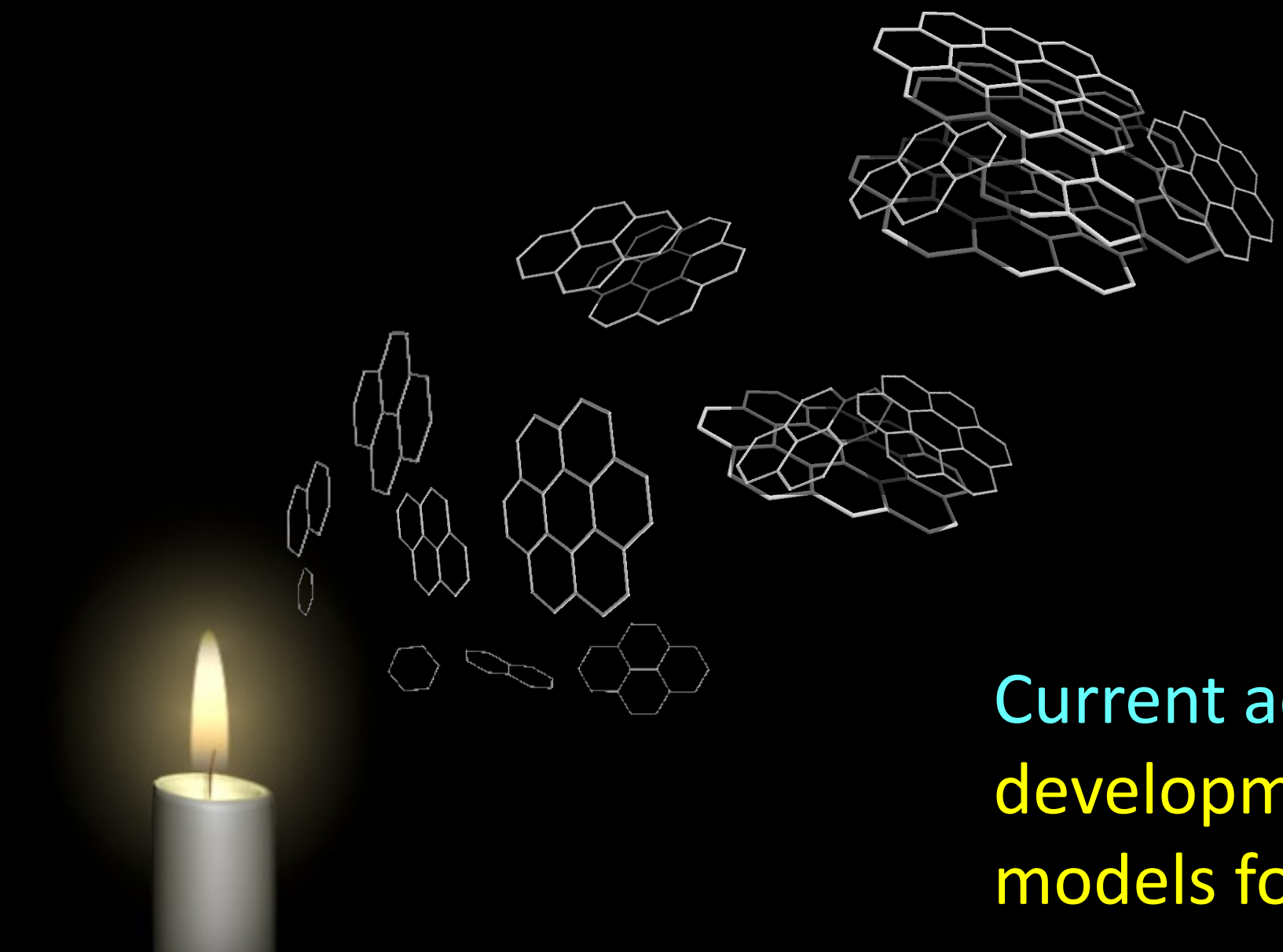
AREAS OF INTEREST

Michael Frenklach, *Mechanical Engineering*

- Combustion model development
- Predictive modeling, UQ
- Data-model system for on-demand computing

