques and methods to use to begin the optimization process
- The optimization itself of the PFR model
- Common problems to avoid and keys for successful model building and optimization of reactors.

Introduction

Modeling reactors is a staple procedure for all chemical engineers. It is one of the many competencies that belong only to chemical engineers due to the wide array of topics that is brings in. Topics include reaction kinetics, thermodynamics, heat transfer, fluid mechanics, and often separations. This paper only focuses on the kinetics, thermodynamics, and heat transfer of design a reactor. Fluid mechanics can be a huge portion of model designing since stirring is a complex and important phenomenon for CSTR's as well as pressure control for PFR's. Separations can also be involved if the reaction produces multiple phases, and the separation of these phases are favorable.

There is a three-step process in order to model and then optimize a reactor. First is the simulation of the model using physics-based principles as well as initializing the variables. This can either be the longest or shortest step. Depending on the desired complexity, a model can be based on about 5 or 6 variables and parameters, or it can be about 30. This model had a whole portion of calculating the overall heat transfer coefficient until it became too hard on the optimizer. There are many complex equations and relationships that go into finding every variable so determining the level of complexity for a model is important. The next step is a sensitivity analysis on the model with a change of inputs. This can be done in multiple ways such as a moving horizon estimator, looping through the model with a set change of inputs, or even a guess and check can work. This part can save a lot of hard work and frustration in the optimization portion if the estimations are precise and how good analysis. The last part is the optimization which includes adjusting parameters to maximize a desired product. This is very involving since a lot of tweaking needs to be done in order hewn in on the desired value.

Theory

This reaction contains one primary reaction with a side-reaction after one of the products is formed. The first reaction is as followed:

$$C_3H_6O \rightarrow C_2H_2O + CH_4$$

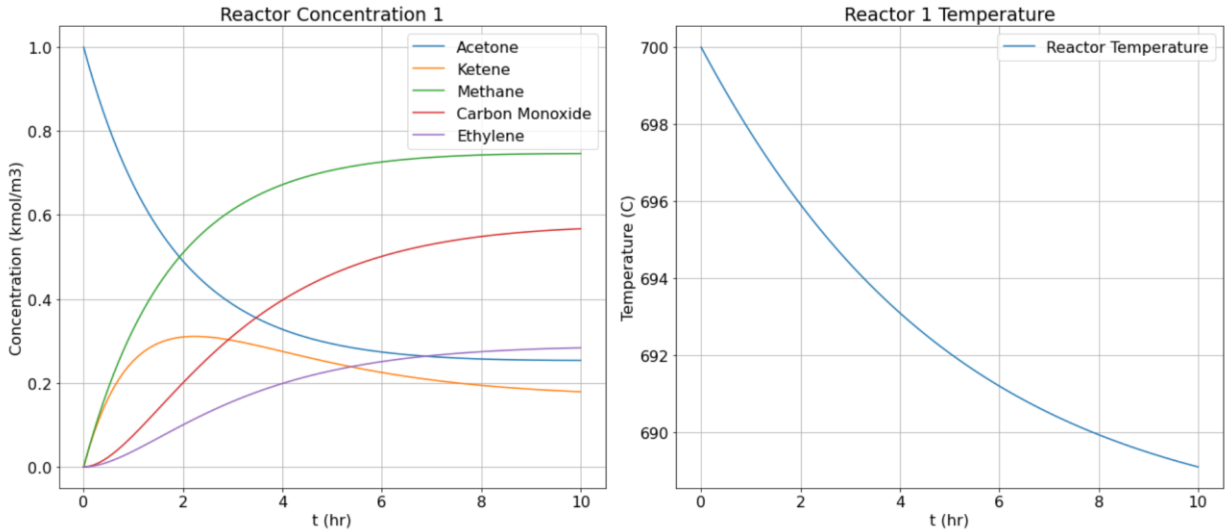
Methane and ketene are both produced with one mole to each mole of acetone. This is a rather simple reaction that gets much more complicated as the other reactions begins.

