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

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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

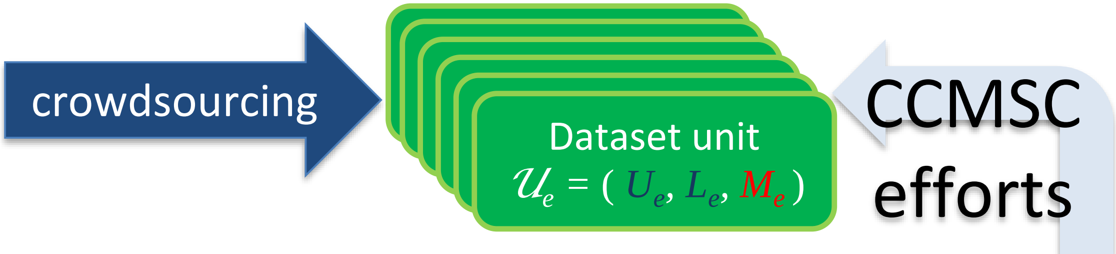
- What is PrIMe?
  - Data Warehouse – repository of experimental records
  - Applications – aid in development of predictive models

- 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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    </dataPoint>
  - <dataPoint id="dp2">
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      <x2>0.144</x2>
    </dataPoint>
  - <dataPoint id="dp3">
```

CCMSC Coal Database

primekinetics.org

github.com/oreluk/coalDB

CCMSC Coal Database

Options

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
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Data Groups Found: 2710

Plot Data

Filter by Coal Name

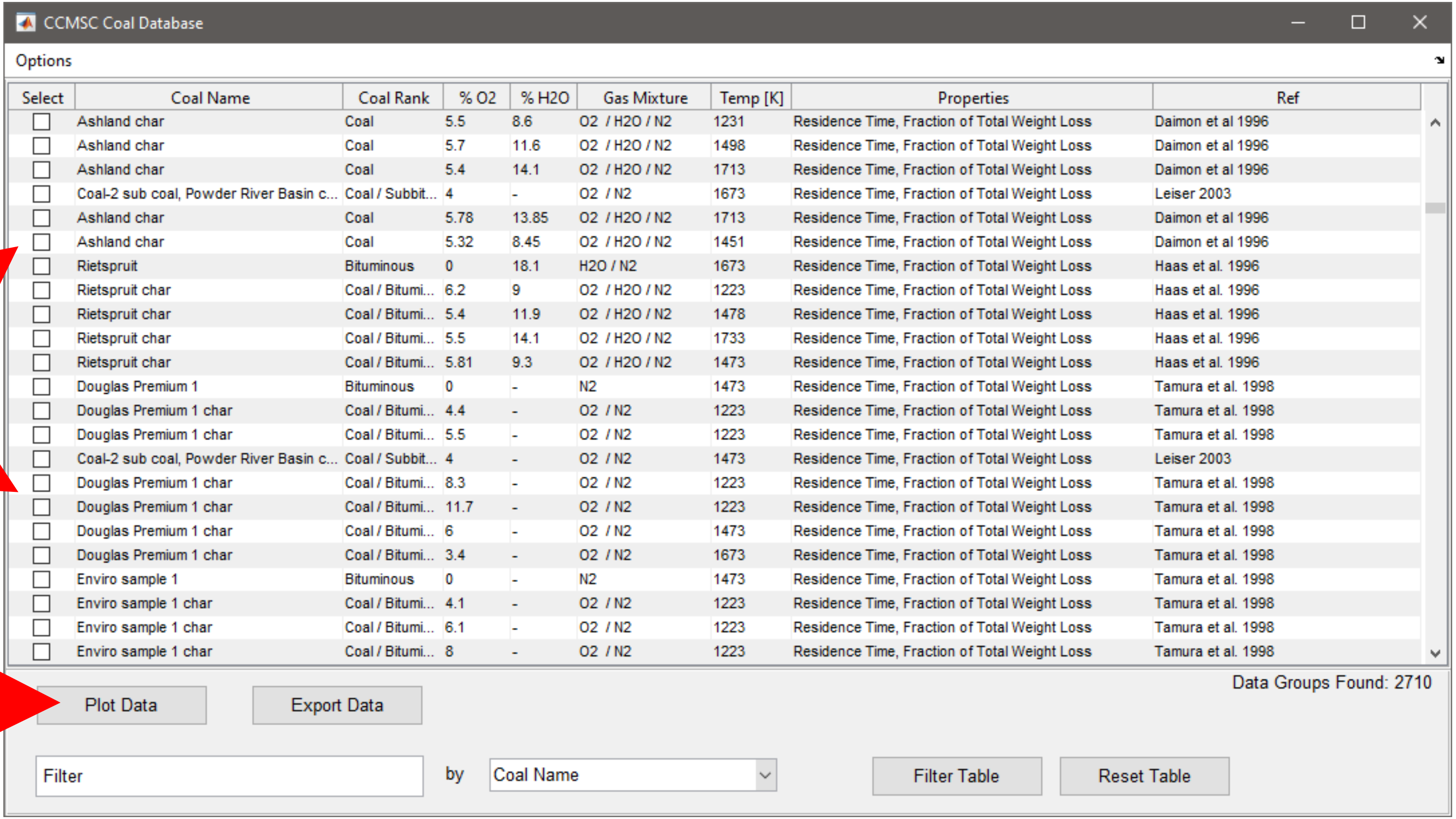
Filter Table

Reset Table

CCMSC Coal Database

Select Experiments

Plot & Export Data



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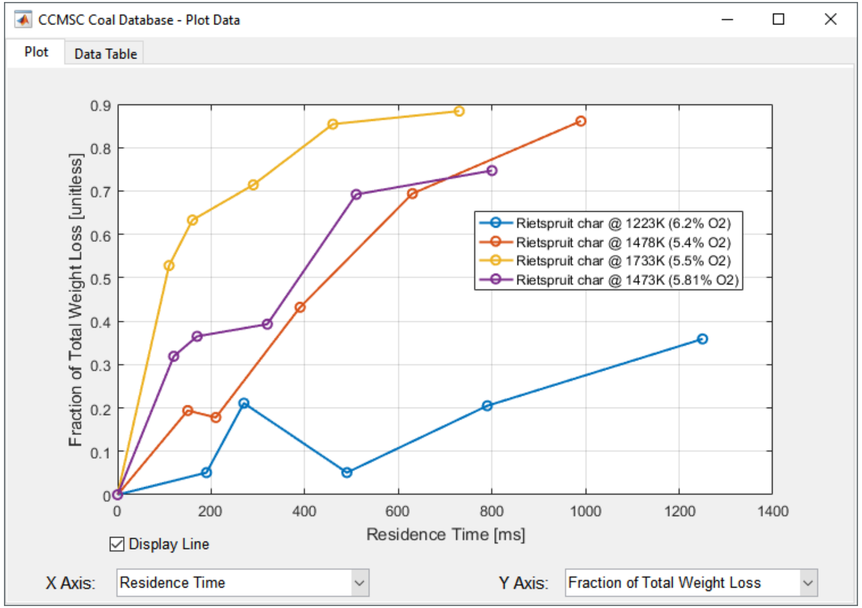
