

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

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CARBON CAPTURE  
MULTIDISCIPLINARY  
SIMULATION CENTER

# Overview

- Introduction
- Giving structure to experimental data
  - PrlMe Data Warehouse
- New PrlMe 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

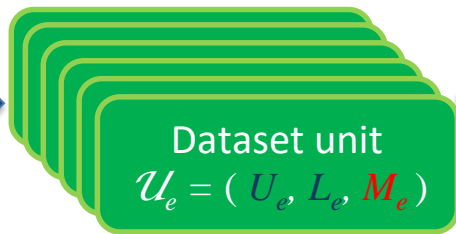


[primekinetics.org](http://primekinetics.org)

- 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

crowdsourcing



CCMSC  
efforts

- 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<sub>2</sub>, %H<sub>2</sub>O, Gas Mixture)

Experiment Types: *Devolatilization, Char oxidation*

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

leveraging existing cloud  
infrastructure and data models

```
<?xml version="1.0"?>
<experiment xsi:schemaLocation="http://purl.org/NET/prime/
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>
  - <property name="length" label="Length" units="m">
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</apparatus>
- <commonProperties>
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  + <property name="temperature" label="T_furnace" units
  + <property name="pressure" label="P" units="atm">
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  <property description="Fraction of Total Weight Loss" r
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    <x2>0</x2>
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  - <dataPoint id="dp2">
    <x1>232</x1>
    <x2>0.144</x2>
  </dataPoint>
  - <dataPoint id="dp3">
```

CCMSC Coal Database
Options

Select	Coal Name	Coal Rank	% O2	% H2O	Gas Mixture	Temp [K]	Properties	Ref
<input type="checkbox"/>	Ashland char	Coal	5.5	8.6	O2 / H2O / N2	1231	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
<input type="checkbox"/>	Ashland char	Coal	5.7	11.6	O2 / H2O / N2	1498	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
<input type="checkbox"/>	Ashland char	Coal	5.4	14.1	O2 / H2O / N2	1713	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
<input type="checkbox"/>	Coal-2 sub coal, Powder River Basin c...	Coal / Subbit...	4	-	O2 / N2	1673	Residence Time, Fraction of Total Weight Loss	Leiser 2003
<input type="checkbox"/>	Ashland char	Coal	5.78	13.85	O2 / H2O / N2	1713	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
<input type="checkbox"/>	Ashland char	Coal	5.32	8.45	O2 / H2O / N2	1451	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
<input type="checkbox"/>	Rietspruit	Bituminous	0	18.1	H2O / N2	1673	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
<input type="checkbox"/>	Rietspruit char	Coal / Bitumi...	6.2	9	O2 / H2O / N2	1223	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
<input type="checkbox"/>	Rietspruit char	Coal / Bitumi...	5.4	11.9	O2 / H2O / N2	1478	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
<input type="checkbox"/>	Rietspruit char	Coal / Bitumi...	5.5	14.1	O2 / H2O / N2	1733	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
<input type="checkbox"/>	Rietspruit char	Coal / Bitumi...	5.81	9.3	O2 / H2O / N2	1473	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
<input type="checkbox"/>	Douglas Premium 1	Bituminous	0	-	N2	1473	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Douglas Premium 1 char	Coal / Bitumi...	4.4	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Douglas Premium 1 char	Coal / Bitumi...	5.5	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Coal-2 sub coal, Powder River Basin c...	Coal / Subbit...	4	-	O2 / N2	1473	Residence Time, Fraction of Total Weight Loss	Leiser 2003
<input type="checkbox"/>	Douglas Premium 1 char	Coal / Bitumi...	8.3	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Douglas Premium 1 char	Coal / Bitumi...	11.7	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Douglas Premium 1 char	Coal / Bitumi...	6	-	O2 / N2	1473	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Douglas Premium 1 char	Coal / Bitumi...	3.4	-	O2 / N2	1673	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Enviro sample 1	Bituminous	0	-	N2	1473	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Enviro sample 1 char	Coal / Bitumi...	4.1	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Enviro sample 1 char	Coal / Bitumi...	6.1	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Enviro sample 1 char	Coal / Bitumi...	8	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998

