Providing structure to experimental data: A large scale heterogeneous database for collaborative model validation

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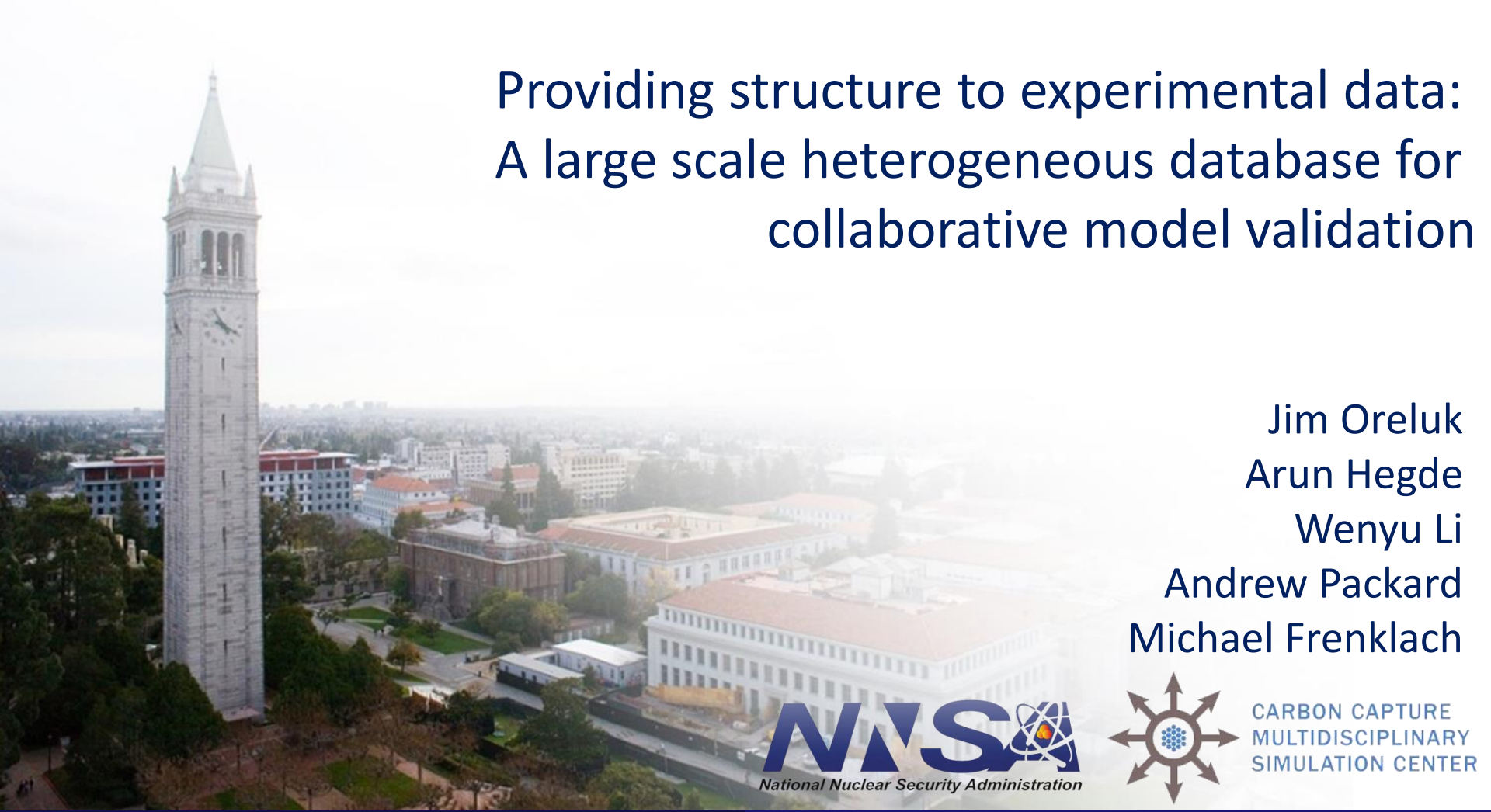

National Nuclear Security Administration

CARBON CAPTURE MULTIDISCIPLINARY SIMULATION CENTER

Overview

- Introduction
- Giving structure to experimental data
  - PrIMe Data Warehouse
- New PrIMe application
  - front-end application to the CCMSC coal database (filter, visualization, and export data)
- Bound-to-Bound Data Collaboration workflow for model validation
- Summary

Introduction

- Predictive modeling starts with validation
- Experimental data stored in various file formats
  - CSV, Excel, tab delimited, ASCII, etc.
  - **No standard**
- Each record requires specialized knowledge of how the data was stored
  - Can be an incomplete record of experiment with missing information
- We would like automated access to data
  - Without structure, query requests are quickly intractable across a diverse collection of data
- Efficiently discover validation data to incorporate in the model validation process

Providing Structure to Experimental Data

primekinetics.org

- What is PrIMe?
  - Data Warehouse – repository of experimental records
  - Applications – aid in development of predictive models
- Transformation of information into a usable form
- PrIMe's data models use XML schemas to provide structure
  - Contains **complete** information of an experiment
  - Experimental data is stored in XML or HDF5 files
- Storage of raw experimental data and derived properties
  - Ability for instrumentation modeling

CCMSC Coal Database for V/UQ

- International Flame Research Foundation, Livorno, Italy
- Sandia National Laboratory, Livermore, CA

269 Solid Fuels & Blends

Fossil, Biomass, Sludge, Waste, Char

2710 Data Groups collected from 1016 Records

Varying Conditions (Temperatures, $\%O_2$, $\%H_2O$, Gas Mixture)

Experiment Types: *Devolatilization, Char oxidation*

In collaboration with Salvatore Iavaron and Alessandro Parente, Université Libre de Bruxelles

