PROCESS MODELING USING OPENMODELICA
SUMMER INTERNSHIP 2025 REPORT

UNDER

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Submitted by

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Contents

Chapter 1

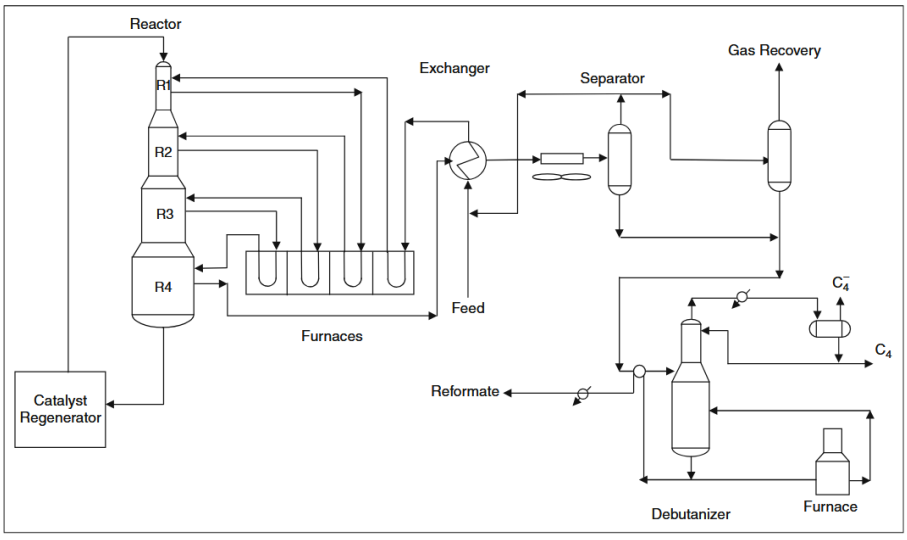
Introduction to Continuous Catalytic Reformer

1.1 Overview of CCR

The Continuous Catalytic Reformer, CCR is a technology used to performing Catalytic Naphtha Reforming. It is the best possible available technology to do Naphtha Reforming, it gives superior quality products than its competitors, Semi Regenerative Catalytic Reforming (SRCR) and Cyclic Regenerative Cataylic Reforming (CRCR).

The CCR carries out the most fundamental process in oil refining, which is the conversion of low octane number (ON) gasoline, to higher octane number gasoline [1]. The advantage of increasing ON of gasoline is that it burns cleaner with very little pollution, which is desired [2]. Apart from that, the CCR process is also responsible for providing a very clean source of Hydrogen (95%). Sometimes when a CCR cannot satisfy its demand of Hydrogen, external Hydrogen generation is involved. This is very expensive. Hence, increasing the 'internal' generation of Hydrogen in CCRs can reduce the cost, and reduce the overall carbon footprint.

1.2 Process carried out in CCR

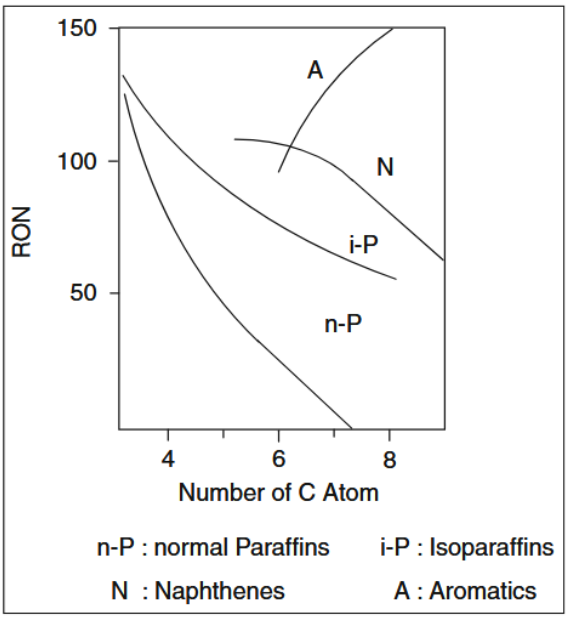


It is the conversion of C_7 - C_{10} with low octane numbers to aromatics, paraffins and iso- paraffins with high Research Octane Numbers (RONs). It

