10th U.S. National Combustion Meeting:

Validation and uncertainty quantification analysis (VUQ) of a char oxidation model

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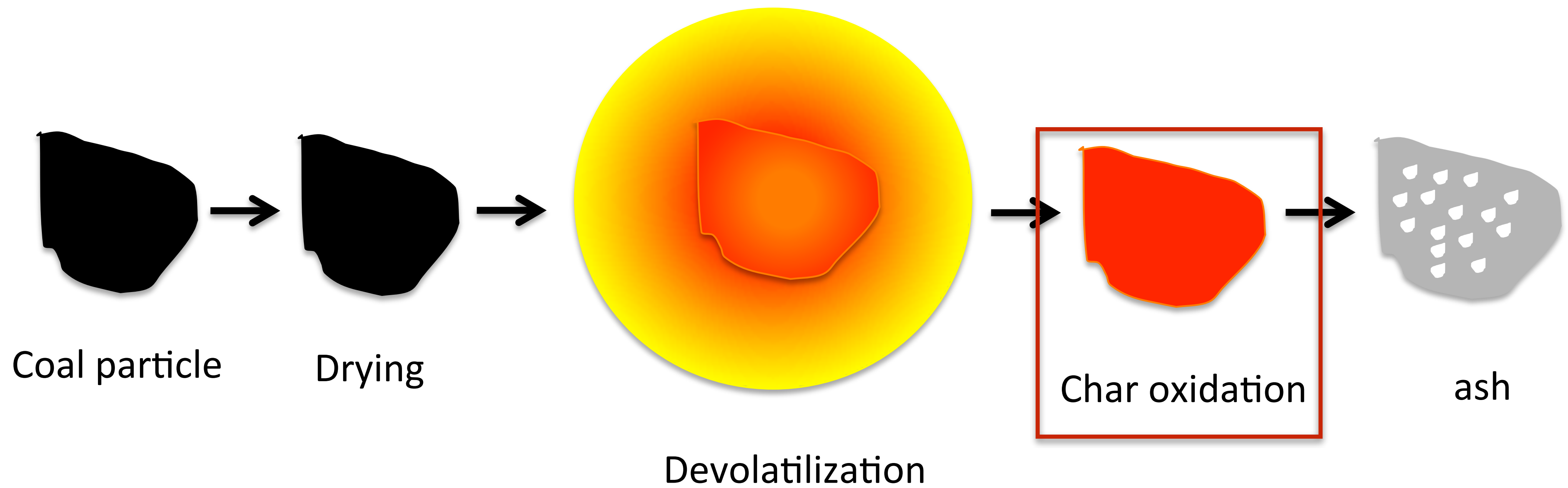
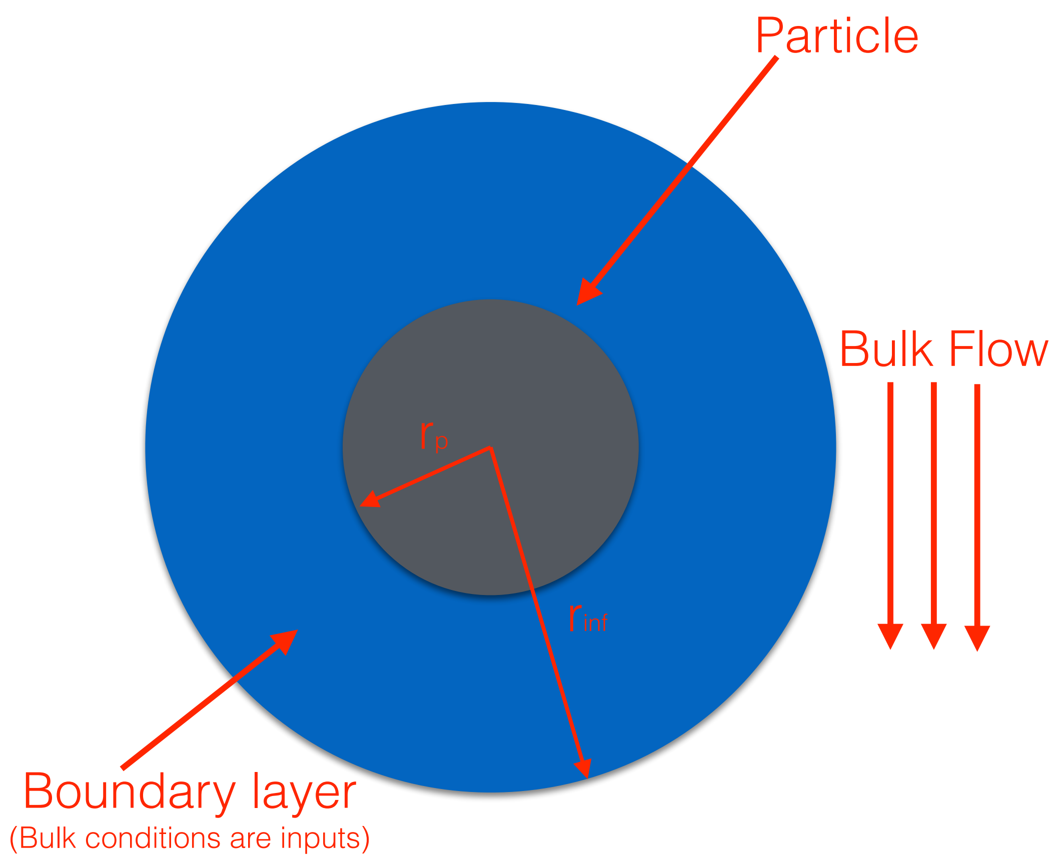
Char oxidation

Char oxidation is the last stage of the coal combustion process. It is the slower stage of the process and can take place in the whole combustion space.



- Involved in calculations of temperature and gas composition.