leveraging existing cloud infrastructure and data models

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xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
  <copyright>©primekinetics.org 2017</copyright>
  <bibliographyLink primeID="b00019060" preferredKey="Leis
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    <kind>drop-tube furnace</kind>
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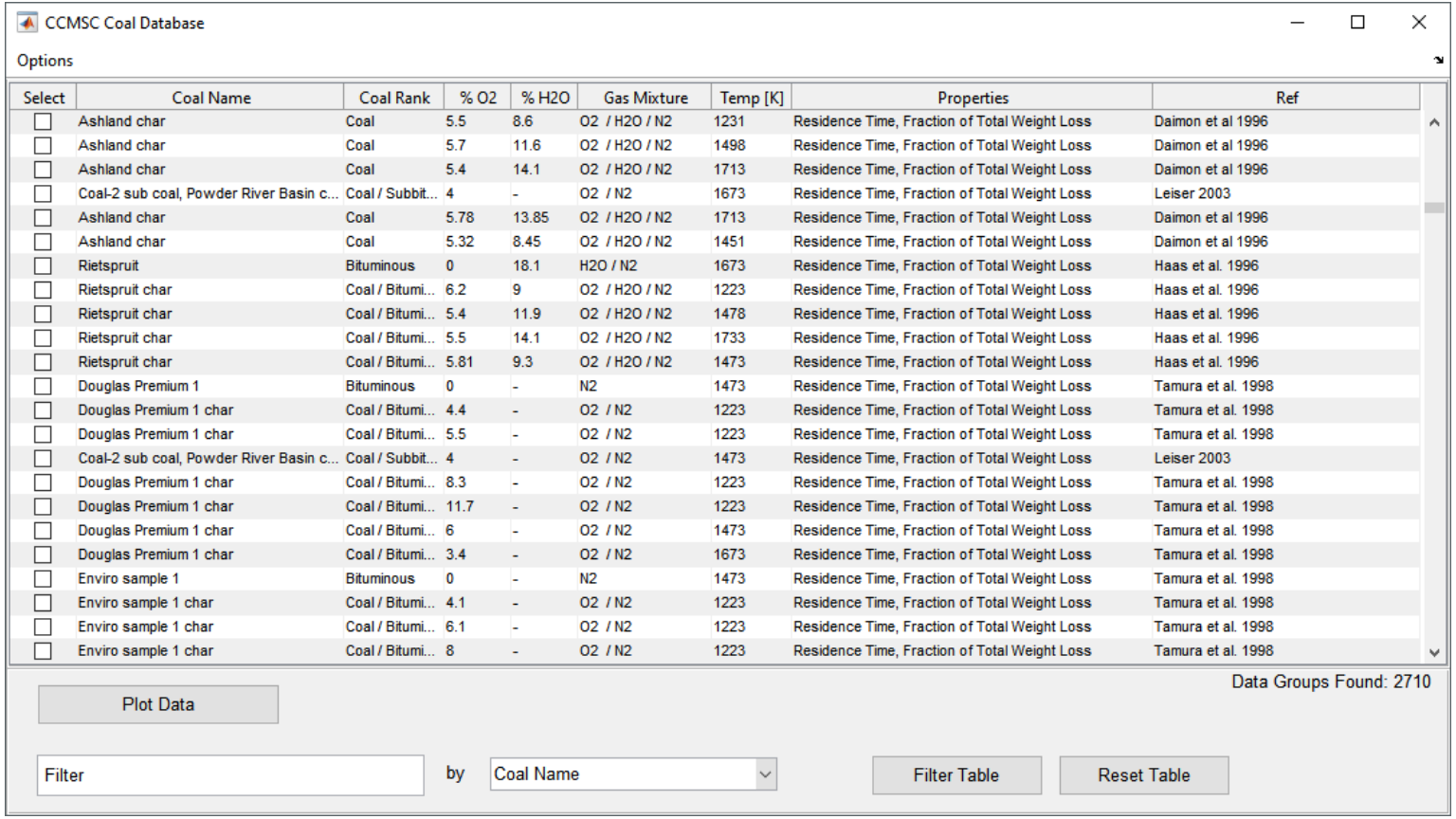
CCMSC Coal Database

primekinetics.org **github.com/oreluk/coalDB**



Select	Coal Name	Coal Rank	% O2	% H2O	Gas Mixture	Temp [K]	Properties	Ref
☐	Ashland char	Coal	5.5	8.6	O2 / H2O / N2	1231	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
☐	Ashland char	Coal	5.7	11.6	O2 / H2O / N2	1498	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
☐	Ashland char	Coal	5.4	14.1	O2 / H2O / N2	1713	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
☐	Coal-2 sub coal, Powder River Basin c...	Coal / Subbit...	4	-	O2 / N2	1673	Residence Time, Fraction of Total Weight Loss	Leiser 2003
☐	Ashland char	Coal	5.78	13.85	O2 / H2O / N2	1713	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
☐	Ashland char	Coal	5.32	8.45	O2 / H2O / N2	1451	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
☐	Rietspruit	Bituminous	0	18.1	H2O / N2	1673	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
☐	Rietspruit char	Coal / Bitumi...	6.2	9	O2 / H2O / N2	1223	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
☐	Rietspruit char	Coal / Bitumi...	5.4	11.9	O2 / H2O / N2	1478	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
☐	Rietspruit char	Coal / Bitumi...	5.5	14.1	O2 / H2O / N2	1733	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
☐	Rietspruit char	Coal / Bitumi...	5.81	9.3	O2 / H2O / N2	1473	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
☐	Douglas Premium 1	Bituminous	0	-	N2	1473	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
☐	Douglas Premium 1 char	Coal / Bitumi...	4.4	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
☐	Douglas Premium 1 char	Coal / Bitumi...	5.5	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
☐	Coal-2 sub coal, Powder River Basin c...	Coal / Subbit...	4	-	O2 / N2	1473	Residence Time, Fraction of Total Weight Loss	Leiser 2003
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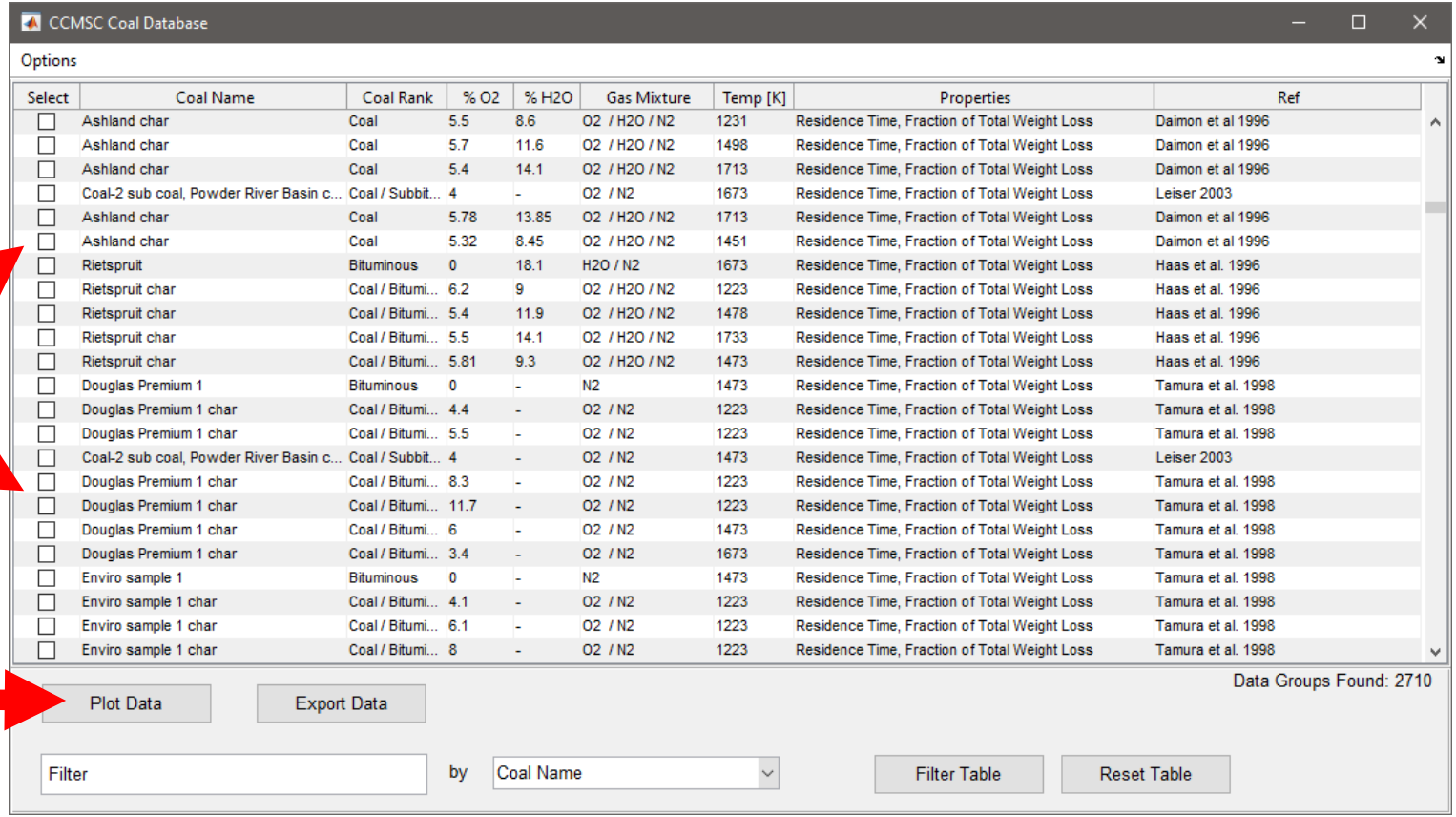
☐	Douglas Premium 1 char	Coal / Bitumi...	11.7	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
☐	Douglas Premium 1 char	Coal / Bitumi...	6	-	O2 / N2	1473	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
☐	Douglas Premium 1 char	Coal / Bitumi...	3.4	-	O2 / N2	1673	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
☐	Enviro sample 1	Bituminous	0	-	N2	1473	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
☐	Enviro sample 1 char	Coal / Bitumi...	4.1	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
☐	Enviro sample 1 char	Coal / Bitumi...	6.1	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
☐	Enviro sample 1 char	Coal / Bitumi...	8	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998