is a highly *Endotermic* Process which requires a lot of supply of energy. The feed consists of Heavy Treated Naphtha. It is distillated into Light Naphtha and Heavy Naphtha. The Heavy Naphtha consists of C_7 - C_{10} and is fed to the CCR, which is the beginning of the reforming process.

The catalyst used in CCR process is a bifunction catalyst consisting of a platinum metal on chlorinated alumina. There are several reactions which occur in this process, all of them are organic reactions. The fastest reactions such as paraffin isomerization and naphthenes decomposition occur in the top part of the CCR, where as slower reactions take place in the bottom part. A continuous heat supply is employed to the CCR reactors because the reactions are highly endothermic in nature and require constant heat supply.

The relation of Number of hydrocarbon vs RON according to the nature and characteristics is given below.



Here we aim to achieve the maximum RON through reforming process in Continuous Catalytic Reformer.

Chapter 2

Literature Study

My approach towards modeling the CCR involved referring research papers and listing down key findings from each. They helped shape my thinking and gave a starting point. I shall list the key findings and summarize what I learnt exactly from each research paper.

Fahim, M.A., Al-Sahhaf, T.A. and Elkilani, A. (2009) Fundamentals of Petroleum Refining. Elsevier.
Key findings:

- The characteristics of feed entering CCR. It consists of Heavy Naphtha since the light Naphta undergoes isomerization and removal of C_6. The heavy naphtha is then processed in the CCR.
- The reactions undergone in CCR. They consist of dehydrogenation of cyclohexanes, paraffin dehydrogenation, dehydrocyclization, isomerization. Isomerization occurs fastest, hence it takes place in the topmost reactor. Reactions such as dehydrocyclization take place very slowly, hence they take place in the lowest reactor. This paper also stated background on reaction kinetics
- Information about the catalyst. The catalyst is bifunctional, consisting of platinum metal on chlorinated alumina. Some reactions use the platinum metal site, such as dehydrogenation reactions. Some reactions such as isomerization reactions use the chlorinated site
- This book helped build the fundamental chemical understanding required to begin modeling from first principles.

Polovina, S. et al. (2018) 'Modeling a Reaction Section of a Commercial Continuous Catalytic Reformer', 32(5), pp. 6378–6396. Available at: `https://doi.org/10.1021/acs.energyfuels.7b03897`.
Key Findings:

- The improvement of Naphtha Reforming process. First it started with Semi-Regenerative catalytic reforming (SRCR), CRCR (Cyclic- Regenerative Catalytic reforming) and CCR (Continuous Catalytic Reforming). All of them have one aspect in common, improvement of yield by avoid catalyst coking. The CCR has the least catalytic coke deposition which keeps the yield higher.
- Process description. The explanation of entire CCR process, this helped me gain a deep understanding of the process. I aim to model the moving bed radial flow reactor.

- This paper helped contextualize the industrial importance and benefits of using a CCR over other methods.

Vathi, G.P. and Chaudhuri, K.K. (1997) 'Modelling and simulation of commercial catalytic naphtha reformers', The Canadian Journal of Chemical Engineering, 75(5), pp. 930–937.
Key Findings:

- The paper presents an early model for catalytic reformers, focusing on industrial scale implementation and practical considerations.
- It uses simplified assumptions to model the reaction network and reactor behavior using available plant data.
- It provided insight into how older methods approached reactor modeling with limited computational resources.

