



THE OHIO STATE UNIVERSITY

---

**DE-FE-0029093: Heat Integration Optimization and Dynamic Modeling Investigation for Advancing the Coal Direct Chemical Looping Process**

**Dikai Xu**

Andrew Tong (PI), L.-S. Fan (Co-PI)

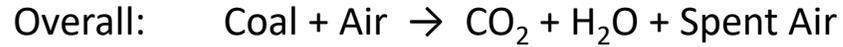
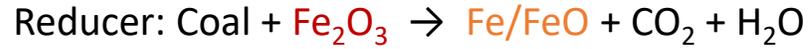
Department of Chemical and Biomolecular Engineering

THE OHIO STATE UNIVERSITY

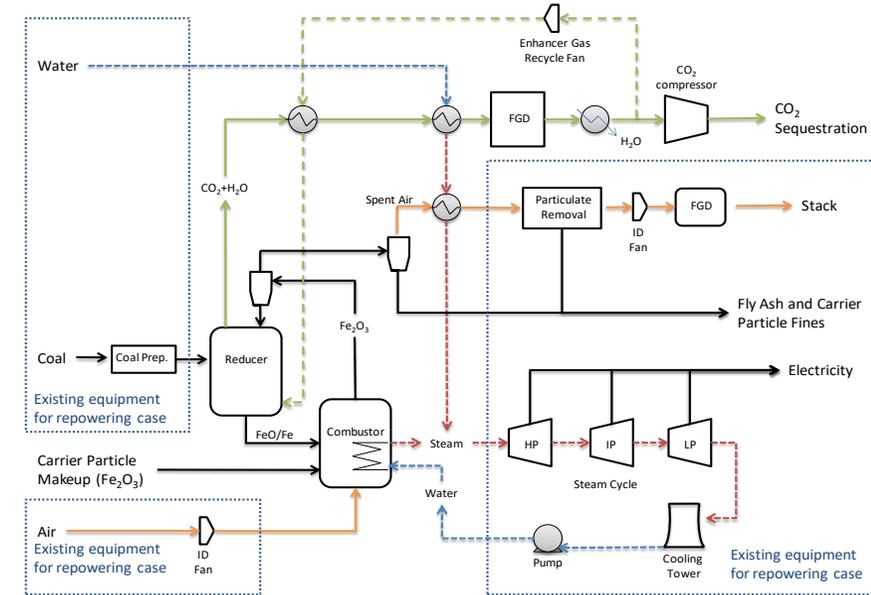
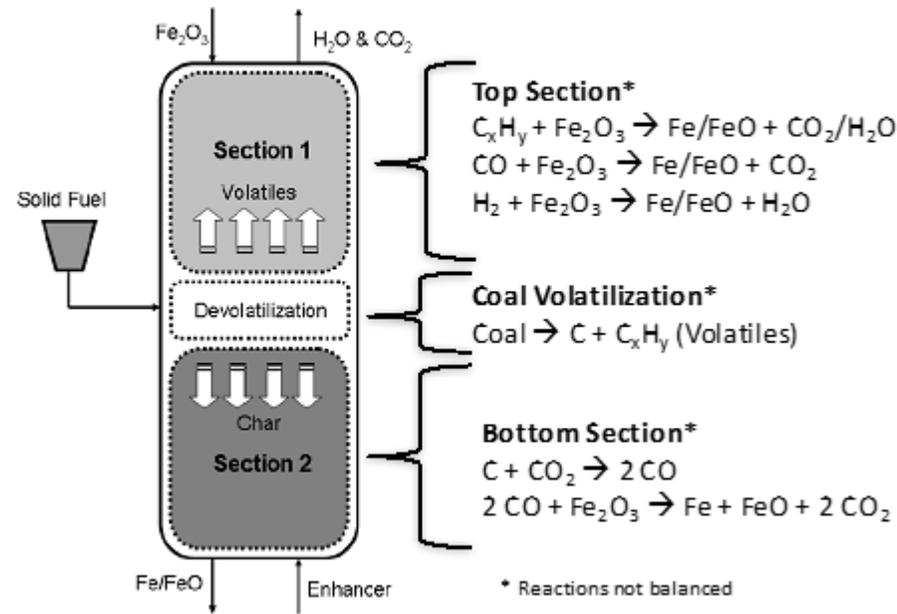
NETL Project Review Meeting | August 15<sup>th</sup>, 2018