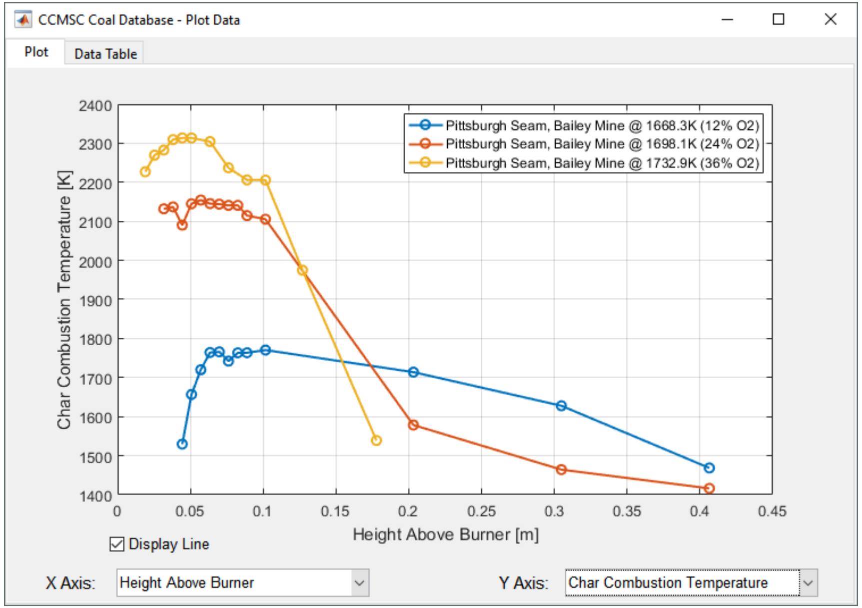
CCMSC Coal Database

Fraction of Weight Loss



Char Temperature



Char Oxidation Example

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

Features:

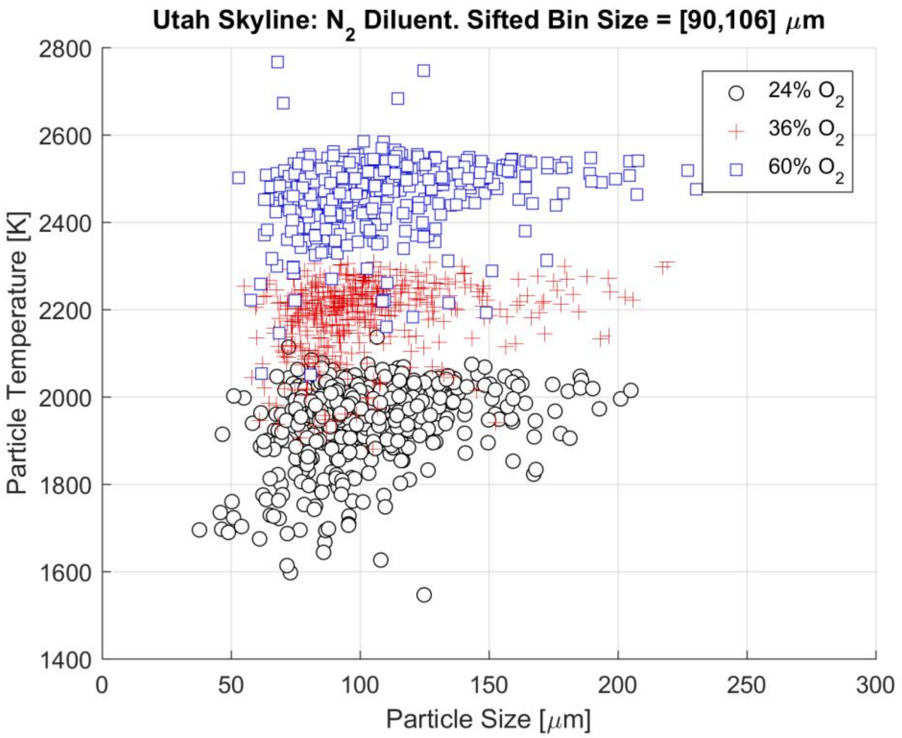
CO_2 or N_2 diluent

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

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

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Feeley, Seiler, Packard, Frenklach. *J. Phy. Chem. A*, 2004, 108, 9573-9583.

