Detailed Coal Combustion Modeling Extended to Oxy-coal Conditions

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Additional Information

- Holland, Troy, Fletcher, Thomas H., Global Sensitivity Analysis for a Comprehensive Char Conversion Model in Oxy-fuel Conditions, *Energy and Fuels* 2016
- Holland, Troy, Fletcher, Thomas H., Comprehensive Model of Single Particle Pulverized Coal Combustion Extended to Oxy-Coal Conditions, *Energy and Fuels* 2017
- Holland, T. M., K. Sham Bhat, Marcy, P., Gattiker, J., Kress, J., Fletcher, T, Extension and Calibration of a Coal Char Thermal Annealing Model, *in preparation*

Acknowledgements

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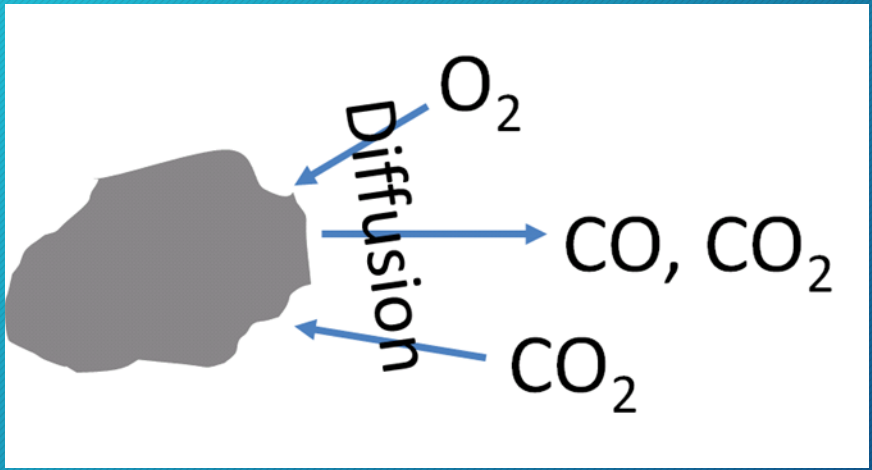
Necessity of a detailed char model

- This work is in support of a PSAAP-2 project
  - Push exascale computing
  - Produce a highly detailed simulation of an industrial pulverized coal boiler (with quantified uncertainty)
- Many complex processes drastically change coal conversion and energy release depending on ambient conditions and coal structure
- Goal: create a detailed model that captures data, then propagate important aspects in a surrogate model

Coal Particle Combustion

- Initial heating
- Devolatilization/swelling
- Char conversion
  - Mode of burning
  - Swelling
  - Annealing
  - Kinetics
  - Porosity
  - Thiele modulus
  - Devolatilization impact
  - Built on CBK=>iterations=>CCK=>CCK/oxy



Sensitive Submodels: Mode of burning

- A simple method to balance particle diameter and density
- Generally effective in the past with simple heuristics
- Not sufficient for oxy-coal conditions
  - Very intense O_2 conditions
  - Non-neglible H_2O and CO_2 gasification

$$\frac{m}{m_0} = \left(\frac{m}{m_0}\right)^{\alpha} \left(\frac{d}{d_0}\right)^{3}$$

O_2 %	Black Thunder			North Antelope			Pittsburgh 8			Utah Skyline		
	O_2	CO_2	H_2O	O_2	CO_2	H_2O	O_2	CO_2	H_2O	O_2	CO_2	H_2O
12%	0.72	0.25	0.03	0.82	0.16	0.02	0.89	0.09	0.02	0.82	0.15	0.03
24%	0.79	0.18	0.03	0.85	0.13	0.02	0.87	0.11	0.02	0.82	0.14	0.03
36%	0.83	0.15	0.03	0.86	0.11	0.02	0.87	0.11	0.03	0.85	0.12	0.04

Shaddix and Molina, Proceeding of the Combustion Institute 32 (2009)

Sensitive Submodels: Mode of burning

O_2 %	Black Thunder			North Antelope			Pittsburgh 8			Utah Skyline		
	O_2	CO_2	H_2O	O_2	CO_2	H_2O	O_2	CO_2	H_2O	O_2	CO_2	H_2O
12%	0.72	0.25	0.03	0.82	0.16	0.02	0.89	0.09	0.02	0.82	0.15	0.03
24%	0.79	0.18	0.03	0.85	0.13	0.02	0.87	0.11	0.02	0.82	0.14	0.03
36%	0.83	0.15	0.03	0.86	0.11	0.02	0.87	0.11	0.03	0.85	0.12	0.04

