Fluid Catalytic Cracking (FCC) Training Problem: Part 1

September 2016

CPFD Software LLC
10899 Montgomery Blvd. NE, Suite A
Albuquerque, NM 87111
+1.505.275.3849
www.cpfd-software.com

Background Information

- An FCC riser is used to "crack" large hydrocarbon molecules into smaller molecules suitable for use in fuels. This reaction occurs on the surface of solid catalyst particles that flow through the riser

- This model uses a *four-lump* model in which the hydrocarbons present are divided into four groups:

  - Gas oil: heavy **gas** compounds being cracked (MW = 400 g/mol)

  - Gasoline: product **gas** compounds (100 g/mol)

  - Gas: light **gas** compounds (50 g/mol)

  - Coke: **solid** carbon that is deposited on the catalyst and causes the catalyst to become deactivated (12 g/mol)

- The gas oil is injected as a liquid spray which quickly vaporizes. In this model, we assume that the gas oil enters the model as a vapor for simplicity.

- The gas-particle mixing, amounts of coke on the catalyst, and riser temperatures are important factors to consider

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FCC geometry

- Riser geometry is contained within the "fcc_riser.stl" file. The dimensions of the file are in millimeters

- Oil feeds are not included in the geometry. These will be modeled with point source injections

- Catalyst is fed through the large pipe near the bottom

21.1 meters
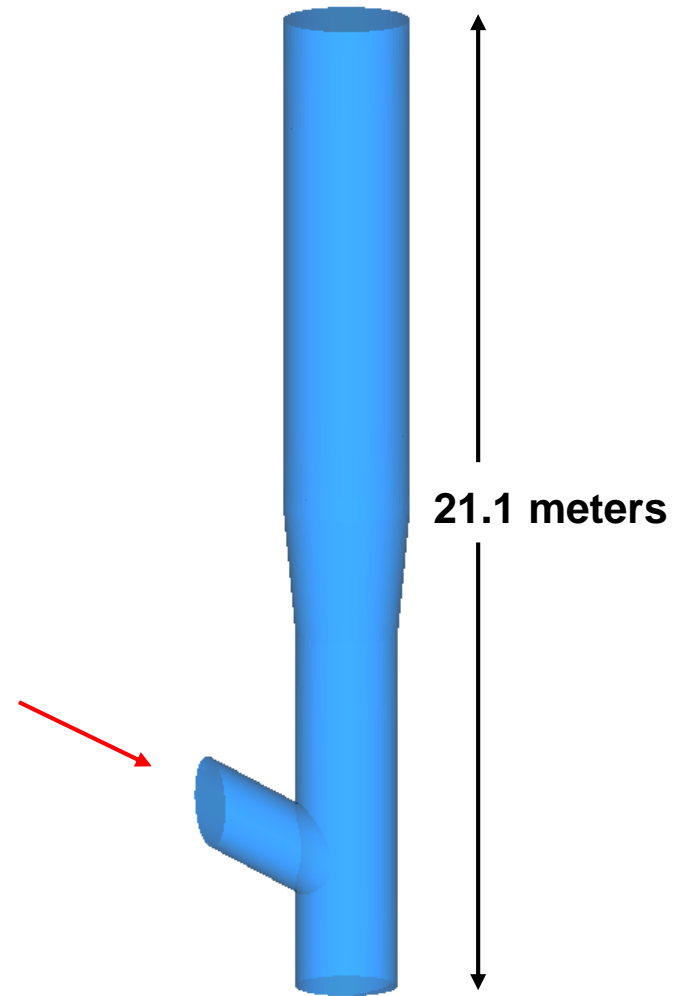
Boundary Conditions
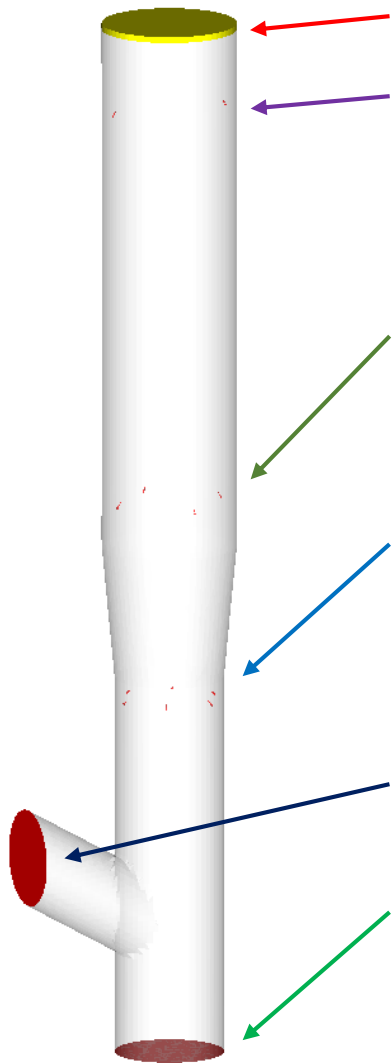
- **Riser outlet**– The pressure riser outlet is maintained at **166.7 kPa**.