Data Groups Found: 2710

by

# CCMSC Coal Database

Options

Select	Coal Name	Coal Rank	% O2	% H2O	Gas Mixture	Temp [K]	Properties	Ref
<input type="checkbox"/>	Ashland char	Coal	5.5	8.6	O2 / H2O / N2	1231	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
<input type="checkbox"/>	Ashland char	Coal	5.7	11.6	O2 / H2O / N2	1498	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
<input type="checkbox"/>	Ashland char	Coal	5.4	14.1	O2 / H2O / N2	1713	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
<input type="checkbox"/>	Coal-2 sub coal, Powder River Basin c...	Coal / Subbit...	4	-	O2 / N2	1673	Residence Time, Fraction of Total Weight Loss	Leiser 2003
<input type="checkbox"/>	Ashland char	Coal	5.78	13.85	O2 / H2O / N2	1713	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
<input type="checkbox"/>	Ashland char	Coal	5.32	8.45	O2 / H2O / N2	1451	Residence Time, Fraction of Total Weight Loss	Daimon et al 1996
<input type="checkbox"/>	Rietspruit	Bituminous	0	18.1	H2O / N2	1673	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
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<input type="checkbox"/>	Rietspruit char	Coal / Bitumi...	5.4	11.9	O2 / H2O / N2	1478	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
<input type="checkbox"/>	Rietspruit char	Coal / Bitumi...	5.5	14.1	O2 / H2O / N2	1733	Residence Time, Fraction of Total Weight Loss	Haas et al. 1996
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<input type="checkbox"/>	Douglas Premium 1	Bituminous	0	-	N2	1473	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Douglas Premium 1 char	Coal / Bitumi...	4.4	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Douglas Premium 1 char	Coal / Bitumi...	5.5	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Coal-2 sub coal, Powder River Basin c...	Coal / Subbit...	4	-	O2 / N2	1473	Residence Time, Fraction of Total Weight Loss	Leiser 2003
<input type="checkbox"/>	Douglas Premium 1 char	Coal / Bitumi...	8.3	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Douglas Premium 1 char	Coal / Bitumi...	11.7	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Douglas Premium 1 char	Coal / Bitumi...	6	-	O2 / N2	1473	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Douglas Premium 1 char	Coal / Bitumi...	3.4	-	O2 / N2	1673	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Enviro sample 1	Bituminous	0	-	N2	1473	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Enviro sample 1 char	Coal / Bitumi...	4.1	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Enviro sample 1 char	Coal / Bitumi...	6.1	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998
<input type="checkbox"/>	Enviro sample 1 char	Coal / Bitumi...	8	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Tamura et al. 1998

Plot Data      Export Data

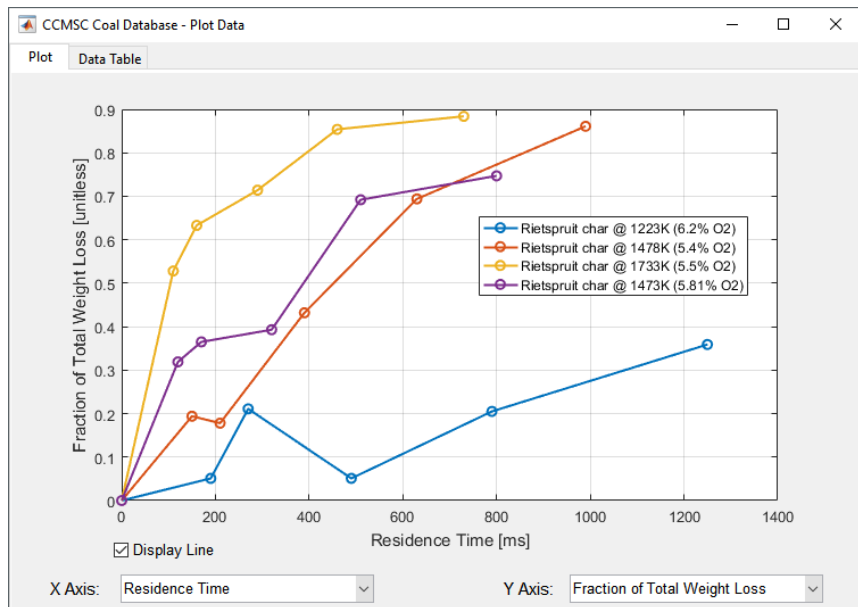
Filter  by  Filter Table      Reset Table

