Task 6 Development of a High Fidelity Proxy Model

NATIONAL ENERGY TECHNOLOGY LABORATORY

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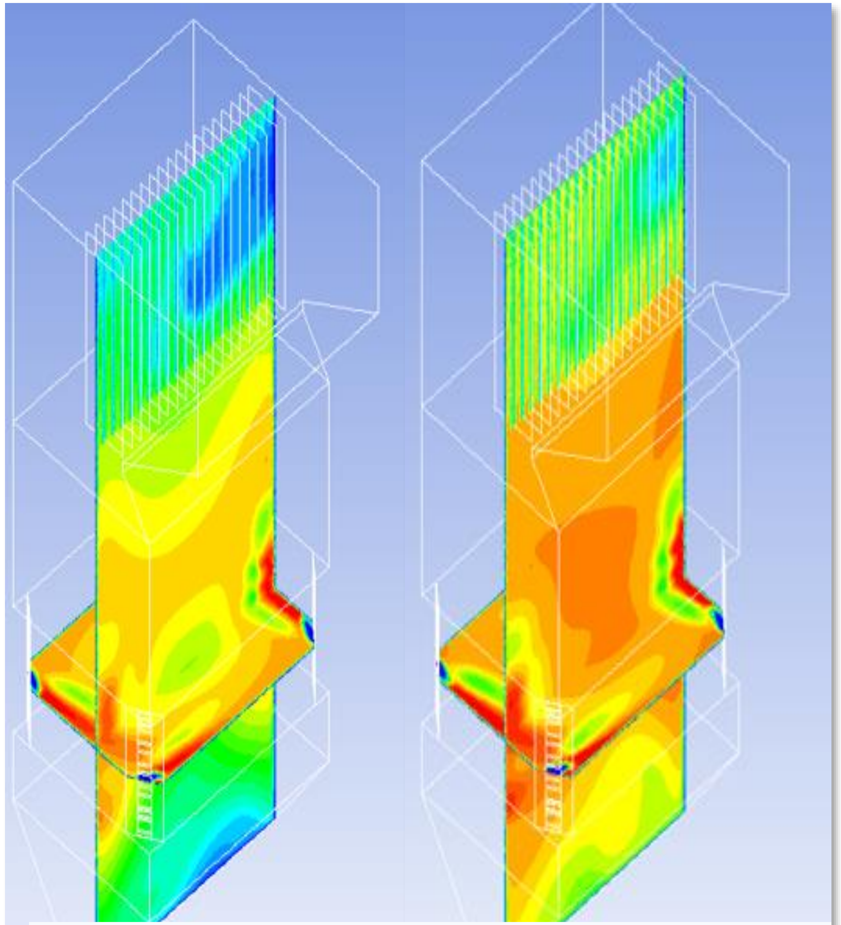
Prof Mohaghegh, A. Aboaba, Y. Martinez, and D. Keller (WVU)

September 30, 2020

Agenda

Development of an Industrial Scale High Fidelity Proxy Model

- Motivation and Goal
- Overview of Approach and Deliverables
- Recap previous results
- Variation in multiple parameters during partial load operation
  - CFD and proxy model results
- Extension of proxy model transient applications
- Details of accomplishments with potential spillover affects into other industries.
- Proxy model uses in various industry and benefits of the technology.
- Path forward.

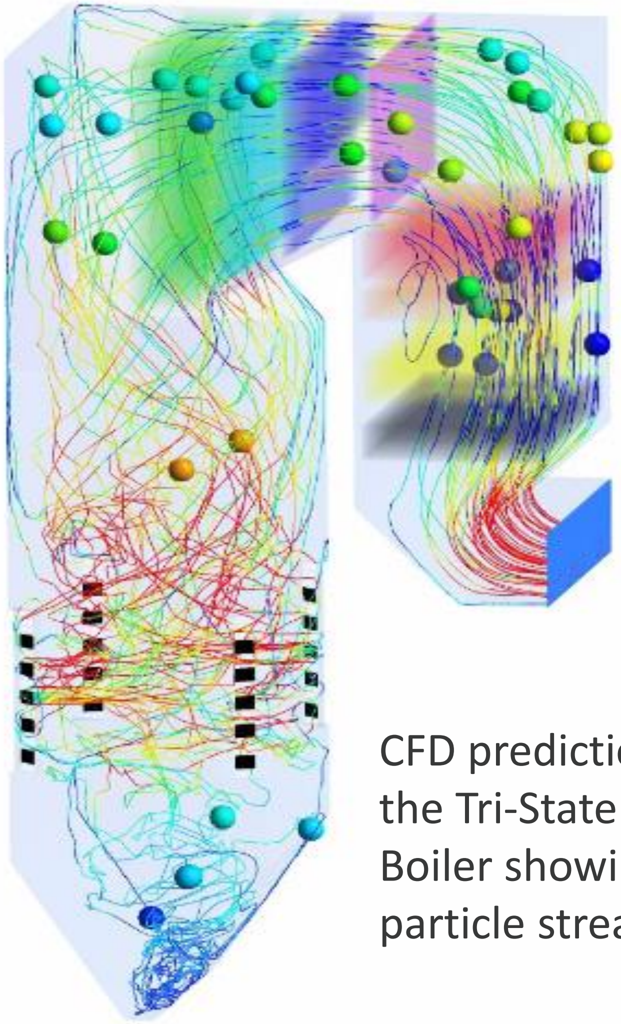


Escalante Tri-State Boiler 40% Full Load (left) and Full Load (right): Gas Temperature Predictions

Motivation & Goal

Motivation: Common practice to use Computational Fluid Dynamic (CFD) models for high fidelity information at a device scale level.

- Steep learning curve
- Large computational resources and time
- Difficult to quantify uncertainties in model predictions
- Difficult to disseminate modeling results
- Never deployed or used directly in the field

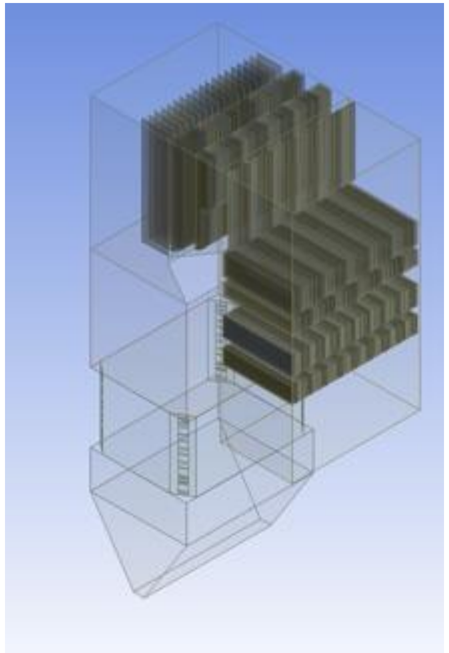


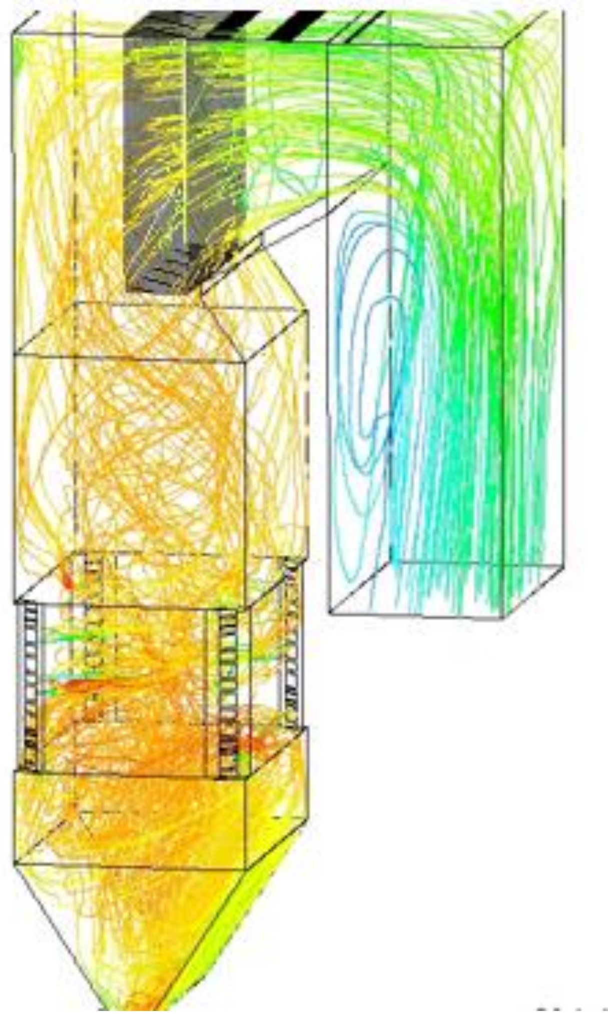
CFD predictions of the Tri-State 245 MW Boiler showing particle streamlines

Motivation & Goal

Goal: Develop a CFD based fast running high fidelity proxy model of an industrial scale boiler.

- Expertise in CFD not required
- Fast running almost real time
- Proxy model could be deployed on basic operating systems (desktop, laptop, tablet)
- Easy to use by engineers in the field
- Could be applied to multiple industrial areas



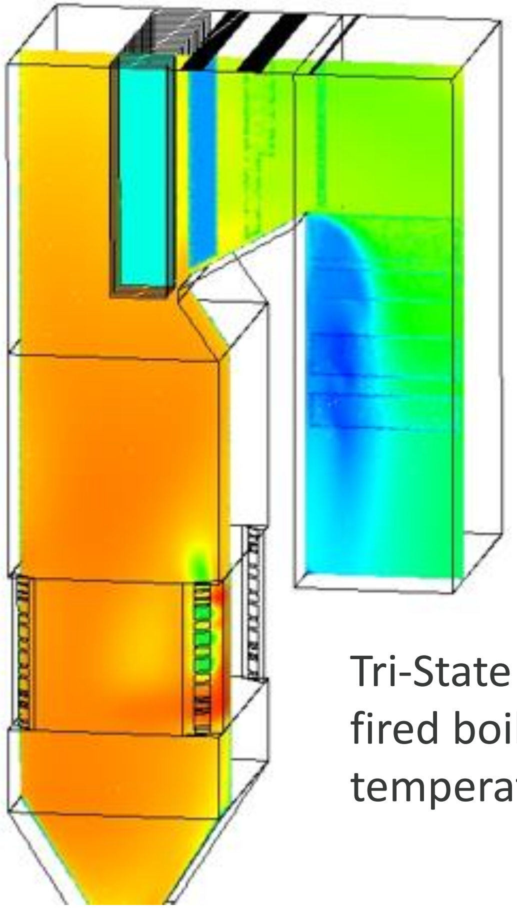


Approach and Deliverables

Leverage the fidelity inherent in a CFD model and recent advances in artificial intelligence (AI) and machine learning (ML) to develop a pr model from three dimensional CFD data.