- **Slurry Back Wash** – Slurry back wash (95 wt.% gas oil, 5 wt.% steam) enters through two (2) nozzles near top of riser at a rate of **0.84 kg/s**, velocity of **0.06 m/s**, and temperature of **364.9 K**. Slurry back wash nozzles are located 19.3 m from the riser bottom and are angled 60° upward.

- **MTC** – A mix of 94 wt.% gas oil and 6 wt.% gasoline enters through four (4) *mixed temperature control* nozzles at a rate of **21.78 kg/s**, velocity of **1 m/s**, and temperature of **364.9 K**. MTC nozzles are located 11.25 m from the riser bottom and are angled 60° upward.

- **Feed Oil** – Gas oil enters through six (6) nozzles at a rate of **232.8 kg/s**, a velocity of **73.2 m/s**, and a temperature of **491.9 K**. The gas oil feed consists of 88.5 wt.% gas oil, 5 wt.% gasoline, and 6.5 wt.% steam. Feed oil nozzles are located 7.221 m from the riser bottom and are angled 45° upward.

- **Catalyst** – Regenerated catalyst enters at a rate of **1740 kg/s** and a temperature of **973 K**. The catalyst is brought in with **0.65 kg/s** of steam.

- **Bottom Steam** – Steam enters the bottom of the riser at a rate of **0.82 kg/s** and a temperature of **633 K**.

Heat transfer

- In this thermal and reacting problem, particle – fluid heat transfer is an important consideration and a different heat transfer correlation is occasionally used for FCC catalyst.

- Use the single particle Nusselt number correlation for Fluid-particle heat transfer recommended by Kunii and Levenspiel in *Fluidization Engineering*

$$Nu_p = \frac{h \, d_p}{k_f} = 2 + 1.2 Re^{0.5} Pr^{0.33}$$

- Visit the Barracuda Support Site at www.cpfd-software.com for more discussion on heat transfer correlations

Particle-Fluid Heat Transfer

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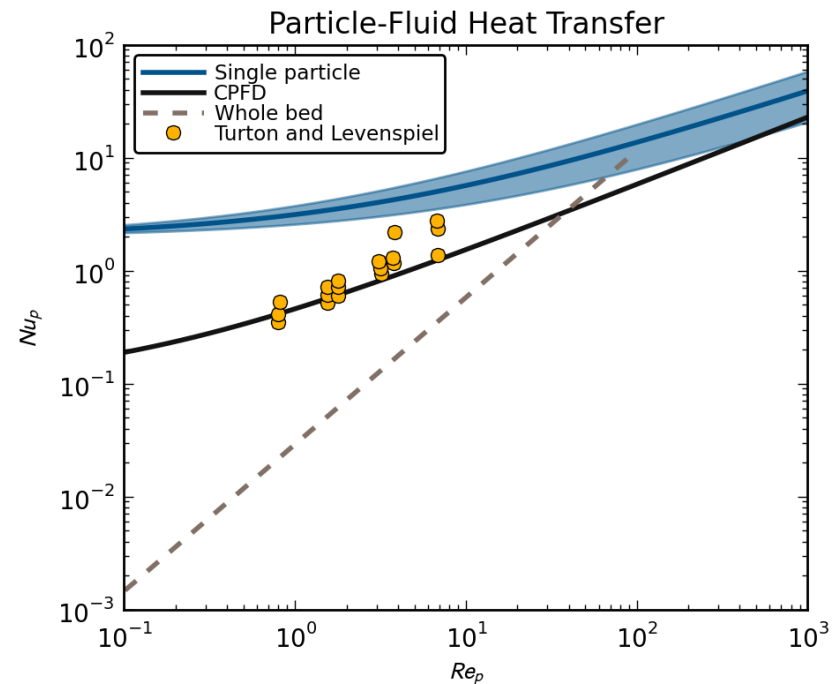
Base Materials

- The following materials are needed in the model.   Important properties are given.