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

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

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

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

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

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

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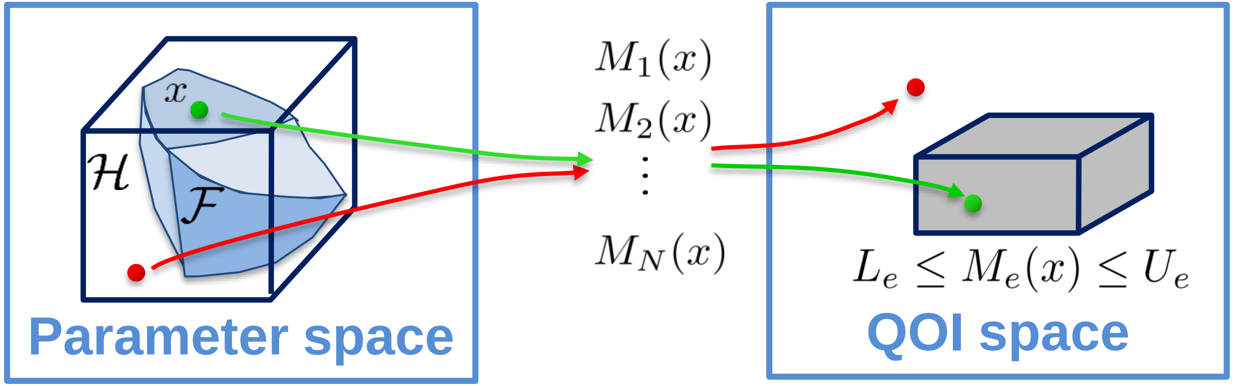


B2BDC Model Validation Workflow

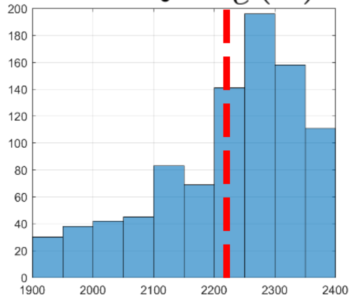
Uncertain Parameters

$x \in \mathcal{H}$

Scenario Parameters, $x_{s,e}$

Char Oxidation Model
(Instrument + Physics)

$\mathrm{QOI}_e(x)$



Particle Temperature