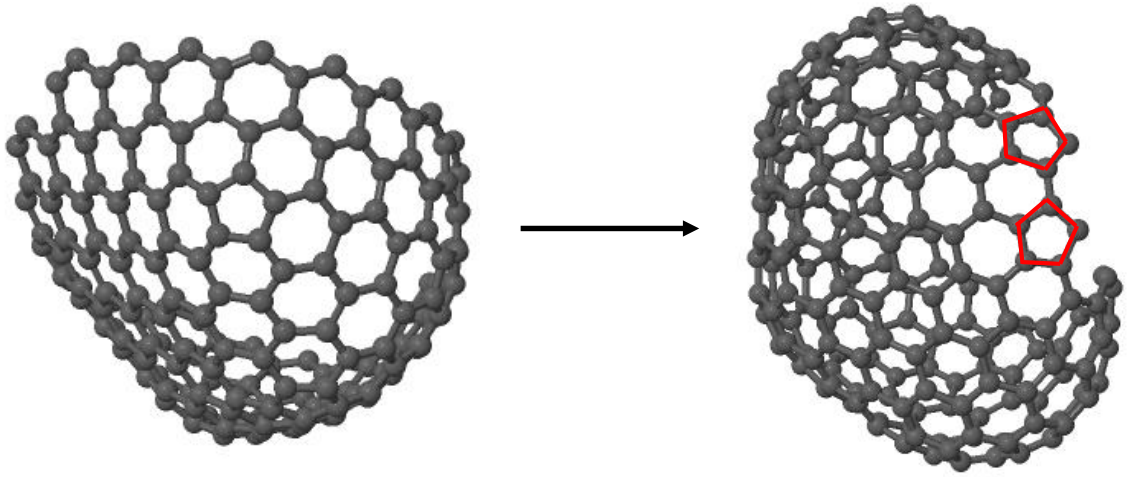
COMBUSTION



Expertise in
model development
of soot oxidation:
-chemistry
-particle dynamics

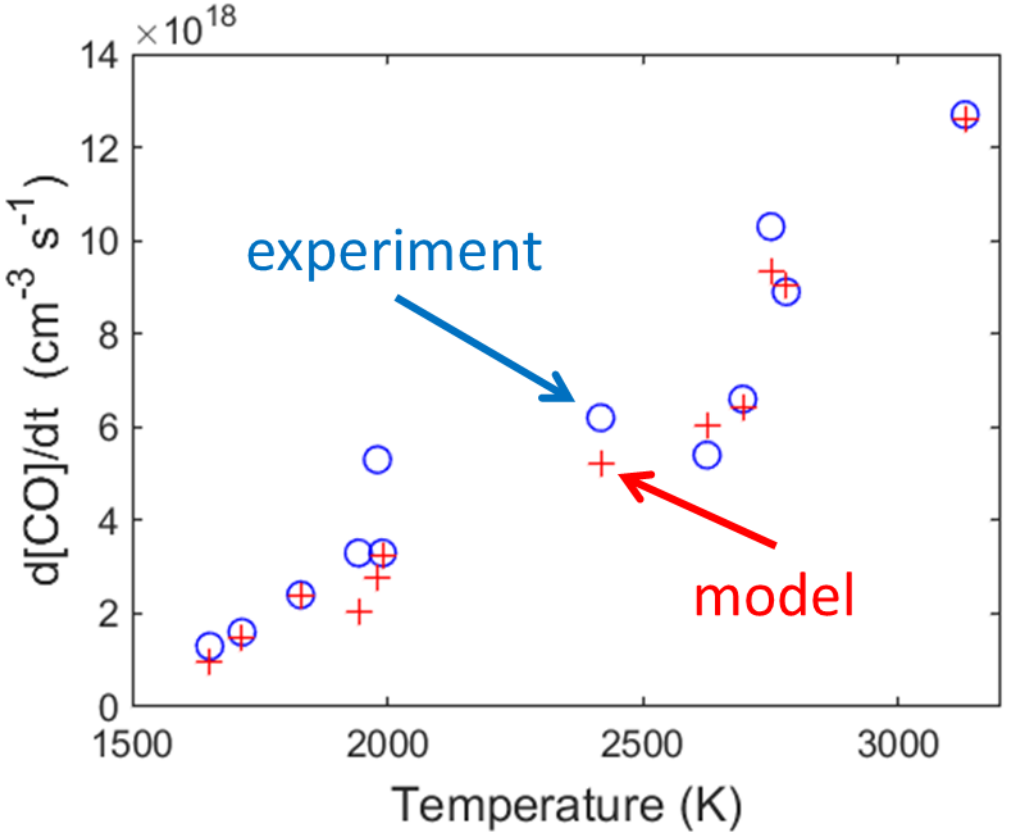
Current activity:
development of reduced-order
models for carbon oxidation