Iranshahi, D. et al. (2014) 'Modeling of naphtha reforming unit applying detailed description of kinetic in continuous catalytic regeneration process', Chemical Engineering Research and Design, 92(9), pp. 1704–1727. Available at: https://doi.org/10.1016/j.cherd.2013.12.012.
Key Findings:

- A comprehensive description of the method used to model the CCR. The paper proceeds in making a kinetic model in the beginning. The kinetic model consists of a reaction network. The network has 32 components and 85 reactions. The stoichiometry of the components have been taken into account. This increases the accuracy of the results
- 2D equations of heat, material balance and pressure drop is given. This helped obtain an understanding in the radial and the axial direction of the moving bed radial flow reactor. It also gave rise to a comprehensive catalyst deactivation model.
- A small description of the method of solving of equations. The method applied to solve equations in this paper is finite difference method. The equations are integrated through each reactor to describe the molar flow and physical properties along the length and breadth of the reactor
- This was the most critical paper for my modeling work and served as the basis for my reaction network and equations.

Mahdavian, M., Fatemi, S. and Fazeli, A. (2010) 'Modeling and Simulation of Industrial Continuous Naphtha Catalytic Reformer Accompanied with Delumping the Naphtha Feed', International Journal of Chemical Reactor Engineering, 8(1). Available at: https://doi.org/10.2202/1542-6580.1859.
Key Findings:

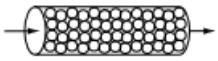
- This paper was put in reference by the above paper. It consists of equations of the CCR in 1D. Since this was less complex, I chose to study this paper for the heat and material balances equations in 1D.
- The paper considers less components and equations hence I chose to stick to the above paper for reaction kinetics and study.
- I learned the representation of mass and energy balance equations in 1D. Since they were in 1D, they were reduced from a PDE to ODE and involved only the axial direction.
- The paper ignored catalyst deactivation model due to axial consideration only, in the axial direction the behavior of catalyst is approximated to be the same.
- It helped me identify which modeling assumptions were reasonable for simplification without large accuracy loss.

Chapter 3

Modeling of a CCR

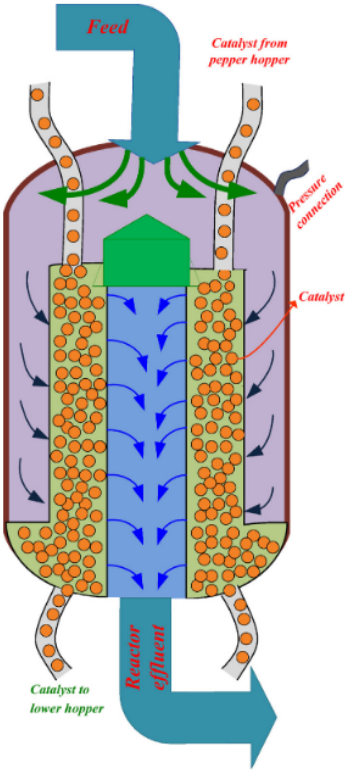
3.1 Process

My initial week after understanding the CCR was a modeling. I did brainstorming, referred to research papers I have stated in my literature study and tried to find methods which I could use for modeling the CCR. I referred back to my knowledge of Chemical Reaction Engineering. In the course, I was taught about Plug Flow Reactors, Packed Bed Reactors, and Continuously Stirred tank- reactor. After reading about CCRs, and PBRs. I figured if CCRs could be modeled as a packed bed reactor as the diagram of a PBR look like this:



PBR Results

In case of a PBR, The inlet stream goes from the top and the outlet stream leaves from the bottom, which is similar to the behavior of a CCR. The Structure of a single CCR reactor looks like this:



There is a catalyst stream which enters from the top and settles into

spaces in the reactor. Inlet feed is dispersed and it moves through the catalyst causing faster reactions and then the reactor effluent is collected. This process is done 4 times (in 4 reactors). Hence, I aimed to model only one reactor in CCR unit successfully, after which the other 4 would be modeled automatically.