CCMSC Coal Database

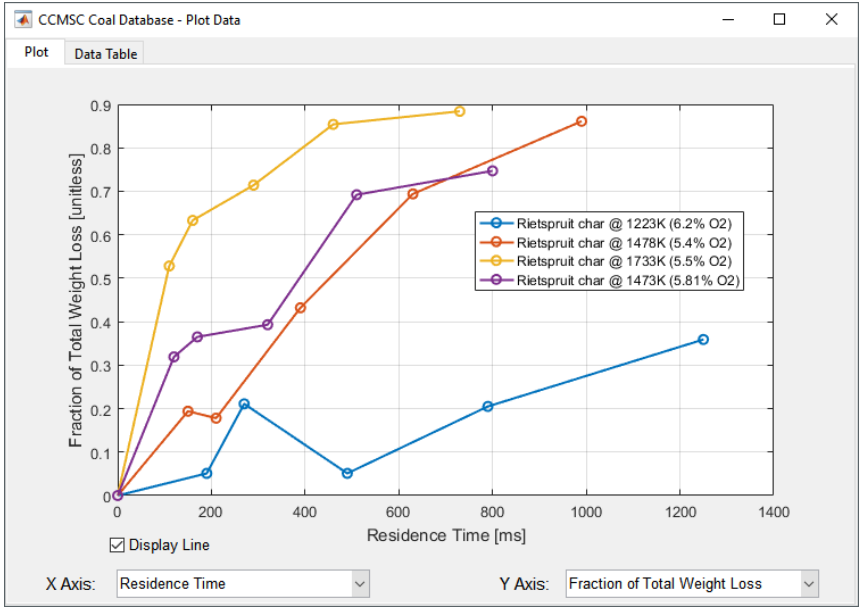
Select Experiments

Plot & Export Data

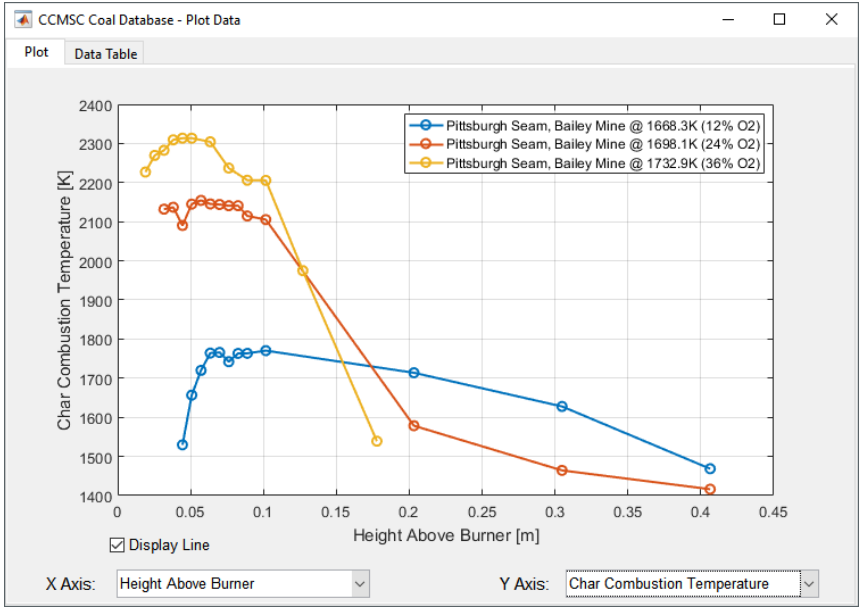


CCMSC Coal Database

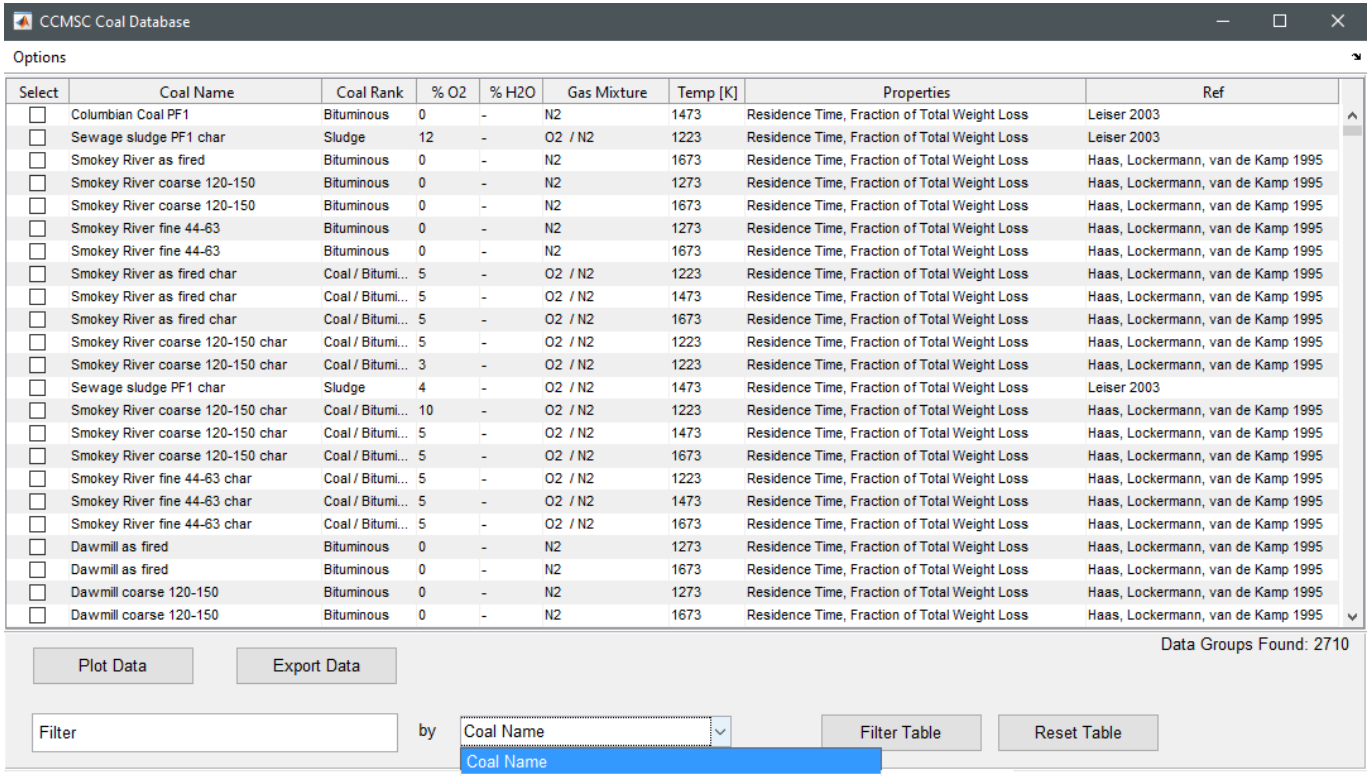
Fraction of Weight Loss