# OSU Coal Direct Chemical Looping Process

Main reactions:



## Reducer Reactor Design

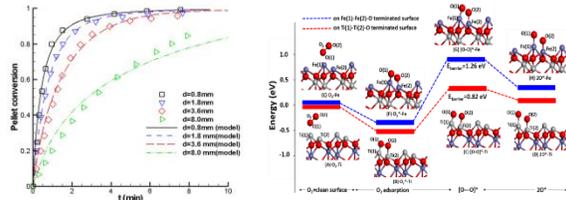


	CDCL Plant
Coal Feed, kg/h	205,358
CO <sub>2</sub> Capture Efficiency, %	96.5
Net Power Output, MW <sub>e</sub>	550
Net Plant HHV Efficiency, %	35.6
Cost of Electricity, \$/MWh	102.67
<b>Increase in Cost of Electricity, %</b>	<b>26.8</b>

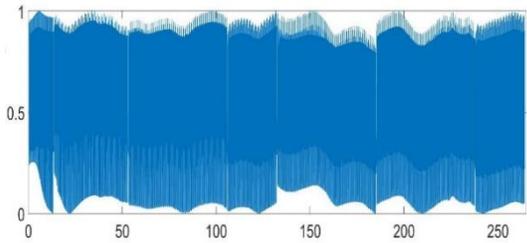
# OSU Chemical Looping Evolution

## Laboratory Studies

### Reduction Kinetics and Mechanism



### Oxygen Carrier Reactivity (TGA)



TGA

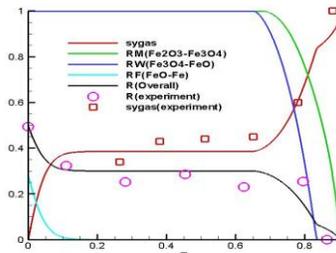


Fixed Bed

1993