Approach and Deliverables:

- **Develop a CFD model of the NETL B6 combustion rig (complete**
- **Develop a proxy model of the NETL B6 combustion rig (complete**
- **Develop a CFD model of an industrial scale boiler (completed)**
- **Develop a proxy model of an industrial scale boiler over a single parameter of interest (completed)**
- **Develop a proxy model of an industrial scale boiler over multiple parameters of interest (completed)**
- **Conduct sensitivity analysis using proxy model to predict optimal performance (in-progress)**
- **Submit manuscript of the sensitivity analysis (in-progress)**
  - Data Driven Proxy Model Development for a Tangentially Fired Coal Boiler under Partial Load Operation
- **Develop a proxy model for transient applications (in-progress)**



Tri-State 245 MW tangentially fired boiler. CFD prediction of temperature through the boiler

NETL Proxy Model Approach

ParaView
Parallel Visualization Application

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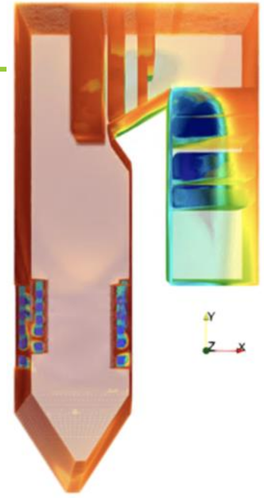
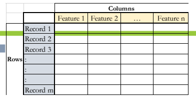
Actual Data .vtk file



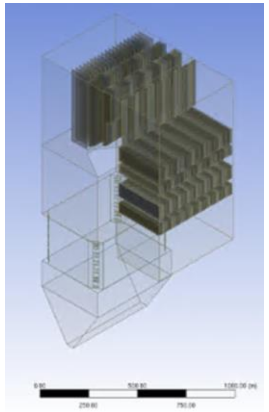
Prediction Data .vtk file



Blind

ANSYS FLUENT

- CFD Simulation runs (32)



Text Files

SPYDER

Deployment

Data Collection

Export Data from FLUENT

- Input Data
- Output data
- System's detail Geometry
- Boundary Conditions

Build Database

- Feature Generation:
  - Geometry
  - Boundary Condition
- Unsupervised Learning
- Reading and importing data (text files) into Python

Modules

- Pandas
- Numpy

Modules

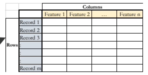
- Skfuzzy
- Numpy

Data Preparation

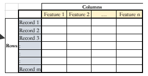
	Columns			
	Feature 1	Feature 2	…	Feature n
Record 1				
Record 2				
Record 3				
Rows :				
:				
:				
Record m				

Database

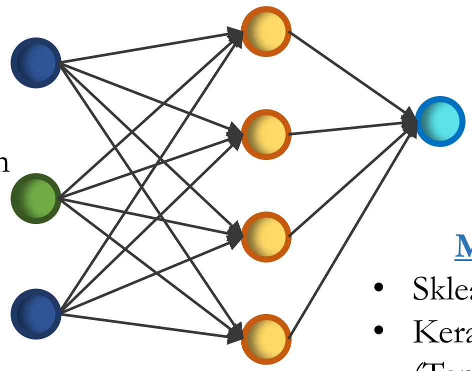
Smart Proxy Development



Training & Calibration



Validation



Target Output

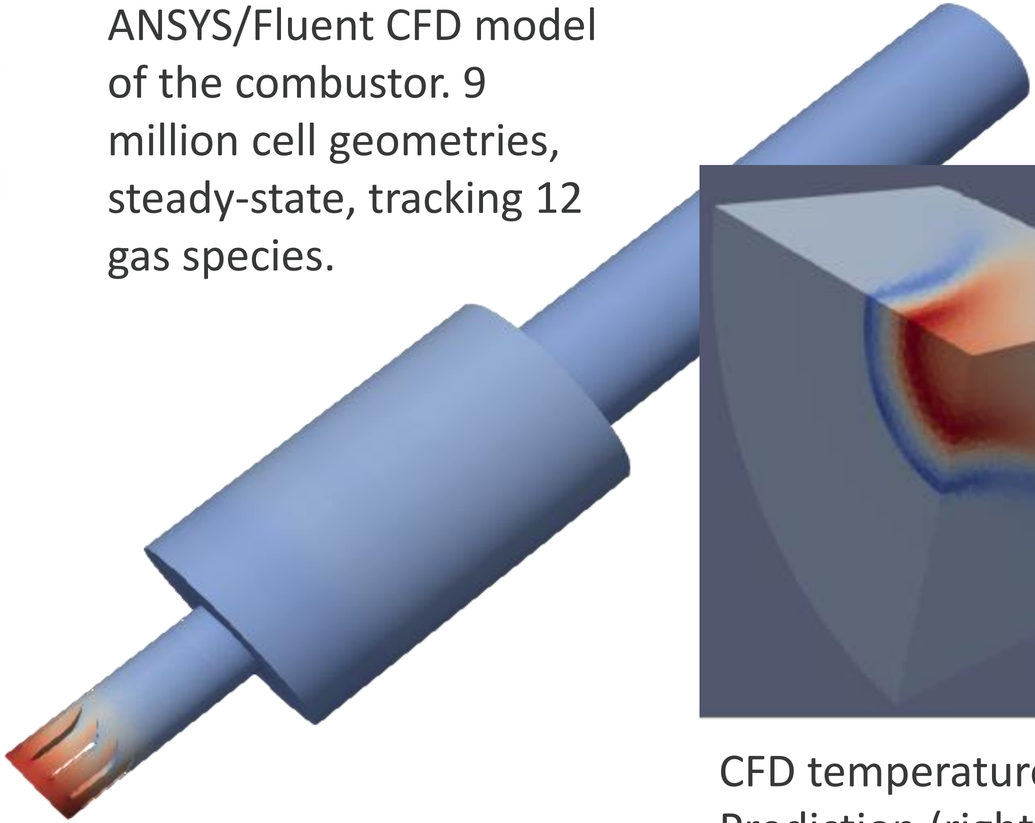
Modules

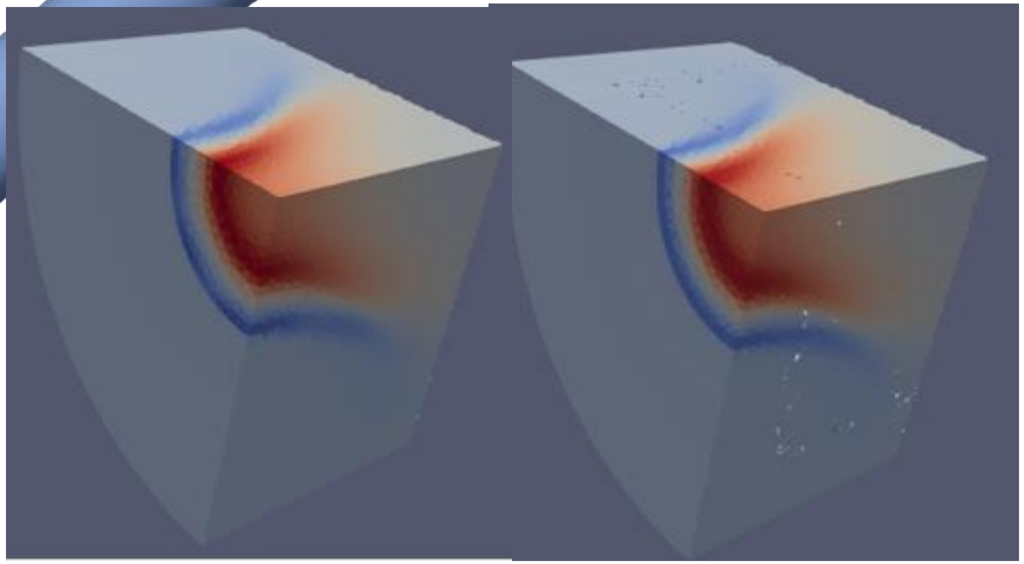
- Sklearn
- Keras (Tensorflow)

NETL Proxy Model: B6 Combustion Rig

NETL B6 combustion rig was used to investigate the effect of fuel interchangeability on combustion performance (Natural Gas w/wo Propane)

ANSYS/Fluent CFD model of the combustor. 9 million cell geometries, steady-state, tracking 12 gas species.





CFD temperature prediction (left) and proxy model Prediction (right) both show excellent agreement experiments. Similar agreement with pressure, velocities and gas species.