RECENT RESULTS



t = 5 ms

t = 6.8 ms



Five-member rings form due to oxidation and become embedded in the graphene layer forming unreactive zigzag edges that cause the oxidation rate to decrease over time.

Singh, Mebel, Frenklach, *J. Phys. Chem A* (2015).

The Carbon-Capture Multidisciplinary Simulation Center

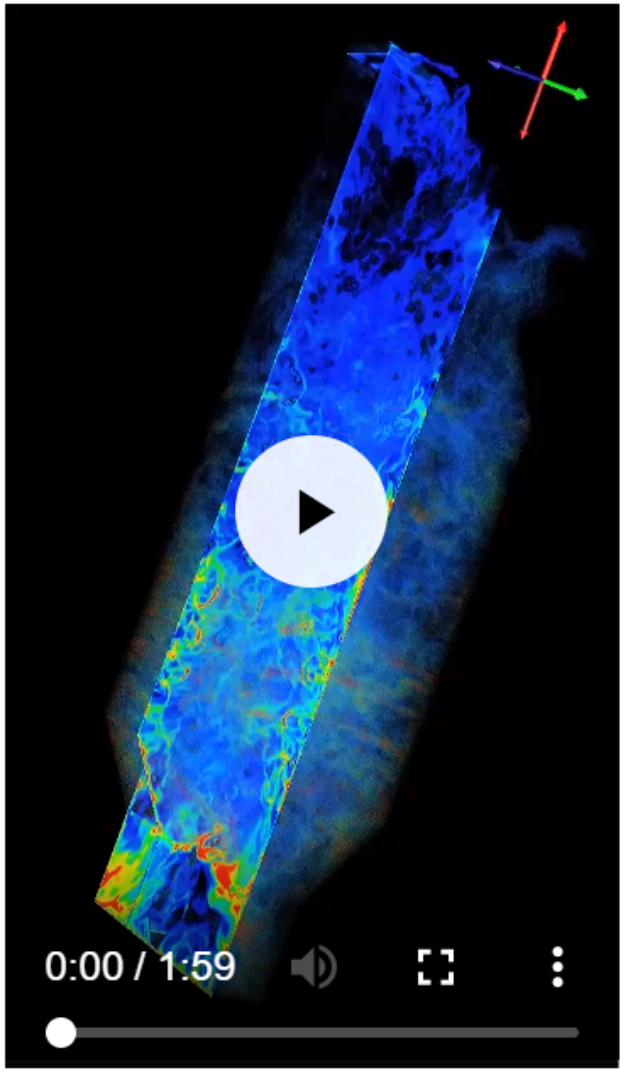
The Carbon-Capture Multidisciplinary Simulation Center (CCMSC) is demonstrating exascale computing with V&V/UQ to more rapidly deploy a new technology for providing low cost, low emission electric power generation to meet the growing energy needs of the U.S. We are using a hierarchal validation approach to obtain simultaneous consistency between a set of selected experiments at different scales embodying the key physics components (large eddy simulations, multiphase flow, particle combustion and radiation) to predict performance in a 350MWe oxy-fired boiler.

To solve this problem, we are developing the following tools:

1. exascale computing software that will be regularly released through open-source licensing,
2. tools for V&V/UQ for use with other large applications with expensive function evaluations and sparse/expensive experimental data, and
3. new advances in computational fluid dynamics, multiphase reacting flow and radiative heat transfer.

The CCMSC is funded by the Predictive Science Academic Alliance Program.