Reacting Particle and Boundary Layer (RPBL) model



$Reaction$	$A[mol, cm^2, s]$	$E[kJ/mol]$
$C_b + C_s + O_2 \rightarrow CO + C(O)_s$	$3.3x10^{15}$	167.4
$C(O)_s + C_b \rightarrow CO + C_s$	$1.0x10^8$	0.0
$C_s + O_2 \rightarrow C(O_2)_s$	$9.5x10^{13}$	142.3
$C(O_2)_s + C_b \rightarrow CO_2 + C_s$	$1.0x10^8$	0.0
$C_s + CO_2 \rightarrow CO + C(O)_s$	$variable$	251.0
$C_s + H_2O \rightarrow H_2 + C(O)_s$	$variable$	222.0

- Computes transient-state conditions for a spherical, constant-diameter, reacting, porous char particle and its reacting boundary layer.
- Transport of gaseous species uses Maxwell-Stefan multicomponent approach.
- Homogeneous gas phase reactions are estimated with a syngas mechanism.
- Heterogeneous reactions are calculated with a six-step reaction mechanism.
- Computes carbon consumption, uses Bhatia and Perlmutter model to estimate surface area evolution.
- Solves one energy equation for the gas and one for the particle.
- Physical properties depend of the fractions of ash and carbon and on void fraction.

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RPBL model equations

Energy equations

Transient term

$$\frac{dT_{g,i}}{dt} = \frac{1}{\rho_{t,i} c_{p\,g,i} V_i}\left[-[(AF_{cond})_{i+1/2} - (AF_{cond})_{i-1/2}] - [(AF_h)_{i+1/2} - (AF_h)_{i-1/2}] - V_i \rho_{t,i} \sum_{k=1}^{Kg} h_{k,i} \frac{dY_{k,i}}{dt} + S_i \right.$$

Conduction

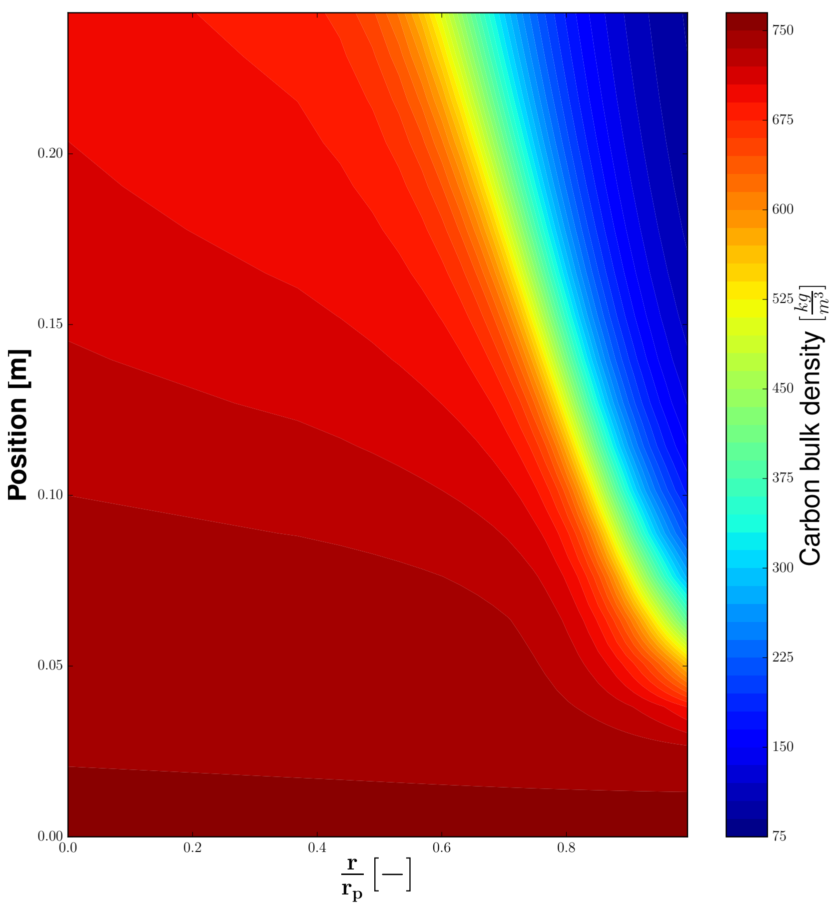
Enthalpy

Heat exchange between solid and gas

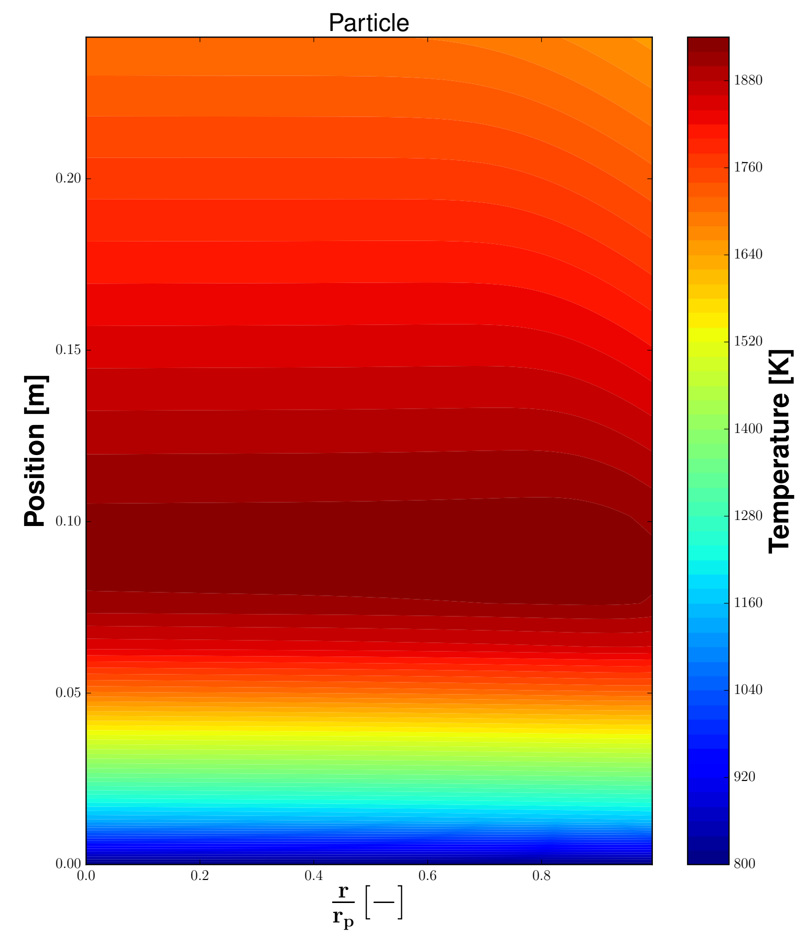
$$\frac{dT_{p,i}}{dt} = \frac{1}{\rho_{bulk\,p,i} c_{p\,p,i} V_i}\left[-[(AF_{cond,p})_{i+1/2} - (AF_{cond,p})_{i-1/2}] - h_{c_b,i}\dot{s}_{c_b,i}\sigma_{r,i} V_i - S_i \right]$$