Sensitive Submodels: Model of burning

- More advanced method adapted from Haugen et al.
- Balance diameter and density based on a weighted effectiveness factor
- Compute a new "mode of burning" at each time step
- Enforce the law of conservation of mass

$$\frac{dr_p}{dt} = \frac{dm_p}{dt} \frac{1-\eta}{4\pi r_p^2 \rho_p}$$

$$\frac{d\rho_p}{dt} = \frac{dm_p}{dt} \frac{\eta}{V_p}$$

(Haugen et al., 2014; Haugen et al., 2015)

Sensitive Submodels: Particle Swelling

- Swelling can be drastic or minimal depending on coal character and heating conditions
- An incorrect swelling model results in incorrect heat and mass transfer
- Swelling at the very high heating rates of practical combustion has typically been incorrectly modeled by ignoring the very substantial impact of heating rate on bubble formation and popping
- The correlation for coal type was also woefully inadequate

Sensitive Submodels: Particle Swelling

$$\left(\frac{d}{d_0}\right)_{HHR} = s_{var}\left(\frac{\dot{T}_{base}}{\dot{T}}\right)^{c_{HR}} + s_{min}$$

$$s_{min} = \left(FC_{ASTM} + A_{ASTM}\right)^{1/3}$$

(Shurtz et al., 2011; Shurtz et al., 2012)

Correlation	Applicable Range
$s_{var} = 1.69\frac{\sigma+1}{M_\delta} - 0.0309$	$0.018 \leq \frac{\sigma+1}{M_\delta} < 0.207$
$s_{var} = -3.37\frac{\sigma+1}{M_\delta} + 1.01$	$0.207 \leq \frac{\sigma+1}{M_\delta} \leq 0.301$
$s_{var} = 0$	$\frac{\sigma+1}{M_\delta} < 0.018\ or\ \frac{\sigma+1}{M_\delta} > 0.301$
$c_{HR} = -191\left(\frac{\sigma+1}{M_\delta}\right)^2 + 68.9\frac{\sigma+1}{M_\delta} - 5.16$	$0.106 < \frac{\sigma+1}{M_\delta} < 0.254$
$c_{HR} = 0$	$\frac{\sigma+1}{M_\delta} < 0.106\ or\ \frac{\sigma+1}{M_\delta} > 0.254$

(Shurtz et al., 2011; Shurtz et al., 2012)

Sensitive Submodels: Thermal Annealing

- The most sensitive submodel
- Drastically different based on heating rate, coal type, and peak particle temperature
- Probably responsible for most of the difficulty in finding coal-general kinetic correlations
- Two distinct phases
  - The massive physical and chemical changes due to devolatilization
  - The lesser changes due to gradual carbon sheet re-ordering and loss of defects

Sensitive Submodels: Thermal Annealing

$$\frac{df_i}{dt} = -A_d * exp\left(\frac{-E_{A_{anneal},i}}{RT}\right) * f_i$$

$$E_a = f(\mu, \sigma, Tr_1, Tr_2)$$

$$\mu = f(HR, NMR, T_{peak})$$

$$\sigma = f(NMR)$$

Sensitive Submodels: Kinetic Parameters

- 8 step system
- All steps tied to R3 and R7 via correlations
- For any given coal, 4 kinetic parameters contain plenty of flexibility (usually 2 are adequate)