Looking at the above two diagrams, I figured the CCR could be approximated to a PBR and continued with the modeling of a *CCR using a PBR technique*. Based on this thought, my literature study resumed and I found very helpful research papers which did the modeling using modelling softwares such as *Aspen and AspenPlus*, some did the modeling using *MATLAB*

3.2 Challenges Faced

The modeling technique given in Research papers included 2D modeling of a CCR. The models took into consideration, both the horizontal and vertical changes, which made the equations fairly complex. To avoid the extra complexity, I referred research papers which depicted 1D modeling of a CCR using PBR technique. That was the starting point, after which I proceeded to OpenModelica modeling of a CCR. I used 1D equations referred in [8]

Chapter 4

Open Modeling in OpenModelica

4.1 Setup

The reactions and equations were in place, after which I could start writing the code for the modeling in OpenModelica, an open-source causal modeling software. The equations I used are listed as follows:

$$\frac{dF_i}{dw} = \sum_{j=1}^{85} r_j \cdot (StCo)_{j,i}, \quad i = 1to32 \tag{4.1}$$

This equation depicts the flowrate of component i after all the reactions have been carried out. There are 32 components and 85 reactions in the model I have considered. It is the *material balance equation*.

To account for temperature and pressure drops, I used the following equation:

$$\frac{dT}{dw} = \frac{\sum_{i=1}^{85}(-\Delta H_i) \cdot r_i}{\sum_j F_j C_{p_j}} \tag{4.2}$$

The temperature equation accounts for the change in enthalpies for all 85 reactions and the heat capacities of the molar flow rates.

The research paper which I have used to get all the equations is *Modeling and Simulation of Industrial Continuous Naphtha Catalytic Reformer Accompanied with Delumping the Naphtha Feed*.

Simulation Setup

- Model used: `DASSL`
- Tolerance: `1e-6`
- Start time: `0`
- End time: `500`
- Time interval: `0.002`

4.2 Process

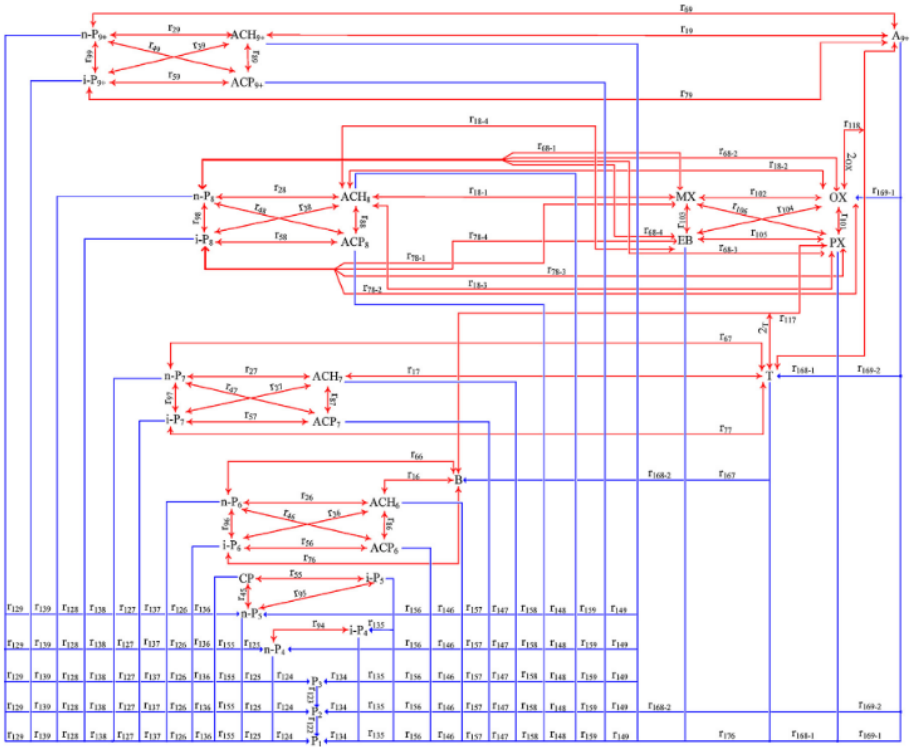


Fig. 2 – Reaction network scheme for naphtha reforming process.

