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Modeling of an Industrial Riser in the Fluid Catalytic Cracking Unit

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Abstract: Problem statement: The aim of this study is to obtain a model that can simulate the performance of an industrial fluid catalytic cracking unit in steady state. **Approach:** The reactions in the riser occur in a transported bed with the fluid and the solids in ideal plug flow. One of the main advantages of the model is that it does not include any partial differential equations. This facilitates the solution of the equations and makes the model particularly suitable for control studies. **Results:** To simulate the FCC riser, the four-lump model involved gas oil, gasoline, light gas and coke (to predict the Gas oil conversion and the product distribution) has been developed. **Conclusion:** Simulation studies are performed to investigate the effect of changing various process variables, such as temperature, catalyst circulation rate and gasoil feed rate. The calculated data of the product distribution were agreed well with the experimental results.

06-606 Computational methods in process engineering

Project Report

Review and Study of Modelling of an Industrial Riser in the Fluid Catalytic Cracking Unit

Mehran Heyari, Habib Ale Ebrahim and Bahram Dabir (2010). Modeling of an Industrial Riser in the Fluid Catalytic Cracking Unit. American Journal of Applied Sciences 7 (2): 221-226, 2010.

Contents

1. Background

The objective of the report is to study the Operation of FCC unit riser, along with modelling and analysis of the system of Ordinary Differential Equation system, with linear boundary condition. The mathematical model developed in the paper selected was used for steady state simulation of Fluidized Catalytic Cracker Riser and analysis of various mathematical methods used for analysis. The reactions in riser occur in transported bed with fluid and solids in Plug flow reactor. Four lump models are used, which include temperature, catalyst circulation rate and gas oil feed rate.

The primary processing of crude oil gives fractions such as gasoline, kerosene, gas oil and heavy residue. FCC unit is used for converting high molecular weight hydrocarbons into lower molecular weight hydrocarbons by cracking operation.

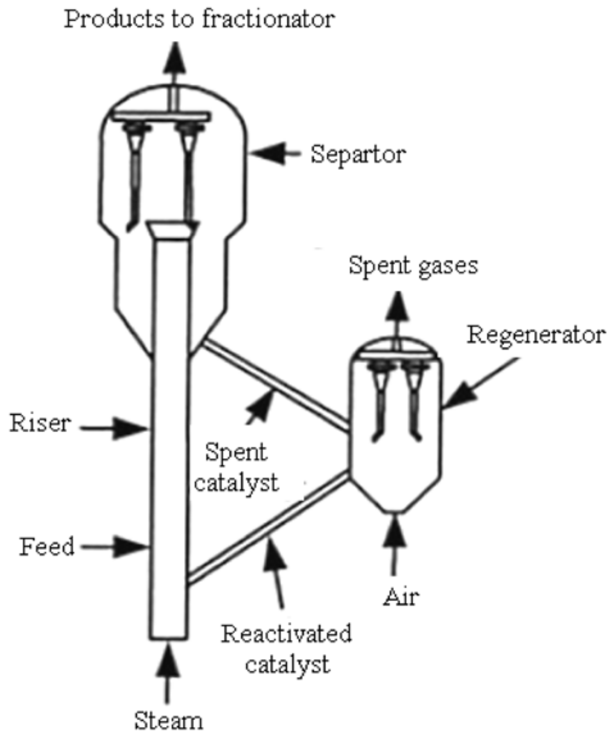
Control of FCC unit is a challenging task and the high economic incentive drives the research in this field. Less production of coke and efficient cracking distinguishes the FCC unit from conventional Thermal cracking unit. The FCC unit consists of reactor and regenerator system where the feed from vacuum distillation unit is cracked in order to obtain desirable hydrocarbons.

FCC unit temperature is critical in operation of the system and it has to be controlled inorder to avoid any abnormal combustion in the reactor.

Fluidized Catalytic Cracker consists of reactor and regenerator. The feed entering the reactor zone of FCC is cracked to lighter hydrocarbons and coke using zeolite catalyst.

Temperature in the regenerator is controlled to avoid uncontrolled combustion. Zeolite catalyst is used for cracking which is recirculated between the reactor and regenerator.

Steam is provided in the bottom of the riser, where the cracking reaction takes place.



The objective of the report is modelling and optimization of the riser using the mathematical model provided in the paper.