$$C_2H_2O \rightarrow CO + \frac{1}{2}C_2H_4$$

As ketene is formed, it also decomposes into carbon monoxide and ethylene. Each reaction just needs the one reactant to occur since both are decomposition reactions. This fortunately makes the rates of each reaction very simple where it could be much more complicated like if a catalyst were present. The complex part of this model is found in attempting to maximize ketene as it is being decomposed. Which temperatures and flowrates are needed to achieve that balance and flexibility? How the reaction works and its nuances should be the main priority while the model is being built since it governs how values change.

Simulation

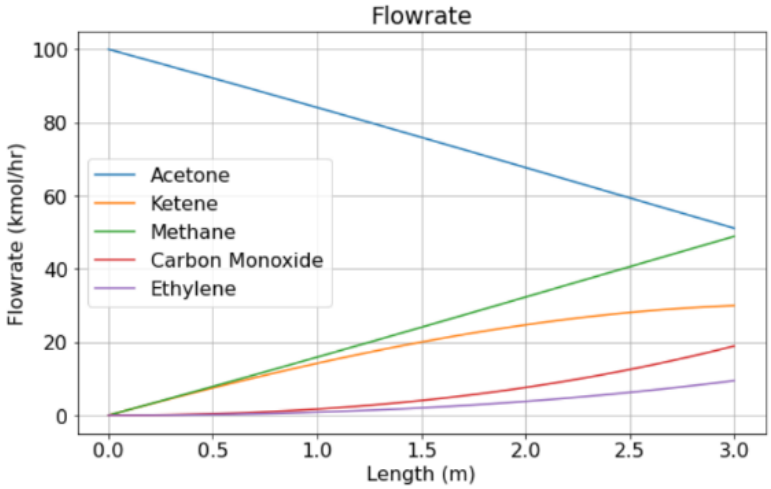
This simulation model is based on multiple reactions occurring in a Plug-Flow Reactor. This is the reactor of choice since all the species are gas and temperature control is easy enough in this case. We also want to take advantage of taking the mixture out of the reactor quickly to minimize the product of unwanted by-products. Extensive amounts of time were used in modeling the CSTR model as with this reaction since at first the PFR model seemed to complex. The model assumed unsteady state as well as some initial conditions for the reactor. The results are below.

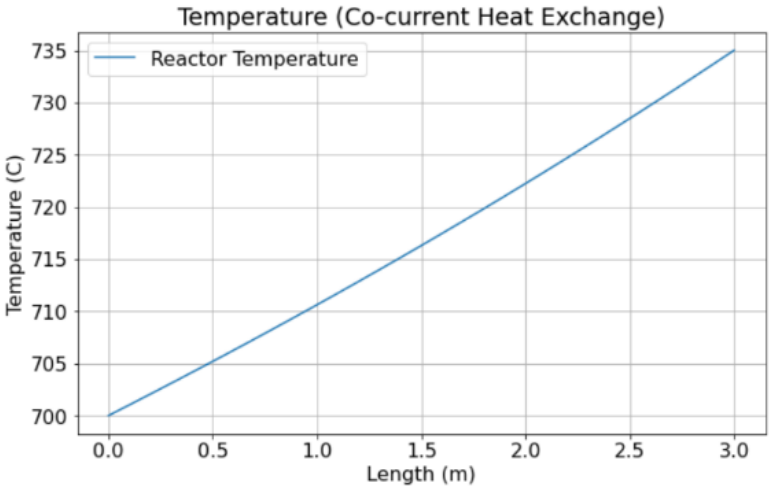


This model shows the weakness in a CSTR since the steady state value will converge to a lower composition of ketene than what is desired.