In my first task, I recorded the data given for the reaction network. For reversible reactions, reaction constant, and equilibrium constant parameters were given. For the irreversible reactions, reaction constant parameters were given. I made a 85x32 stoichiometric coefficient matrix to record for the moles of the component in each reaction. If the components were the reactants, they were assigned with a (-) sign, if they were the products, they were assigned with a (+) sign.

Secondly, in the *equation* section in OpenModelica, I calculated the Reaction constants and equilibrium constants for all the reactions, which enabled in finding the rates. Thus, all the 85 rates were found and I could proceed with the modeling of the reaction.

The rates were calculated using the partial pressure technique. Initially I assumed a mole fraction quantity of the components. In the calculations, the mole fractions were expressed as

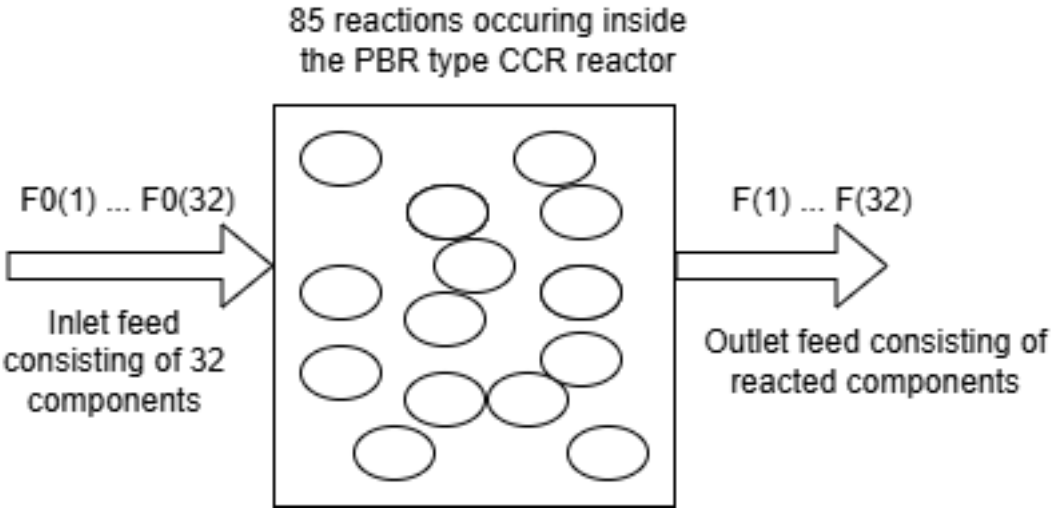
$$\frac{flowrateofcomponent}{totalflowrate} \tag{4.3}$$

Hence the final rate equation I used in all the calculations is:

$$r_i = k_i \left(\frac{F_i}{\sum F_i}\right)(P)^{StoCo(product)} - \frac{\left(\frac{F_i}{\sum F_i}\right)(P)^{StoCo(reactant)}}{K_i} \tag{4.4}$$