The problem is presented with Ordinary Differential Equations and linear boundary conditions. The ordinary differential equations have been analyzed for Stability and Sensitivity. 4^{th} Order Range Kutta method, Eulers Method and Adam's Method was used for solving the ODE equations and the computational time of various methods and stability of results were compared.

The linear algebraic equation was solved using Newtons method and number of steps to convergence was recorded. The result was compared with Python Scipy package fsolve.

The four lump model involves gas oil, gasoline, light gas and coke.

The study has been conducted as three sections, which is outlined in Study Objectives & Strategy.

It has been assumed as cracking of gas oil is a second order reaction and cracking of gasoline is a first order reaction.

2. Lump Mathematical model used for simulation:

System of Differential Equations solved by **Euler's Method, 4th order Range Kutta method and Python build-in solver (using Adam's method)**

1. Gas Oil: $\frac{dy_A}{dz} + \frac{\phi_R A_R(1-\varepsilon)\rho_s L_R}{F_{gR}}[K_{AB} + K_{AC} + K_{AD}]y_A^2 = 0$
2. Gasoline: $\frac{dy_B}{dz} + \frac{\phi_R A_R(1-\varepsilon)\rho_s L_R}{F_{gR}}[(K_{BC} + K_{BD})y_B - K_{AB}y_A^2] = 0$
3. Light Oil Hydrocarbon: $\frac{dy_D}{dz} + \frac{\phi_R A_R(1-\varepsilon)\rho_s L_R}{F_{gR}}[K_{BD}y_B + K_{AD}y_A^2] = 0$
4. Coke: $\frac{dy_C}{dz} + \frac{\phi_R A_R(1-\varepsilon)\rho_s L_R}{F_{gR}}[K_{BC}y_B + K_{AD}y_A^2] = 0$

Linear Equation for Boundary Condition solved using **Newtons Method (implemented manually) and Powell's Hybrid method** as implemented in the HYBRJ algorithm in MINPACK using Python odeint fsolve.

Boundary condition evaluation at Z = 0, is done for estimating the entrance temperature (T_R), given by the relation:

$$F_S C_{PS}(T_R - T_S) + F_{gL} C_P{}^L{}_{gL}(T_{vap} - T_f) + F_{gL} C_P{}^V{}_{gL}(T_R - T_{vap}) + F_{gL}\Delta H_{Vap} + F_{ds} C_{Pds}(T - T_{ds}) = 0$$

3. Variables used in simulation

i. Input Variables in Simulation

1. Steam Temperature (Ts)
2. Gas oil vaporization temperature (T_gasvap)
3. Gas Oil Vaporization Temperature (Hvap)
4. Rate Constant
    a. Gasoil to gasoline (K0_ab)
    b. Gas oil to coke (K0_ac)
    c. Gasoline to light gases (K0_ad)
    d. Gasoline to coke (K0_bc)

    e. Gas oil to light gases (K0_bd)
5. Decay Constant (alpha_0)
6. Inlet flow rate (Q_overall)
7. Feed Temperature (Feed_T)
8. Catalyst Temperature (Cat_T)
9. Riser Diameter (d_R)
10. Superficial velocity (v_s)
11. Activation Energy
    a. Activation energy of coke (for deactivation) (E_coke)
    b. Activation energy of Gas oil to gasoline (E_ab)
    c. Activation energy of gasoil to light gasses (E_bd)
    d. Activation energy of gas oil to coke (E_ac)
    e. Activation energy of gasoline to light gases (E_ad)
    f. Activation energy of Gasoline to coke (KE_bc)
12. Enthalpy of reaction
    a. Gas oil to gasoline (Hab)
    b. Gasoil to light gasses (Hbd)
    c. Gas oil to coke (Hac)
    d. Gasoline to light gases (Had)
    e. Gasoline to coke (Hbc)
13. Heat Capacity
    a. Gas oil (Cp_gasoil)
    b. Gasoline (Cp_gasoline)
    c. Light Gas (Cp_Lightgas)
    d. Coke (Cp_coke)
    e. Steam (Cp_steam)
14. Riser Length (L_r)
15. Catalyst porosity-ε (e)
16. Fluidized Bed Density (rh_s)

ii. <u>Estimated variables in simulation</u>

1. Decay coefficient (alpha)
2. Function for decay of catalyst activity due to coke decomposition (phi)
3. Rate Coefficient
    a. Gasoil to gasoline (Kab)
    b. Gas oil to coke (Kac)
    c. Gasoline to light gases (Kad)

   d. Gasoline to coke (Kbc)
   e. Gas oil to light gases (Kbd)
4. Residence Time (t_c)

4. Study Objectives & Strategy

The simulation and study has been done as 3 sections, which are outlined below:

Section 1:

- The solution to the differential equations has been solved using Adam's method, Eulers method & Range Kutta Method .The computational time, solution stability and solution pattern has been compared and analyzed.