NETL Proxy Model of an Industrial Scale Boiler

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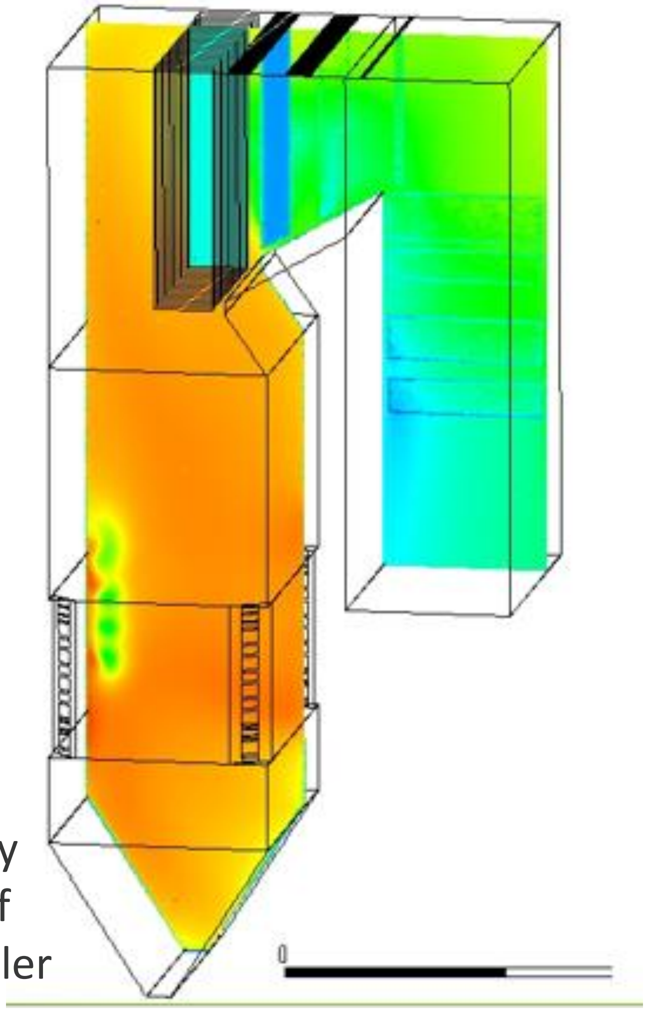
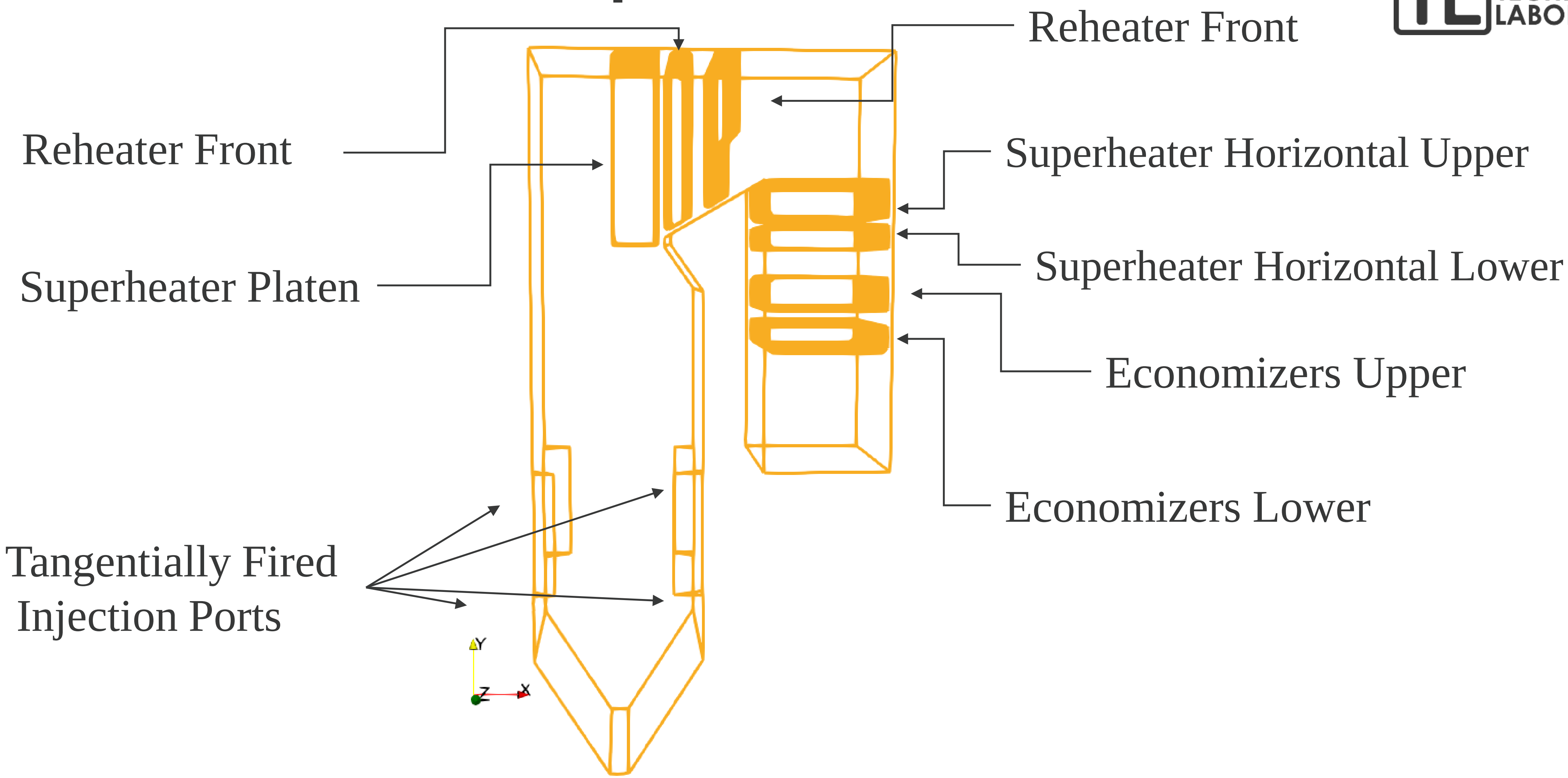
- Partner with industry to ensure relevance of the proxy modeling effort.
  - CRADA with Tri-State Generation & Transmission
  - MOU with NTPC (commercial scale boiler in India)
  - Upper management discussions with ANSYS/Fluent to determine area of collaboration
  - Longview Power Plant Morgantown WV



Tri-State 245 MW tangentially fired boiler. CFD prediction of temperature through the boiler