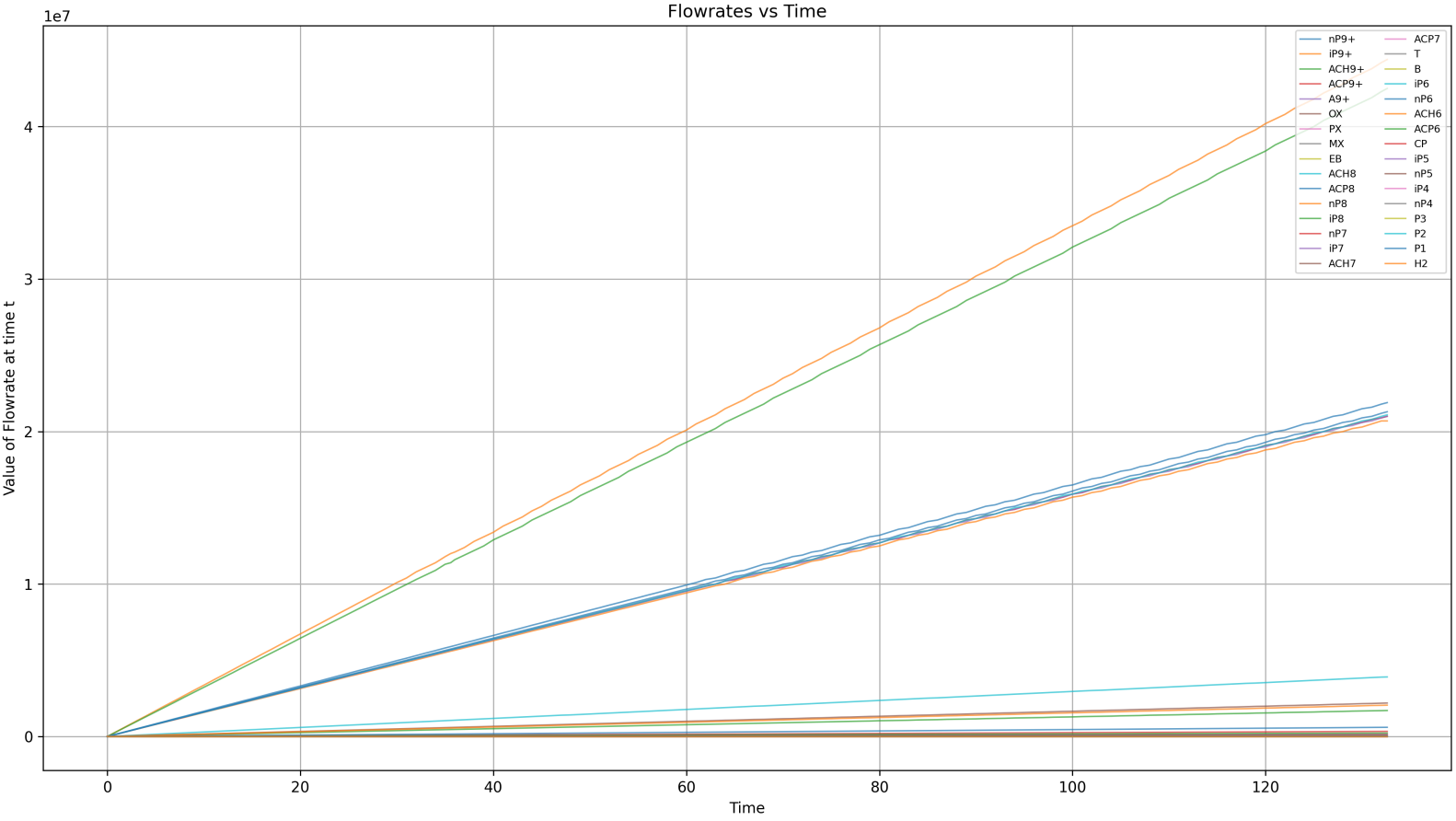
Now after inputting all the parameter I was able to finally code all the equations in the *equations* section.

Next I had to decide the parameter on whose basis the temperature, flowrate and pressure will be calculated. Normally, openmodelica calculates parameters based on the time. The parameters had to be tweaked in the simulation setup, so that they represented the weight of the catalyst. The simulation ended based on the z value, which is the area of cross section of the CCR. As soon as the area crosses the total area, the simulation ends.