  Linear boundary conditions were solved by Newtons method, which was manually implemented in Python and Powell's Hybrid method was implemented in the HYBRJ algorithm in MINPACK using Python odeint fsolve. This algorithm uses dogleg step.

  The Hybrid algorithm retains the fast convergence of Newton's method but will also reduce the residual when Newton's method is unreliable.

  The results obtained from the simulation was studied and analyzed for any discrepancy to data provided in publication referred. As part of this the following parameters were analyzed graphically and compared with following data from publication referred:
  - Concentration Profile
  - Riser Temperature Profile
  - Conversion of Feed
  - Yield for varying inlet flow rate
  - Yield vs conversion
  - Gasoline flow rate vs feed inlet temperature
  -

Section 2:

- Sensitivity analysis of the system was done to identify and understand the variables having nontrivial effect on results.
- The variables with considerable effect on the system was identified. These parameters were considered during the system optimization studies conducted in Section 3.
- The variables were assumed to be independent to each other for the analysis.

Section 3:

- The identified variables to be minimized and maximized were studied to understand the pattern of solution. The correlation and dependence of independent parameters on dependent parameters were studied and the following variations have been analyzed:

- Variation of Feed temperature on riser temperature and product flow
- Variation of feed flow rate in riser temperature
- Variation of Riser Height on Product Flow
- Gasoline production at varying inlet flow rate for different riser height.

5. Summary of Solver Observations:

Equations Solved	Method Used	Solving Time / Number of Iterations	Solution Stability / Accuracy	Discussion
Ordinary Differential Equations	Adam's Method (Odeint Solver build – in Python Scipy)	*0.0052 sec / 878*	NA	The computational time is lowest for Adam's method.
	4^{th} order Range Kutta Method	*0.0405 sec / 900*	The solution is stable. Attached graphs for the same.	4^{th} order Range Kutta Method takes maximum computational time. This is due more number of variable evaluations in the simulation when compared to Eulers Method.
	Eulers Method	*0.0189 sec / 900*	The solution is stable. Attached graphs for the same.	Eulers method takes the lower computational time for the same number of steps due to less variable evaluations in each step when compared to Range Kutta Method. Since the system of ODEs is not stiff and has good convergence properties Euler's method provided accurate solution with less computational time than Range Kutta Method
Linear Algebraic Equation (Boundary Condition)	Odeint fsolve	*14 iterations*	The solution converges to a stable solution.	14 iterations was required to get a converged solution by using Powell's Hybrid method.
	Newtons Method	*1 iteration*	The solution is accurate to fsolve precision.	Since the profile is linear the solution reaches convergence in 1 iteration.

6. Results and Discussion:

i. Solution of Ordinary Differential Equations using Odient:

Scipy odeint solver evaluates the equation for stiffness and selects the method accordingly. BDF solver is used for stiff system and Adam's method is used for non stiff system. As it can be found in attached code, the odeint function has evaluated the function as non stiff and has therefore used Adam's method. The solution obtained is stable and is similar to results obtained in publication referred for obtaining the data set.

ii. Solution of Ordinary Differential Equations using Range Kutta Method:

The solution set and graphs obtained from Range Kutta Method is identical to Odient. The system is stable for 4th order Range Kutta Method.

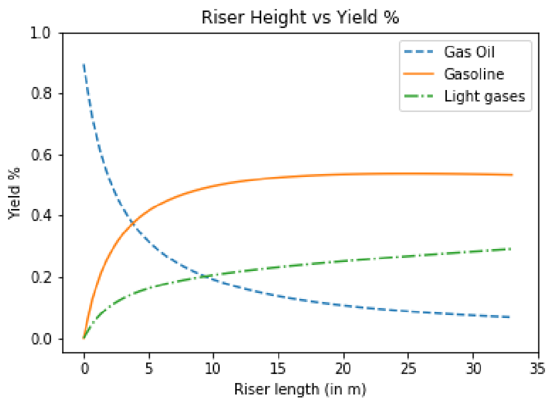
iii. Solution of Ordinary Differential Equations using Eulers Method:

The solution set and graphs obtained from Eulers Method is identical to Odient. The system is stable for Eulers Method.