- The steam and Nitrogen are available in the base materials library. The other components will need to be created.

Name	State	Density	MW	Δ Hf	Heat Capacity	Viscosity	Therm Cond
-	-	kg/m3	g/mol	J/kg	J/kg/K	kg/m/s	W/m/K
Catalyst base	Solid	1620	102	0	1150		
Coke	Solid	1200	12.5	0	1150		
Gas	Gas		50	-75000	1040	1.66E-05	0.025
Gas Oil	Gas		400	-745000	3300	5.00E-05	0.025
Gasoline	Gas		100	-550000	1040	1.66E-05	0.025
Steam	Gas	Available in base material library					
N2	Gas						

Catalyst Properties

- **Close pack volume fraction:** 0.58

- **Catalyst Density** – 1620 kg/m^3

- **Catalyst Diameter** – Use the FCC_PSD.sff provided

- **Initial coke on catalyst** – 0.1 wt%

- **Heat capacity** – 1150 J/kg/K

- **Particle Drag model** – EMMS-based model of Yang et al (2003)

Yang, N., Wang, W., Ge, W., and Li, J. (2003). CFD simulation of concurrent-up gas-solid flow in circulating fluidized beds with structure-dependent drag coefficient. *Chemical Engineering Journal*. 96: 71-80.
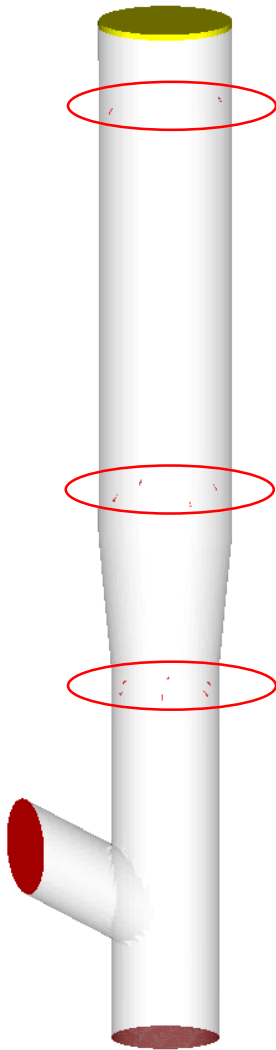
Initial entry of catalyst into empty riser during simulation start-up

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Point source nozzle locations

Slurry back wash

MTC

Feed Oil

- Locations are contained in csv files for the feed oil, MTC, and slurry back wash nozzles

- These are imported by clicking the "Import" button at the bottom of the Injection BC Editor.

Reaction Chemistry

A four lump cracking model is being used in this work. The kinetics have been adapted from the kinetics used by Nayak et al (2005). The **four-lump model** assumes that there are four hydrocarbon components in the system: Gas oil, Gasoline, Gas, and Coke

$$\text{GasOil} \xrightarrow{r_1} 4 \text{ Gasoline} \quad r_1 = \frac{3.589 \times 10^6 \, s^{-1} \cdot RT\theta_{\text{Cat}}}{P\theta_f} \exp\left(-\frac{8222.3 \text{ K}}{T}\right)[\text{GasOil}]^2 \varphi$$

$$\text{GasOil} \xrightarrow{r_2} 8 \text{ Gas} \quad r_2 = \frac{2.541 \times 10^7 \, s^{-1} \cdot RT\theta_{\text{Cat}}}{P\theta_f} \exp\left(-\frac{10748.1 \text{ K}}{T}\right)[\text{GasOil}]^2 \varphi$$

$$\text{GasOil} \xrightarrow{r_3} 32 \text{ Coke} \quad r_3 = \frac{6.791 \times 10^4 \, s^{-1} \cdot RT\theta_{\text{Cat}}}{P\theta_f} \exp\left(-\frac{7779.65 \text{ K}}{T}\right)[\text{GasOil}]^2 \varphi$$

$$\text{Gasoline} \xrightarrow{r_4} 2 \text{ Gas} \quad r_4 = 885.72 s^{-1} \theta_{\text{Cat}} \theta_f^{-1} \exp\left(-\frac{6350.7 \text{ K}}{T}\right)[\text{Gasoline}]\varphi$$