$$2C + O_2 \rightarrow C(O)_\alpha + CO \quad (R1)$$

$$C + O_2 + C(O)_\alpha \rightarrow C(O)_\alpha + CO_2 \quad (R2)$$

$$C(O)_\alpha \rightarrow CO \quad (R3)$$

$$CO_2 + C \leftrightarrow C(O)_\beta + CO \quad (R4)$$

$$C(O)_\beta \rightarrow CO \quad (R5)$$

$$C + H_2O \leftrightarrow C(O)_\gamma + H_2 \quad (R6)$$

$$C(O)_\gamma \rightarrow CO \quad (R7)$$

$$C + 2H_2 \rightarrow CH_4 \quad (R8)$$

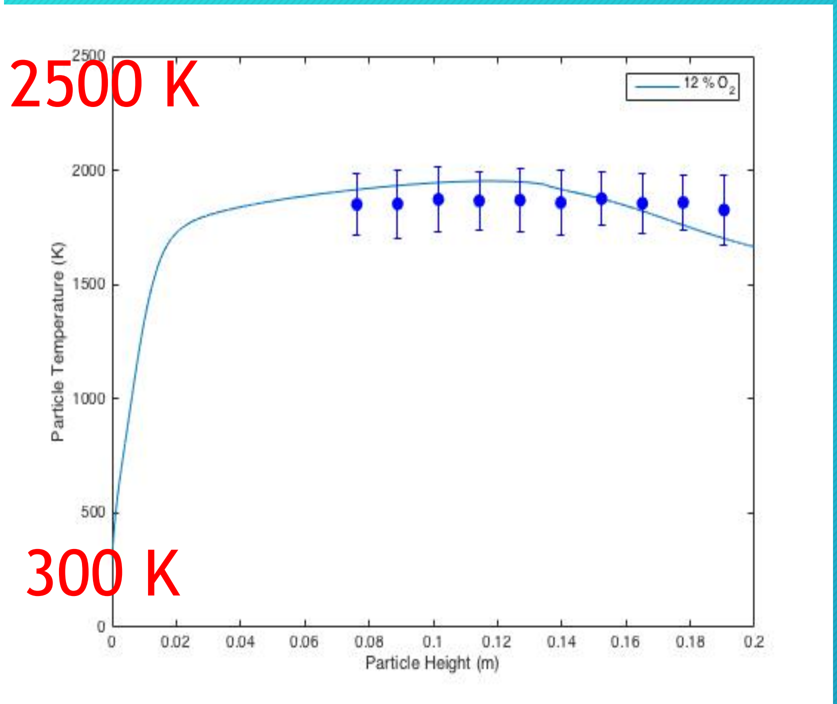
$$R_{C-O_2} = \frac{k_1 k_2 P_{O_2}^2 + k_1 k_3 P_{O_2}}{k_1 P_{O_2} + \frac{k_3}{2}}$$

$$R_{C-CO_2} = \frac{k_4 P_{CO_2}}{1 + \frac{k_4}{k_5} P_{CO_2} + \frac{k_{4r}}{k_5} P_{CO} + \frac{k_6}{k_7} P_{H_2O} + \frac{k_{6r}}{k_7} P_{H_2}}$$

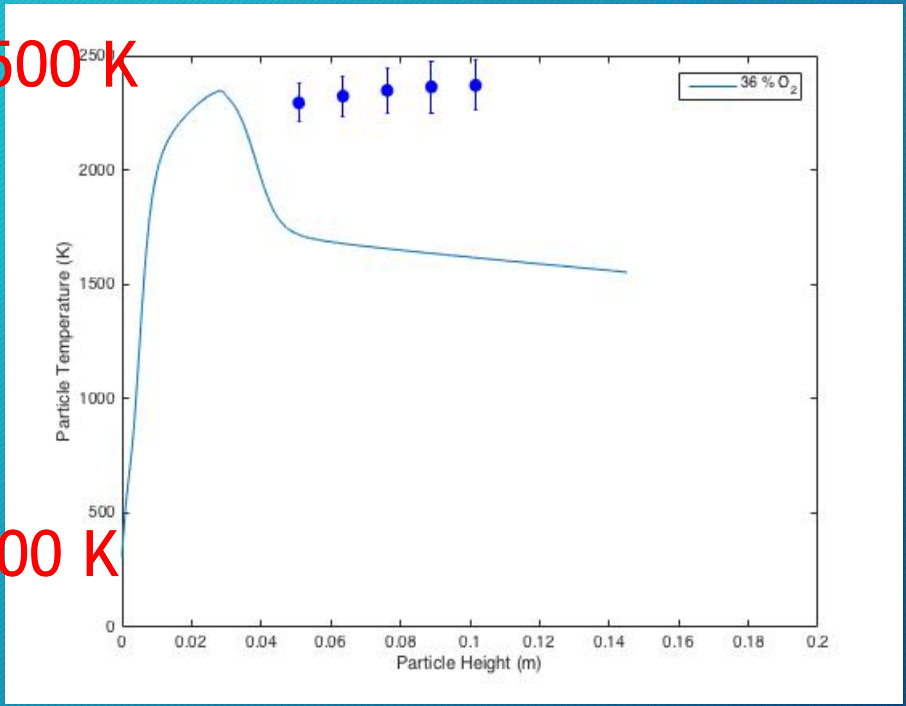
$$R_{C-H_2O} = \frac{k_8 P_{H_2O}}{1 + \frac{k_4}{k_5} P_{CO_2} + \frac{k_{4r}}{k_5} P_{CO} + \frac{k_6}{k_7} P_{H_2O} + \frac{k_{6r}}{k_7} P_{H_2}}$$