Data Groups Found: 2710

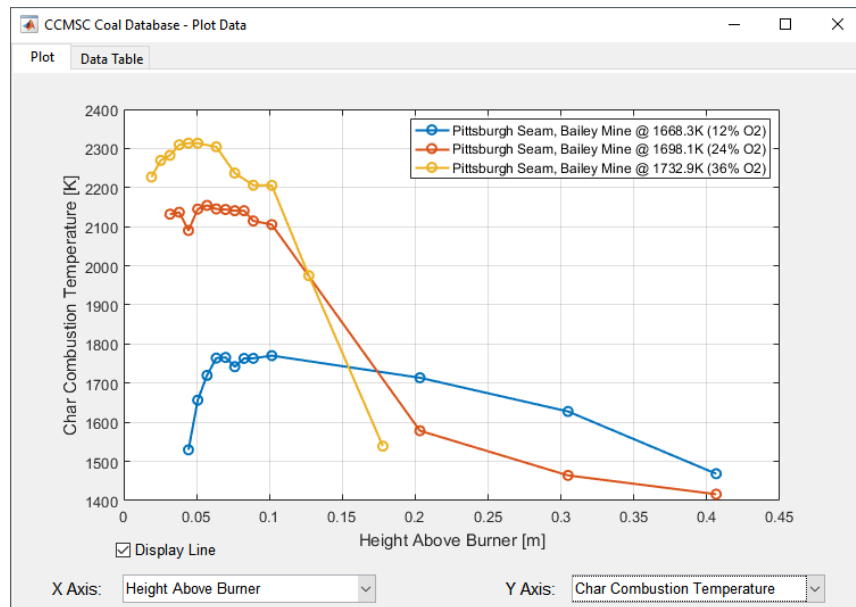
Select Experiments

Plot & Export Data

## Fraction of Weight Loss



## Char Temperature





# Char Oxidation Example

CCMSC Coal Database

Options

Select	Coal Name	Coal Rank	% O2	% H2O	Gas Mixture	Temp [K]	Properties	Ref
<input type="checkbox"/>	Columbian Coal PF1	Bituminous	0	-	N2	1473	Residence Time, Fraction of Total Weight Loss	Leiser 2003
<input type="checkbox"/>	Sewage sludge PF1 char	Sludge	12	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Leiser 2003
<input type="checkbox"/>	Smokey River as fired	Bituminous	0	-	N2	1673	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River coarse 120-150	Bituminous	0	-	N2	1273	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River coarse 120-150	Bituminous	0	-	N2	1673	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River fine 44-63	Bituminous	0	-	N2	1273	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River fine 44-63	Bituminous	0	-	N2	1673	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River as fired char	Coal / Bitumi...	5	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River as fired char	Coal / Bitumi...	5	-	O2 / N2	1473	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River as fired char	Coal / Bitumi...	5	-	O2 / N2	1673	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River coarse 120-150 char	Coal / Bitumi...	5	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River coarse 120-150 char	Coal / Bitumi...	3	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Sewage sludge PF1 char	Sludge	4	-	O2 / N2	1473	Residence Time, Fraction of Total Weight Loss	Leiser 2003
<input type="checkbox"/>	Smokey River coarse 120-150 char	Coal / Bitumi...	10	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River coarse 120-150 char	Coal / Bitumi...	5	-	O2 / N2	1473	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River coarse 120-150 char	Coal / Bitumi...	5	-	O2 / N2	1673	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River fine 44-63 char	Coal / Bitumi...	5	-	O2 / N2	1223	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River fine 44-63 char	Coal / Bitumi...	5	-	O2 / N2	1473	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Smokey River fine 44-63 char	Coal / Bitumi...	5	-	O2 / N2	1673	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Dawmill as fired	Bituminous	0	-	N2	1273	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Dawmill as fired	Bituminous	0	-	N2	1673	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Dawmill coarse 120-150	Bituminous	0	-	N2	1273	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995
<input type="checkbox"/>	Dawmill coarse 120-150	Bituminous	0	-	N2	1673	Residence Time, Fraction of Total Weight Loss	Haas, Lockermann, van de Kamp 1995

Plot Data      Export Data

Data Groups Found: 2710

Filter  by  Filter Table      Reset Table

- Coal Name
- Coal Rank
- Coal - % Carbon Dry Ash Free (Greater Than Value)
- %O2 (Greater Than Value)
- %H2O (Greater Than Value)
- Gas Mixture
- Temperature (Greater Than Value)