CCMSC Coal Database

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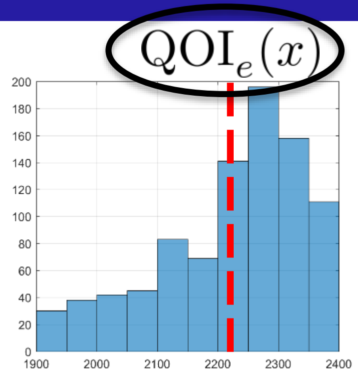

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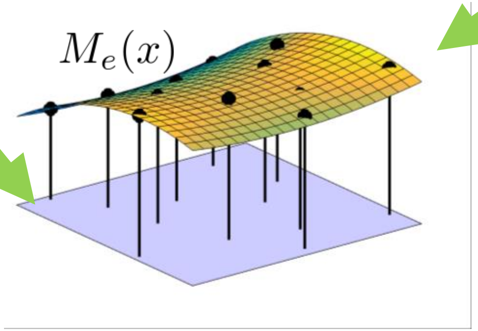

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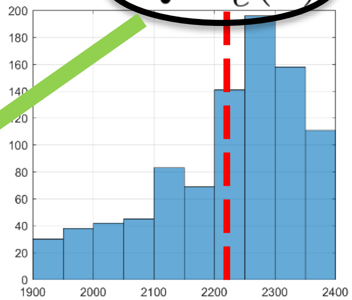

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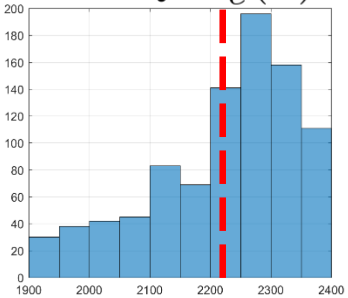

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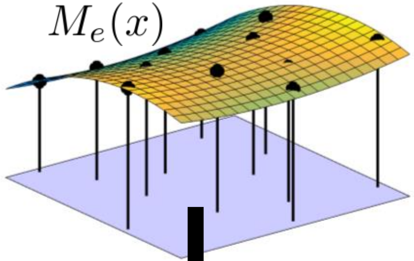


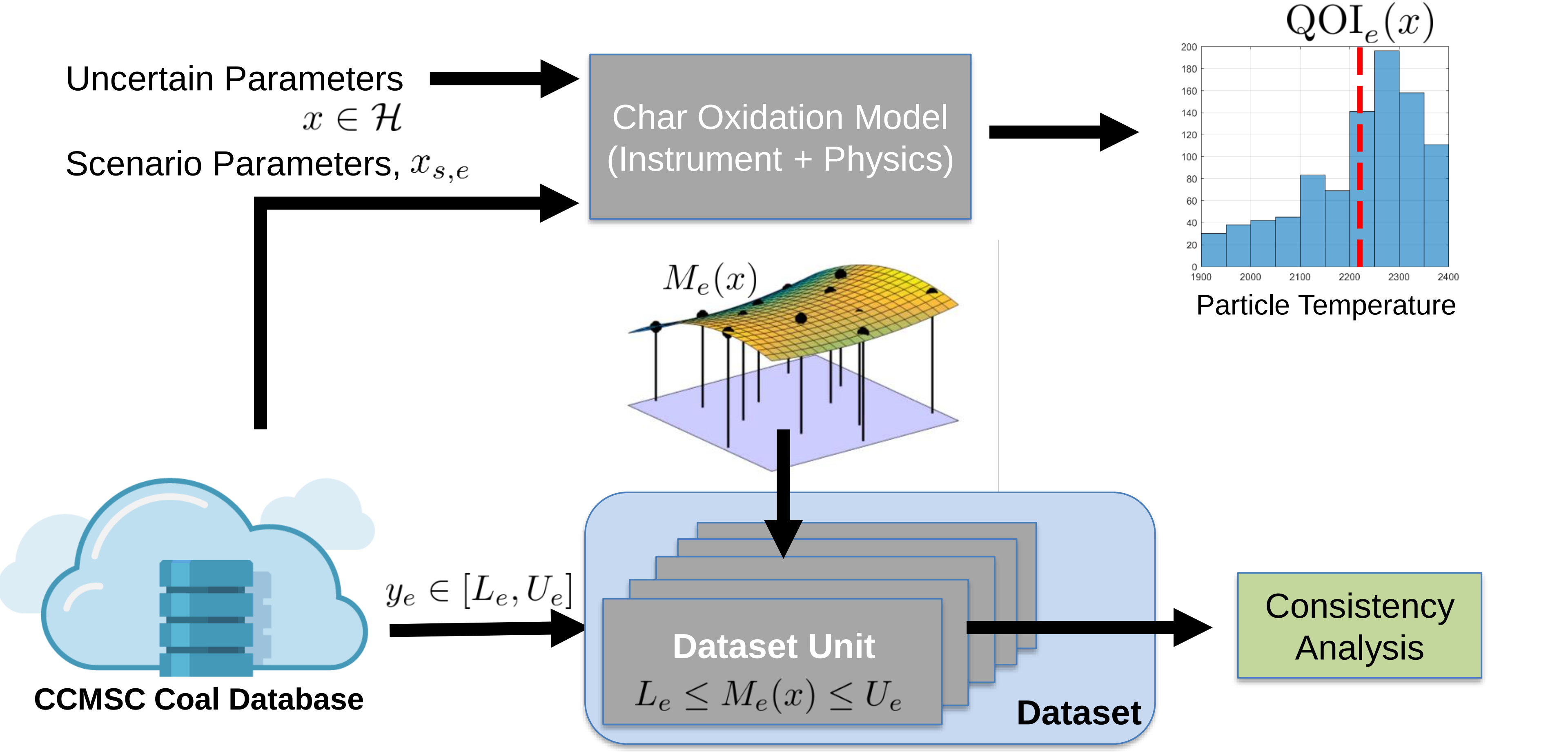
CCMSC Coal Database

$y_e \in [L_e, U_e]$

Dataset Unit

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