(Niksa et al., 2003; Liu and Niksa, 2004) (Shurtz and Fletcher, 2013)

CCK Result for Black Thunder

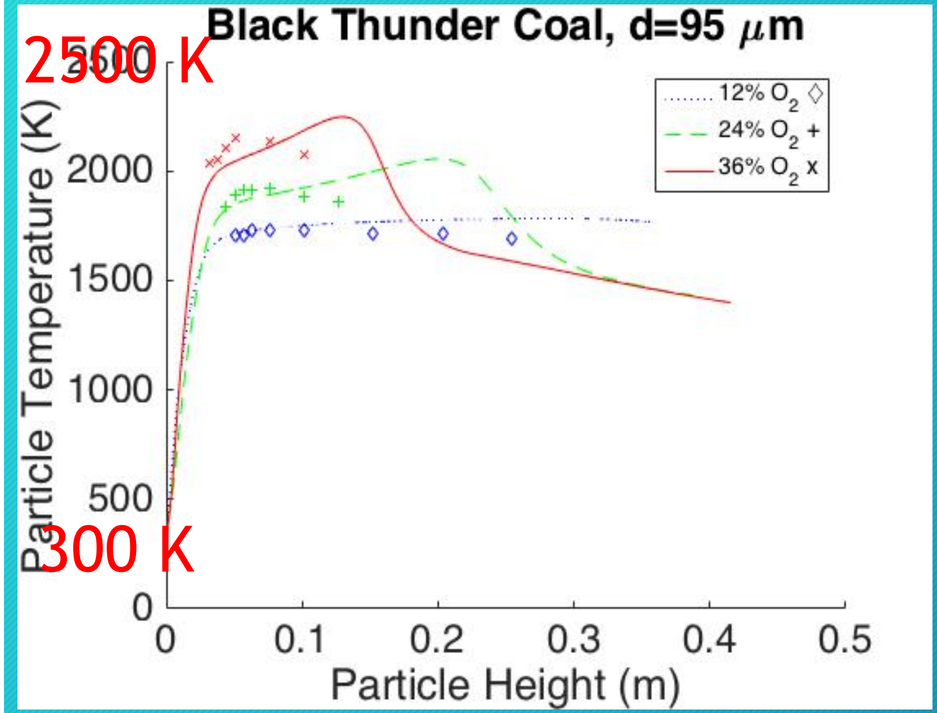


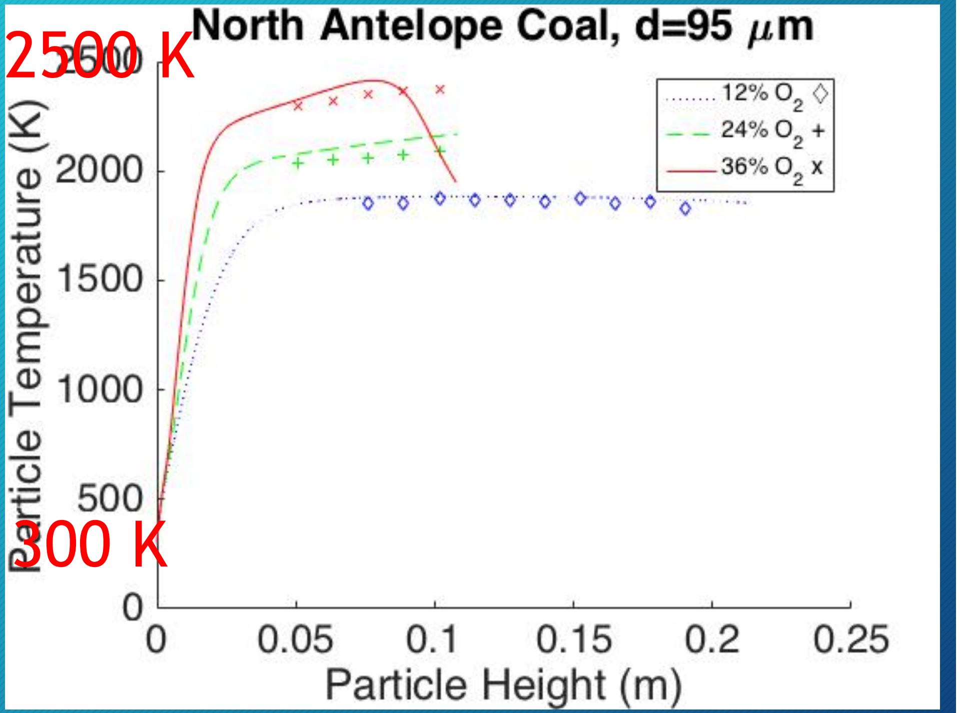
T_p vs height for Black Thunder in 12% O_2 2 Standard deviations from the mean T_p