# Char Oxidation Example

CCMSC Coal Database

Options CCMSC Coal Database

Select Options

Select	Coal Name	Coal Rank	% O2	% H2O	Gas Mixture	Temp [K]	Properties	Ref
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 24	-	-	O2 / N2	-	Height Above Burner, Particle Velocity	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 24	-	-	O2 / N2	-	Height Above Burner, Gas Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 24	-	-	O2 / N2	-	Height Above Burner, Devolatilization Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 24	-	-	O2 / N2	-	Height Above Burner, Char Combustion Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 36	-	-	O2 / N2	-	Height Above Burner, Particle Velocity	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 36	-	-	O2 / N2	-	Height Above Burner, Gas Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 36	-	-	O2 / N2	-	Height Above Burner, Devolatilization Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 36	-	-	O2 / N2	-	Height Above Burner, Char Combustion Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 24	-	-	O2 / CO2	-	Height Above Burner, Particle Velocity	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 24	-	-	O2 / CO2	-	Height Above Burner, Gas Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 24	-	-	O2 / CO2	-	Height Above Burner, Devolatilization Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 24	-	-	O2 / CO2	-	Height Above Burner, Char Combustion Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 36	-	-	O2 / CO2	-	Height Above Burner, Particle Velocity	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 36	-	-	O2 / CO2	-	Height Above Burner, Gas Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 36	-	-	O2 / CO2	-	Height Above Burner, Devolatilization Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Black Thunder Seam, WY	Subbituminous 36	-	-	O2 / CO2	-	Height Above Burner, Char Combustion Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Pittsburgh Seam, Bailey Mine	Bituminous 24	-	-	O2 / N2	1698.1	Height Above Burner, Particle Velocity	Shaddix et al. 2009
<input type="checkbox"/>	Pittsburgh Seam, Bailey Mine	Bituminous 24	-	-	O2 / N2	1698.1	Height Above Burner, Gas Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Pittsburgh Seam, Bailey Mine	Bituminous 24	-	-	O2 / N2	1698.1	Height Above Burner, Devolatilization Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Pittsburgh Seam, Bailey Mine	Bituminous 24	-	-	O2 / N2	1698.1	Height Above Burner, Char Combustion Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Pittsburgh Seam, Bailey Mine	Bituminous 36	-	-	O2 / N2	1732.9	Height Above Burner, Particle Velocity	Shaddix et al. 2009
<input type="checkbox"/>	Pittsburgh Seam, Bailey Mine	Bituminous 36	-	-	O2 / N2	1732.9	Height Above Burner, Gas Temperature	Shaddix et al. 2009
<input type="checkbox"/>	Pittsburgh Seam, Bailey Mine	Bituminous 36	-	-	O2 / N2	1732.9	Height Above Burner, Devolatilization Temperature	Shaddix et al. 2009

Plot Data Export Data

Filter 20 by %O2 (Greater Than Value) Filter Table Reset Table

Data Groups Found: 1910

# Char Oxidation Example

The screenshot displays the CCMSC Coal Database application. The main window shows a table with columns for 'Coal Name', 'Coal Rank', '% O2', '% H2O', 'Gas Mixture', 'Temp [K]', 'Properties', and 'Ref'. The table lists various coal samples, including Pittsburgh Seam, Bailey Mine and North Antelope. A filter is applied to the '% H2O' column, showing a value of 10. The interface includes a 'Filter' sidebar on the left, a 'Data Groups Found: 1878' indicator at the bottom right, and buttons for 'Plot Data', 'Export Data', 'Filter Table', and 'Reset Table'.

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

Data Groups Found: 1878

Filter: 10 by %H2O (Greater Than Value) [Filter Table] [Reset Table]

# Char Oxidation Example

The screenshot displays the CCMSC Coal Database application. The main window shows a table with columns: Select, Coal Name, Coal Rank, % O2, % H2O, Gas Mixture, Temp [K], Properties, and Ref. The table lists various coal samples with their respective properties. A filter is applied to the 'Gas Mixture' column, showing 'N2'. The bottom right corner of the interface displays 'Data Groups Found: 942', which is circled in red. Other interface elements include 'Options', 'Select', 'Filter', 'Plot Data', 'Export Data', 'Filter Table', and 'Reset Table' buttons.

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

Data Groups Found: 942

# Char Oxidation Example

The screenshot displays the CCMSC Coal Database application window. The interface includes a search bar with the text "utah skyline" and a dropdown menu set to "Coal Name". Below the search bar are buttons for "Plot Data", "Export Data", "Filter Table", and "Reset Table". A table of coal data is visible, with columns for "Select", "Coal Name", "Coal Rank", "% O2", "% H2O", "Gas Mixture", "Temp [K]", "Properties", and "Ref". The table contains 19 rows of data, all for "Utah Skyline" coal, with varying ranks (Bituminous 24, 36) and gas mixtures (O2 / H2O / N2). A red circle highlights the text "Data Groups Found: 198" in the bottom right corner of the window.

Select	Coal Name	Coal Rank	% O2	% H2O	Gas Mixture	Temp [K]	Properties	Ref
<input type="checkbox"/>	Utah Skyline	Bituminous	24	14	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	24	14	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	24	14	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	24	14	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	24	14	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis
<input type="checkbox"/>	Utah Skyline	Bituminous	36	10	O2 / H2O / N2	-	Height above Burner, Particle Velocity, Particle Size, ...	Ethan Hecht Thesis

# Char Oxidation Example

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

Features:

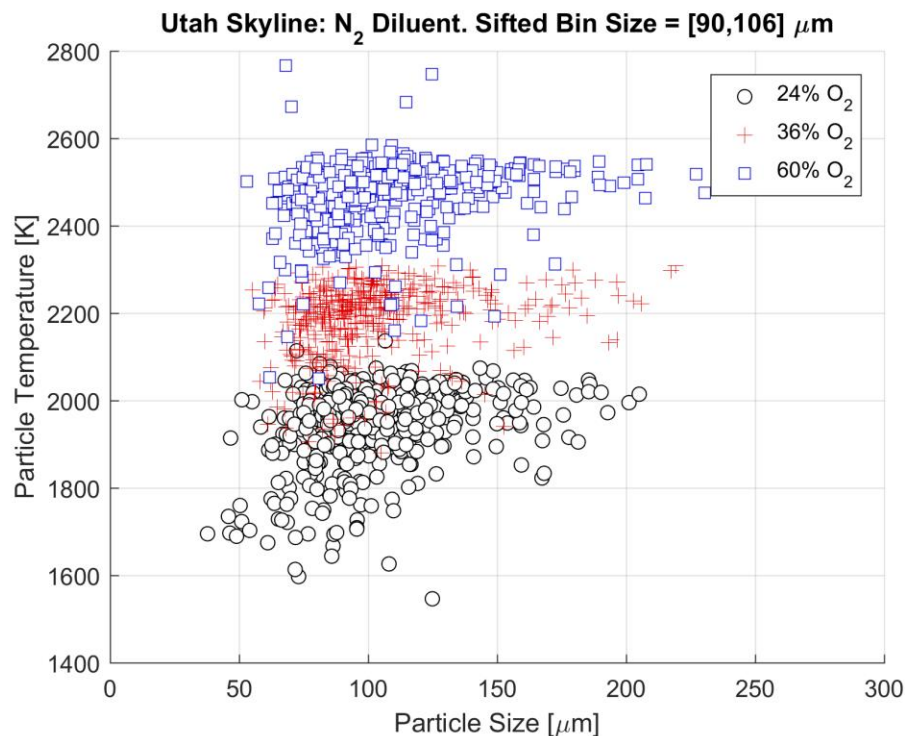
CO<sub>2</sub> or N<sub>2</sub> diluent

Initial Particle Diameter: 53 – 150  $\mu\text{m}$

O<sub>2</sub>: 24 – 60%

H<sub>2</sub>O: 10 – 16%

Validation data at 399 different gas conditions & heights above burner



# Bound-to-Bound Data Collaboration (B2BDC)

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

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

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

---

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

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

# Bound-to-Bound Data Collaboration (B2BDC)

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

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

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

---

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

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



# Bound-to-Bound Data Collaboration (B2BDC)

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

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

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

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

# Bound-to-Bound Data Collaboration (B2BDC)

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

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

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

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

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

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

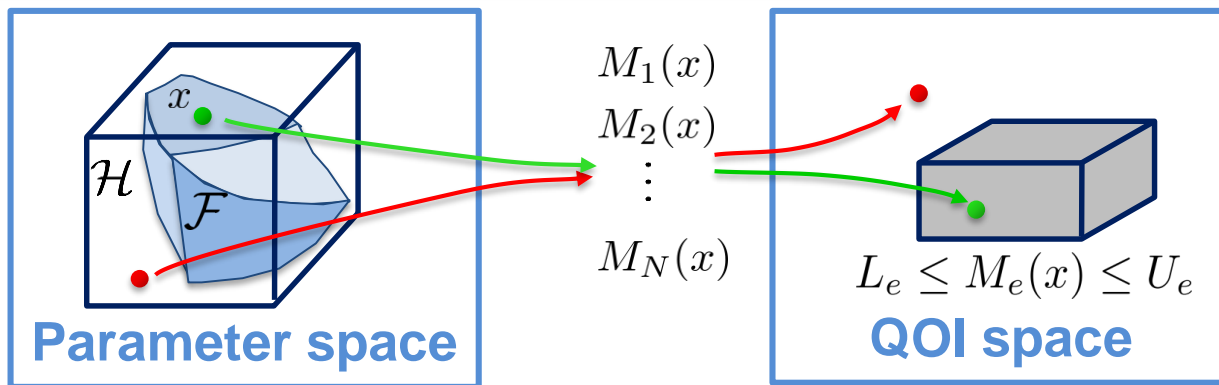
$\gamma \geq 0$  : Consistent Dataset

$\gamma < 0$  : Inconsistent Dataset

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

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

for  $e = 1, \dots, N$ .



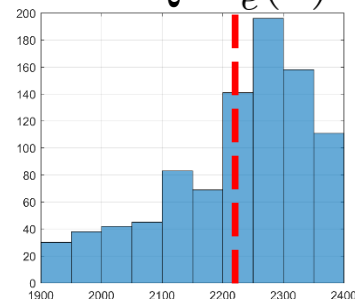
# B2BDC Model Validation Workflow

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

Scenario Parameters,  $x_{s,e}$

Char Oxidation Model  
(Instrument + Physics)