Tri-State Boiler Components



NETL CFD Model of Tri-State Boiler

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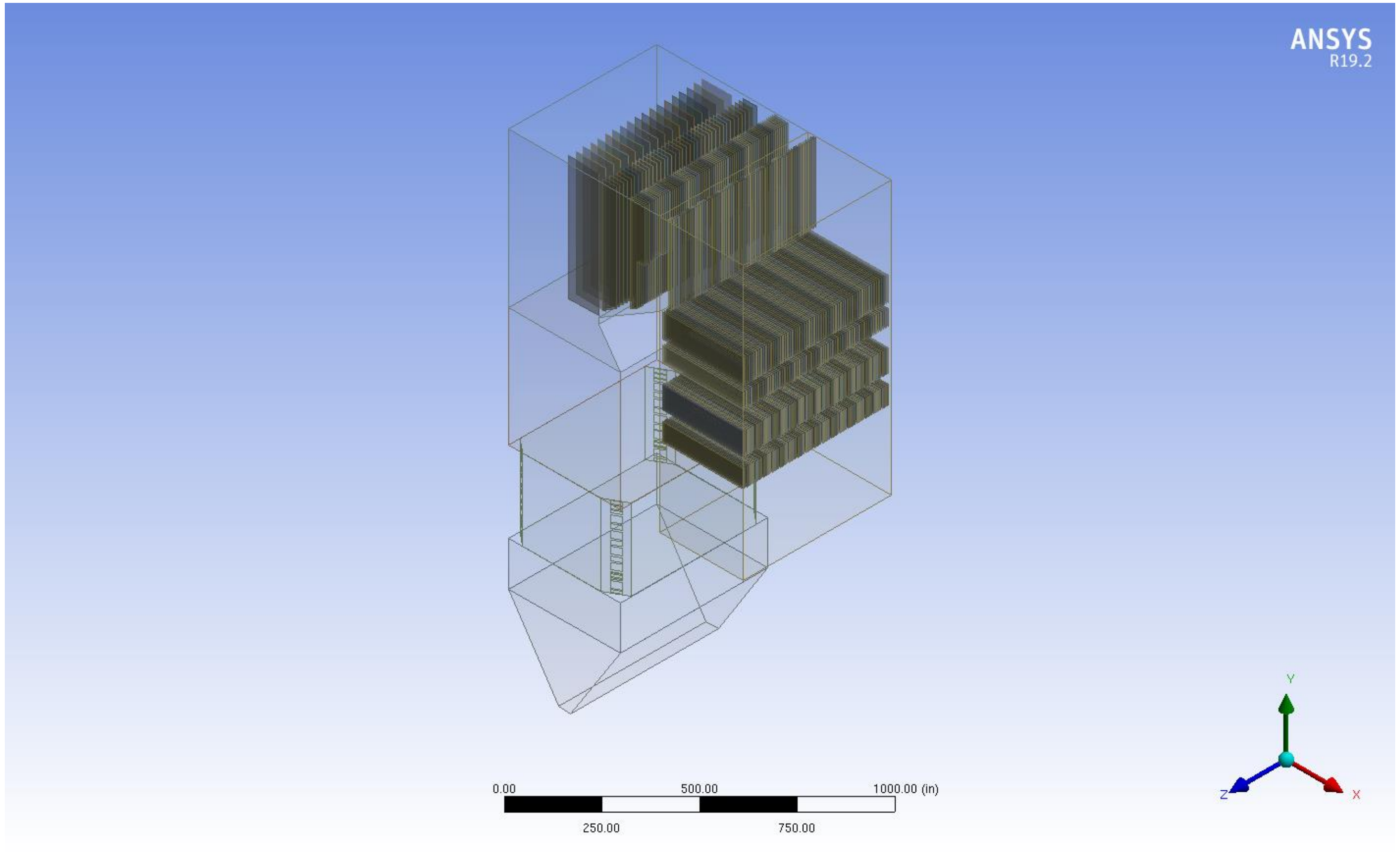
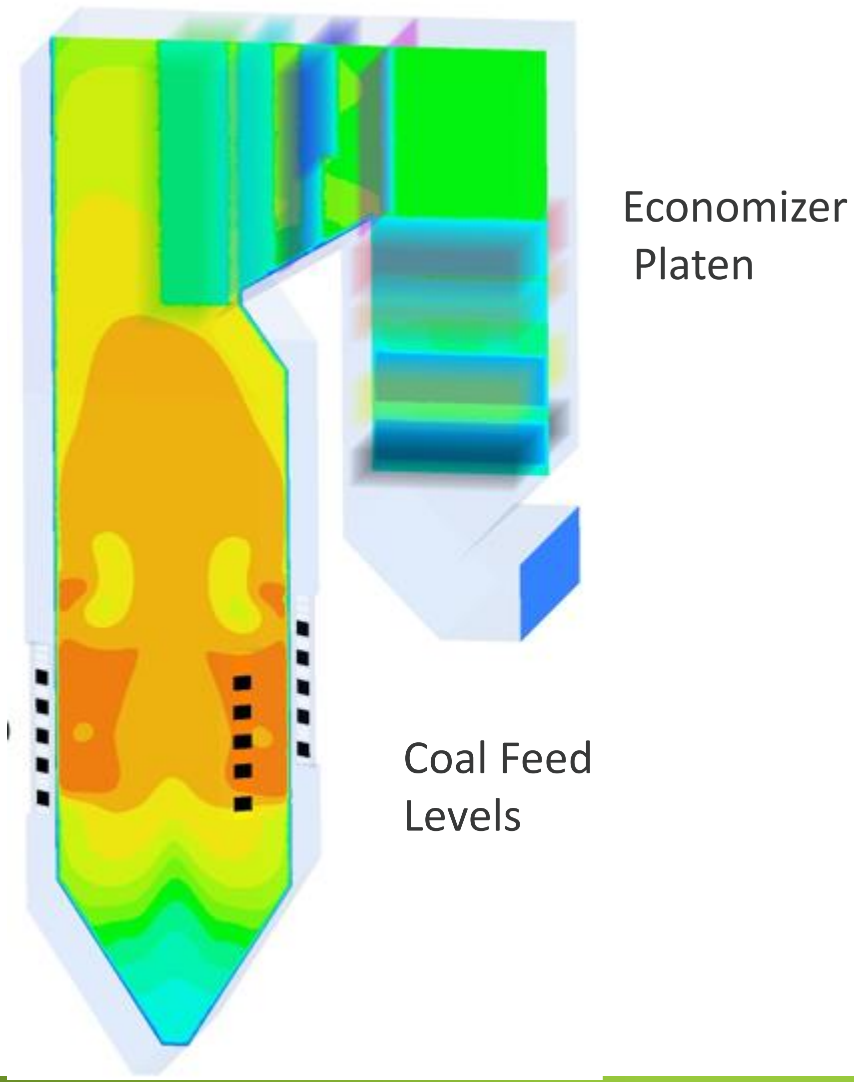
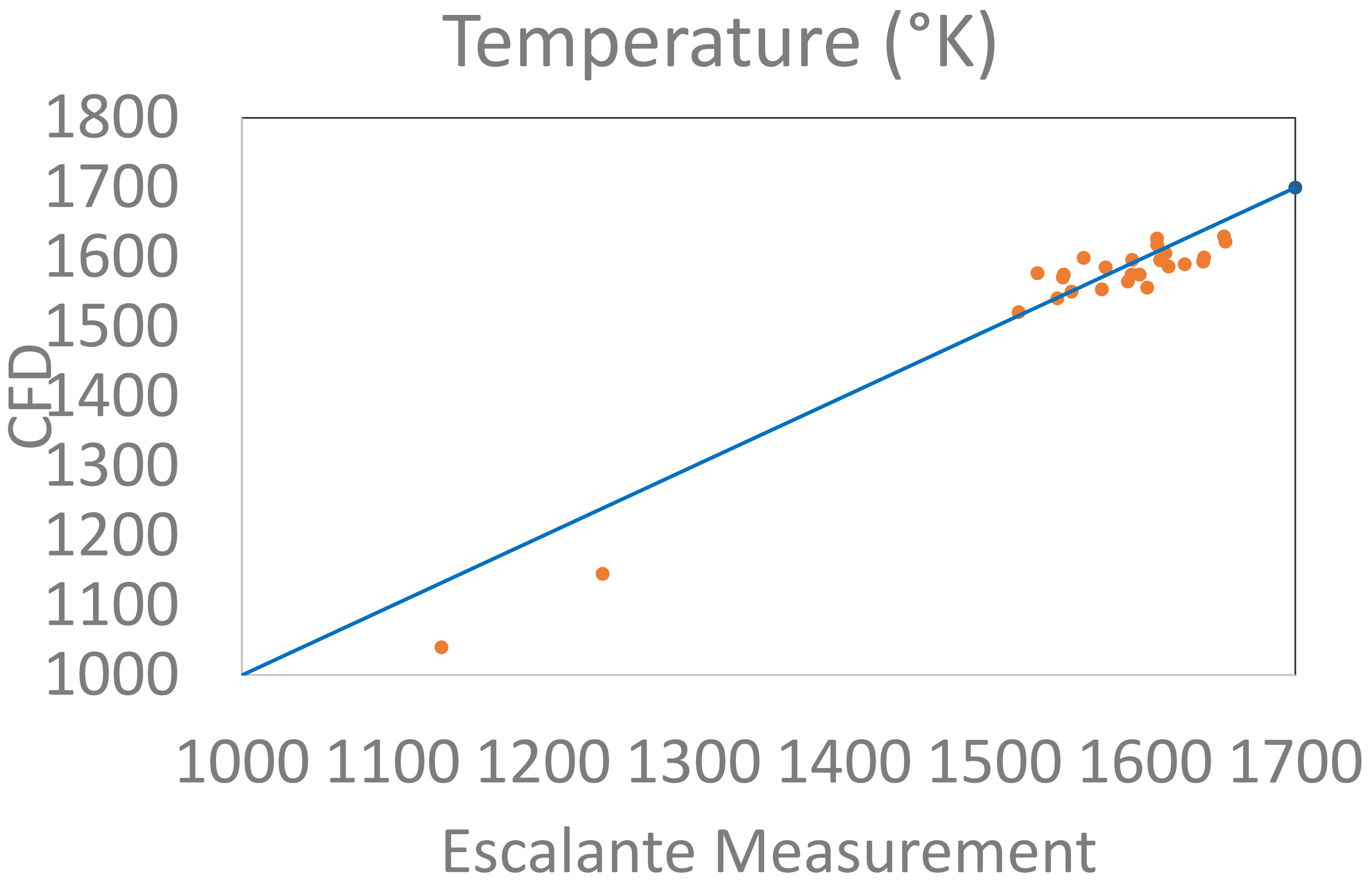
- **CFD Model Fluent**
  - ~4M Computational Cells
  - Steady-state DPM model
  - Radiative Heat Transfer
  - Moisture Release
  - Pyrolysis/Devolatization
  - Char Oxidation Model
  - Gas-phase combustion
  - Realizable k-epsilon
- **Develop Proxy Model Under Turndown Conditions**
  - Base (100% Load), 80%, 60%, 50% and 40%



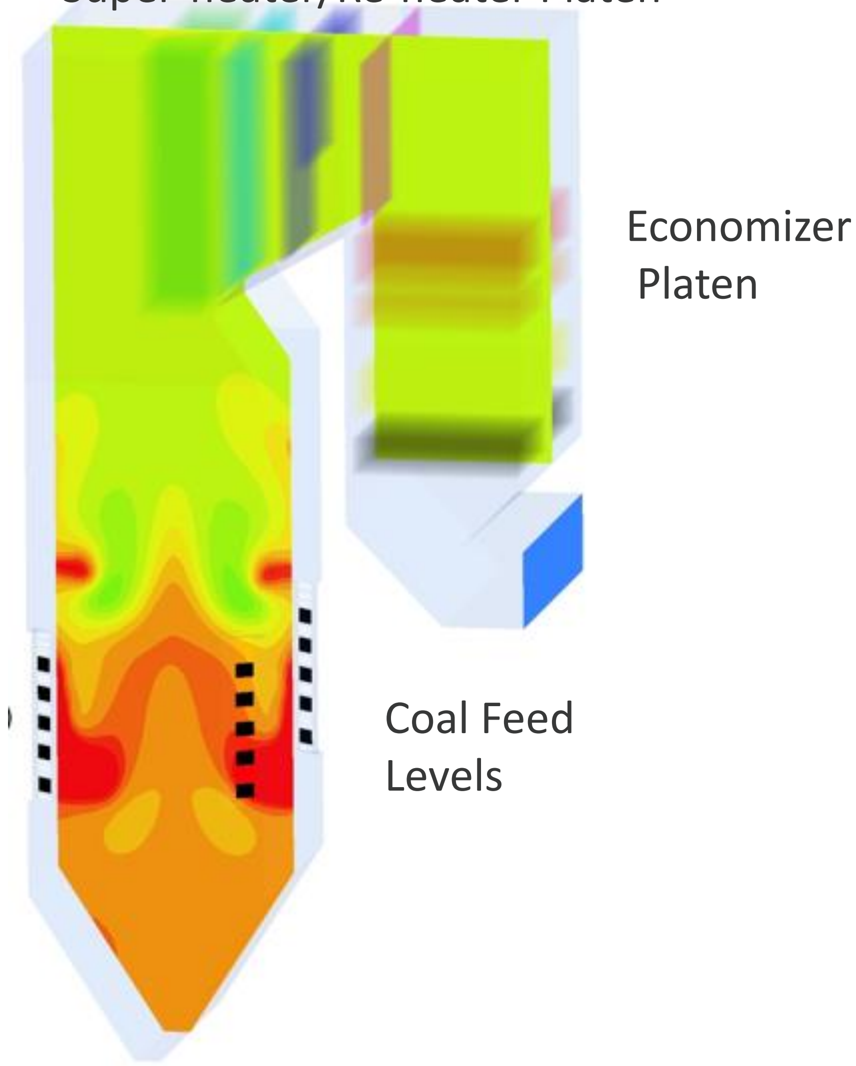
CFD Predictions vs Plant Data (Temperature)