## Bench Testing

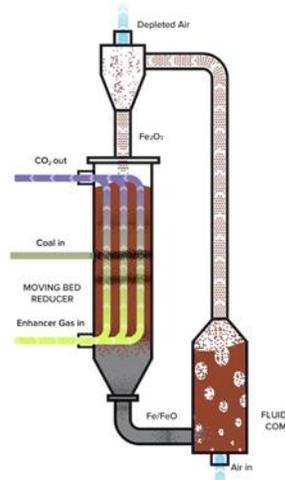
### Moving Bed Model and Results



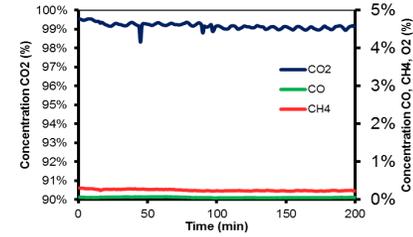
2.5 kW<sub>th</sub> Reducer

## Sub-Pilot Testing

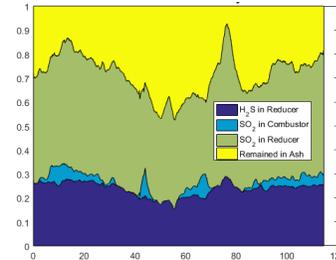
### Integrated Design



### Reduce Gas Profile



### Sulfur Balance



25 kW<sub>th</sub> CDCL Unit

## Pilot Plant Demonstration



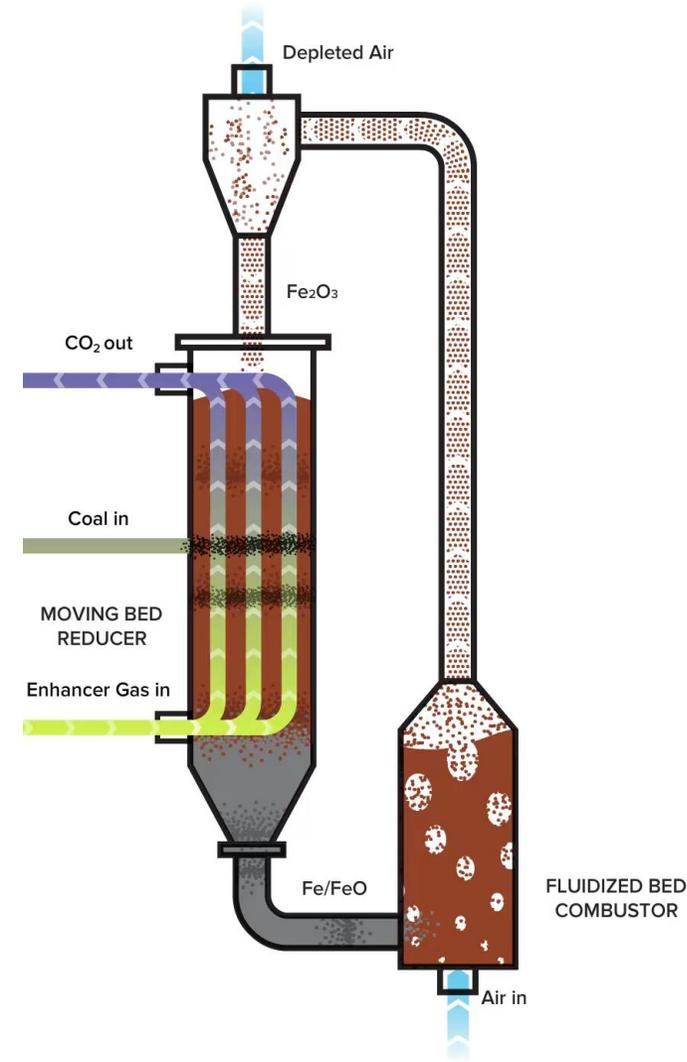
250 kW<sub>th</sub> CDCL Unit

2013 to present

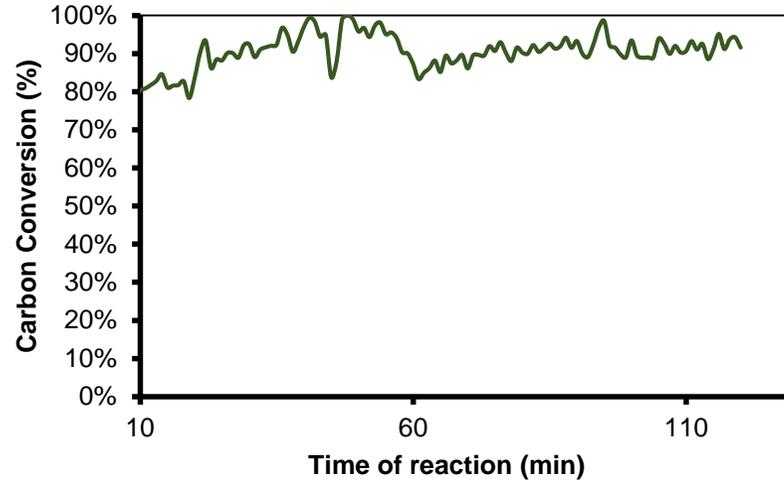


# OSU Coal Direct Chemical Looping Process

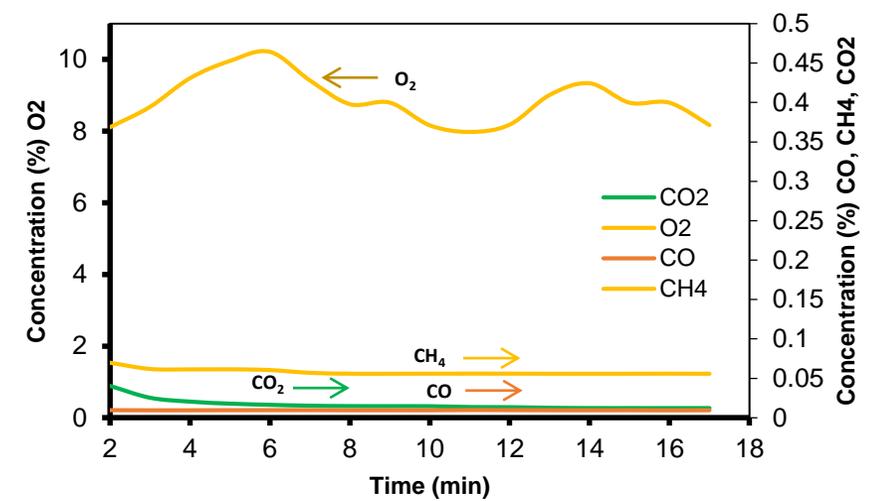
## 200-Hour Continuous Operation at 25kW<sub>th</sub> Sub-pilot Scale