T_p vs height for Black Thunder in 36% O_2 2 Standard deviations from the mean T_p

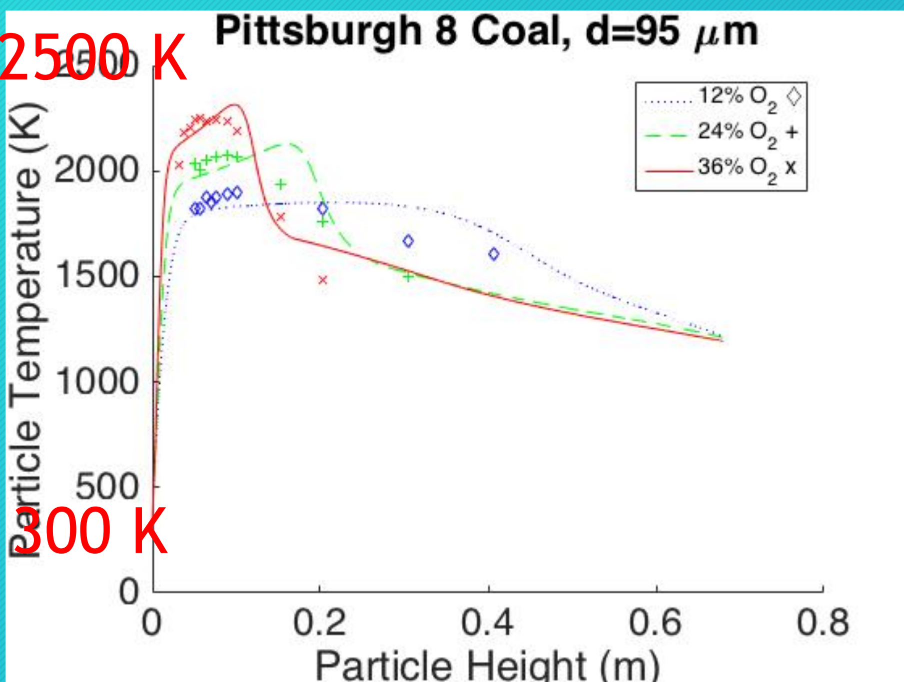
CCK/oxy 95 micron Diameter Result

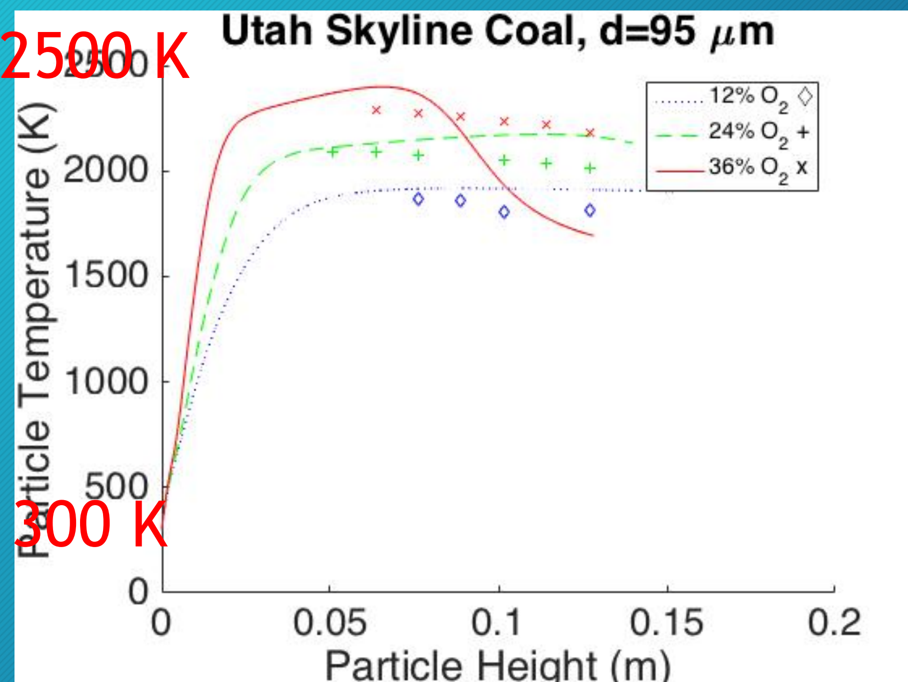




Initial raw coal diameter

CCK/oxy 95 micron Diameter Result



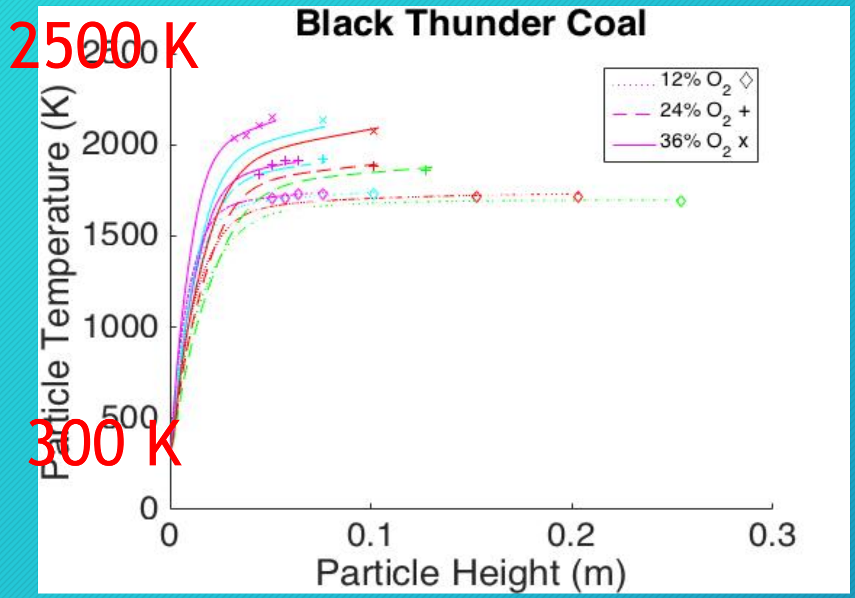


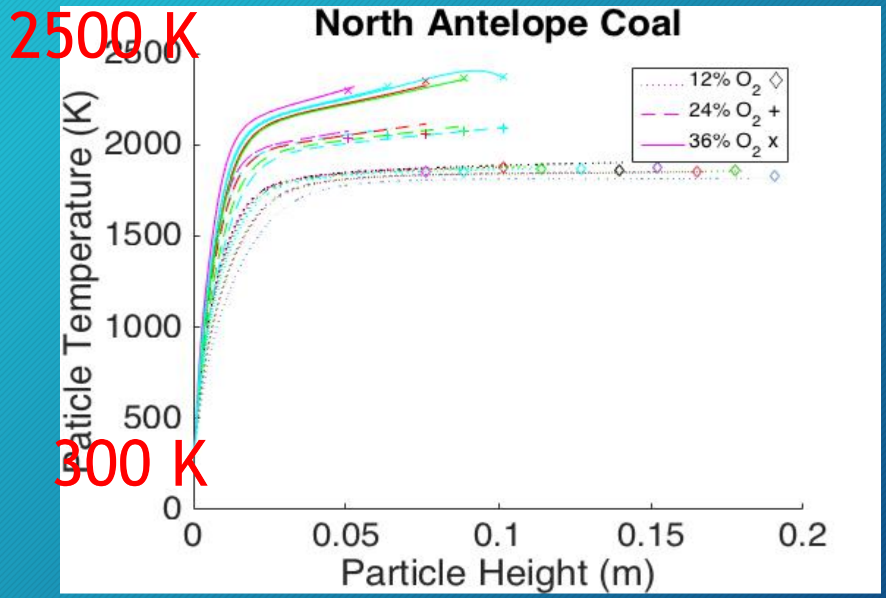
Initial raw coal diameter

CCK/oxy Result with Correct Diameter

- Each observed data point is the average of several hundred observations at a specific observation height
- Each observed particle has a specific diameter and temperature, and the hundreds of observations form a particle distribution
- The particle distribution is clearly different between observation heights, and shows a clear trend (larger particles are preferentially observed at later observation heights)
- The detection system is sensitive to particle emissions, so larger, hotter particles are preferentially observed
- As smaller particles burn out, the observed particles come from a skewed sample of the original distribution