$QOI_e(x)$



Particle Temperature



CCMSC Coal Database

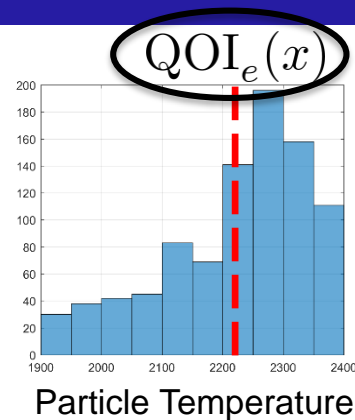
# B2BDC Model Validation Workflow

Uncertain Parameters

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

Scenario Parameters,  $x_{s,e}$

Char Oxidation Model  
(Instrument + Physics)



CCMSC Coal Database

# B2BDC Model Validation Workflow

Uncertain Parameters

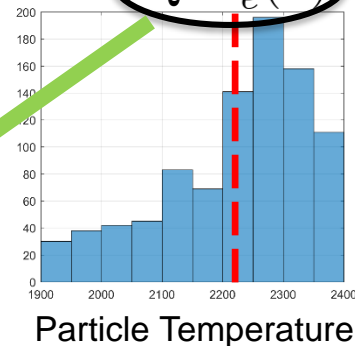
$$x \in \mathcal{H}$$

Scenario Parameters,  $x_{s,e}$

Char Oxidation Model  
(Instrument + Physics)

$$M_e(x)$$

$$QOI_e(x)$$



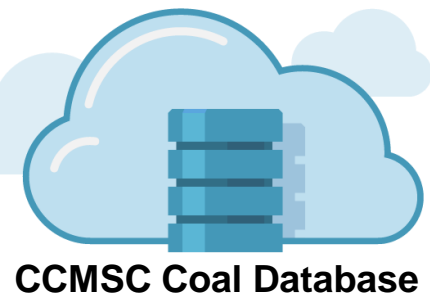
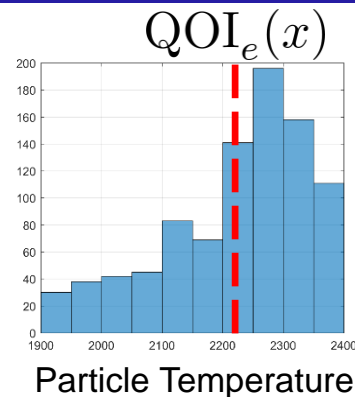
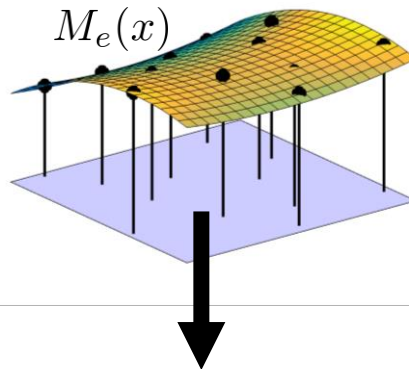
CCMSC Coal Database

# B2BDC Model Validation Workflow

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

Scenario Parameters,  $x_{s,e}$

Char Oxidation Model  
(Instrument + Physics)



$y_e \in [L_e, U_e]$

Dataset Unit

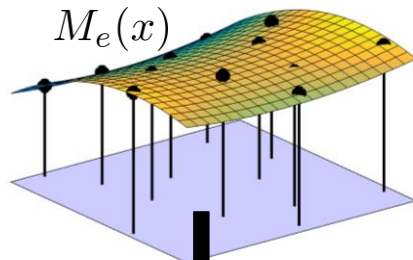
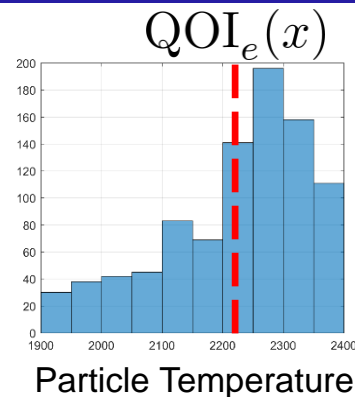
$$L_e \leq M_e(x) \leq U_e$$

# B2BDC Model Validation Workflow

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

Scenario Parameters,  $x_{s,e}$

Char Oxidation Model  
(Instrument + Physics)