So the preferred model of choice is the PFR. This PFR with have a cooling method since high temperatures will cause Ketene to decompose into Carbon Monoxide and Ethylene. Will all of that said, the following variables are listed below:

Constants	Variables	Fixed Values	Manipulated	Controlled
Hf,	Fa	Fa0	Ta	Cb
U	Fc	T0		T
A	Fd			
Ea	Fe			

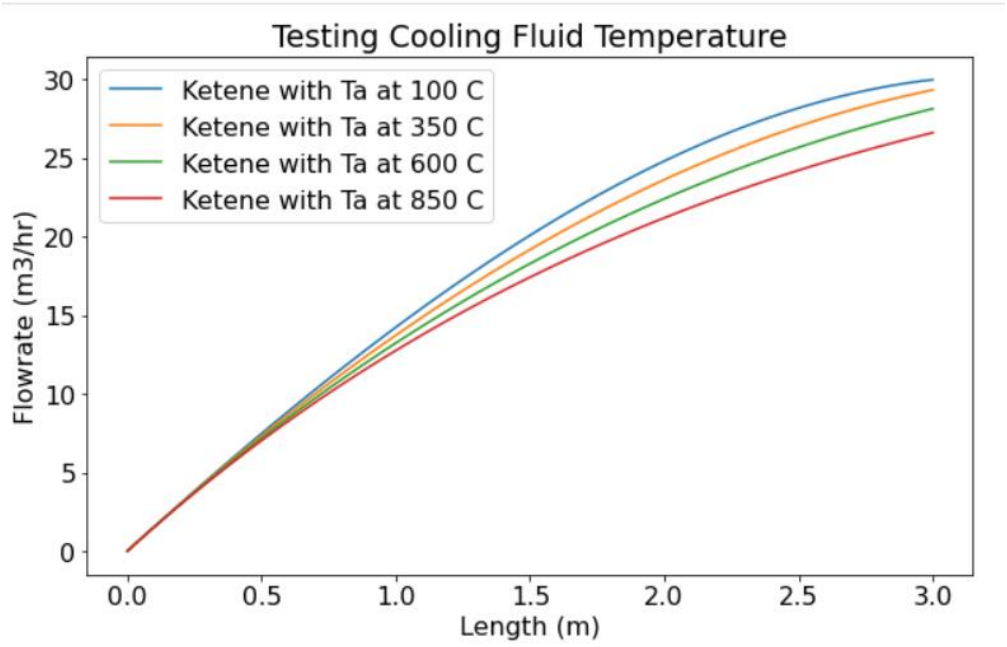




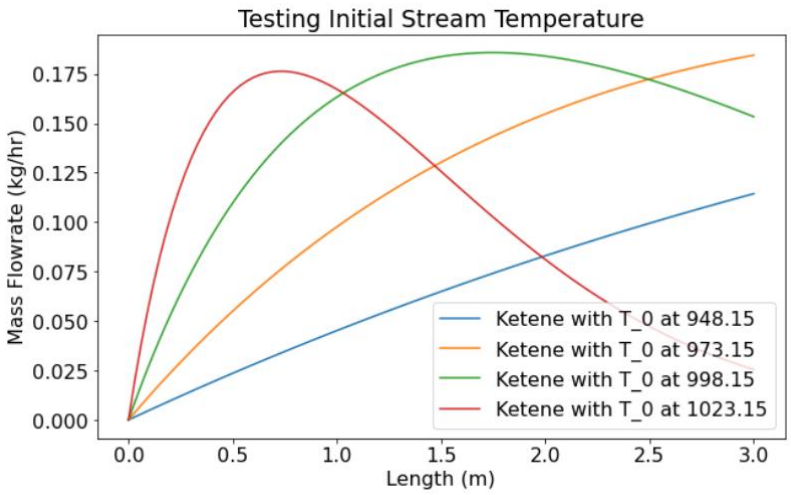
On the left is shown Figure 1 which are the simulation results. We based this model off of a HYSYS simulation to hewn in better on values such as overall heat transfer coefficient. Even in this first simulation, the results are promising and fairly optimized already. A yield of about 30 kmol/hr is fairly high in this case and it might be difficult to optimize it even further.