Since the system of ODEs is not stiff and has good convergence properties Eulers method provided accurate solution with less computational time than Range Kutta Method.

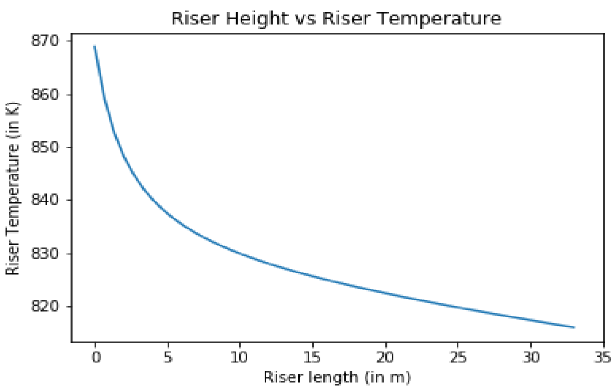
iv. Solution obtained using solvers (4th Order Range Kutta, Eulers Method & Adam's method)

Riser Height vs Yield



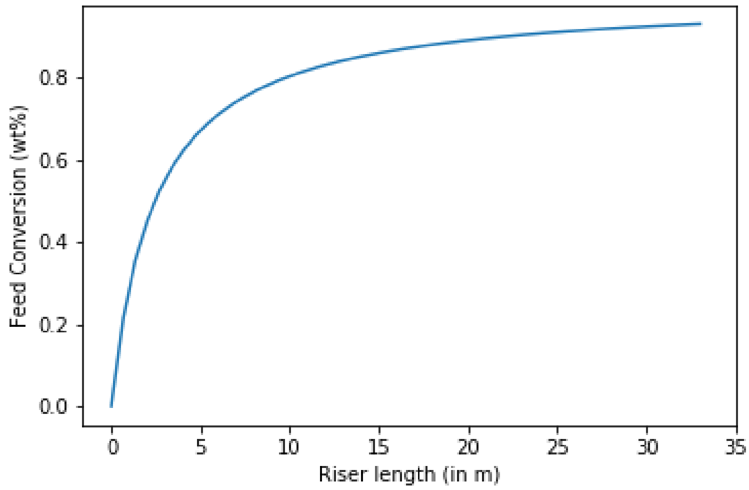
The result indicates that the yield obtained for the riser is at a length of 20 m after which the Gas oil will be reacting to be converted to Light Gases, which is also a desirable product in the system.

Riser Height vs Riser Temperature



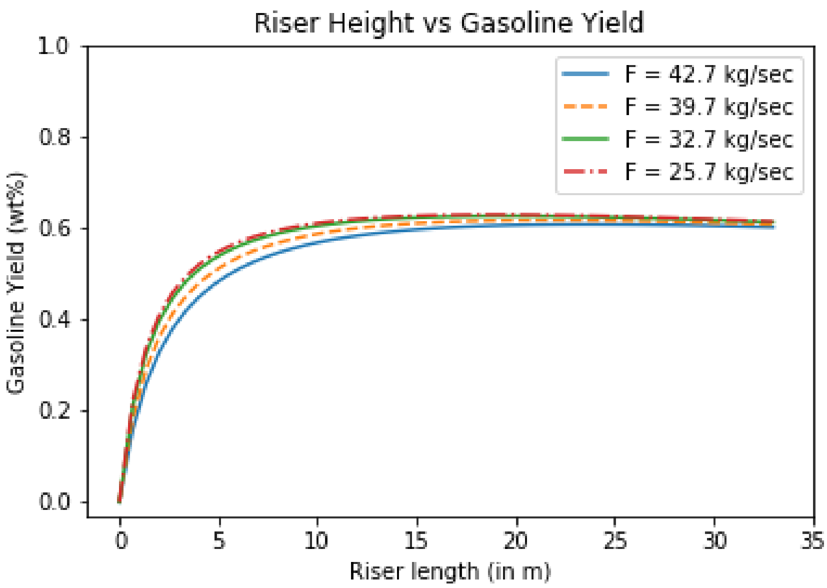
The cracking reaction is endothermic and therefore the temperature in the riser decreases as the reaction proceeds along the length of the reactor.