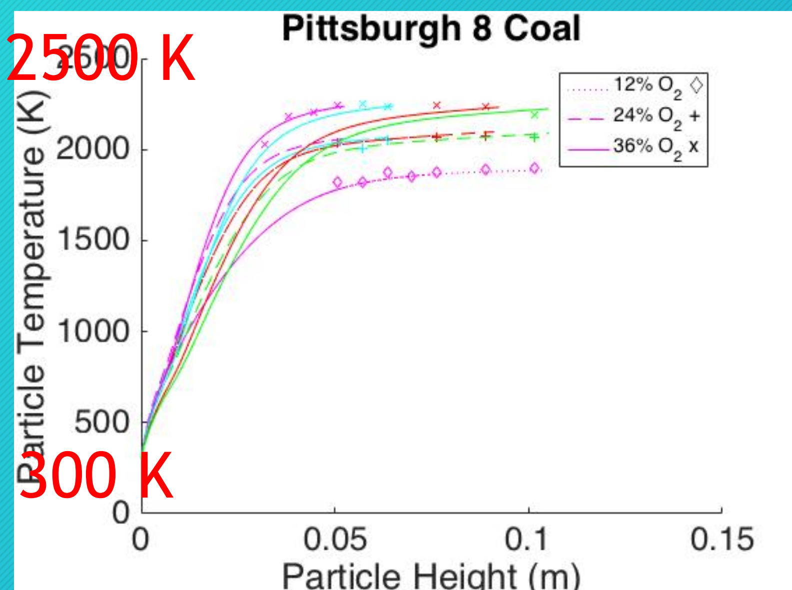
CCK/oxy Result with Correct Diameter

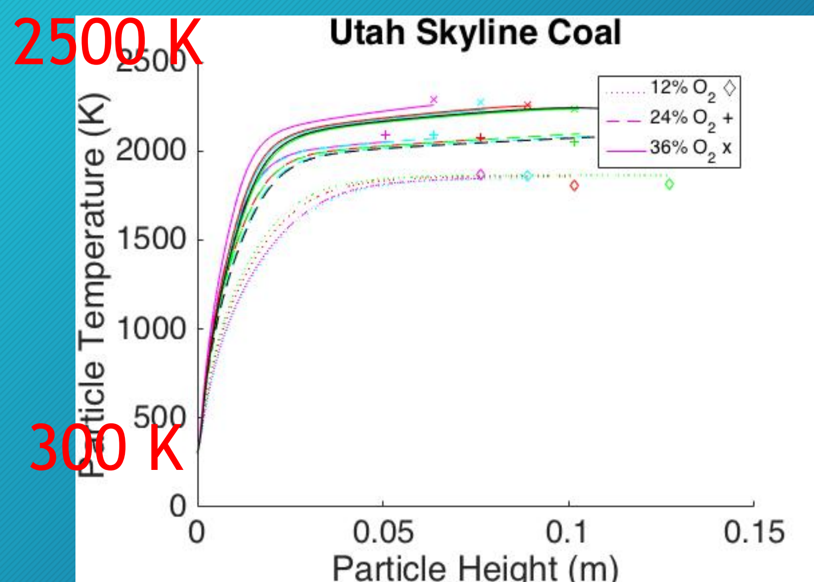




Post-swelling diameters of char at each height (from data)