Estimation/Sensitivity Analysis

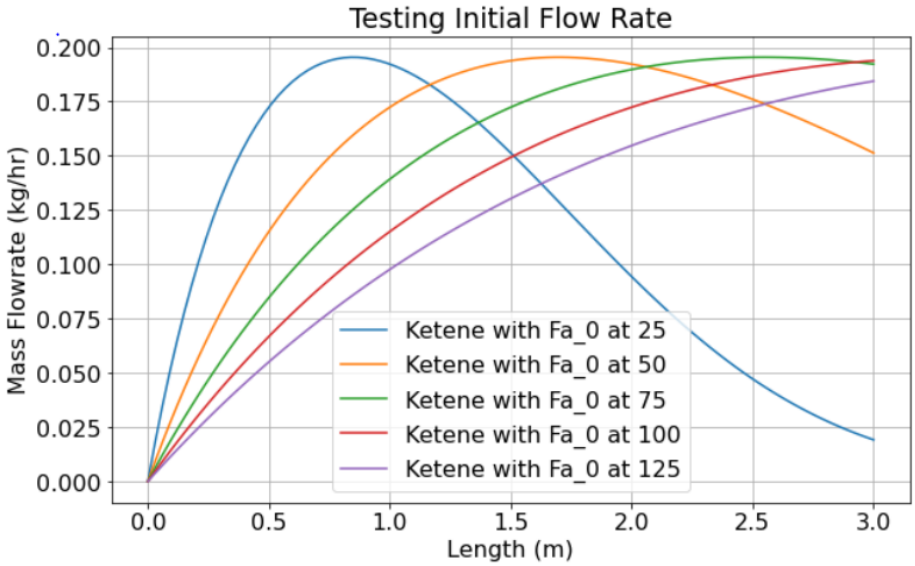
For this model, many of the parameters were known are should just be chosen. Having that in mind, it felt better to focus on the sensitivity aspect of our controlled variables and determine which parameters effect the most. There are three figures that are tell a different story in how concentration of Ketene can be maxed. Below is the figure showing varying cooled fluid temperatures. This cool fluid is low-pressure steam. Since the reaction is running at such a high temperature, steam can be used as a coolant. In this case, there is actually very little change in yield as the cooling temperature changes drastically. This shows that this would not function very well as a manipulated variable in order to control the reaction



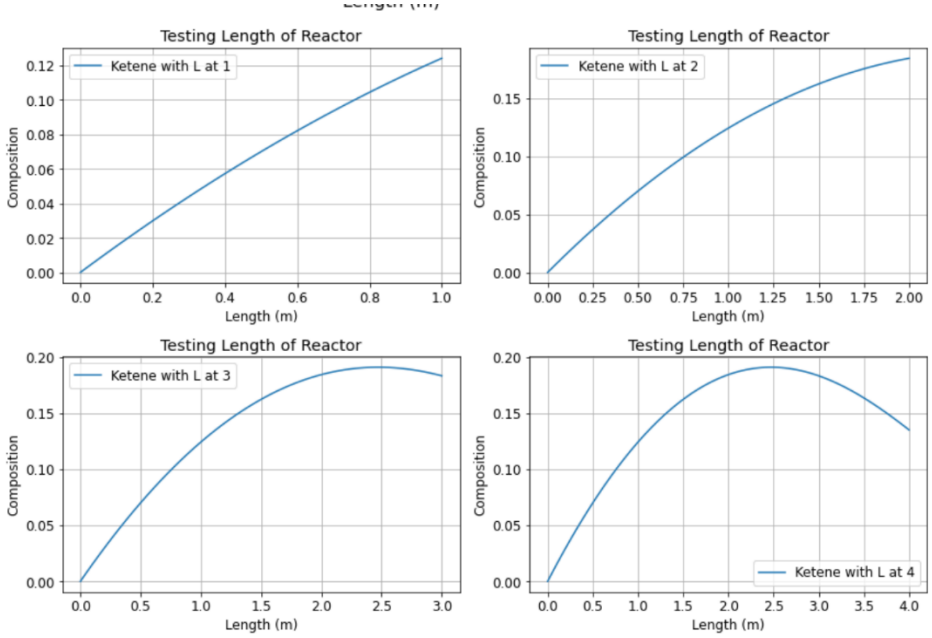
The next figure shows plots that vary by changing the initial steam temperature. Here it is shown that Ketene is drastically changed by these adjustments would play a huge role in controlling ketene if it was used. This makes sense because initial streams temperatures act as a beginning trajectory and therefore heavily influence the other streams and quantities near it. In the figure below, it shows that a starting temperature of about 700 C would product the best yield and that is already what the stream is setup to be.