B2BDC Model Validation Workflow



Validation through consistency

Model Form

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

Transport

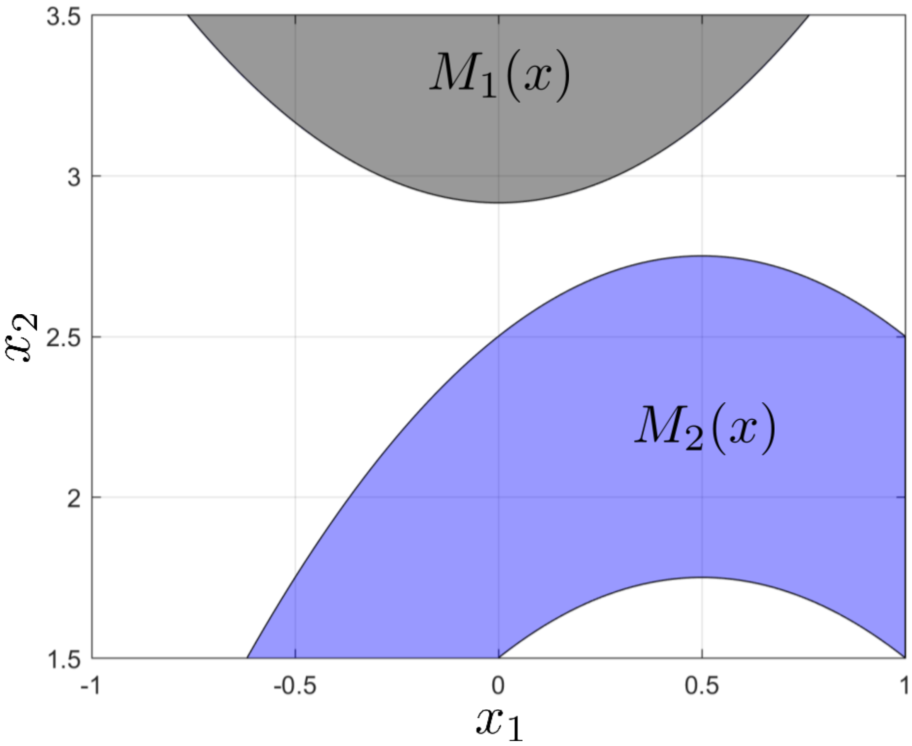
- Diffusion of oxidizer to particle surface
- Diffusion of products from particle surface

Scalar consistency measure:

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

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.



Iavarone et al. *Energy Procedia*, 120 (2017): 500-507.

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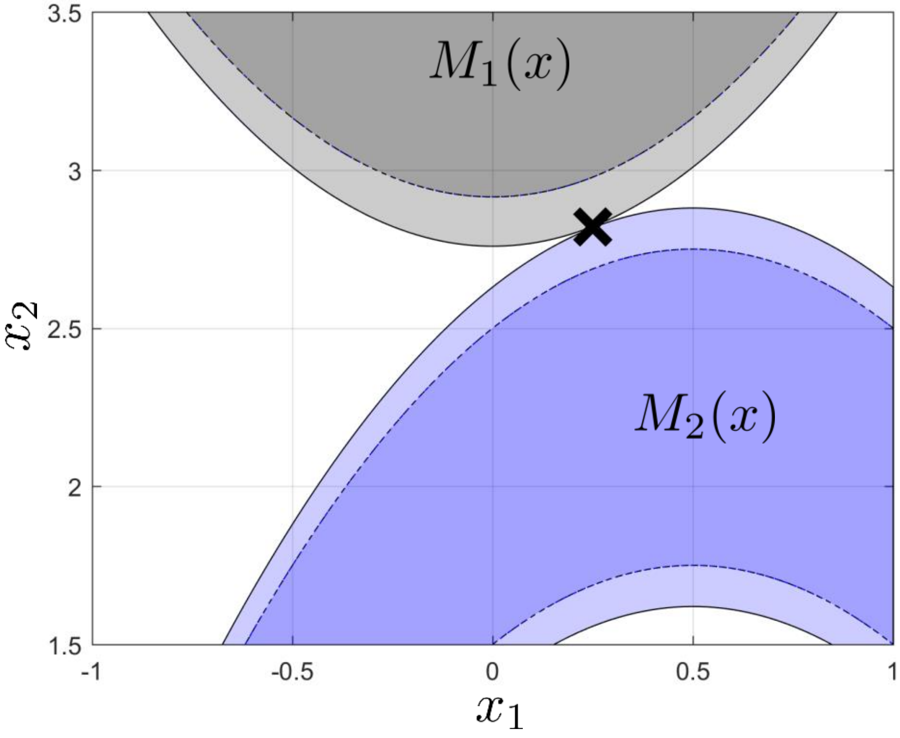


Validation through consistency

Model Form

Uncertain Kinetic Parameters