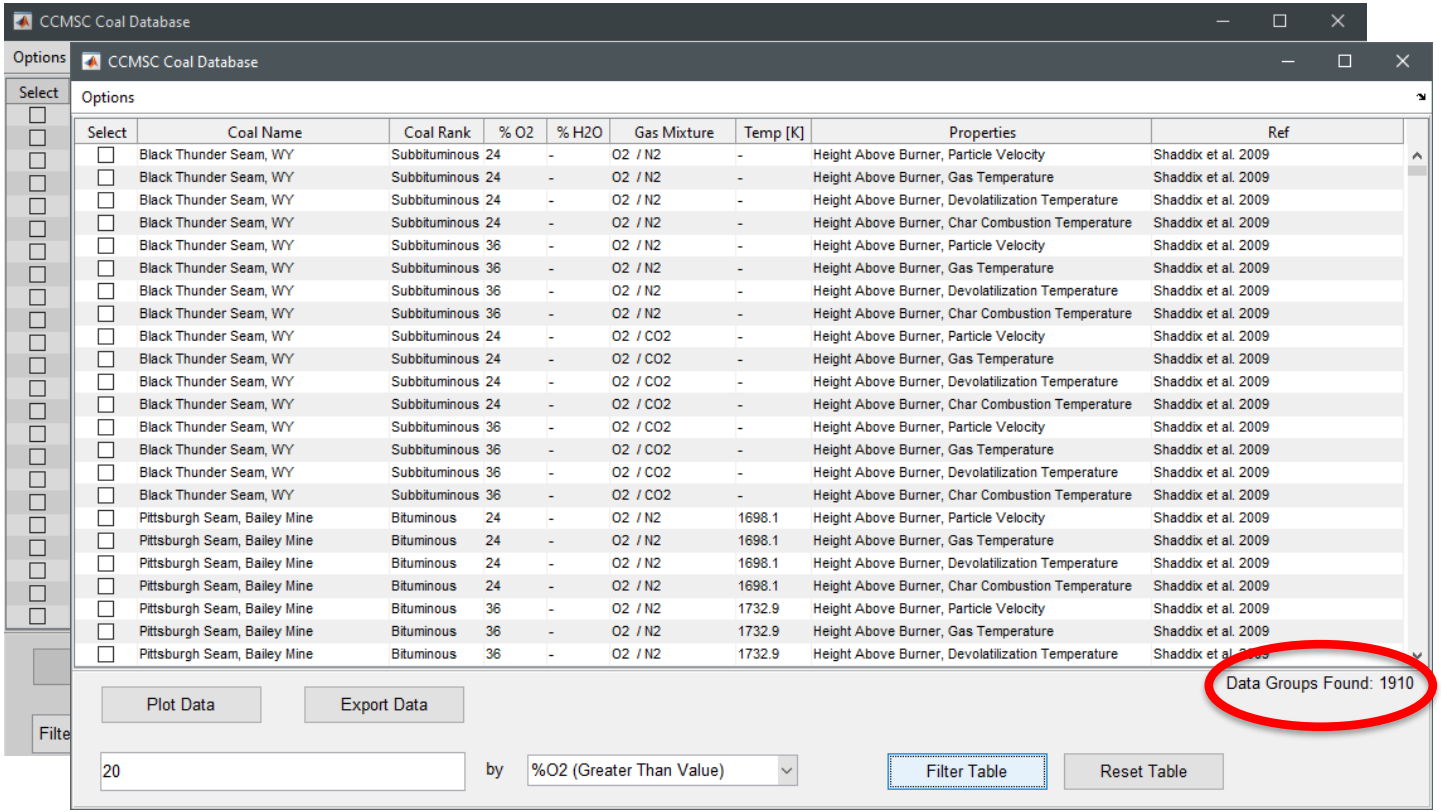
Char Temperature



Char Oxidation Example



Char Oxidation Example



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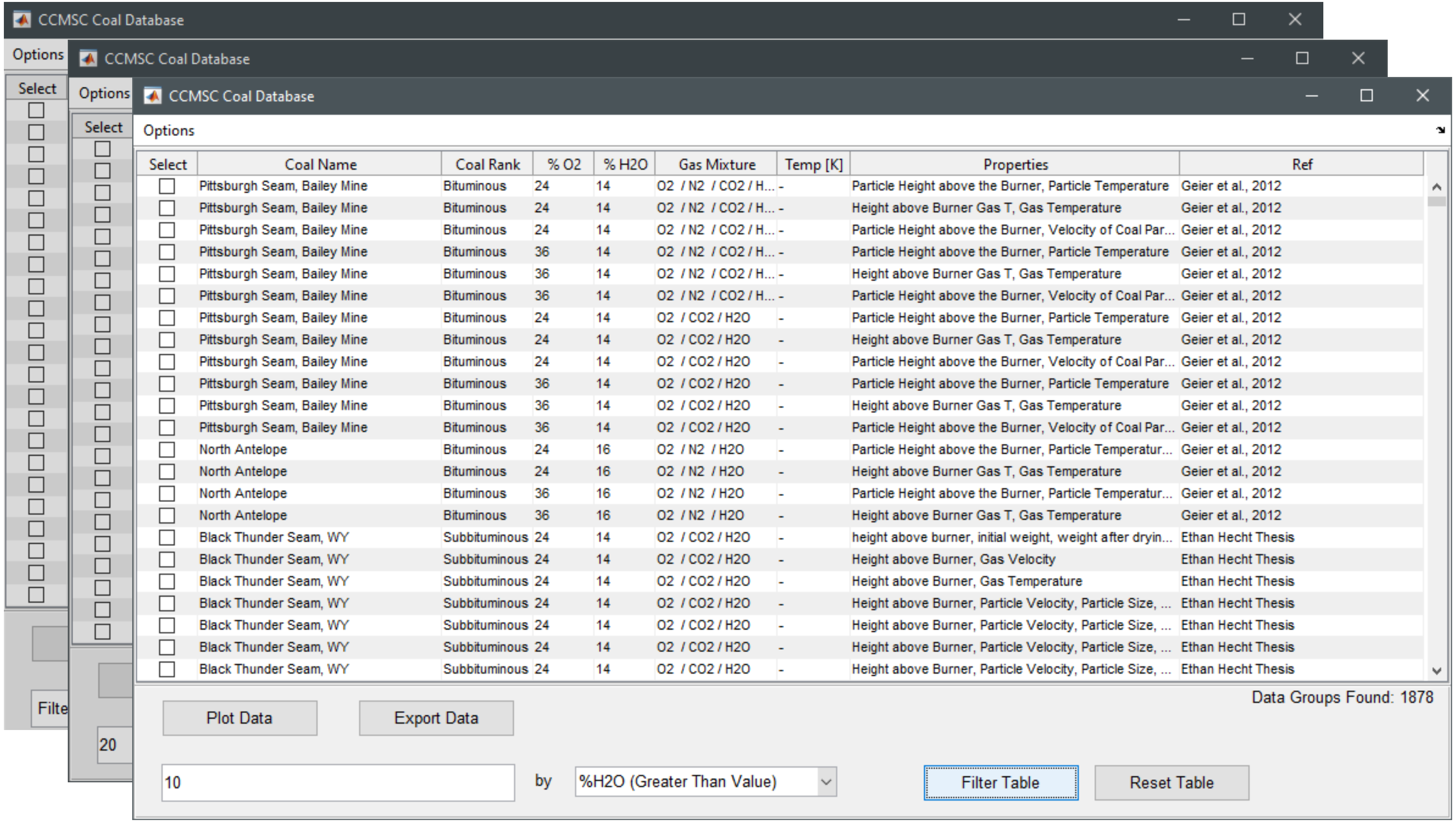