The next figure shows the curves of adjusting for initial flow rate of acetone in the feed stream. Since Acetone is the only reactant entering the system, it is a very important variable to consider as it starts the whole reaction. Maybe, this flow rate would be able to change dynamically but in general it is just to be picked as a fixed value. Looking at this graph, it is clear to see that around 80 to 100 shows to produce the right amount of ketene. The other's curves start off tall and then find themselves disappointed at the result.



The last figure shows how the length of the reactor can affect the overall production of ketene. This shows that the length of the reactor has an optimal value found between 1 and 4 meters given the other parameters are constant. This shows us that the length should be around 3 to 4 in order to achieve the optimal result.



Optimization

For this model, the overall objective was to maximize the composition of Ketene coming out of the reactor. We saw in the estimation report that many parameters will adjust this level. The parameters of focus to optimize the composition of Ketene will be length/volume or reactor, and the overall heat transfer coefficient. The volume and length of the reactor is a parameter in this model since this would be a model to use for the design of a reactor. This optimization will help the design to find out the optimal size of the reactor. The overall heat transfer coefficient is a parameter that could change before a design and after. This coefficient is affected by many variables such as material, flowrate, type of coolant. A later optimization model could be used to optimize the flowrate for an existing reactor that has already been built. In that case, optimizing ketene production would be through adjusting parameters that are easy to change during production. Some variables include initial flow rate, initial temperature, and temperature of cooling fluid. This model was prepared to handle both cases but after countless revisions, it seemed unnecessary and challenging to achieve.

The optimization worked in the end but not without work and struggle to go with it. Due to the number of equations and their complexity, the optimizer had a hard time converging onto an answer at times. There are many controlled variables such as multiple species and temperature, as well as many manipulated/fixed variables to adjust. The method that made it simpler and easier for the optimizer was by adjusting the COST for the flowrate of ketene and messing with the bounds for many if not all variables. A common problem that arose was the optimizer would simply find a solution where the variable was on a bound. Adjusting those bounds was tricky since some had obvious bounds while others were unknown. This figure below shows plots of each species composition before optimization.

```
Coolant Temperature: 397.15 K
Volume of Reactor: 3.927 m3
Length of Reactor: 5.000 m
Overall Heat Transfer Coefficient: 53125.0 kJ/m2-K
Composition of Ketene: 0.10368685848
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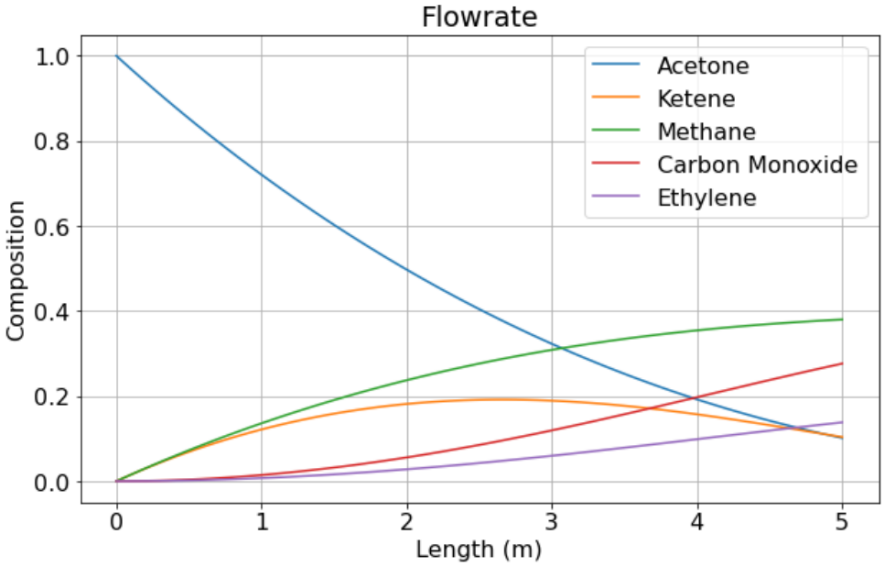

The unoptimized values for each variable to adjust are shown above on the graph (volume and length are connected). We can see on the graph that there is room for improvement. There is a part where Ketene composition peaks at about 2.8 m and the optimizer should adjust for that. The other dance that the optimizer will have to do is the balance between coolant temperature and overall heat transfer coefficient. Both affect one another and it may complicate the optimization. If economics were involved, then extra weight could be added to prefer one method over the other. After much (and I mean a lot) configuration and testing, the optimization was found. In the figure below shows the optimization results.