Learn More ▶



Announcements

V/UQ Winter School, January 16-26, 2018

The Institute for Clean & Secure Energy (ICSE), in conjunction with the Carbon Capture Multidisciplinary Simulation Center (CCMSC) would like to announce the creation of the V/UQ Winter School, held at the Silverado Lodge at the Canyons Resort in Park City, UT January 16-26, 2018. Registration and hotel information is available on the linked flyer.

Research Highlights

CARBON CAPTURE MULTIDISCIPLINARY SIMULATION CENTER

International Collaborations

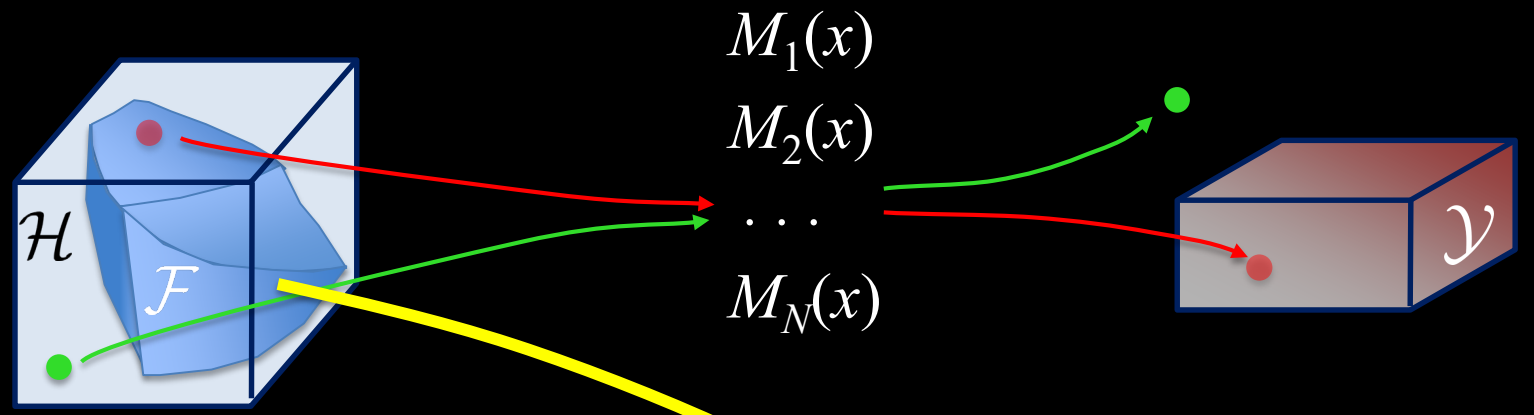
The need to reduce CO2 emissions is global, and the CCMSC is fostering international collaborations in support of its mission to demonstrate exascale computing with V&V/UQ to more rapidly