$y_e \in [L_e, U_e]$

Dataset Unit

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

Dataset

Consistency  
Analysis

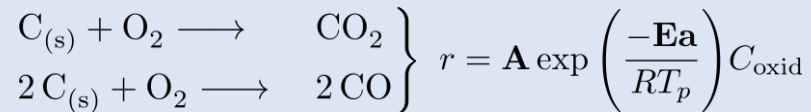


CCMSC Coal Database



# Validation through consistency

## Model Form



## Transport

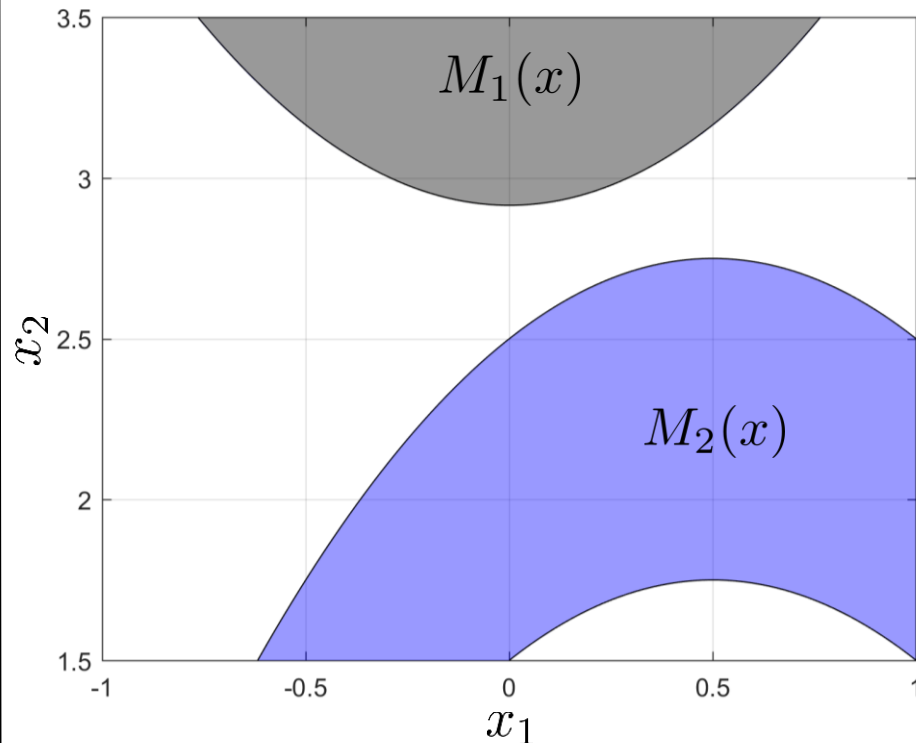
- Diffusion of oxidizer to particle surface
- Diffusion of products from particle surface

## Scalar consistency measure:

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

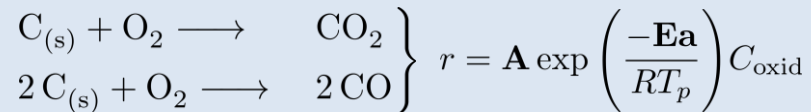
If **all** constraints are expanded by at least 26% the inconsistency can be resolved.

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



# Validation through consistency

## Model Form



## Transport

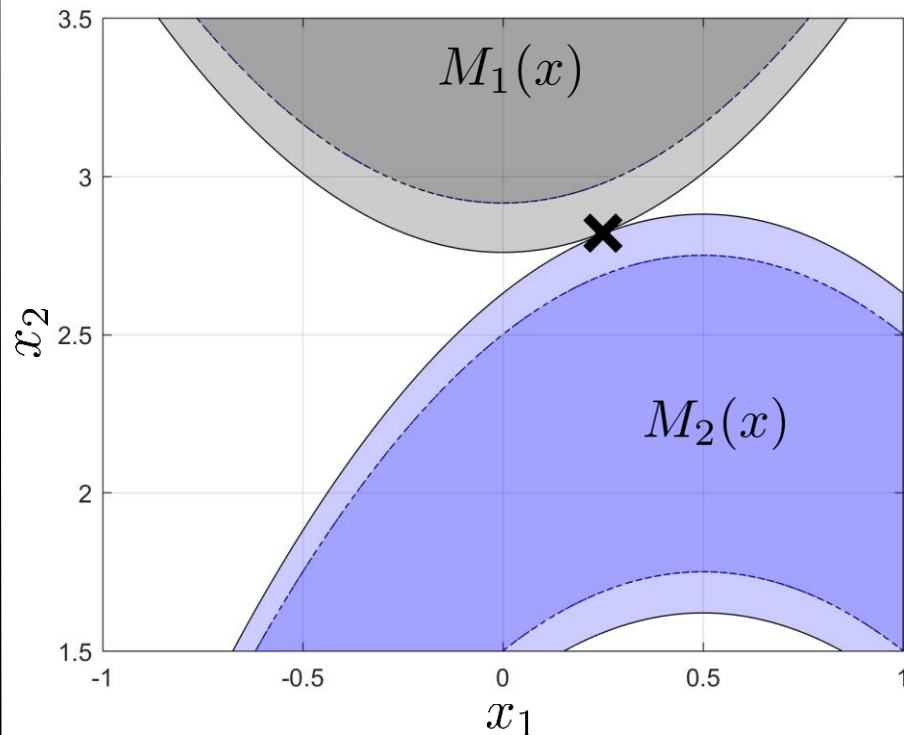
- Diffusion of oxidizer to particle surface
- Diffusion of products from particle surface

## Scalar consistency measure:

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

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.