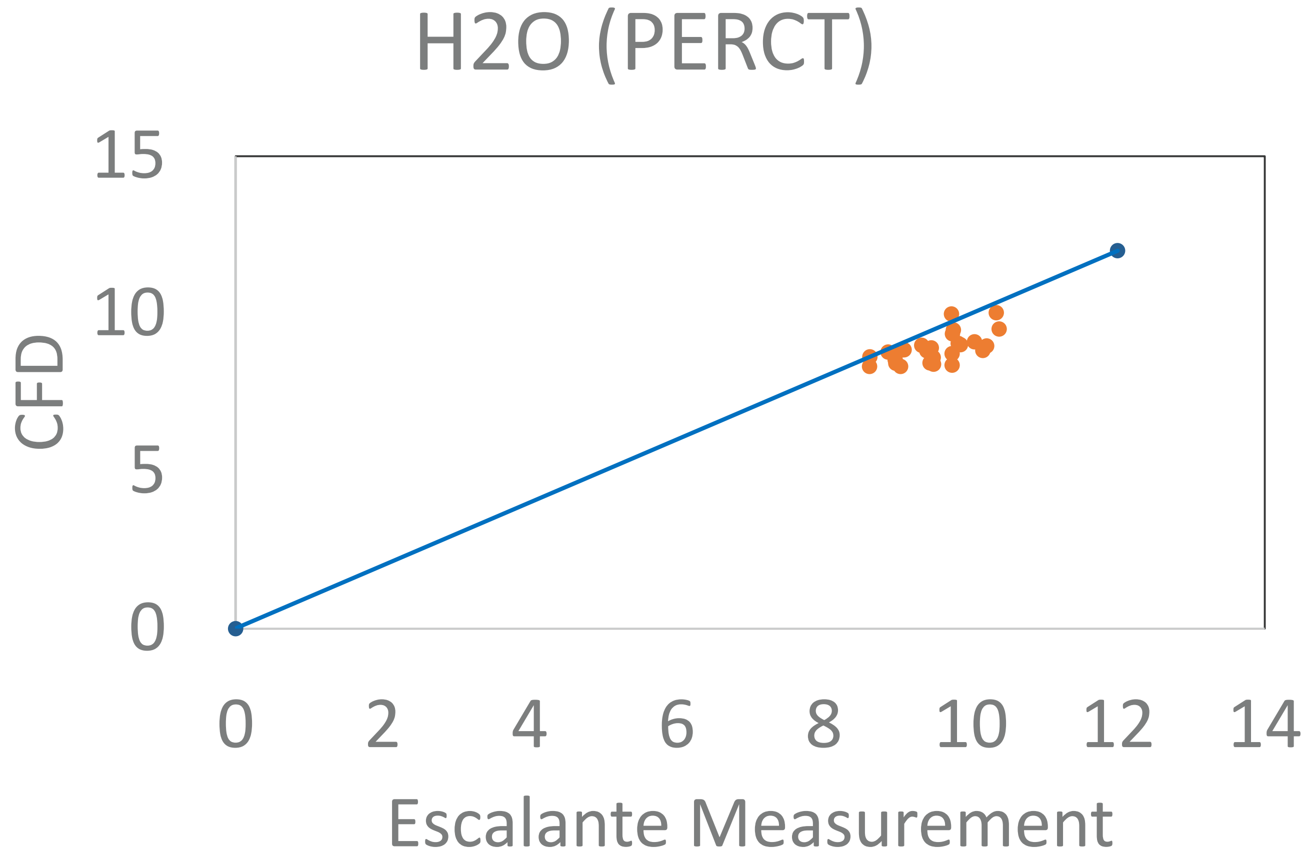
Super-heater/Re-heater Platen



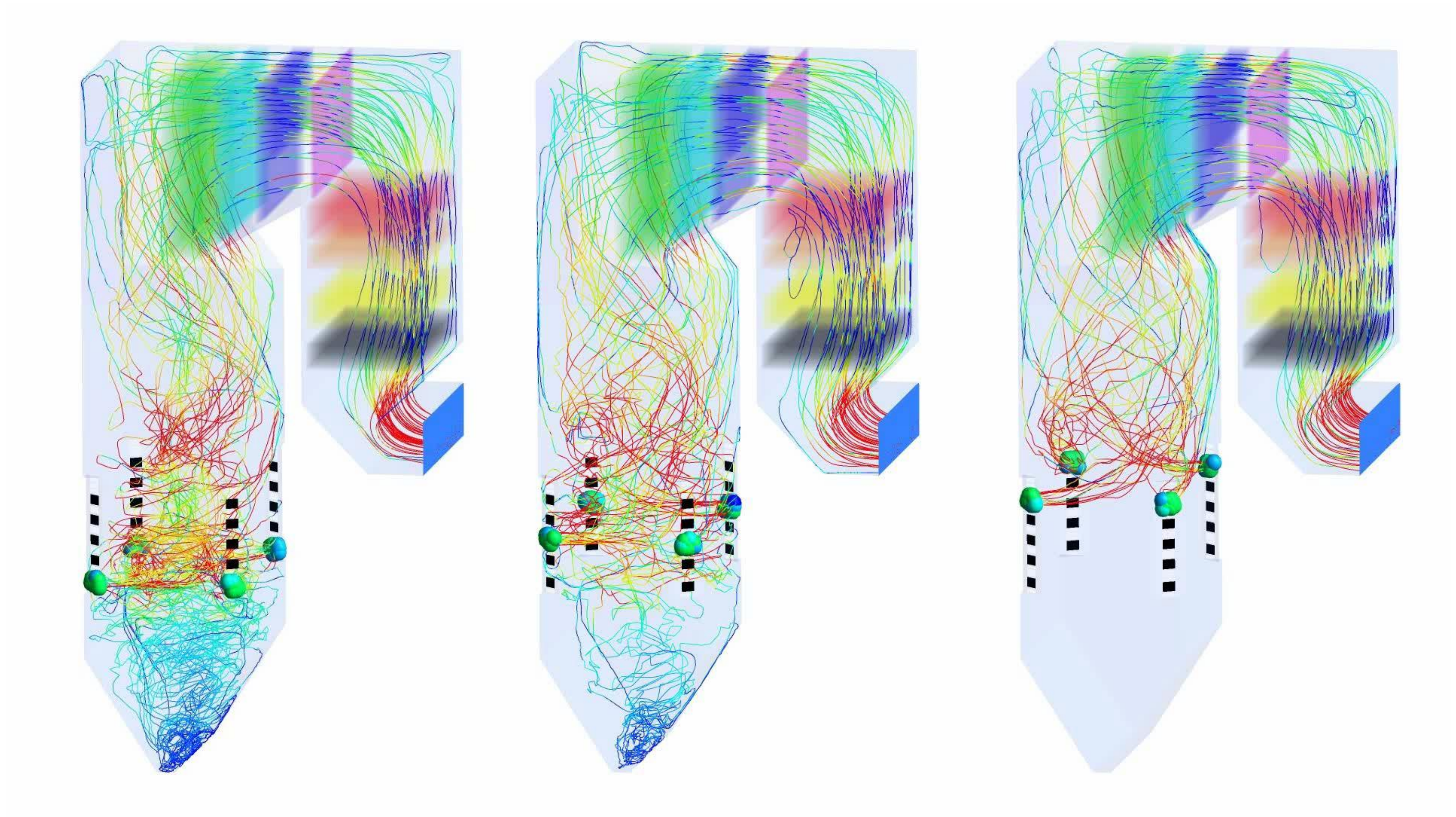


CFD Predictions vs. Plant Data (Moisture)





Fidelity of the NETL CFD Tri-State Model



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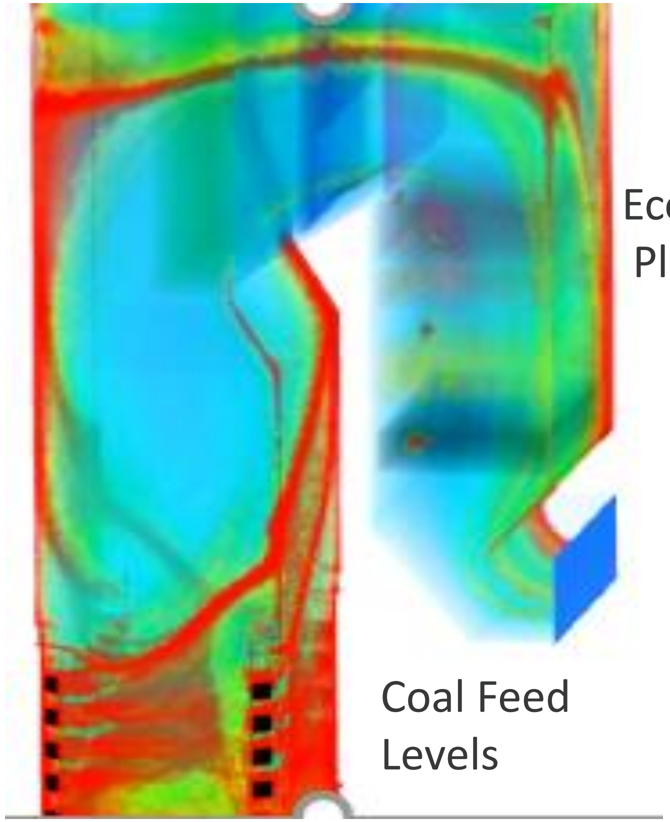
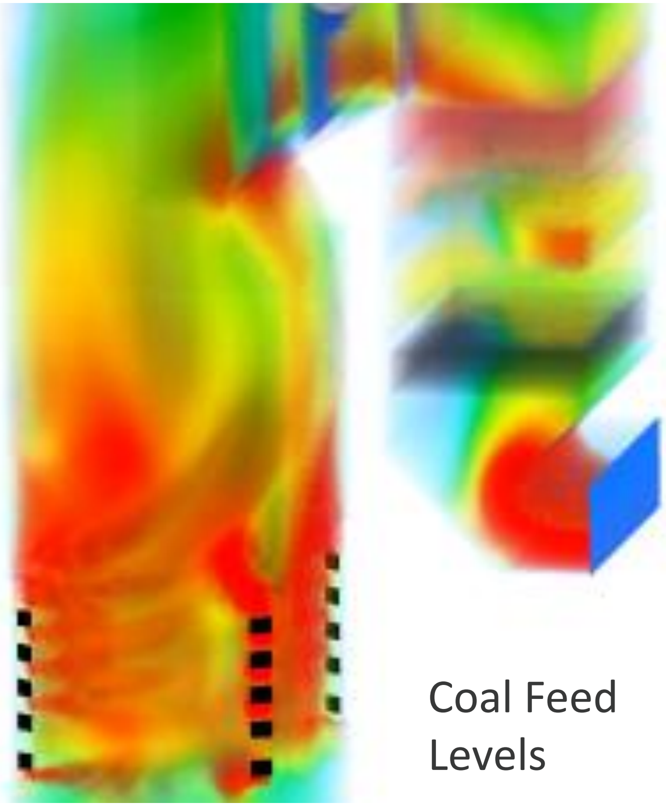


Economizer Platen

Coal Feed Levels

Left particle concentration right velocity magnitude predicted by the NETL CFD model.