Riser Height vs Feed Conversion

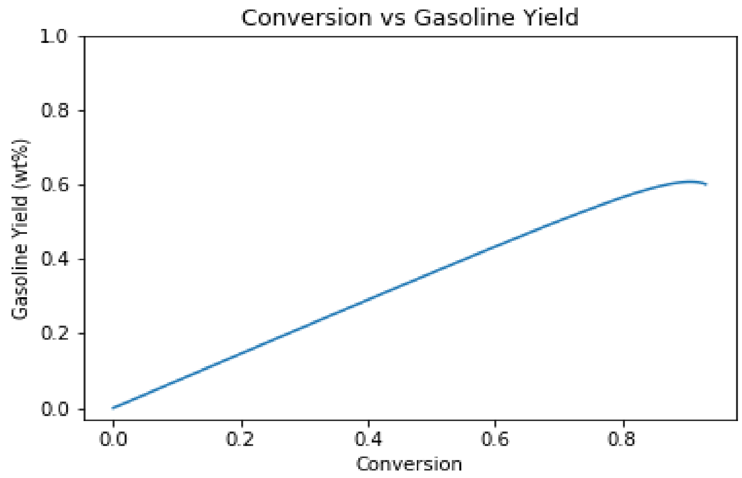


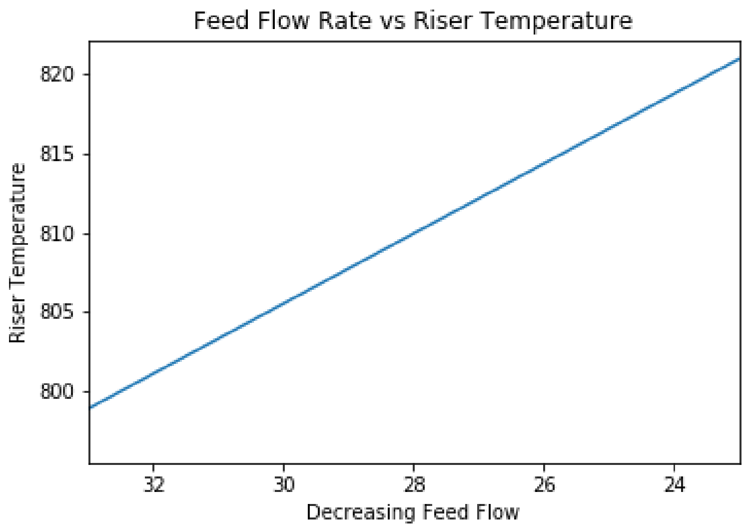
As intepreted from the Yield of various components along the riser length , the feed conversion is reaches the maximum at 35 m along the riser length.

Riser Height vs Gasoline Yield



It can be noted from the plot that the gasline yield in the system decreases with increase in flow rate of feed, due to reduction in conversion in the riser.

Riser Height vs Gasoline Yield

The maximum gasoline yield was obtained around 90 % conversion of the feed, this is critical to optimizing removal of gasoline from the riser at the highest conversion.

Riser Height vs Gasoline Yield

With decrease in flow rate of feed the riser temperature increses thereby increasing the rate of cataytic reaction. This is direct confrontnation with Catalyst to gas ratio vs Riser Temperature plot in refered publication.

The results obtained have the same trend and observations as noted in the referred publication and therefore the simulation techniques used is correct and stable.

7. Sensitivity analysis of ODE:

Sensitivity analysis was done to understand how various parameters (design variables) influence the solution of the ordinary differential equation. The parameters are varied to understand the variables having nontrivial effect on results. This will ensure that the results of the system are robust with different imputations. The sensitivity analysis was done for:

i. Maximum Temperature in the reactor

It is crucial to understand the parameters that can be most sensitive in the system. Since increase in maximum temperature in the system can lead to instability of the process which can lead to excess coke formation, effecting the overall performance and efficiency of the system, sensitivity analysis of maximum temperature in the reactor is crucial.

ii. Maximum Flow Rate of Gasoline

Since gasoline flow rate is the critical parameter to be optimized in the system, understanding the variables (‘p’ vector) can be advantageous in understanding the parameters to be adjusted for getting optimum Gasoline flow rate.