RPBL model results

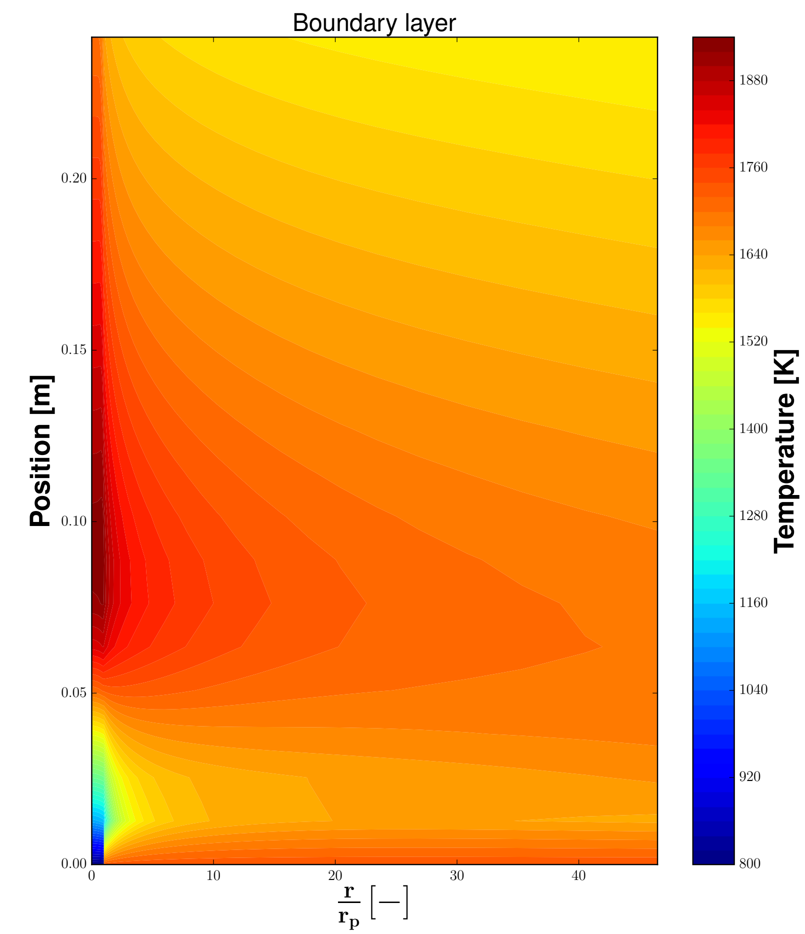
Base case



Carbon burnout



Particle temperature



Gas temperature

N= 60, Np = 30; RPBL solved 781 ODEs

$$\tau = 5,\ \frac{r_{inf}}{r_p} = 53,\ \psi = 8,\ \varepsilon_p = 0.96,\ \lambda_p = 1.33,\ d_p = 95\,\mu m,$$

$$\phi_{initial} = 0.18,\ Y_{c,initial} = 0.98,\ Sgc_{initial} = 8000\,[kg_c/m^2]$$

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Step 1: Selection of quantities of interest (QOIs)

- Particle temperature and velocity (experimental data collected by Hecht).
- Three chars obtained from Illinois #6 (high volatile bituminous coal), Utah Skyline (western bituminous coal), and Black Thunder (subbituminous coal).
- Two environments: O_2 = (24, 36 vol%), H_2O = (14 vol%, balance CO_2.
- Average particle temperature from RPBL is used.