CCK/oxy Result with Correct Diameter

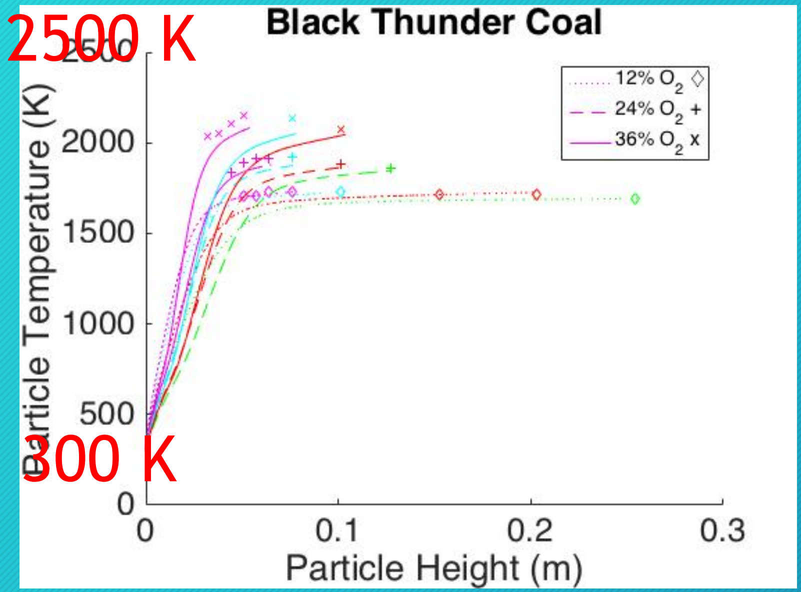




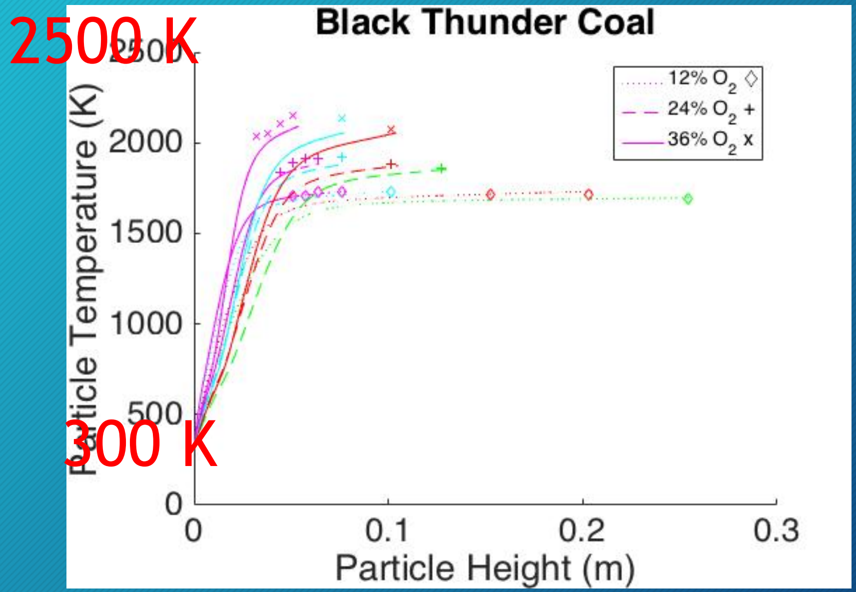
Post-swelling diameters of char at each height (from data)

Observations, Conclusions, and Recommendations

- Improved submodels capture the physics of combustion well (effective fitting and extrapolation)



Extrapolated from 12% O_2 Oxy-coal Data



Extrapolated from 12% O_2 Conventional Data

Observations, Conclusions, and Recommendations

- In general, the model fit the data shockingly well
- The proper initial particle diameter trends are essential
- The annealing model greatly reduces the unpredictability and variability seen due to preparation conditions

Future work

- Potential for a feasible parameter space based solely on coal proximate and ultimate analysis
- Even a naïve correlation of kinetic parameters with NMR parameters has promising results
- More realistic correlations would require an expanded data set and kinetic correlation form

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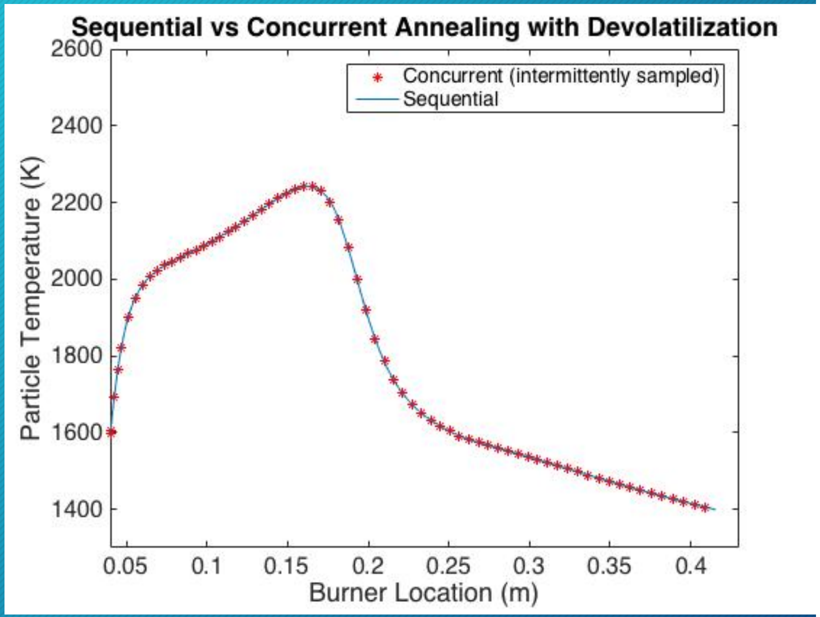
Sensitive Submodels: CPD

- Chemical Percolation Devolatilization
  - Coal structure and heating rate dependent
  - Thoroughly tested to successfully track initial heat-up and devolatilization
  - Volatiles that do not escape cross-link back into the structure of the coal
  - Integrated and verified to play nicely with the other submodels (generally within 0.04 K)



Burner Location