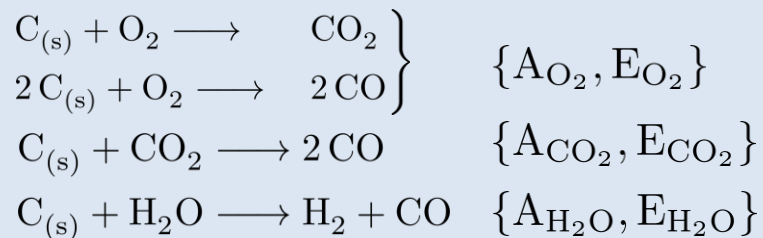


# Validation through consistency

## Model Form

---

### Uncertain Kinetic Parameters



### 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

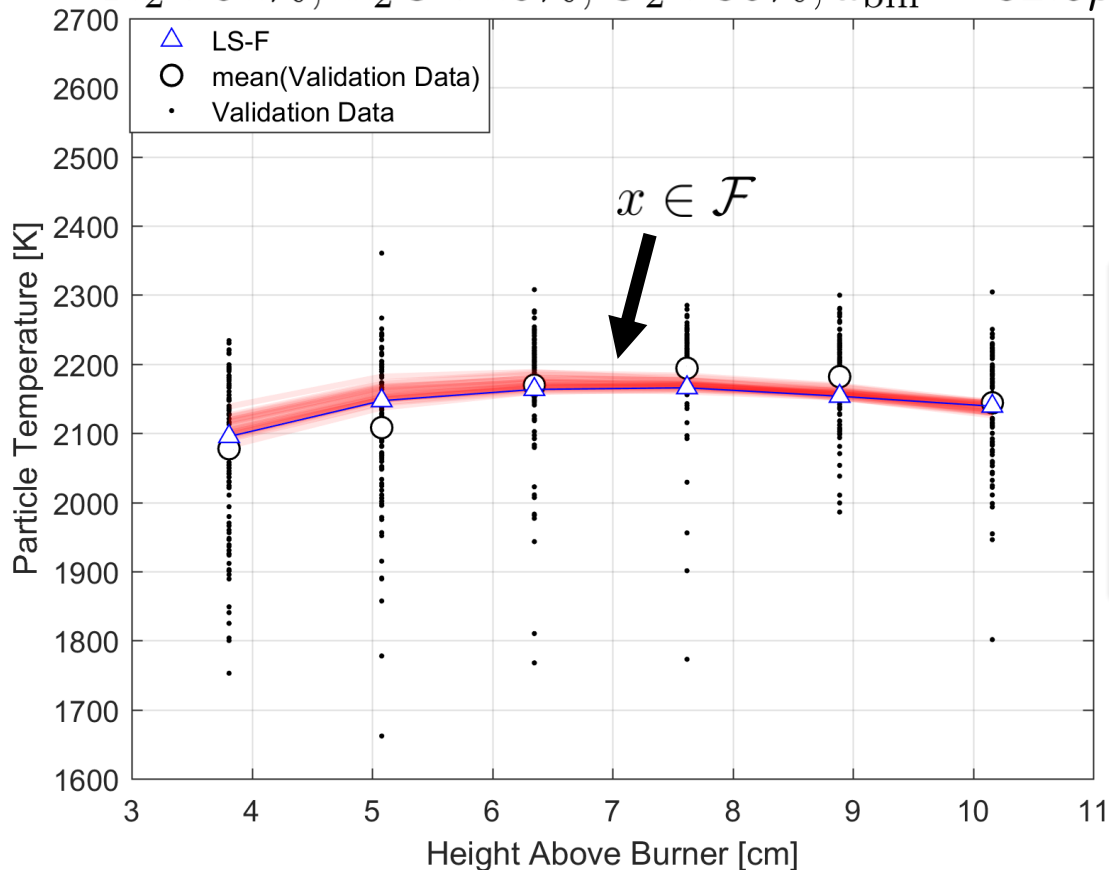
### Scalar consistency measure:

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

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

# Validation through consistency

$\text{N}_2 : 54\%$ ,  $\text{H}_2\text{O} : 10\%$ ,  $\text{O}_2 : 36\%$ ,  $d_{\text{bin}} = 82.5\mu\text{m}$



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

s.t.  $x \in \mathcal{F}$

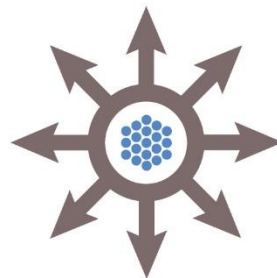
$y_e$  : mean of the validation data

# 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

# Acknowledgements

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CARBON CAPTURE  
MULTIDISCIPLINARY  
SIMULATION CENTER