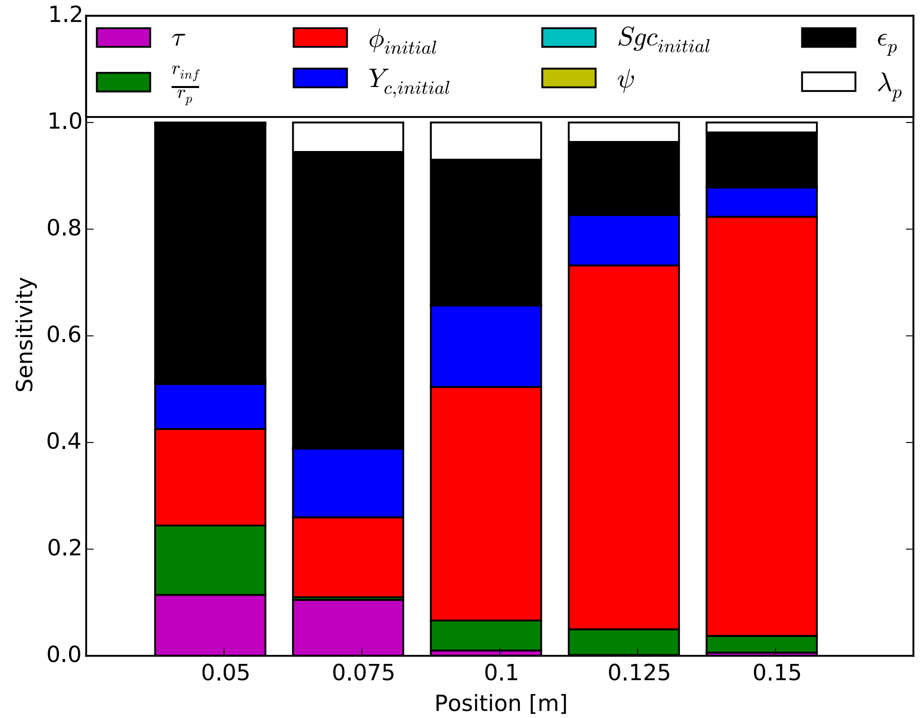
Step 2: Input/Uncertainty Map

Parameter	Priority	Range min	Range max	Nominal value
Numerical Parameters				
N_p	1	15	100	30
N	1	30	200	60
$rtol$	1			1e-4
Model Parameters				
$\tau\,[-]$	6	3	6	
$\frac{r_{inf}}{r_p}\,[-]$	6	50	120	
$\psi\,[-]$	6	3	8	
$\epsilon_p\,[-]$	6	0.1	1	
$\lambda_p\,[\frac{W}{mK}]$	6	0.1	2	
$\rho_{true\,c}\,[\frac{kg}{m^3}]$	1			921
$\rho_{true\,ash}\,[\frac{kg}{m^3}]$	1			2000
$h_{solid\,gas}\,[\frac{W}{m^2K}]$	1			1
Scenario parameters				
$d_p\,[\mu m]$	6	50	160	
$v_g\,[\frac{m}{s}]$	3			From reactor model
$T_g\,[K]$	3			From reactor model
$O_{2,bulk}\,[-]$	3			From reactor model
$H_2O_{bulk}\,[-]$	3			From reactor model
$CO_{2,bulk}\,[-]$	3			From reactor model
$H_{2,bulk}\,[-]$	3			From reactor model
$CO_{bulk}\,[-]$	3			From reactor model
$O_{2,initial}\,[-]$	3			1.00e-3
$H_2O_{initial}\,[-]$	3			1.00e-3
$H_{2,initial}\,[-]$	3			1.00e-3
$CO_{initial}\,[-]$	3			1.00e-3
$CO_{2,initial}\,[-]$	3			0.99
$T_{p,initial}\,[K]$	3			From reactor model
$\phi_{initial}$	6	0.15	0. 7	
$Y_{c,intial}\,[-]$	6	0.5	1	
$Sgc_{initial}\,[\frac{kg}{m^2}]$	6	8000	12000	
$T_w\,[K]$	3			500
$Pressure\,[\frac{kg}{m^2}]$	3			1.00e5

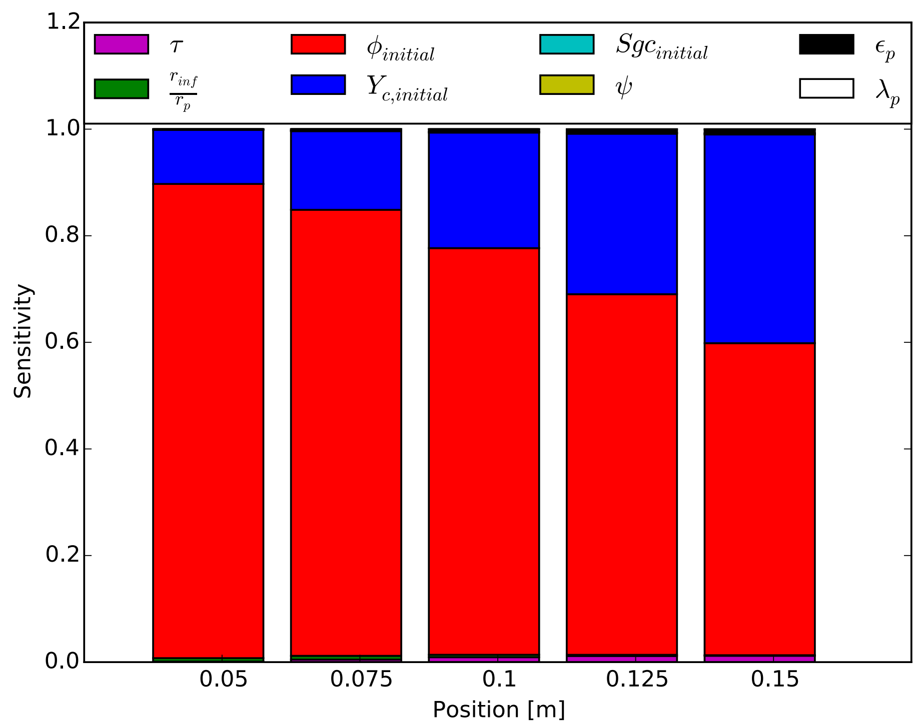
- Sensitivity analysis with eight active parameters for three particle sizes (50 μm, 80 μ*m*, 120 μm)
- Particle size is the ninth parameter
- Test sensitivity of particle temperature and velocity.