$$\text{Gasoline} \xrightarrow{r_5} 8 \text{ Coke} \quad r_5 = 5.3198 \times 10^7 \, s^{-1} \theta_{\text{Cat}} \theta_f^{-1} \exp\left(-\frac{13910.3 \text{ K}}{T}\right)[\text{Gasoline}]\varphi$$
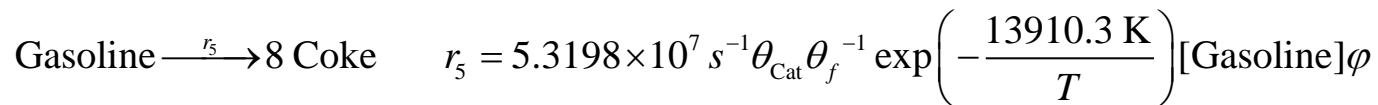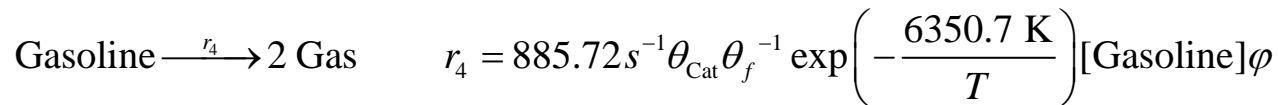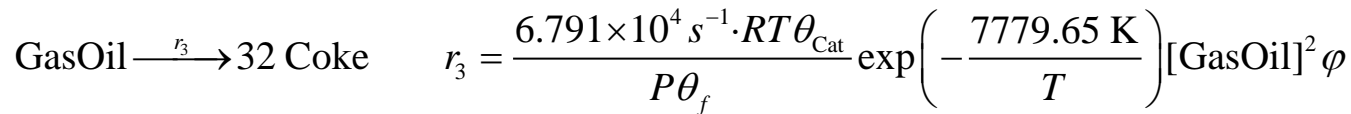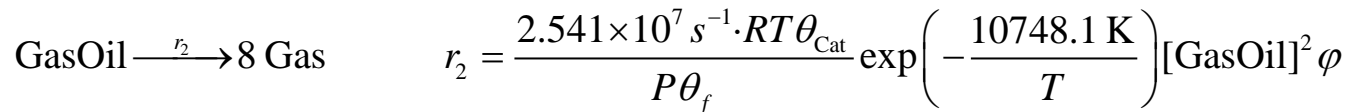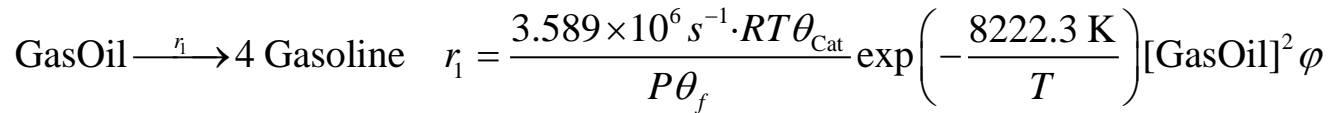
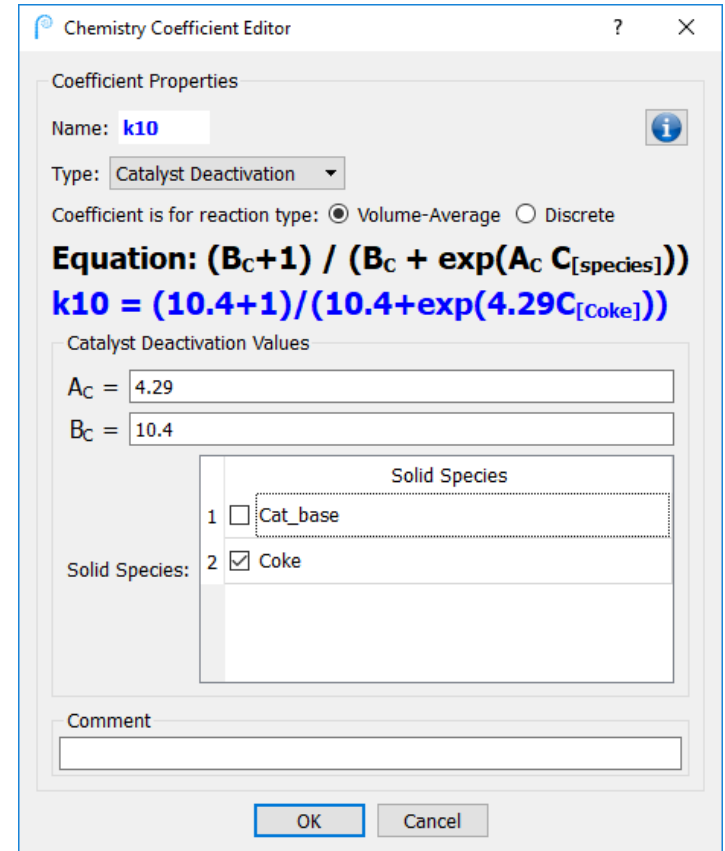Where φ is the catalyst deactivation function (next slide)