Select	Coal Name	Coal Rank	% O2	% H2O	Gas Mixture	Temp [K]	Properties	Ref
☐	Pittsburgh Seam, Bailey Mine	Bituminous	24	14	O2 / N2 / CO2 / H...	-	Particle Height above the Burner, Particle Temperature	Geier et al., 2012
☐	Pittsburgh Seam, Bailey Mine	Bituminous	24	14	O2 / N2 / CO2 / H...	-	Height above Burner Gas T, Gas Temperature	Geier et al., 2012
☐	Pittsburgh Seam, Bailey Mine	Bituminous	24	14	O2 / N2 / CO2 / H...	-	Particle Height above the Burner, Velocity of Coal Par...	Geier et al., 2012
☐	Pittsburgh Seam, Bailey Mine	Bituminous	36	14	O2 / N2 / CO2 / H...	-	Particle Height above the Burner, Particle Temperature	Geier et al., 2012
☐	Pittsburgh Seam, Bailey Mine	Bituminous	36	14	O2 / N2 / CO2 / H...	-	Height above Burner Gas T, Gas Temperature	Geier et al., 2012
☐	Pittsburgh Seam, Bailey Mine	Bituminous	36	14	O2 / N2 / CO2 / H...	-	Particle Height above the Burner, Velocity of Coal Par...	Geier et al., 2012
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☐	Pittsburgh Seam, Bailey Mine	Bituminous	36	14	O2 / CO2 / H2O	-	Particle Height above the Burner, Velocity of Coal Par...	Geier et al., 2012
☐	North Antelope	Bituminous	24	16	O2 / N2 / H2O	-	Particle Height above the Burner, Particle Temperatur...	Geier et al., 2012
☐	North Antelope	Bituminous	24	16	O2 / N2 / H2O	-	Height above Burner Gas T, Gas Temperature	Geier et al., 2012
☐	North Antelope	Bituminous	36	16	O2 / N2 / H2O	-	Particle Height above the Burner, Particle Temperatur...	Geier et al., 2012
☐	North Antelope	Bituminous	36	16	O2 / N2 / H2O	-	Height above Burner Gas T, Gas Temperature	Geier et al., 2012
☐	Black Thunder Seam, WY	Subbituminous	24	14	O2 / CO2 / H2O	-	height above burner, initial weight, weight after dryin...	Ethan Hecht Thesis
☐	Black Thunder Seam, WY	Subbituminous	24	14	O2 / CO2 / H2O	-	Height above Burner, Gas Velocity	Ethan Hecht Thesis
☐	Black Thunder Seam, WY	Subbituminous	24	14	O2 / CO2 / H2O	-	Height above Burner, Gas Temperature	Ethan Hecht Thesis
☐	Black Thunder Seam, WY	Subbituminous	24	14	O2 / CO2 / H2O	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
☐	Black Thunder Seam, WY	Subbituminous	24	14	O2 / CO2 / H2O	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
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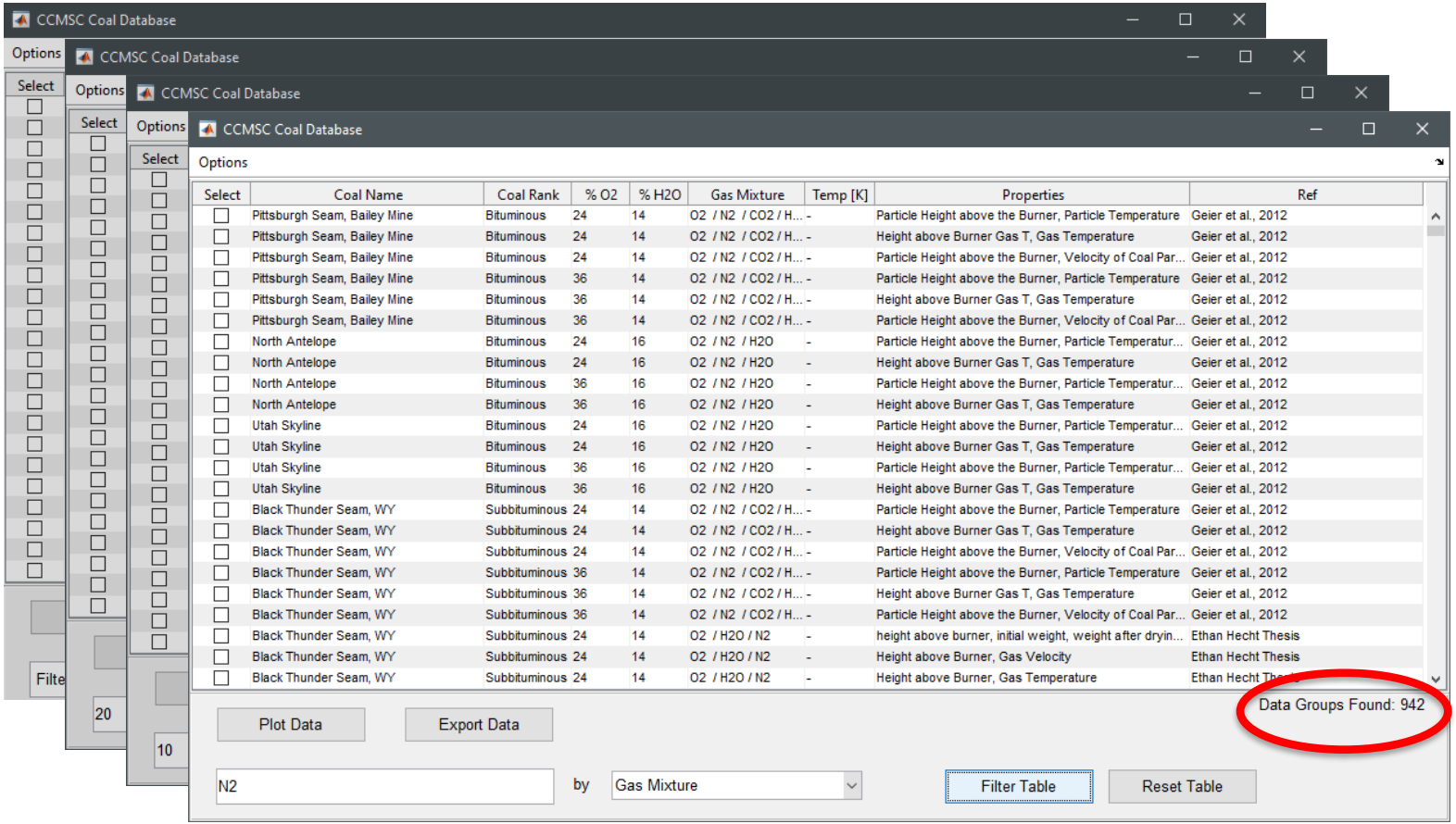
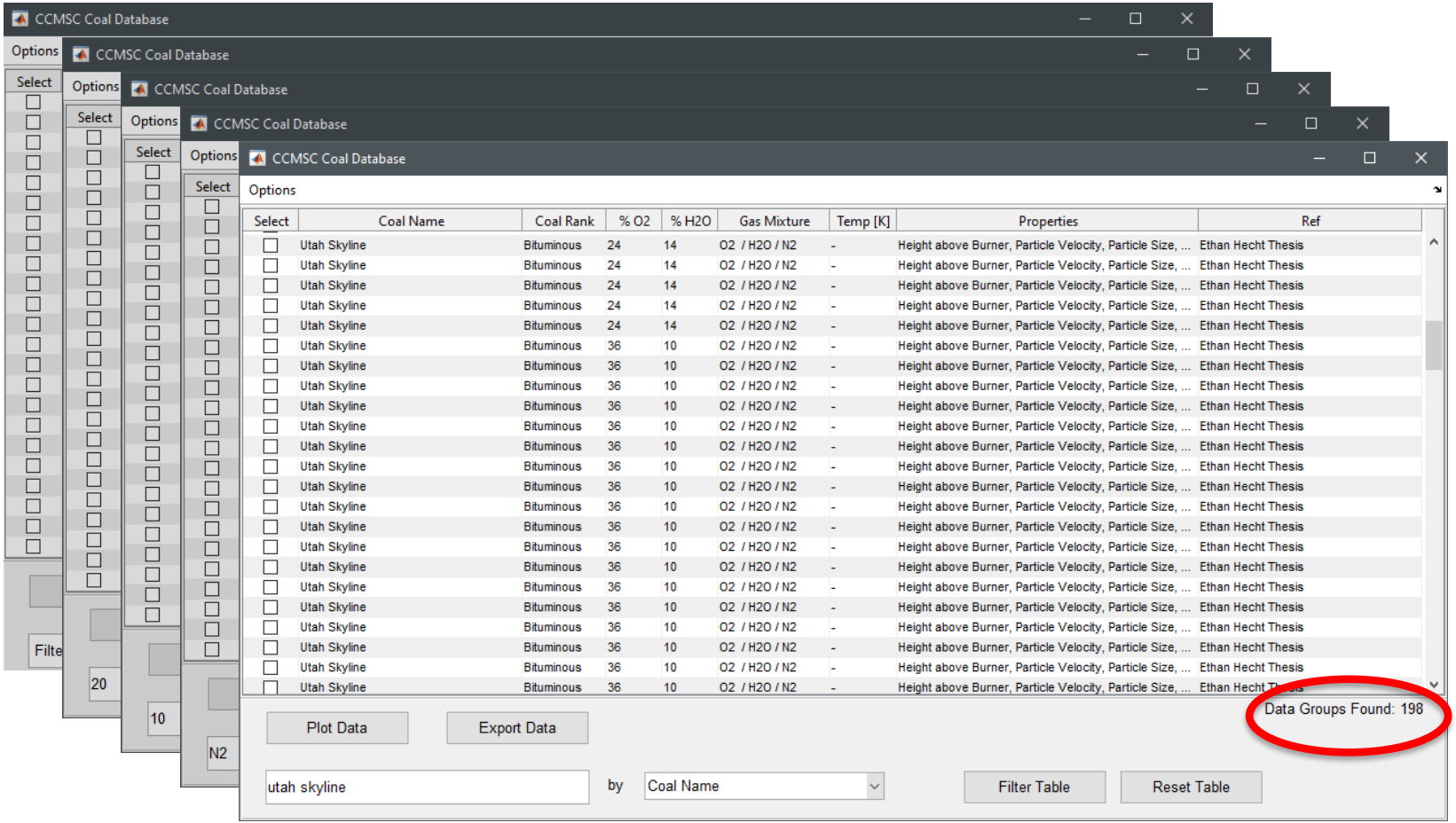
Char Oxidation Example