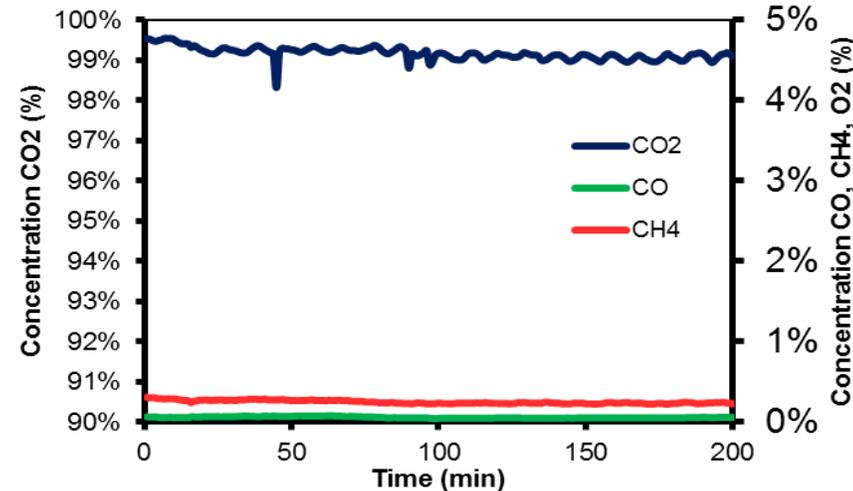
Reducer Carbon Conversion Profile



Combustor Gas Concentration Profile



Reducer Gas Concentration Profile

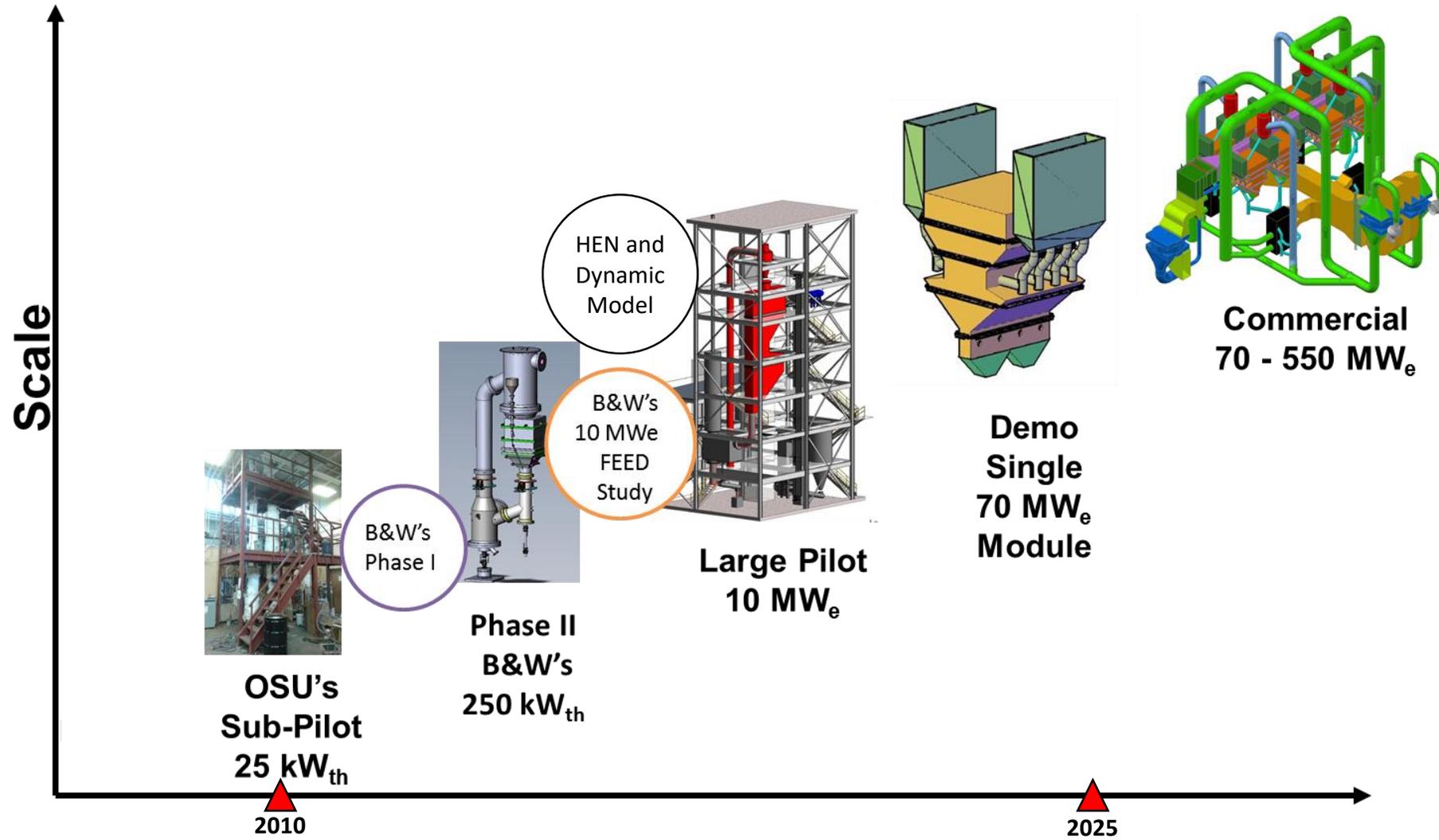


### Sample Data: PRB Process Performance

- Continuous steady carbon conversion from reducer throughout all solid fuel loading (5-25kW<sub>th</sub>)
- <0.25% CO and CH<sub>4</sub> in reducer outlet = full fuel conversion to CO<sub>2</sub>/H<sub>2</sub>O
- <0.1% CO, CO<sub>2</sub>, and CH<sub>4</sub> in combustor = negligible carbon carry over, nearly 100% carbon capture