Nayak, S., Joshi, S., and Ranade, V. (2005). Modeling of vaporization and cracking of liquid oil injected in a gas-solid riser. *Chemical Engineering Science*. 60: 6049-6066.

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Catalyst deactivation function

The catalyst deactivation function is given in the following form:

$$\varphi = \frac{11.4}{10.4 + \exp(4.29 w_c)}$$

where w_c is the weight fraction of coke on the particle. To implement this function in Barracuda VR 17, the catalyst deactivation is entered as a type of rate coefficient.
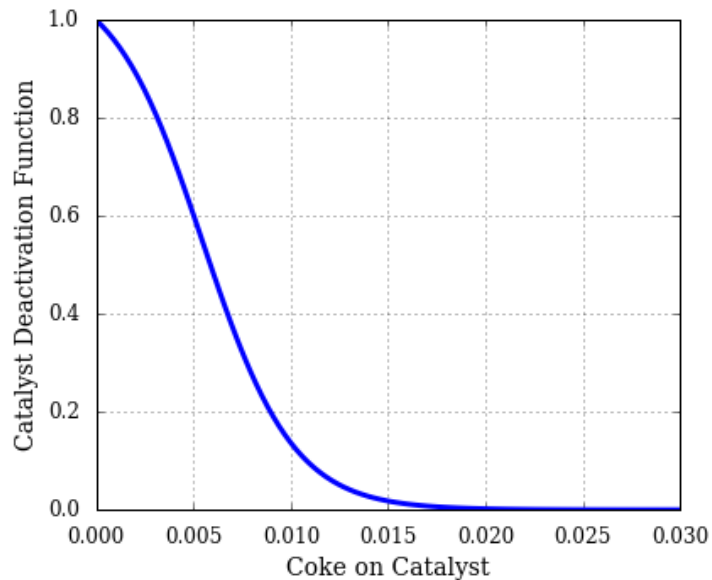
Chemistry Coefficient Editor

Coefficient Properties

Name: **k10**

Type: Catalyst Deactivation ▼

Coefficient is for reaction type: ● Volume-Average ○ Discrete

Equation: $(B_C+1) / (B_C + \exp(A_C C_{[species]}))$

$k10 = (10.4+1)/(10.4+\exp(4.29 C_{[Coke]}))$

Catalyst Deactivation Values

A_C = 4.29

B_C = 10.4

	Solid Species
1 ☐	Cat_base
2 ☑	Coke

Comment

[OK] [Cancel]

Chemistry Implementation Notes

- Volume average chemistry will need to be used for each reaction. Units are mol/m^3 for concentration and mol/m^3/s for the reaction rate

- Reactions of this nature are possible to implement in Barracuda but can be challenging at times.

- Hint: the rate expression for the Gas Oil to Gasoline reaction can be implemented as:

$$R00 = \left((k_0)[GasOil]^2\right) * \left((k_5)\right)$$

where k_0 and k_5 are appropriate rate coefficients

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Considerations for Data Output and Simulation

- We are interested in the temperatures, flow profiles, and gas composition. At a minimum, GMV output should be selected that reflects this

- For gas composition, it is more straightforward to think of the gas compositions in terms of mass. (Mole fractions can become confusing due to the drastically different molecular weights of the base material compounds)

- Catalyst enters at a relatively high volume fraction which can be prone to "backing up" if the gas flow is not high enough. Monitoring this feed rate is recommended.

- 60 seconds of total run time with averaging started at 30 seconds should be sufficient