```
Optimized Coolant Temperature: 120.000 C
Optimized Volume of Reactor: 3.508 m3
Optimized Length of Reactor: 4.467 m
Optimized Overall Heat Transfer Coefficient: 19650.000 kJ/m2-K
Maximized Composition of Ketene: 0.19409901292
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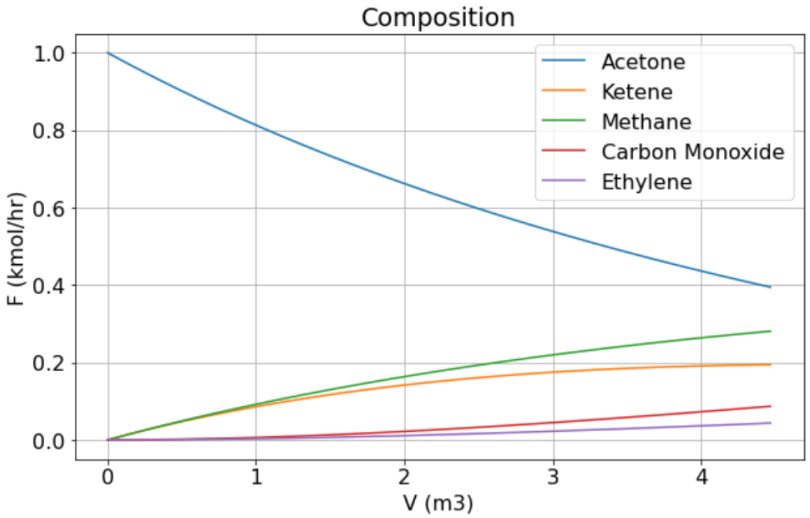

Sometimes the model had a hard time optimizing and the values would end up on the bounds even though it produced a less optimal result. Moving through the bounds with a loop proves this phenomenon since a parameter would optimize to a higher bound where a lesser value would have been more optimal. More work would have to go in to determine the cause of this and place realistic bounds. But overall, this figure shows that it is possible to optimize and find the precise parameters for a reactor.

Conclusion

Overall, this model and project showed the complexities of modeling reactors with many parameters and variables to adjust. The model must be accurate enough to a point to allow the optimizer to do the work to reach the desired yield. This report goes over the simulation of this model as well as the sensitivity analysis attached with the model. The optimization was able to find the parameters to maximize the yield of ketene as it came to a mole fraction of .194, which is a great bit higher than the .103 that it originally was.

Appendix Below