Parameters used for vector ‘p’ of sensitivity analysis are:

Variables	Maximum Gasoline Flow Rate	Maximum Temperature
Steam Temperature (Ts)	0	0.02773245
Gas Oil Vap. Temperature (T_gasvap)	0	0
Gas oil enthalpy of vaporization (Hvap)	0	-0.06164216
Rate Constant		
Gasoil to gasoline (K0_ab)	3.35e-01	0
Gas oil to coke (K0_ac)	-1.03e-03	0
Gasoline to light gases (K0_ad)	-2.47e-01	0
Gasoline to coke (K0_bc)	-1.18646766e-07	0
Gas oil to light gases (K0_bd)	-8.54627524e-02	0
Decay Constant (alpha_0)	6.15018589e-03	0
Inlet flow rate (Q_overall)	**1.08546287e+00**	**-0.49309123**
Feed Temperature (Feed_T)	**-3.07789785e-04**	**0.53548886**
Catalyst Temperature (Cat_T)	0	0
Riser Diameter (d_R)	1.46946351e-04	0
Superficial velocity (v_s)	3.55528553e-02	0
Activation Energy		
Activation energy of coke (for deactivation) (E_coke)	2.43116291e-03	0

Activation energy of Gas oil to gasoline (E_ab)	4.81135550e-03	0
Activation energy of gasoil to light gasses (E_bd)	-9.83351103e-04	0
Activation energy of gas oil to coke (E_ac)	-7.65332317e-06	0
Activation energy of gasoline to light gases (E_ad)	-4.08772910e-03	0
Activation energy of Gasoline to coke (E_bc)	-1.64837364e-09	0
Enthalpy of reaction		
Gas oil to gasoline (Hab)	0	0
Gasoil to light gasses (Hbd)	0	0
Gas oil to coke (Hac)	0	0
Gasoline to light gases (Had)	0	0
Gasoline to coke (Hbc)	0	0
Heat Capacity		
Gas oil (Cp_gasoil)	0	-0.42714508
Gasoline (Cp_gasoline)	0	0
Light Gas (Cp_Lightgas)	0	0
Coke (Cp_coke)	0	0
Steam (Cp_steam)	0	-0.00430399
Riser Length (L_r)	9.72268997e-04	0

iii. Sensitivity analysis observation:

Feed Temperature- With increase in feed temperature the maximum temperature in the reactor is having a positive variation, i.e an increase in temperature. This is not useful for the system and can have adverse effect in the optimized model.

It can also be noted that increase in temperature had a negative variation in gasoline flow which is not desirable.

Therefore it is not advisable to increase the temperature in the reactor. The variation of system parameters with increase in temperature has been studied and analyzed below.

Inlet Flow Rate – With increase in inlet flow rate the there is a negative variation in reactor temperature, which can an advantageous effect in the system.

Similarly with increase in inlet flow rate there has been a positive deviation in Gasoline flow rate. But as noted before the gasoline yield will decrease with increase in inlet flow. The increase in gasoline flow observed here might be due to the increase in overall flow into the riser.

Therefore it is advisable to increase the inlet flow rate into the riser though there might be an overall decrease in gasoline yield in the system. The variation of system parameters with increase in inlet flow rate has been studied and analyzed below.

iv. Python Package used for sensitivity analysis:

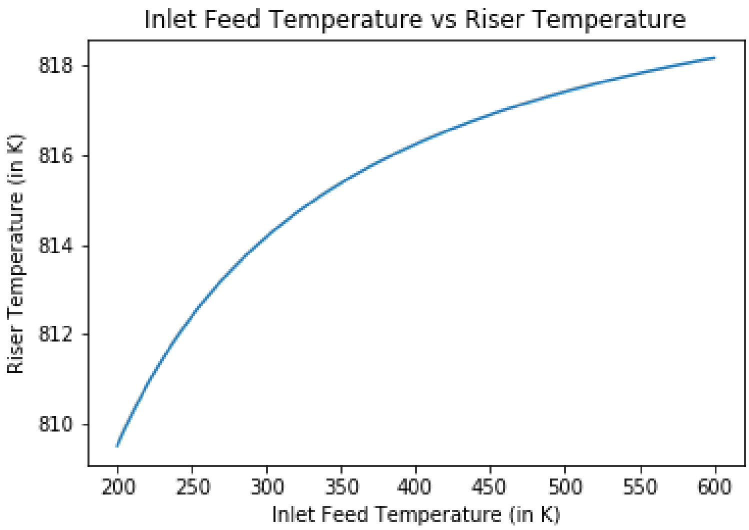
Numdifftools 0.9.20 in python solves automatic numerical differentiation problems in one or more variables. This is used for defining the sensitivity parameters and solving for the sensitivity of system.