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

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

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

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

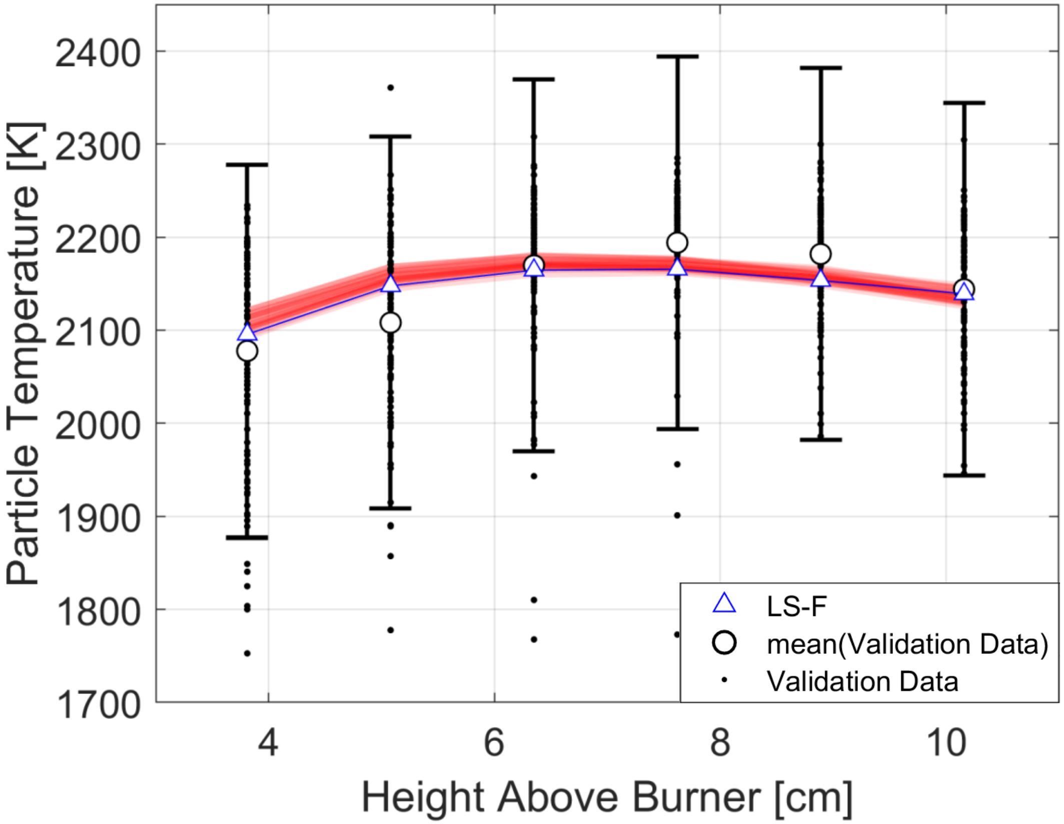
Scalar consistency measure:

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

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

Validation through consistency

$N_2 : 54\%, H_2O : 10\%, O_2 : 36\%, d_{\text{bin}} = 82.5\mu\text{m}$



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

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

Acknowledgements

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