Char Oxidation Example



Char Oxidation Example

Experimental Data of Utah Skyline coal from Sandia's Laminar Entrained Flow Reactor

Features:

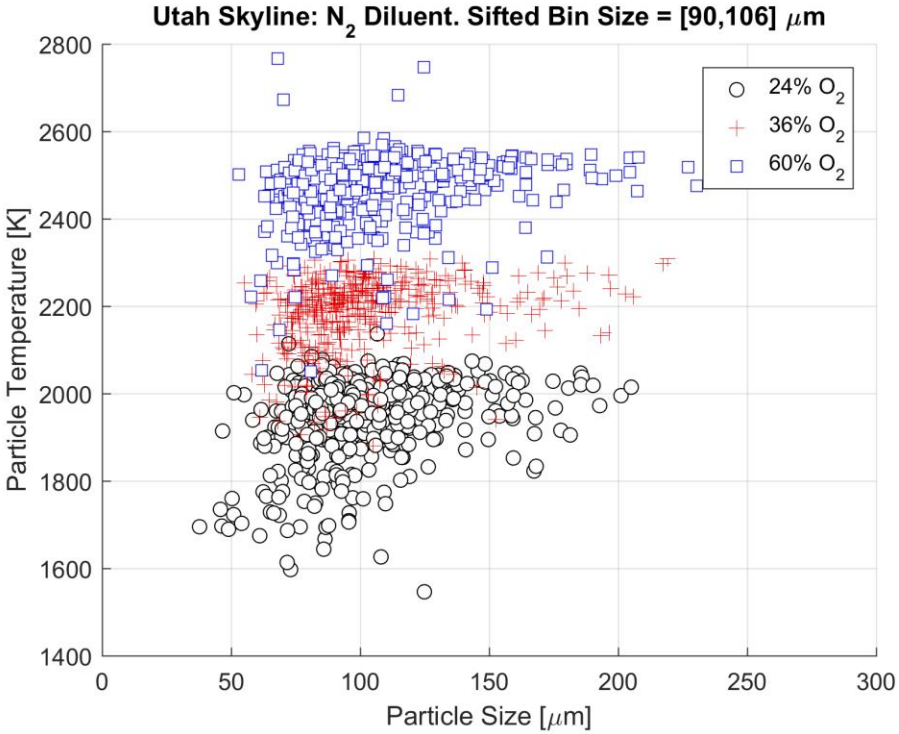
CO_2 or N_2 diluent

Initial Particle Diameter: $53 - 150\mu m$

O_2: $24 - 60\%$

H_2O: $10 - 16\%$

Validation data at 399 different gas conditions & heights above burner



Bound-to-Bound Data Collaboration (B2BDC)

Uncertain parameters: $x \in \mathcal{H} \subseteq \mathbb{R}^n$

$$\mathcal{H} = \{x \in \mathbb{R}^n : l_i \leq x_i \leq u_i,\ i = 1, \ldots, n\}$$

Bounds on QOI model: $L_e \leq M_e(x) \leq U_e,\ \text{for } e = 1, ..., N$

Dataset: $x \in \mathcal{H} \subseteq \mathbb{R}^n$

$$L_e \leq M_e(x) \leq U_e,\ \text{for } e = 1, ..., N$$

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Bounds on QOI model: $L_e \leq M_e(x) \leq U_e$, for $e = 1, ..., N$

Dataset: $x \in \mathcal{H} \subseteq \mathbb{R}^n$

$$L_e \leq M_e(x) \leq U_e,\ \text{for } e = 1, ..., N$$

Feasible set: $$\mathcal{F} = \bigcap_{e=1}^{N} \{x \in \mathcal{H} : L_e \leq M_e(x) \leq U_e\}$$

Bound-to-Bound Data Collaboration (B2BDC)

Scalar consistency measure

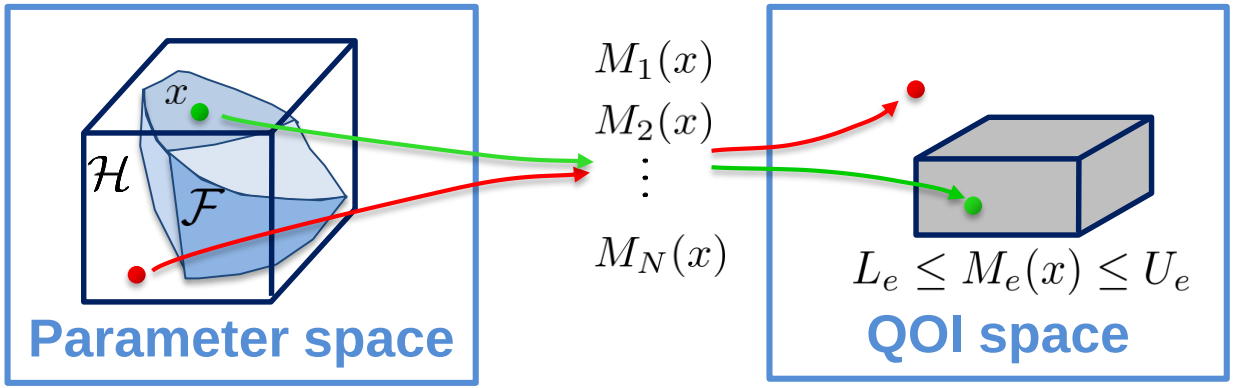
$\gamma \geq 0$: Consistent Dataset

$\gamma < 0$: Inconsistent Dataset

$$C_{\text{Dataset}} = \max_{\gamma, x \in \mathcal{H}} \quad \gamma$$

$$\text{s.t.} \quad L_e + \frac{(U_e - L_e)}{2}\gamma \leq M_e(x) \leq U_e - \frac{(U_e - L_e)}{2}\gamma$$