- Small-size particles $53-60\,\mu m$
- Medium-size particles $75-90\,\mu m$
- Big-size particles $106-125\,\mu m$

Step 2: Input/Uncertainty Map



Particle temperature



Particle velocity

General

- 256 RPBL cases were run.
- Uncertainty Quantification Toolkit (UQTk)
- Use coefficients of first order polynomial chaos surrogate model.
  $d_p = 80\,\mu m\ (75 - 90\mu m)$

Particle temperature

- Most sensitive parameters were $\phi_{initial}$, Y_c, and ϵ_p
- Next were $\frac{r_{inf}}{r_p}$, τ and λ_p
- Least sensitive parameters were $Sgc_{initial}$ and ψ

Particle velocity

- Most sensitive parameters were $\phi_{initial}$, and Y_c

Conclusion

- Five parameters were selected for consistency analysis:
  d_p, $\phi_{initial}$, Y_c, ϵ_p, and $\frac{r_{inf}}{r_p}$

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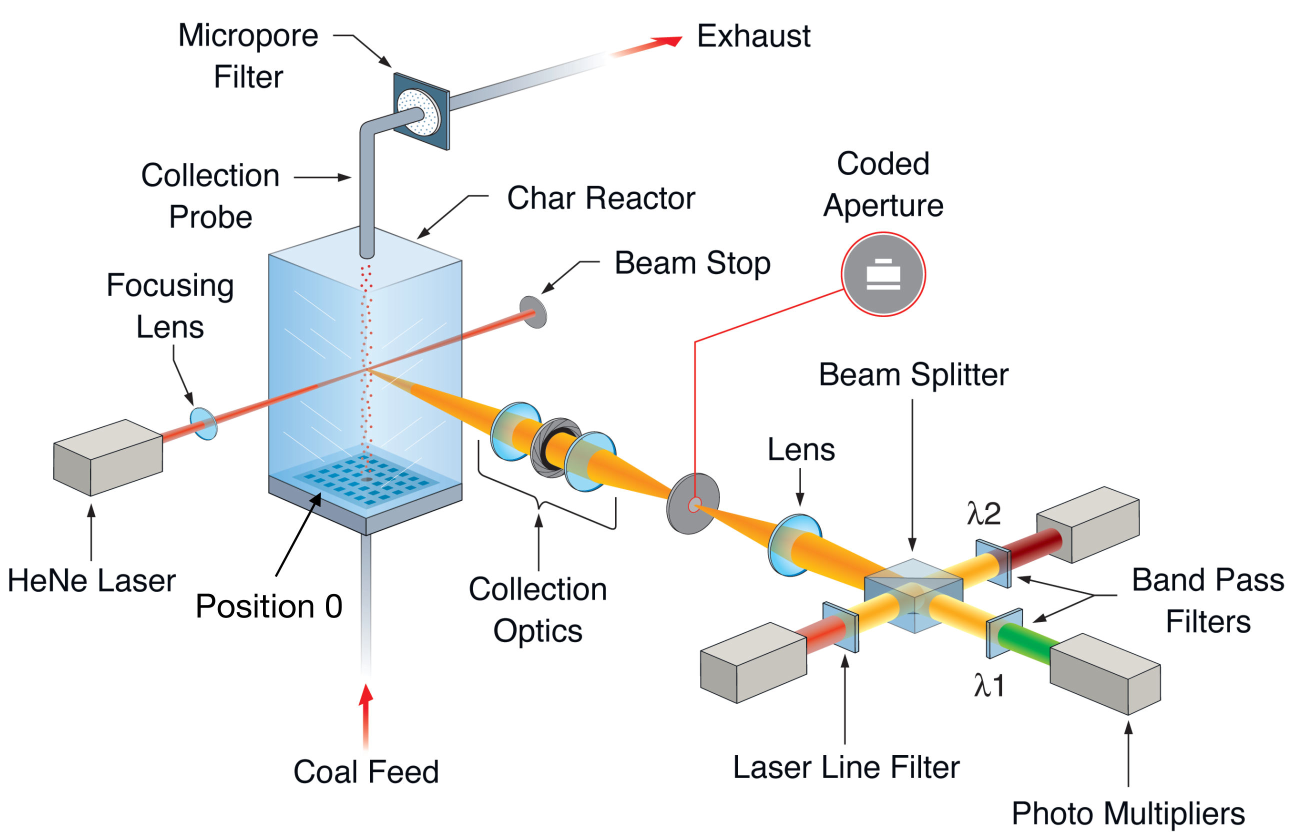
Step 3: Experimental data collection

Laminar, entrained flow reactor at Sandia National Laboratories.



- Three types of measurements: temperature, velocity and size of a single particle.
- Three type of char : Illinois #6 (I6), Utah Skyline (US), Black Thunder (BT).
- Two environment conditions:

