Coal Particle Combustion

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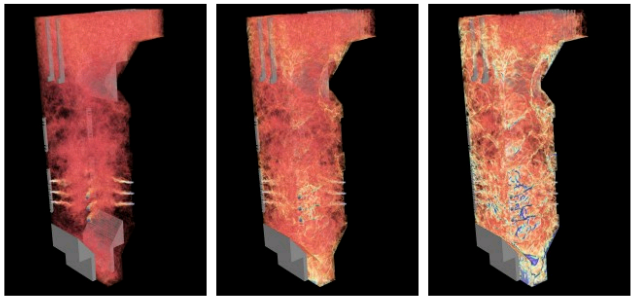


Small (30 μm) particles. Medium (60 μm) particles. Large (90 μm) particles.

Pyrolysis

- CPD model predicts volatiles and tar as function of coal type, T, and dT/dt
- Surrogate pyrolysis model needed

Solution: Modified 2-step

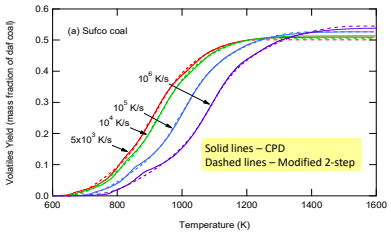
$$\frac{d(\alpha_{coal})}{dt} = -(F_1 k_1 + F_2 k_2)\alpha_{coal}$$

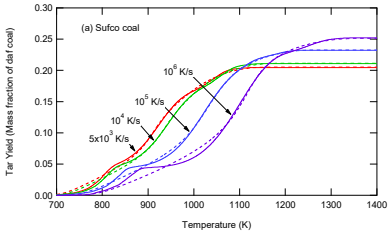
$$\frac{d(\alpha_{vol})}{dt} = (F_1 Y_1 k_1 + F_2 Y_2 k_2)\alpha_{coal}$$

$$F_n = e^{(\sum_{i=0}^{5} c_{i,n}[X_v]^i)}$$

$$\frac{d(\alpha_{tar})}{dt} = \left(F_{1,tar} Y_{1,tar} k_{1,tar} + F_{2,tar} Y_{2,tar} k_{2,tar}\right)\alpha_{coal}$$

- Can fit CPD model predictions of volatiles well for multiple heating rates heating rate





Char Conversion

- Complex surface chemistry
- Heat of rxn
- External and pore diffusion
- Sintering, ash inhibition

$$2C + O_2 \underset{1}{\rightarrow} C(O) + CO$$

$$C + C(O) + O_2 \underset{2}{\rightarrow} CO_2 + C(O)$$

$$C(O) \underset{3}{\rightarrow} CO$$

$$C + CO_2 \underset{4}{\rightarrow} C(O) + CO$$

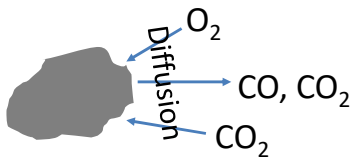
$$C(O) \underset{5}{\rightarrow} CO$$

$$C + H_2O \underset{6}{\rightarrow} C(O) + H_2$$

$$C(O) \underset{7}{\rightarrow} CO$$

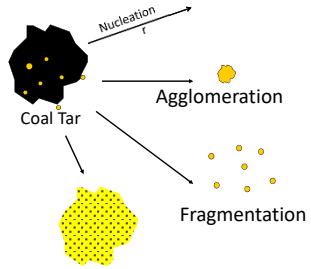
$$C + 2H_2 \underset{8}{\rightarrow} CH_4$$

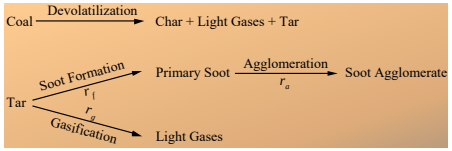
- CBK Features (from Hurt)
  - Decreasing rate with increasing conversion
  - Annealing, ash inhibition
  - Originally included statistical kinetics
  - Effectiveness factor for pore diffusion
  - Particle size distribution
- Char Conversion Kinetics (CCK)
  - Based on CBK/E and CBK/G (from Liu and Niksa)
  - Multiple surface reactions
  - Multi-component transport
  - Random pore model
  - Global sensitivity analysis
  - Generate a surrogate model

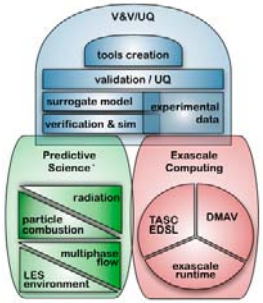


Soot

- Coal tar soot is different than soot from light gases
- Soot in flame regions can radiate significant amount of heat away from flame to walls
- Soot mainly comes from coal tar, but at high temperatures acetylene becomes more important
- Alex Brown's soot model implemented in Arches







Carbon Capture Multidisciplinary Simulation Center (CCMSC) team structure.