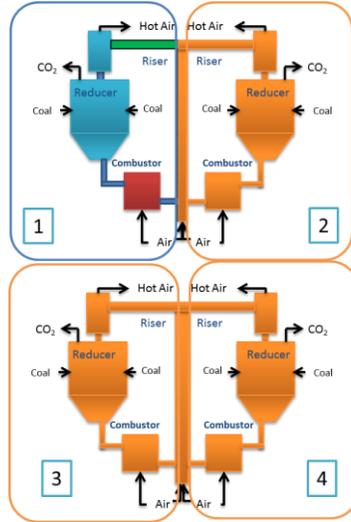


# CDCL Development Pathway



# Scale Up Plan

## Modular Reactor Design



- Chemical looping inherent low capital cost technology
- Reduce risks for large scale-up



Lab Testing

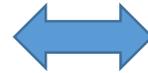


Bench (25 kW<sub>th</sub>)

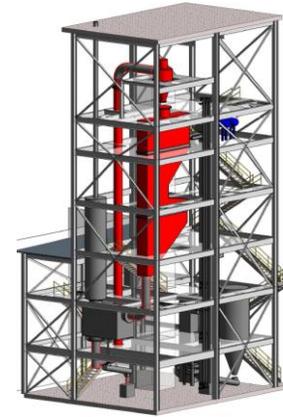


Small Pilot (250<sub>th</sub>)

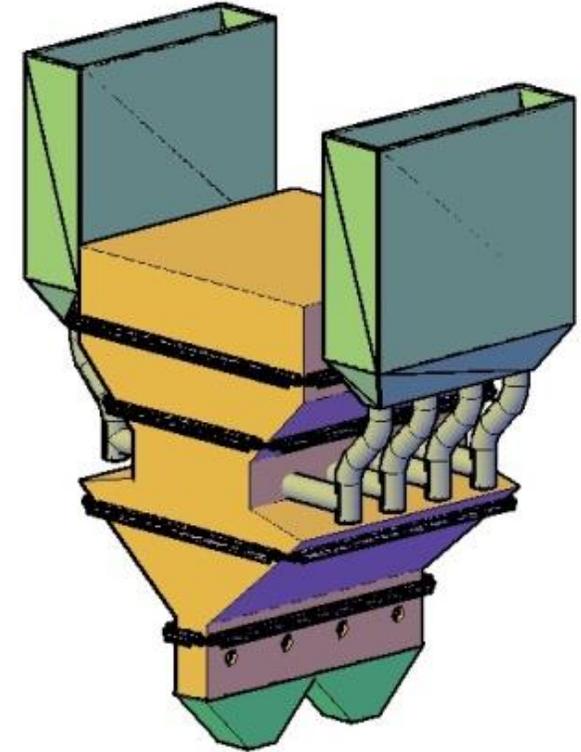
High Risk



100x



Large Pilot (10 MW<sub>e</sub>)