  $O_2\ vol\% = 24,\ 36;\quad H_2O\ vol\% = 14\quad \text{balance}\ CO_2$

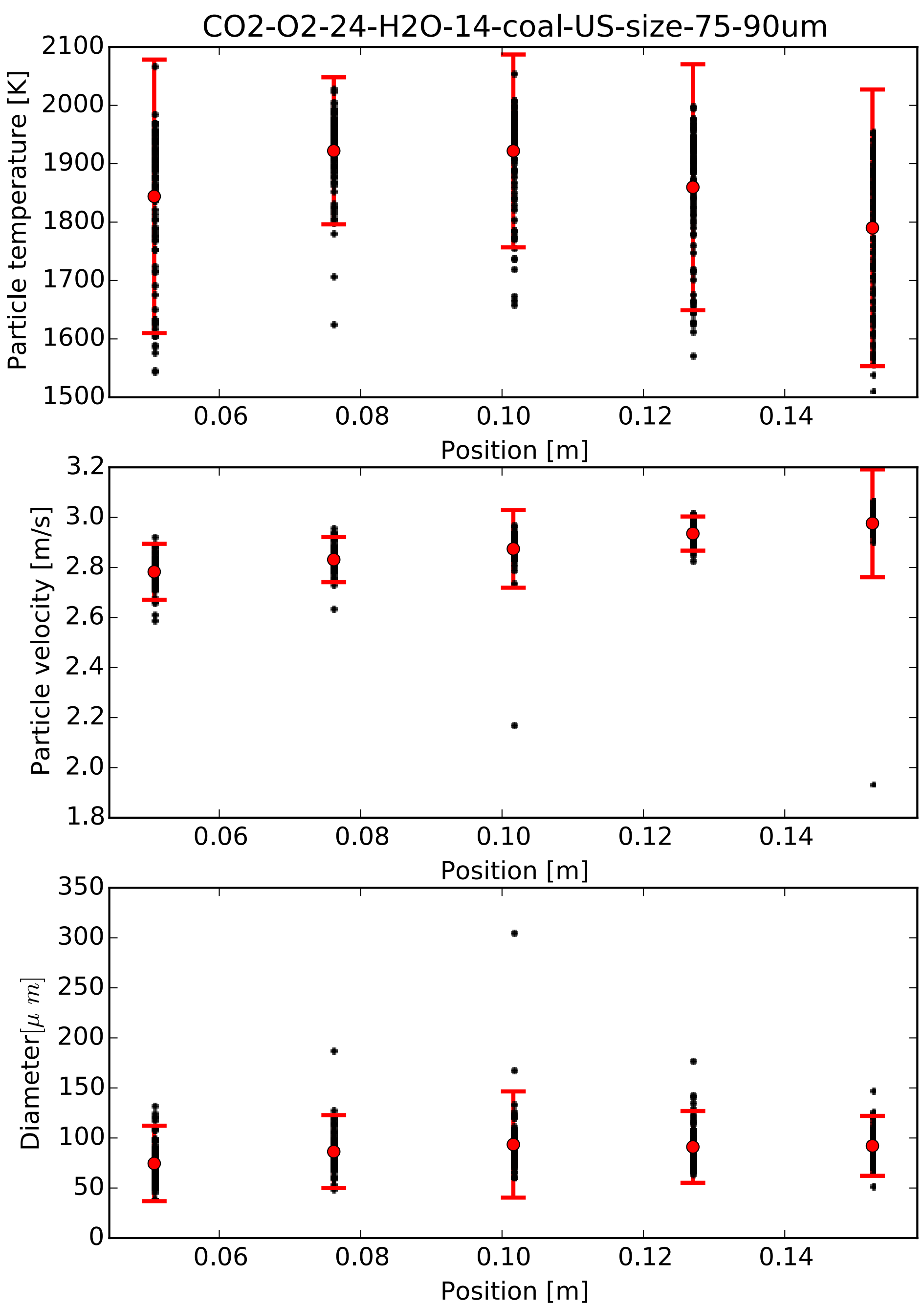
- Six bin sizes :

  53-63 μm, 63-75 μm, 75-90 μm, 90-106 μm, 106-125 μm, and 125-150 μm

- In each position approximately 100 particles are measured.

Step 3: Experimental data collection

Uncertainties in experimental measurements



Systematic error

$$\bar{y} - y_T = \Delta + \beta$$

Sampling error

$$|\beta| \leq t_{\alpha/2,v} \frac{s}{\sqrt{n}}$$

- Systematic error is assumed much smaller than random error.
- Experiment is defined as one char, one environment, and one particle size at all measurement positions in the reactor.
- Sampling error was computed for 36 experiments using a confidence interval of 95 %.

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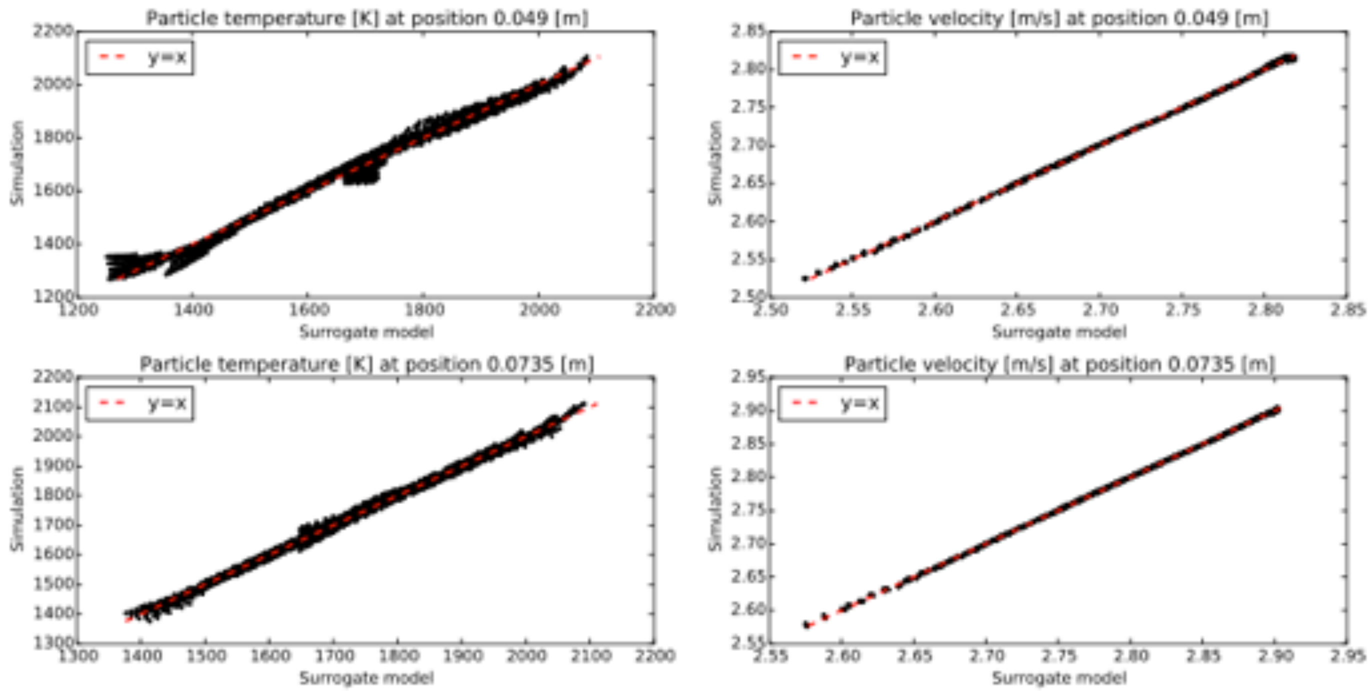
Step 3: Simulation data collection
RPBL model

- RPBL was run using average temperature and velocity profiles from reactor model
- Five parameters were used: d_p, $\phi_{initial}$, Y_c, ϵ_p, and $\frac{r_{inf}}{r_p}$
- Uncertainty Quantification Toolkit (UQTk) was used to produce a design of experiments.
- 10901 cases were run.
- Each case has 60 cells, therefore RPBL is solving 781 ODEs.
- RPBL cases were run on linux cluster at the University of Utah; with 520 cores it was possible to run all cases in one day.