8. Critical parameter optimization plots

Based on the Sensitivity analysis, the following parameters has evaluated for optimized results:

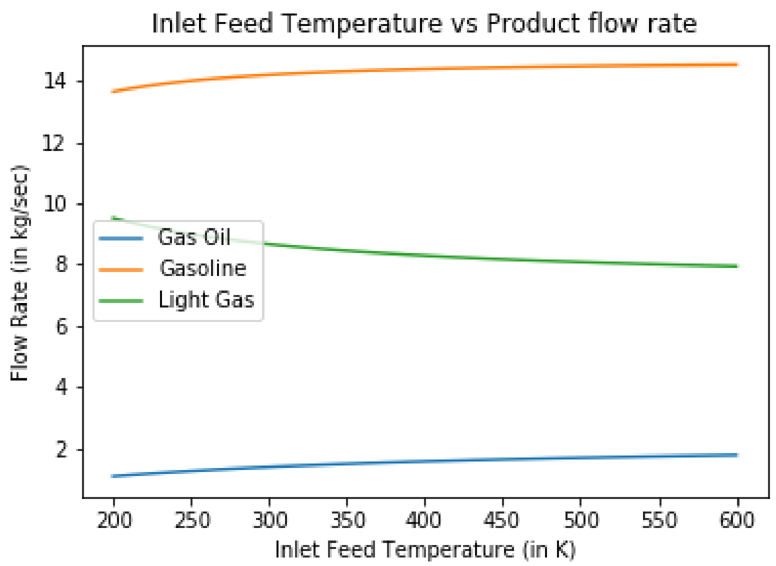
i. Variation of Feed temperature - Riser temperature and Product flow

Variation of inlet feed temperature along the riser length



As observed before , with increase in inlet feed temperarture there has been an increase in temperature along the length of the riser.

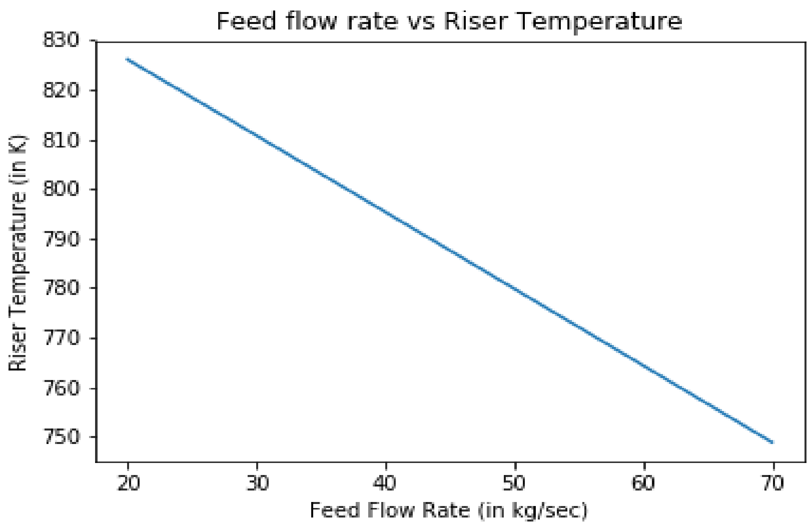
Riser Height vs Gasoline Yield



It can be noted that with increase in inlet feed temperature, the Gasloine flow rate increases upto 400 K beyond which the flow rate remains constant. Therefore increaseing inlet feed temperature does not have a major advantage in increasing the Product flow rate.