Super-heater/Re-heater Platen

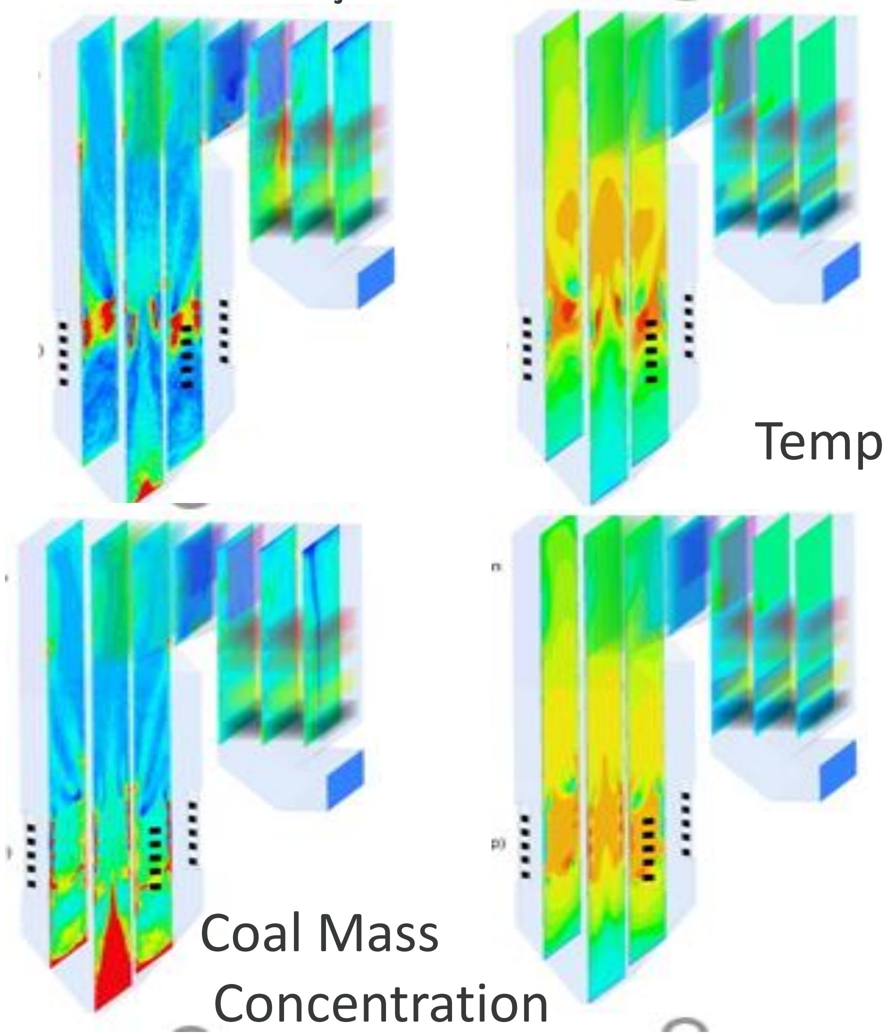


Economizer Platen

Coal Feed Levels

Fidelity of the NETL CFD Tri-State Model

Effect of Coal Injection Levels



- In the top figures coal and primary air are evenly distributed between the top 2 injection layers. In the bottom figures coal and primary air are evenly distributed between all 5 injection layers.
- Injection of coal and primary air at the top 2 injection layers creates a “fire ball” which moves upward allowing more heat to be transferred to the internal super-heater/re-heater platens.
  - The temperature at the bottom part of the boiler drops
  - Less Coal Ash is trapped in the bottom hopper region.
  - Higher temperatures around the burners

NETL Proxy Model Approach

ParaView
Parallel Visualization Application

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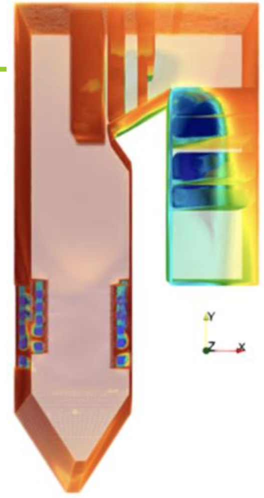
Actual Data
.vtk file

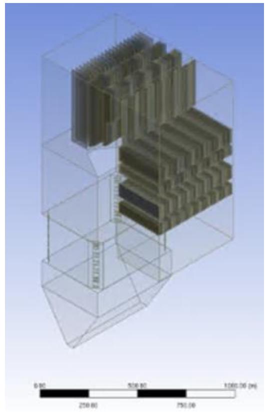
Prediction Data
.vtk file



Blind

- CFD Simulation runs (32)

ANSYS FLUENT



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Training & Calibration

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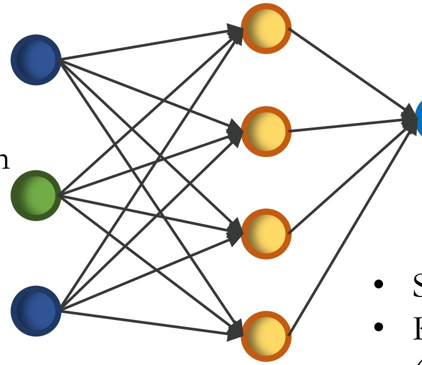
Smart Proxy Development



Target Output

Modules
- Sklearn
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Simulation Matrix to Generate the NETL Proxy Model for Turndown

- **Three out of 19 input parameters are modified in the Tri-State CFD simulations relevant to turn down operating conditions:**
  - Coal flow rate (kg/s)
  - Pulverized air flow (kg/s)
  - Secondary air flow (kg/s)

Input Parameters	Minimum	Maximum
Coal flow rate (kg/s)	0.65	1.67
Pulverized air flow (kg/s)	2.32	3.80
Secondary air flow (kg/s)	2.91	6.53

NETL Proxy Model: Data Partitioning

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Total CFD Runs provided = 32

CFD Runs for:
Training & Calibration = 14
Validation = 3
Blind = 3

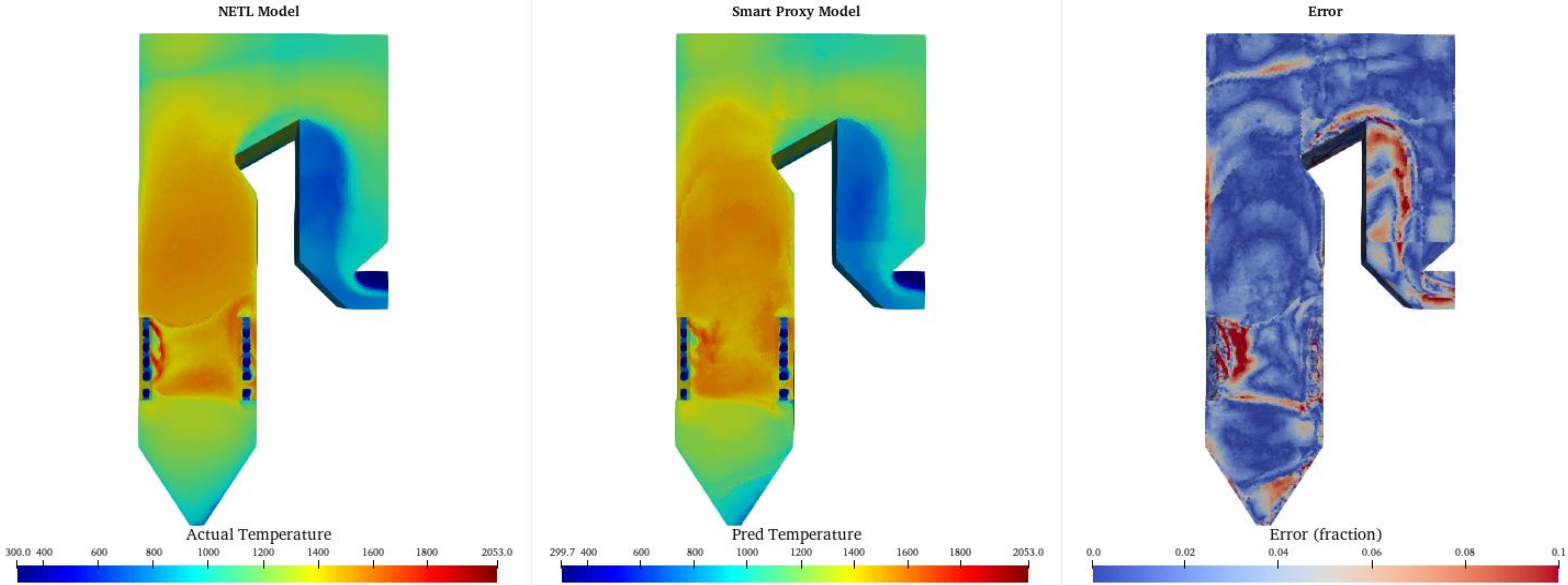
Total CFD Runs not used during this stage of the Proxy Modeling = 12