Step 4: Construction of surrogate models



- Surrogate models for particle temperature and velocity are created for each measurement location.

- PC of order 4 was used for $O_2 = 24\ vol\,\%,\ H_2O = 14\ vol\,\%,\ \text{balance}\ CO_2$ environment; 3125 cases were run.
- PC of order 5 was used for $O_2 = 36\ vol\,\%,\ H_2O = 14\ vol\,\%,\ \text{balance}\ CO_2$ environment; 7776 cases were run.

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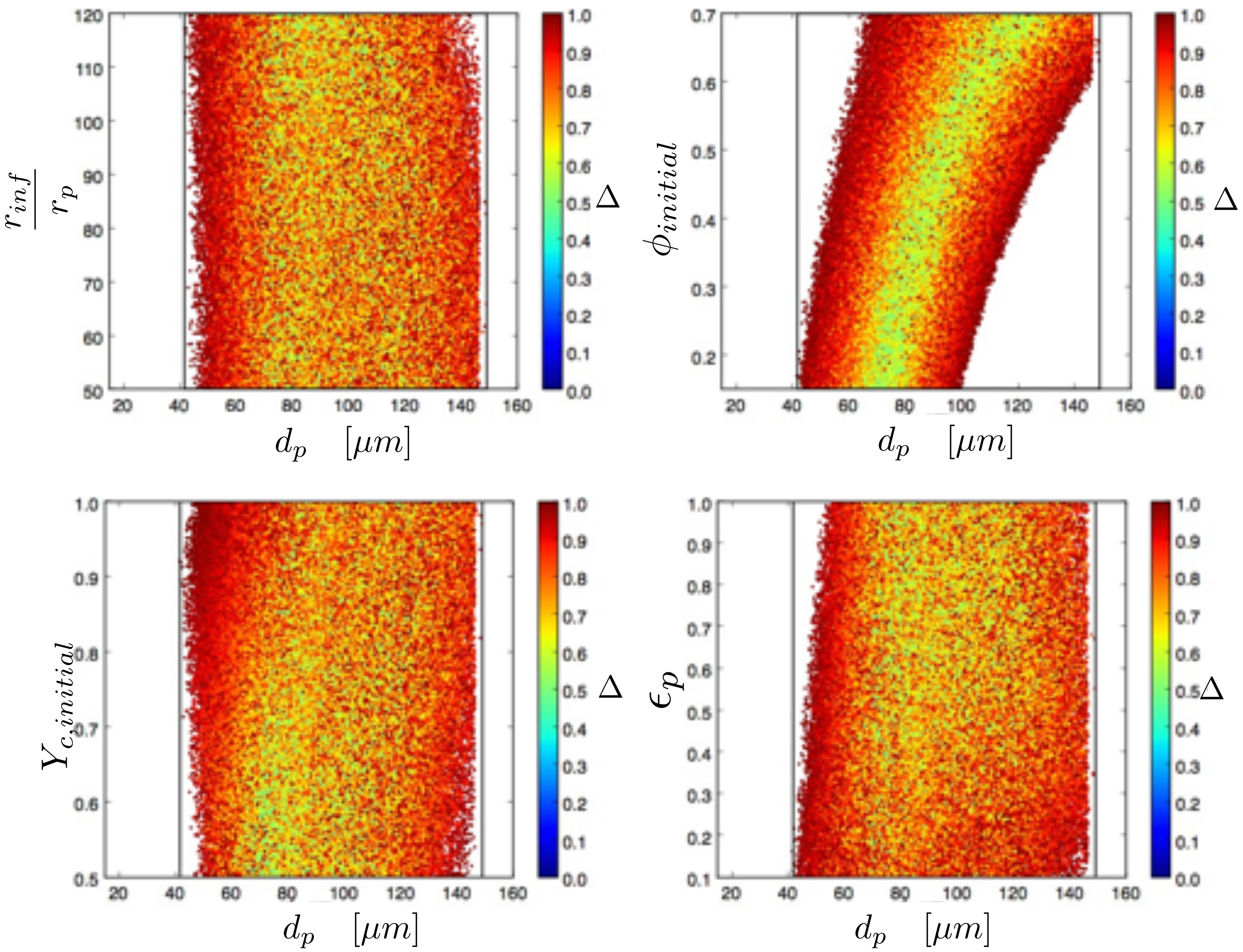
Step 5: Analysis of model outputs

US char $O_2 = 24\ vol\%$, $H_2O = 14\ vol\%$, balance CO_2 environment 75-90 μm size bin



Parameter	Prior range	Consistent range	Nominal value
d_p [μm]	36.9- 146.5	42.0-146.0	75-90
$\phi_{initial}$	0.15 - 0.7	0.15 - 0.7	-
$Y_{c,intial}$ [$-$]	0.5-1	0.5-1	-
$\frac{r_{inf}}{r_p}$ [$-$]	50-120	50-120	-
ϵ_p [$-$]	0.1-1	0.1-1	-

- Consistency analysis was carried out for 36 experiments performed by Hecht.
- Experimental particle size was used as prior range.
- Same set of RPBL data is used for the three chars.