ii. Variation of Feed flow rate - Riser temperature and Product flow

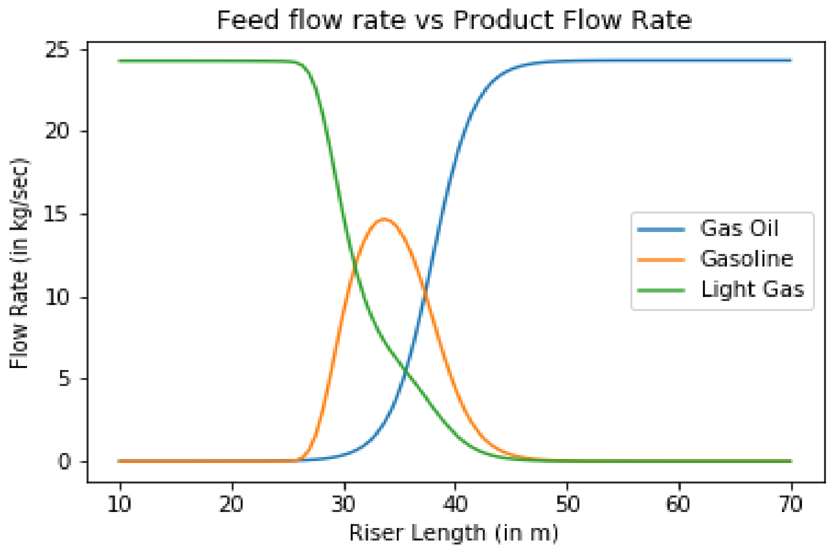
Feed flow rate vs Riser Temperature



As observed by sensitivity analysis, with increase in feed flow rate the riser temperature decreases.

iii. Variation of Riser length on and Product flow

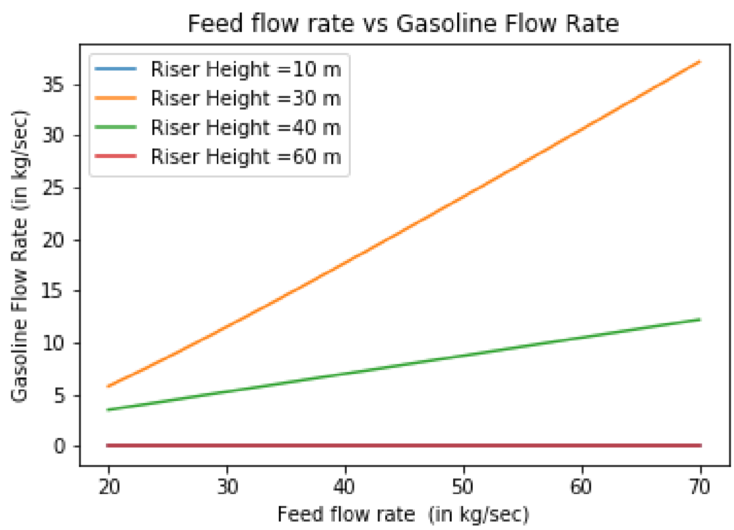
Feed flow rate vs Riser Temperature



It can be noted from the graph that the Gasoline production is maximum at riser height of 33.636 m is required for maximizing the flow rate of Gasoline, which is the desired product.

iv. Gasoline production at varying inlet flow rate for different riser heights

Gasoline production at varying inlet flow rate for different riser height



As it can observed from previous plot the maximum Gasoline production is for riser height in the range of 30 m. But from this interactive plot it can be noted that increase in Gasoline flow is increasing at a higher slope for riser height of 30m.

Conclusion & Recommendation

Section 1:

- The solutions obtained is similar to the results discussed in the publication referred.
- Eulers method, 4th Order Range Kutta method is stable and provides results with the same accuracy as Adams method. The differential equations evaluated are stable for all the methods evaluated and simulation time was almost identical.
- The solution obtained by MINPACK algorithm for linear system solving is identical with Newton system.

Section 2 & Section 3:

- Sensitivity Analysis indicates that increasing feed temperature in the reactor is not desirable as it will decrease the flow rate of desirable product and increase the maximum temperature in the system.
- Increasing flow rate of feed is desirable even though it decreases the gasoline yield as it increases the overall gasoline flow.
- The most efficient reaction in the reactor was for rise height of 33 m and above for which the conversion of light hydrocarbon to coke takes place, thereby decreasing the flow rate of desirable products.

References:

Mehran Heyari, Habib Ale Ebrahim and Bahram Dabir (2010). Modeling of an Industrial Riser in the Fluid Catalytic Cracking Unit. American Journal of Applied Sciences 7 (2): 221-226, 2010.

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APPENDIX 1
PYTHON SIMULATION