Predictive modeling (UQ): Bound-to-Bound Data Collaboration

prior information on uncertain parameters

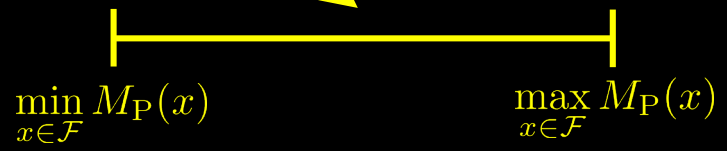
$x \in \mathcal{H}$

space of observed QOIs

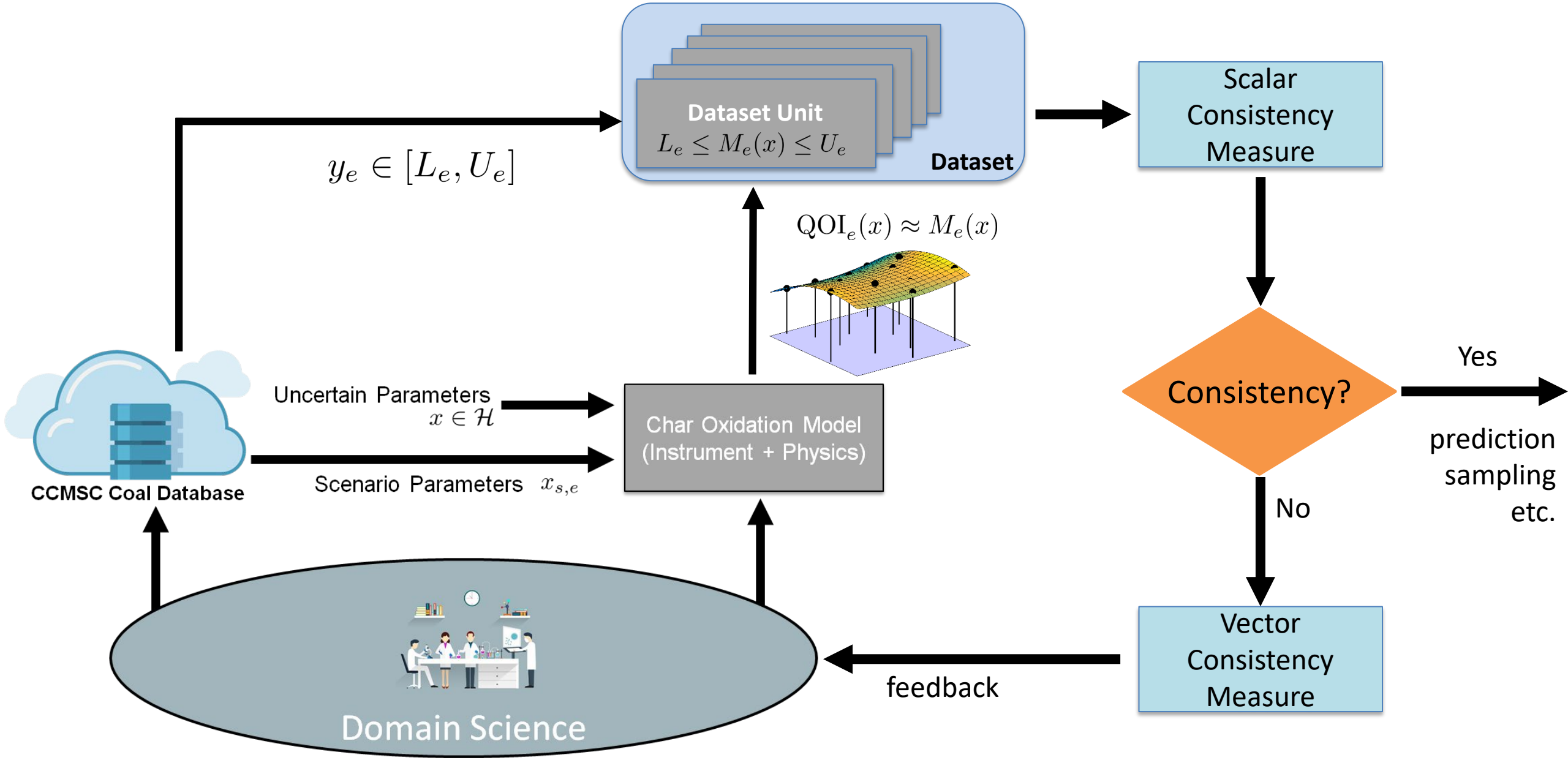


All the ● parameter vectors constitute the *feasible set*

If $\mathcal{F}$ is not empty, make prediction for unmeasured QOI



Model Validation Workflow



New direction: Treating model discrepancy in B2BDC

- model is tentatively correct, suspect experiments
  - experimental bias
  - B2BDC consistency analysis identifies experiments to suspect
- experiments are less suspect than the model
  - model bias

$$y = M(x) + b_{\mathrm{M}} (+ \varepsilon)$$

Providing Structure to Experimental Data

- Experimental data comes in various file formats
  - CSV, excel, tab delimited, ASCII
- Requires knowledge of how the data was stored
- For automated access to data we need structure

primekinetics.org

- What is PrIMe?
  - Data Warehouse – repository of experimental data records
  - Applications – aid in development of predictive models
- PrIMe data models use XML schemas to provide structure
  - Data stored in XML, JSON or HDF5 files
- Ability to store raw experimental measurements
- Publically available validation data

Experimental Data for Model Validation

- 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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