$$\text{for } e = 1, \ldots, N.$$



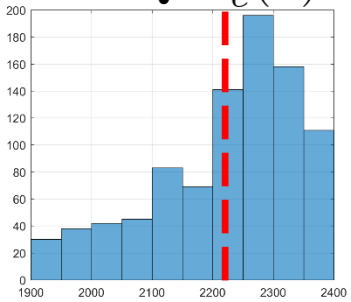
B2BDC Model Validation Workflow

Uncertain Parameters
$x \in \mathcal{H}$

Scenario Parameters, $x_{s,e}$

Char Oxidation Model
(Instrument + Physics)

$\mathrm{QOI}_e(x)$



Particle Temperature

CCMSC Coal Database

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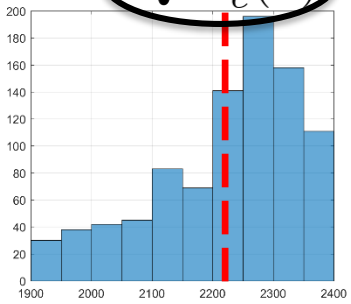

Particle Temperature

CCMSC Coal Database

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Scenario Parameters, x_{s_i}

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(Instrument + Physics)

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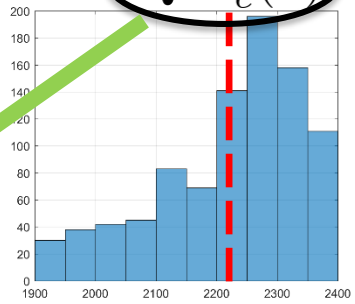
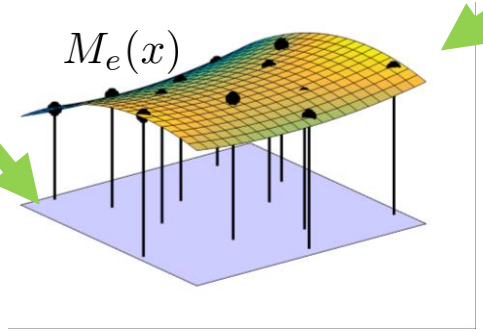


Particle Temperature

$M_e(x)$



CCMSC Coal Database

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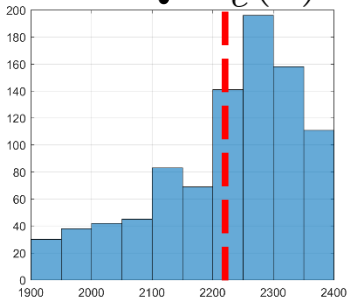

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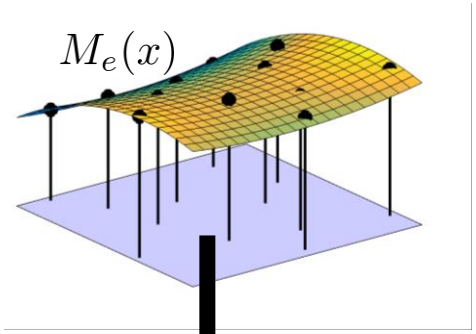

CCMSC Coal Database

$y_e \in [L_e, U_e]$

Dataset Unit

$L_e \leq M_e(x) \leq U_e$

B2BDC Model Validation Workflow

Uncertain Parameters
$x \in \mathcal{H}$

Scenario Parameters, $x_{s,e}$

Char Oxidation Model
(Instrument + Physics)

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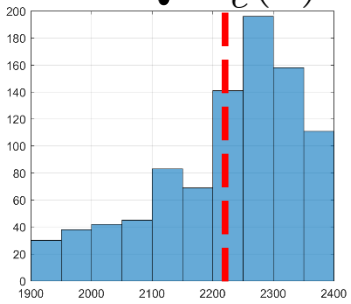

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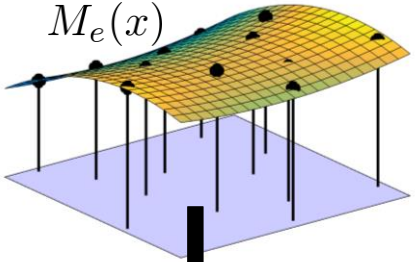


CCMSC Coal Database

$y_e \in [L_e, U_e]$

Dataset Unit
$L_e \le M_e(x) \le U_e$

Dataset

Consistency Analysis

Validation through consistency

Model Form

$$\left.\begin{array}{l} \mathrm{C_{(s)} + O_2 \longrightarrow \quad CO_2} \\ \mathrm{2\,C_{(s)} + O_2 \longrightarrow \quad 2\,CO} \end{array}\right\} \; r = \mathbf{A} \exp\left(\frac{-\mathbf{Ea}}{RT_p}\right) C_{\mathrm{oxid}}$$

Transport

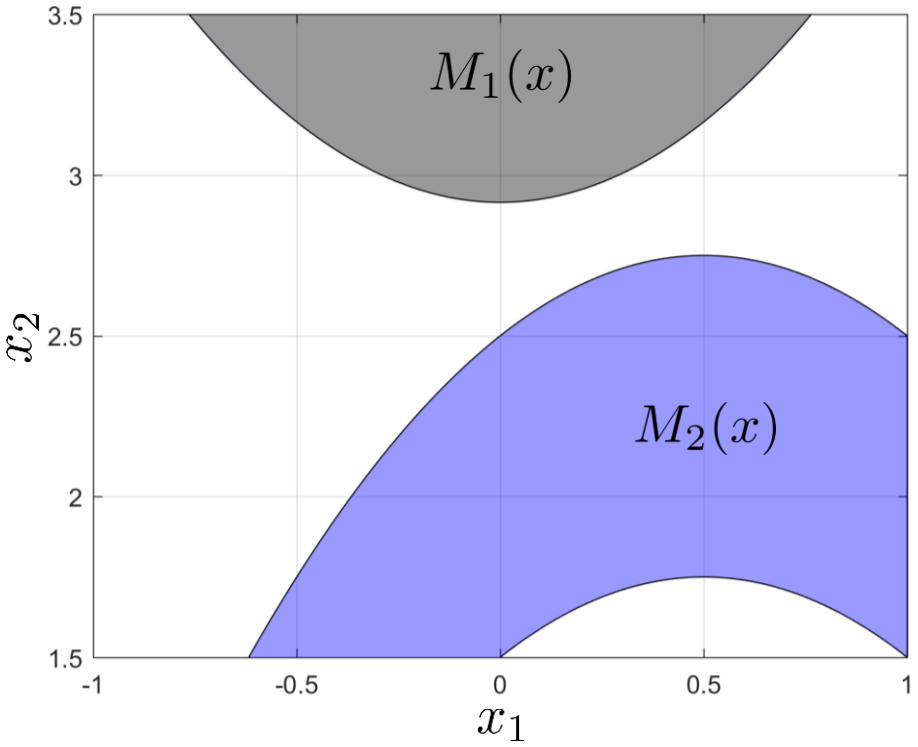
- Diffusion of oxidizer to particle surface
- Diffusion of products from particle surface

Scalar consistency measure:

$$\mathrm{C_{Dataset}} = [-0.26, -0.19]$$

If **all** constraints are expanded by at least 26% the inconsistency can be resolved.