CFD Runs = 4, 5, 10, 14, 15, 17, 18, 21, 25, 30, 31, 32

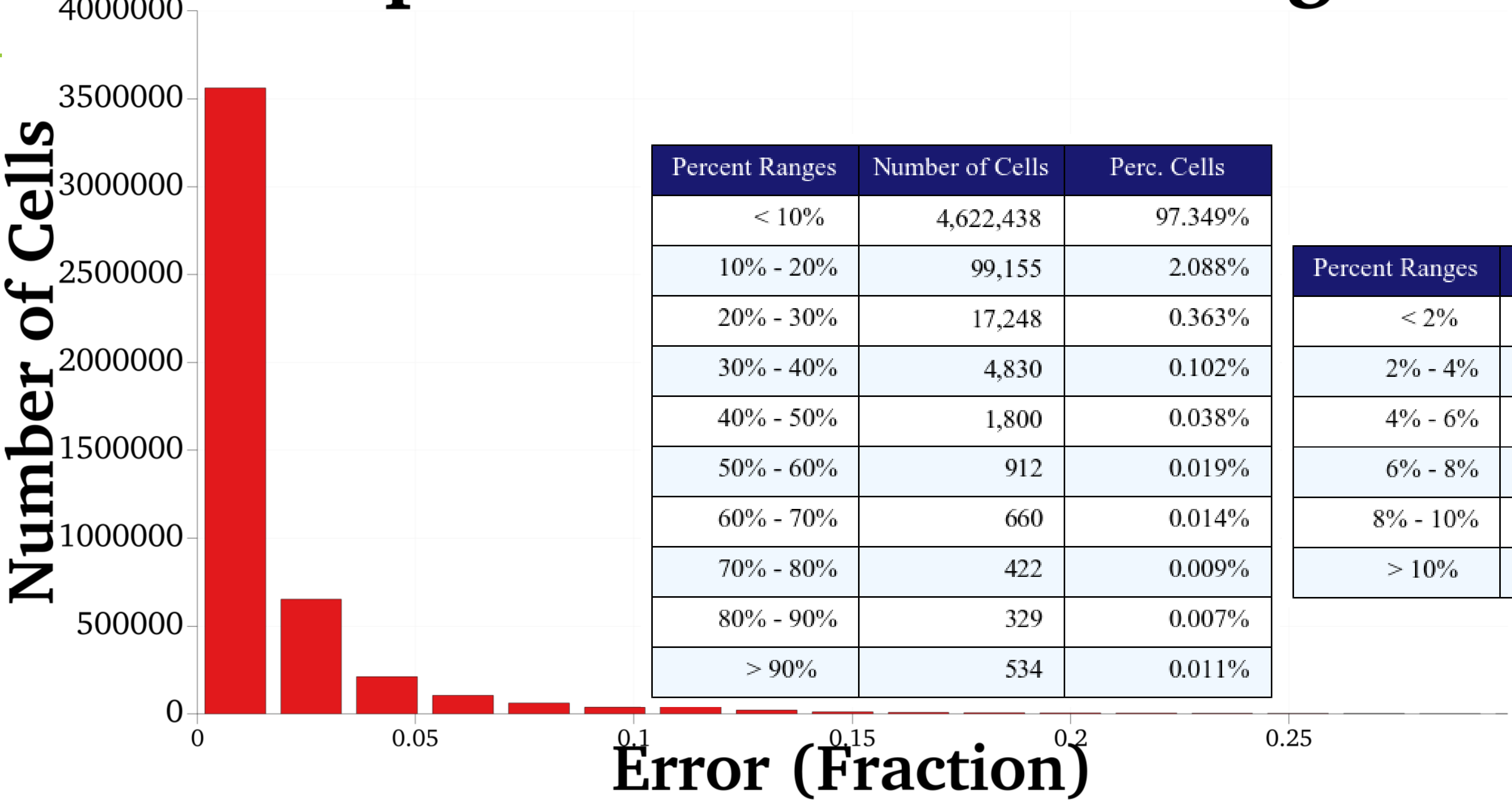
	Training & Calibration	Validation	Blind
MUST BE INCLUDED IN TRAINING	1	24	23
	3	6	11
	8	20	16
	9		
	12		
	13		
	19		
	26		
	28		
	2		
	7		
	22		
	27		
	29		
TOTAL	14	3	3