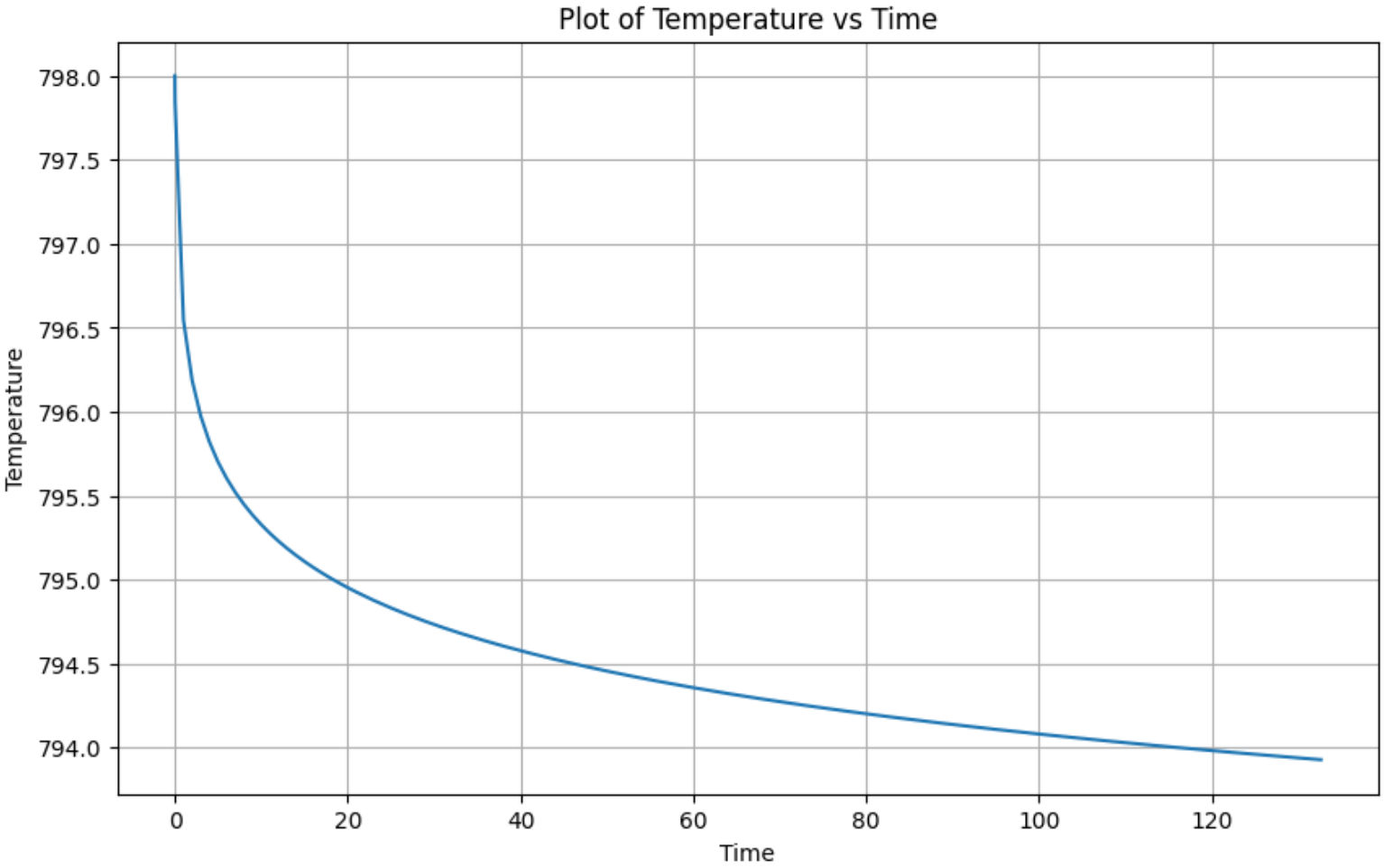
This is the basic diagram of the modeling of a CCR, I have adapted in the steps above.