If **all** constraints are expanded by no more than 19% the inconsistency **cannot** be resolved.



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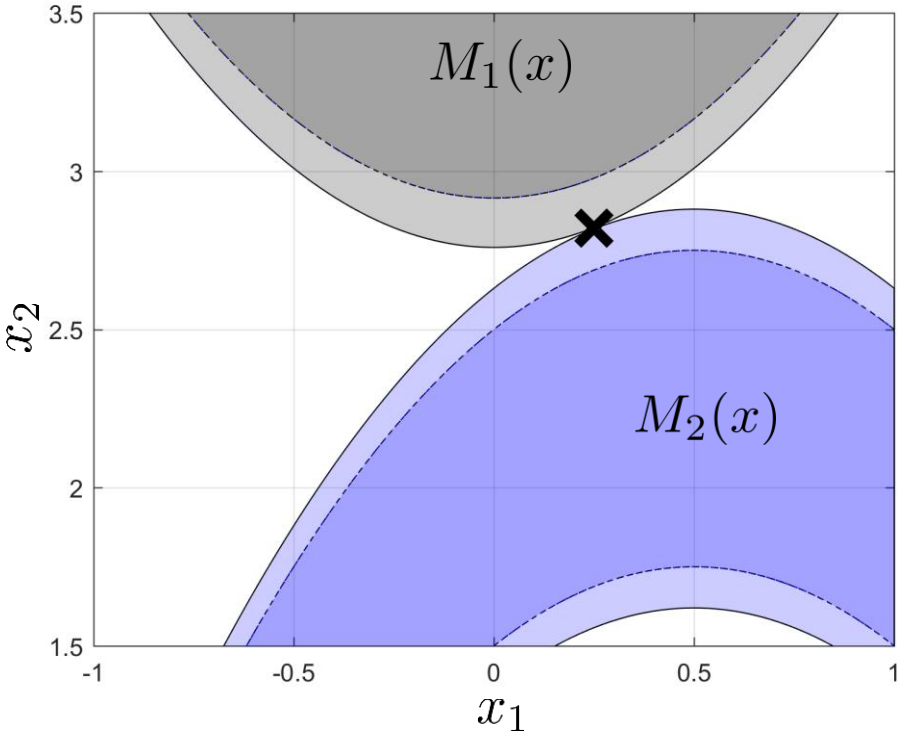


Validation through consistency

Model Form

Uncertain Kinetic Parameters

$$\left.\begin{aligned} \mathrm{C_{(s)} + O_2} &\longrightarrow \mathrm{CO_2} \\ \mathrm{2\,C_{(s)} + O_2} &\longrightarrow \mathrm{2\,CO} \end{aligned}\right\} \quad \{\mathrm{A_{O_2}}, \mathrm{E_{O_2}}\}$$

$$\mathrm{C_{(s)} + CO_2} \longrightarrow \mathrm{2\,CO} \quad \{\mathrm{A_{CO_2}}, \mathrm{E_{CO_2}}\}$$

$$\mathrm{C_{(s)} + H_2O} \longrightarrow \mathrm{H_2 + CO} \quad \{\mathrm{A_{H_2O}}, \mathrm{E_{H_2O}}\}$$

Transport

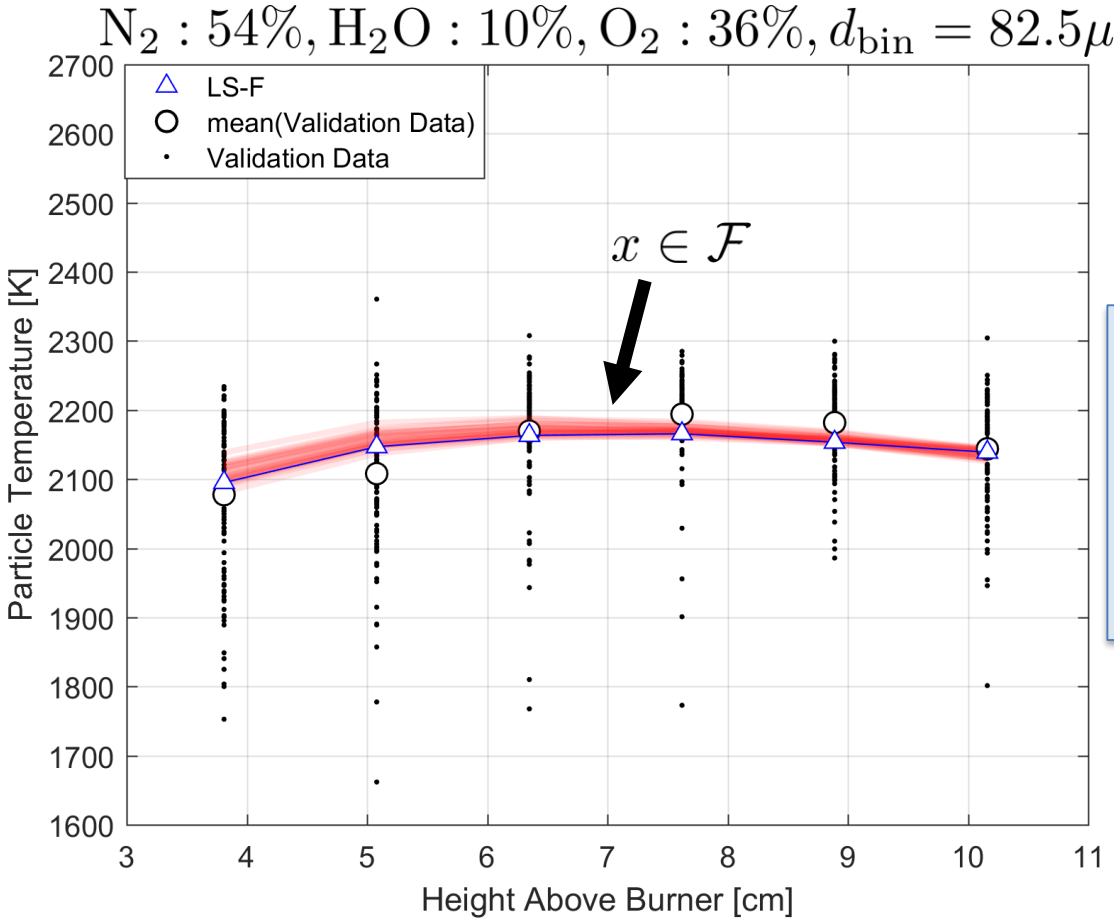
- Diffusion of oxidizer to particle surface
- Diffusion of products from particle surface
- Diffusion of oxidizer through coal particle
  - coal particle is a porous medium with internal surface area

Scalar consistency measure:

$$\mathrm{C_{Dataset}} = [0.06, 0.32]$$

$$\mathcal{F} = \bigcap_{e=1}^{N} \{x \in \mathcal{H} : L_e \leq M_e(x) \leq U_e\}$$

Validation through consistency



$$x_{\text{LS-F}} = \underset{x}{\text{argmin}} \, ||M_e(x) - y_e||_2$$
$$\text{s.t.} \;\; x \in \mathcal{F}$$

y_e : mean of the validation data

Summary

- Developed new data models for coal data
- Easy filtering through a diverse collection of experimental data
- B2BDC based test-bed for exploring parameter and model form uncertainty
  - With a consistent dataset we can do prediction of posterior QOI or parameter bounds, and sample the feasible set for correlations between parameters and QOIs

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