Demonstration of the results from Sample Training CFD Runs

Temperature - Simulation Run 12

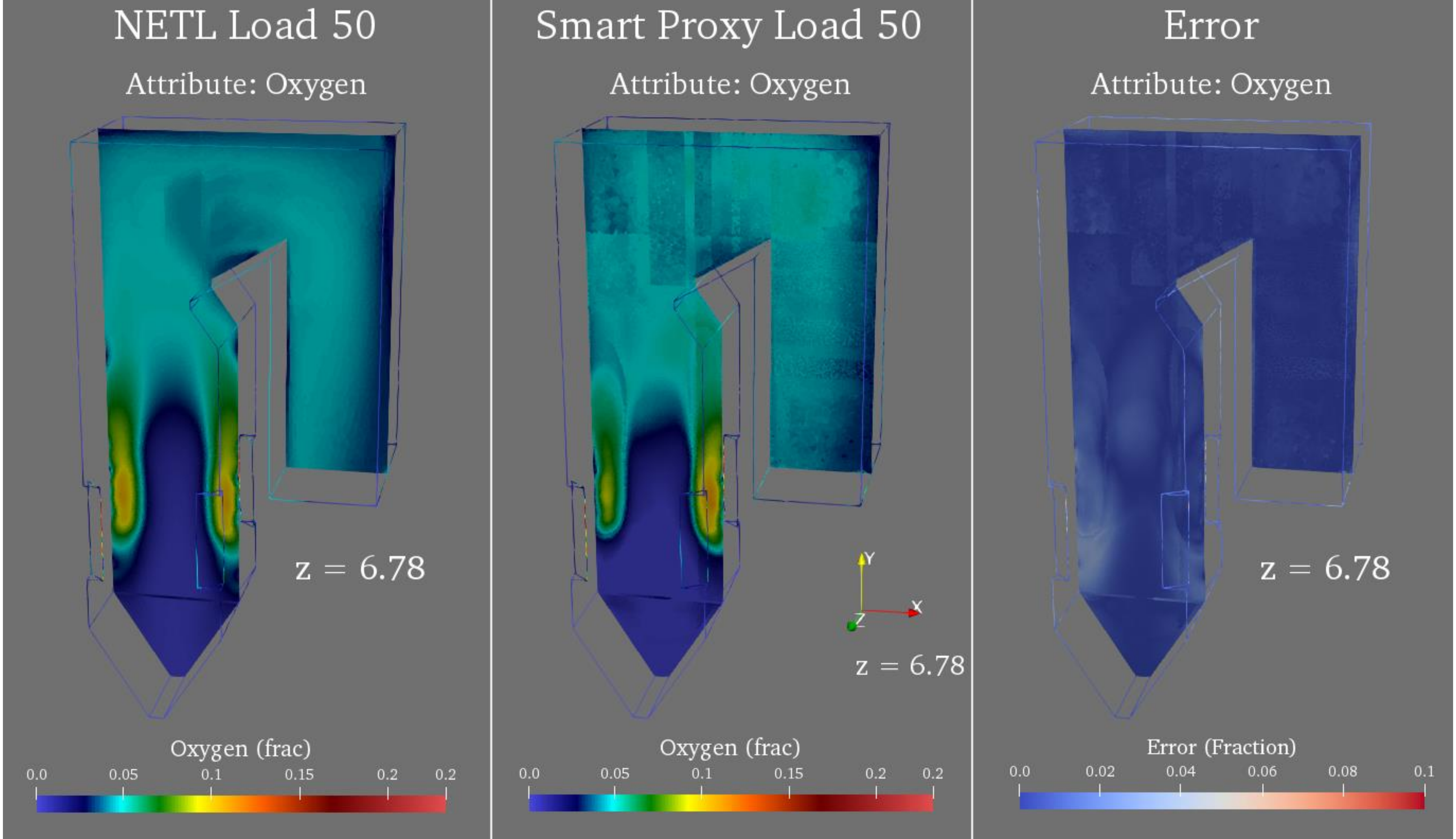


Temperature - Error Histogram

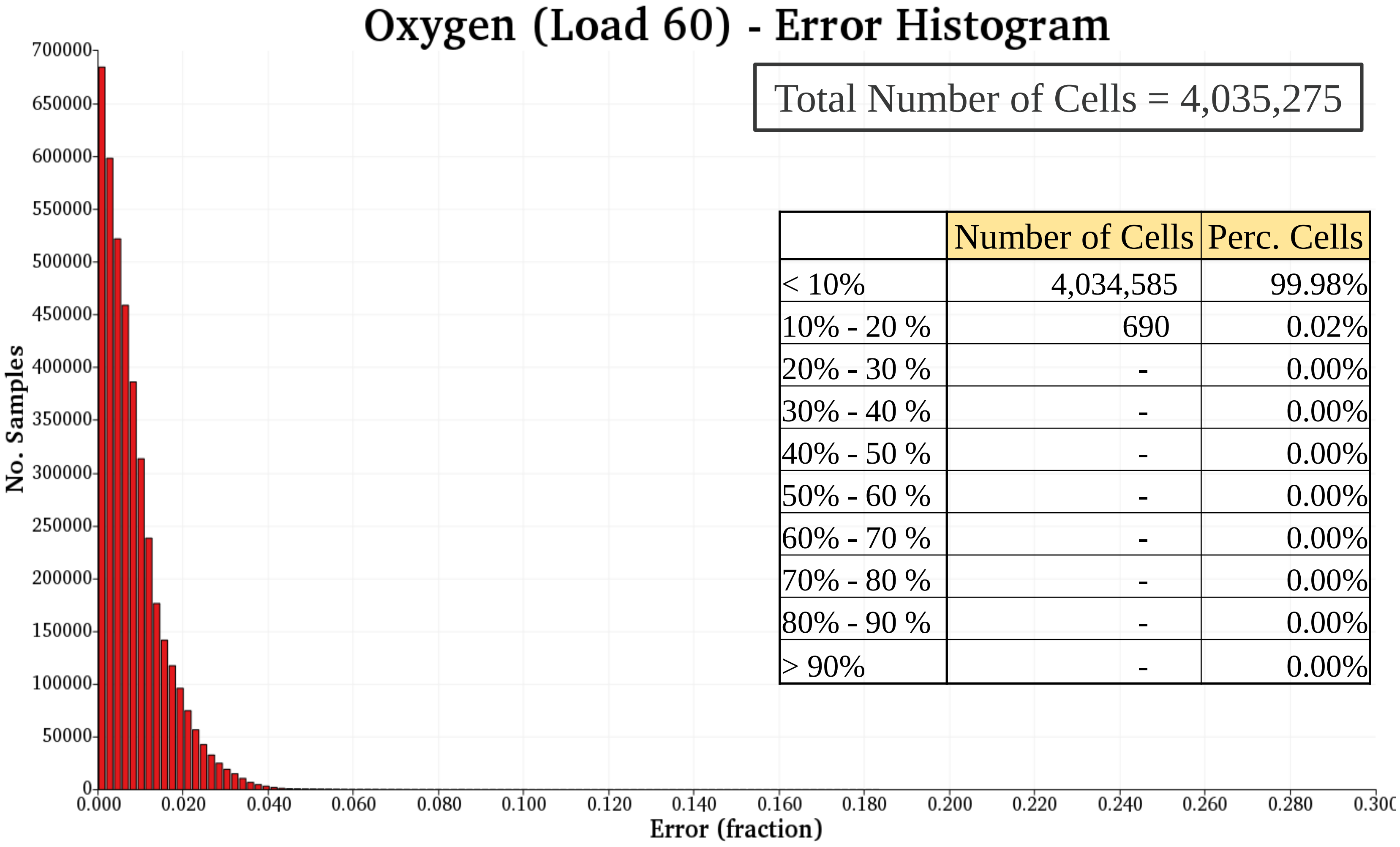


Percent Ranges	Number of Cells	Perc. Cells
< 10%	4,622,438	97.349%
10% - 20%	99,155	2.088%
20% - 30%	17,248	0.363%
30% - 40%	4,830	0.102%
40% - 50%	1,800	0.038%
50% - 60%	912	0.019%
60% - 70%	660	0.014%
70% - 80%	422	0.009%
80% - 90%	329	0.007%
> 90%	534	0.011%

Percent Ranges	Number of Cells	Perc. Cells
< 2%	3,733,161	78.621%
2% - 4%	563,718	11.872%
4% - 6%	184,504	3.886%
6% - 8%	90,013	1.896%
8% - 10%	51,042	1.075%
> 10%	125,890	2.651%


NETL Load 50
Attribute: Oxygen
z = 6.78
Oxygen (frac)
0.0 0.05 0.1 0.15 0.2 0.2
Smart Proxy Load 50
Attribute: Oxygen
Y
X
Z
z = 6.78
Oxygen (frac)
0.0 0.05 0.1 0.15 0.2 0.2
Error
Attribute: Oxygen
z = 6.78
Error (Fraction)
0.0 0.02 0.04 0.06 0.08 0.1

Oxygen (Load 60%) Error Histogram



	Number of Cells	Perc. Cells
< 10%	4,034,585	99.98%
10% - 20 %	690	0.02%
20% - 30 %	-	0.00%
30% - 40 %	-	0.00%
40% - 50 %	-	0.00%
50% - 60 %	-	0.00%
60% - 70 %	-	0.00%
70% - 80 %	-	0.00%
80% - 90 %	-	0.00%
> 90%	-	0.00%

Similar error magnitude and histograms for pressure, gas velocities, gas species

Fidelity of the NETL Proxy Tri-State Model

Temperature

Fidelity of the NETL Proxy Tri-State Model

Oxygen

Extensions of NETL's Proxy Model for Transient Application

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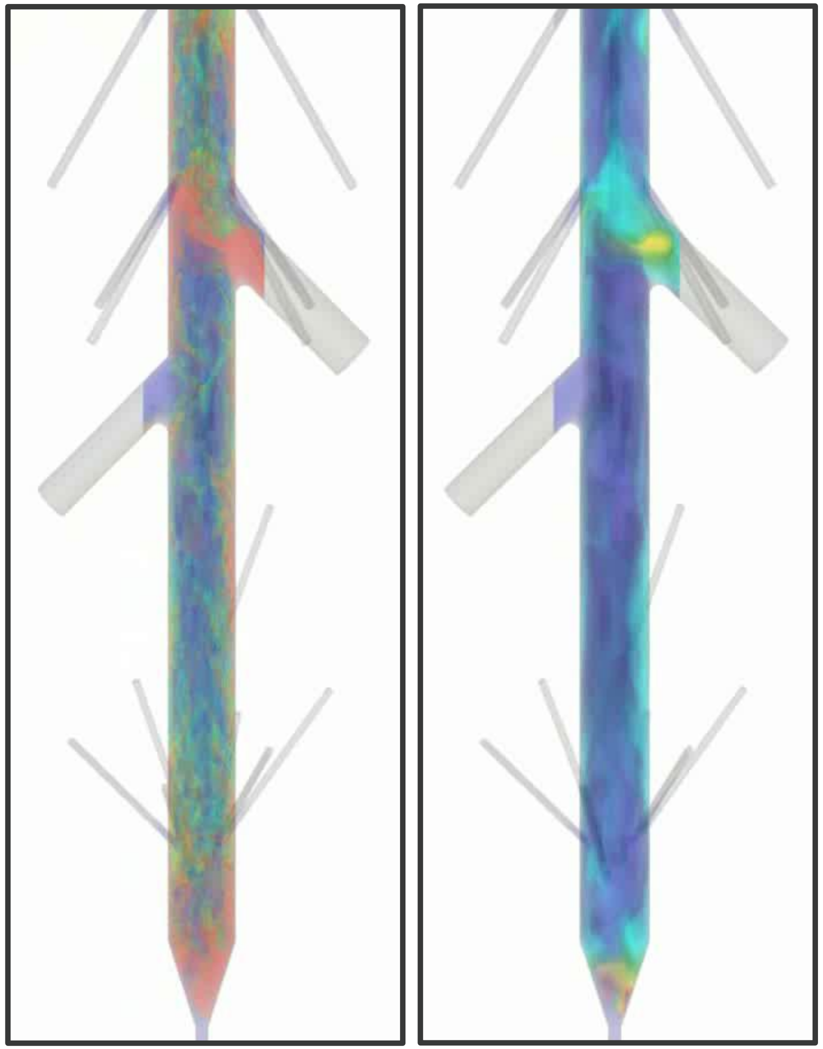
- **Novel machine learning hybrid algorithms built in Google's TensorFlow framework were developed and joined to NETL's MFiX CFD software to improve computational speed and maintain accuracy.**
- **Accomplishments:**
  - Replaced the stiff chemistry solver in MFiX with a machine learned hybrid algorithm that maintains thermochemical accuracy within the flow field and improves chemical solver time (up to 300x over serial LSODA, and 35x over parallel LSODA).
  - C3M 19.1 released in June with support for MLA-STEV solver.
  - Developed a Machine Learning DNN LEQ solver that can outperform state of the art traditional LEQ solvers in both accuracy and time to solution.
- **Impact:**
  - Allows reduction in chemistry, simulation and project time which reduces cost, time, power consumption and improves productivity.
  - Exceptional scaling using GPUs as problem size increases.
  - Achieved Technology Transfer through public release of C3M.
- **Research Partners:**
  - Nvidia, Intel, IBM, Microway

TensorFlow



Owoyele, O., Buchheit, K, Jordan, T., VanEssendelft, D., Accelerating Computational Fluid Dynamics Using TensorFlow, 2018 NETL Workshop On Multiphase Flow Science, 2018

Industrial Extensions of NETL's Proxy Model

- **NETL's proxy model approach in a data driven general approach able to take any steady-state data and reproduce the data over multiple parameters of interest.**
  - Geometry independent, scale independent, runs in near real-time, runs on any basic compute hardware
- **Additional uses of the proxy model.**
  - Operational improvements, diagnostics, prognostics, digital twins, cyber security, virtual sensing, cyber-physical modeling and increased fidelity for process level models
  - Parameter sensitivity analysis, CFD uncertainty quantification, device scale optimization

Path Forward for NETL's Proxy Model

- Develop a CFD model of the NETL B6 combustion rig (completed)
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- Submit manuscript of the sensitivity analysis (in-progress)
  - "Data Driven Proxy Model Development for a Tangentially Fired Coal Boiler under Partial Load Operation"
- Develop a proxy model for transient applications (in-progress)

NETL Products and Accomplishments

- An open-source version of MFiX has been developed MFIX-AI which couples MFiX with Google's TensorFlow accelerated CFD simulations using AI and ML and to allow collaborative research in the area of CFD and AL/ML (e.g., proxy model development)
- High fidelity CFD model of an industrial scale boiler under turndown conditions
- High fidelity proxy model of an industrial scale boiler
- Yong Liu, Mehrdad Shahnam and Chris Guenther, "CFD Simulations of Propane/Natural Gas Blended Fuels Combustion in Gas Turbine," AICHE Annual Meeting, 192d, November 10-15, 2019, Orlando, FL
- Shahab D. Mohaghegh, Mehrdad Shahnam, Ayodeji Aboaba, Yvon Martinez , Chris Guenther, Yong Liu, Anthony Morrow, and Ashley Konya, "Data-Driven Smart Proxy for Computational Fluid Mechanics," Multiphase Flow Science Workshop, Aug 6-8, 2019, Morgantown WV
- Aboaba, A.; Martinez, Y.; Mohaghegh, S.; Shahnam, M.; Guenther, C.; Liu, Y., Smart Proxy Modeling Application of Artificial Intelligence & Machine Learning in Computational Fluid Dynamics, https://www.osti.gov/biblio/1642460, DOI 10.2172/1642460

Thank You

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