4.3 Results



The result obtained is Flowrate of all the praffins, naphthenes, olefins present in the inlet feed, and the number of carbon in each. By observation in the diagram, it is clearly visible that the higher carbons are forming more and the lower carbon concentration is reducing as the feed is going through the reactor. Thus the aim we set out to achieve, conversion of lower number carbon to higher number carbon, is successfully achieved. Lower number carbon is consumed and higher number carbon flowrate increases. It is also observed that the Hydrogen concentration increases too. This is one of the aim of a CCR, and it fulfills the role of *CCR as a main source of clean hydrogen.*

Thus, the flowrates and their characteristic plots check out with the theory of CCR



Since I have considered radial model only, there is very little temperature drop. Actual temperature drop occurs when the stream moves axially across the reactor. The axial temperature drop occurs due to the endothermic nature of reactions. Radial pressure drop is, it is lower at the walls and higher at the centre. In contrast, radial temperature gradients are relatively small and often neglected in simplified models. Regarding pressure, the radial pressure profile shows higher pressure near the center of the reactor and lower pressure near the walls, which is a typical characteristic due to flow distribution and wall friction effects.

The link to the entire code file with all the references is given here

4.4 Code Snippet

```
equation
  der(z) = 0.01;
  for i in 1:m loop
    k[i] = (a[i] - E_R[i]/T);
  end for;
  for i in 1:rev loop
    K[i] = (A[i] - B[i]/T);
  end for;
  for i in 1:n loop
    molarfracs[i] = max(0,(F[i]/flow_rt));
  end for;
  sum_molar = sum(molarfracs[i] for i in 1:n);
  for i in 1:rev loop
    r_forward[i] = product(if final_stoco[j,i]< 0 then
       (molarfracs[j]*P)^abs(final_stoco[j,i]) else 1.0
       for j in 1:n);
    r_reverse[i] = product(if final_stoco[j,i] > 0 then
       (molar_fracs[j]*P)^final_stoco[j,i] else 1.0 for
       j in 1:n);
    rate[i] = k[i] * (r_forward[i] - (1 / K[i]) *
       r_reverse[i]);
  end for;
  for i in rev+1:m loop
    r_irrev[i - rev] = product(if final_stoco[j, i]<0
       then (molarfracs[j]*P)^abs(final_stoco[j, i])
       else 1.0 for j in 1:n);
    rate[i] = k[i] * r_irrev[i - rev];
  end for;
  for j in 1:n loop
    der(F[j]) = if F[j]<=0 then 0 else
       sum(final_stoco[j,i]*rate[i] for i in 1:m);
  end for;
  flow_rt = sum(F[j] for j in 1:n);
  // implemented the energy balance equation
  der(T) = (sum(rate[i]*(dH[i]) for i in 1:m)/
     sum(F[j]*cp[j] for j in 1:n));
  when z >= area then
    terminate("Reached end of reactor.");
  end when;
```

Listing 4.1: OpenModelica code for mass balance

Acknowledgments

Through this internship, I strengthened several concepts and learned how to apply classroom concepts in real world modeling. This expanded my thinking and made me proficient with Chemical Reaction Engineering and Thermodynamics concepts.

The use of open source softwares was new to me. I have always used Python, Matlab for performing programming tasks. But, using tools like DWSIM and OpenModelica for my internship expanded my knowledge in causal modeling and flowsheet making.

I would like to express my sincerest gratitude to Prof. Kannan Moudgalya for providing me an opportunity to work under his guidance and supervision. I would like to thank Mr. Priyam Nayak for his continuous support. He guided me through the entire internship and helped me whenever it was required. I would like to thank the Spoken Tutorials community for such helpful tutorials on DWSIM and OpenModelica. Lastly, I would like to thank Department of Chemical Engineering, IIT Bombay for hosting my internship.

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