$$\frac{|\ y_{m,e}(\mathbf{x}) - y_e\ |}{u_e} \leq 1$$

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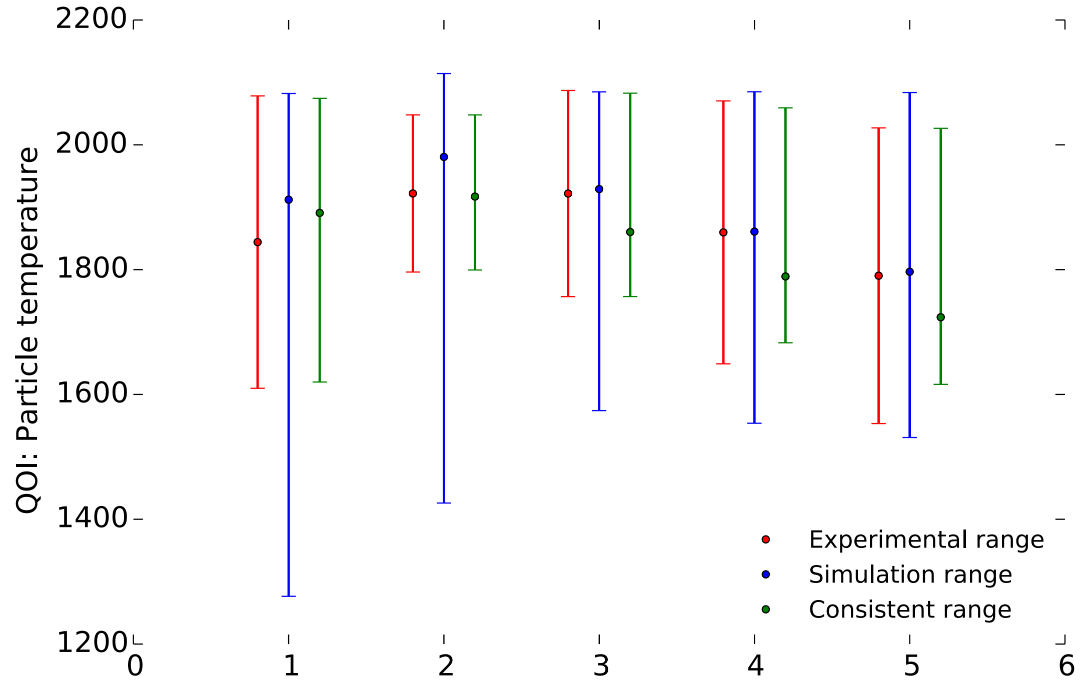
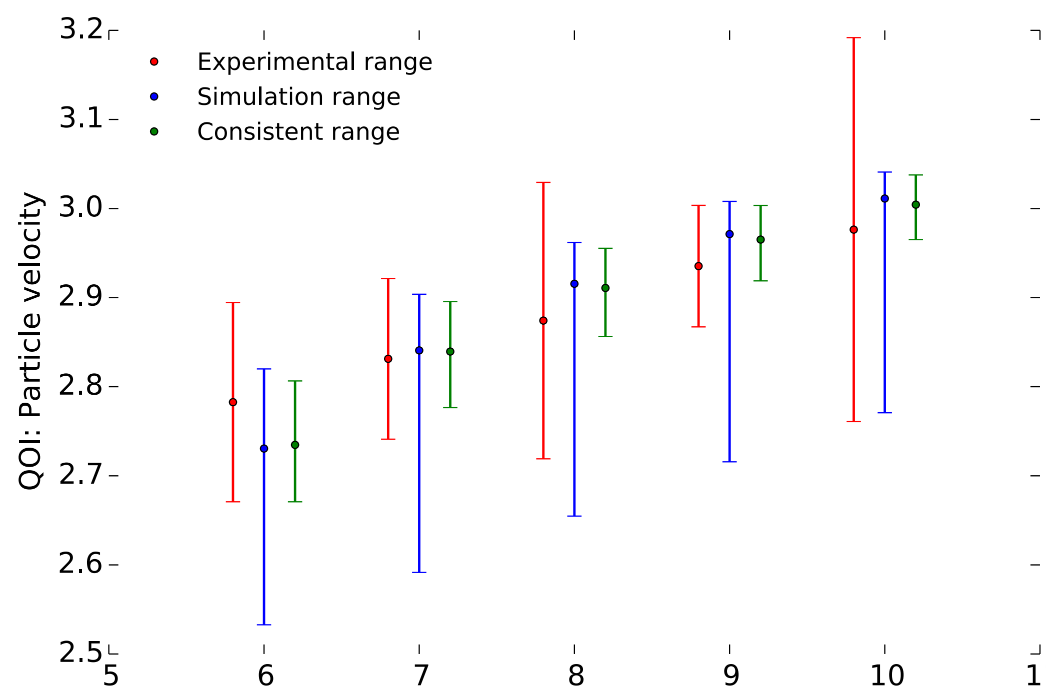
Step 5: Analysis of model outputs

US char $O_2 = 24\ vol\%$, $H_2O = 14\ vol\%$, balance CO_2 environment 75-90 μm size bin





We performed a similar consistency analysis for the other 35 experiments and obtained consistency with all 36 experiments.

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Step 6: Feedback and feed forward

Model

- Transient RPBL model for char oxidation was developed. Assumptions in the formulation include:
  - Diameter of the particle during the combustion process was constant.
  - Gradient of pressure was assumed negligible.
  - Same heterogeneous reaction mechanism was used for all three chars.
- QOIs (particle temperature and velocity) are most sensitive to $d_p, \phi_{initial}, Y_c, \epsilon_p$
  - Consistency was found for 36 experiments if experimental size of particle is used as prior range.
  - Develop models of coal devolatilization that predict void fraction and carbon mass fraction.
  - Use a better classification system for characterizing the size distribution of particles.
- Increase the number of measurements at each position in order to reduce the sampling error.

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