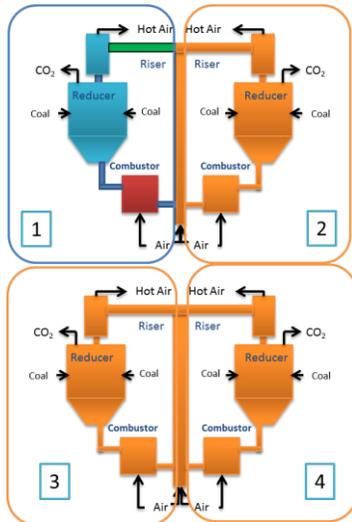
Commercial Offering

Time

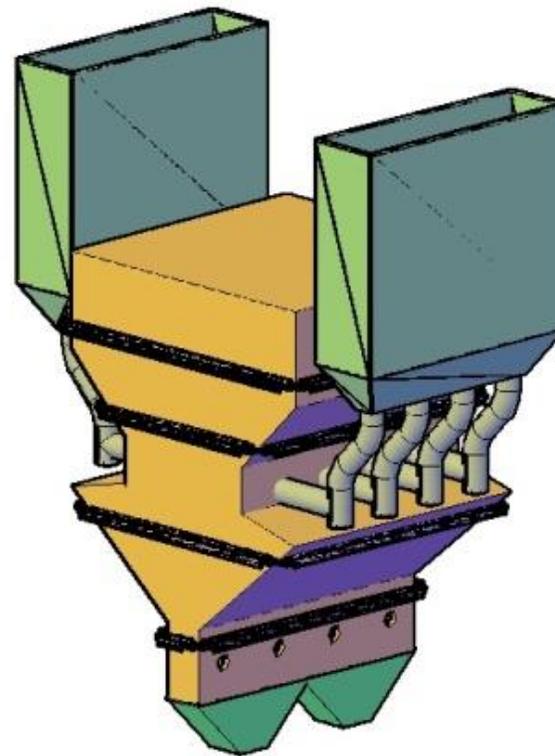


# Scale Up Plan

## Modular Reactor Design



## Challenge: Integrating with Dover Site



Lab Testing



Bench  
(25 kW<sub>th</sub>)

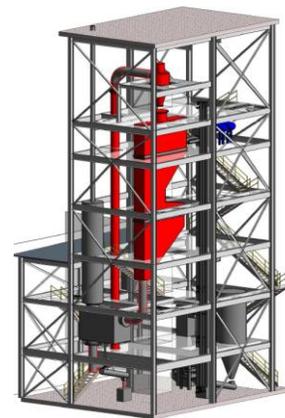


Small Pilot  
(250<sub>th</sub>)

High Risk



100x



Large Pilot  
(10 MW<sub>e</sub>)

Commercial Offering

Time

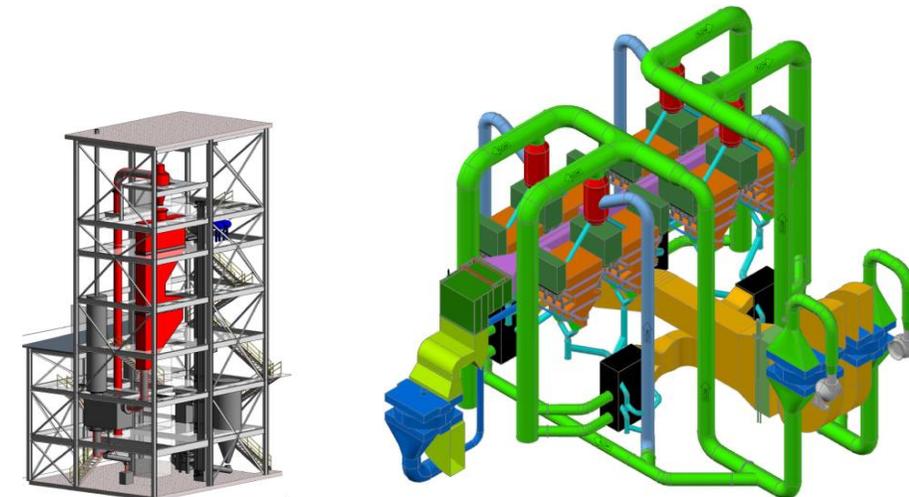


# Project Objective

Reduce risks in the CDCL technology development to enable scale-up and eventual commercialization

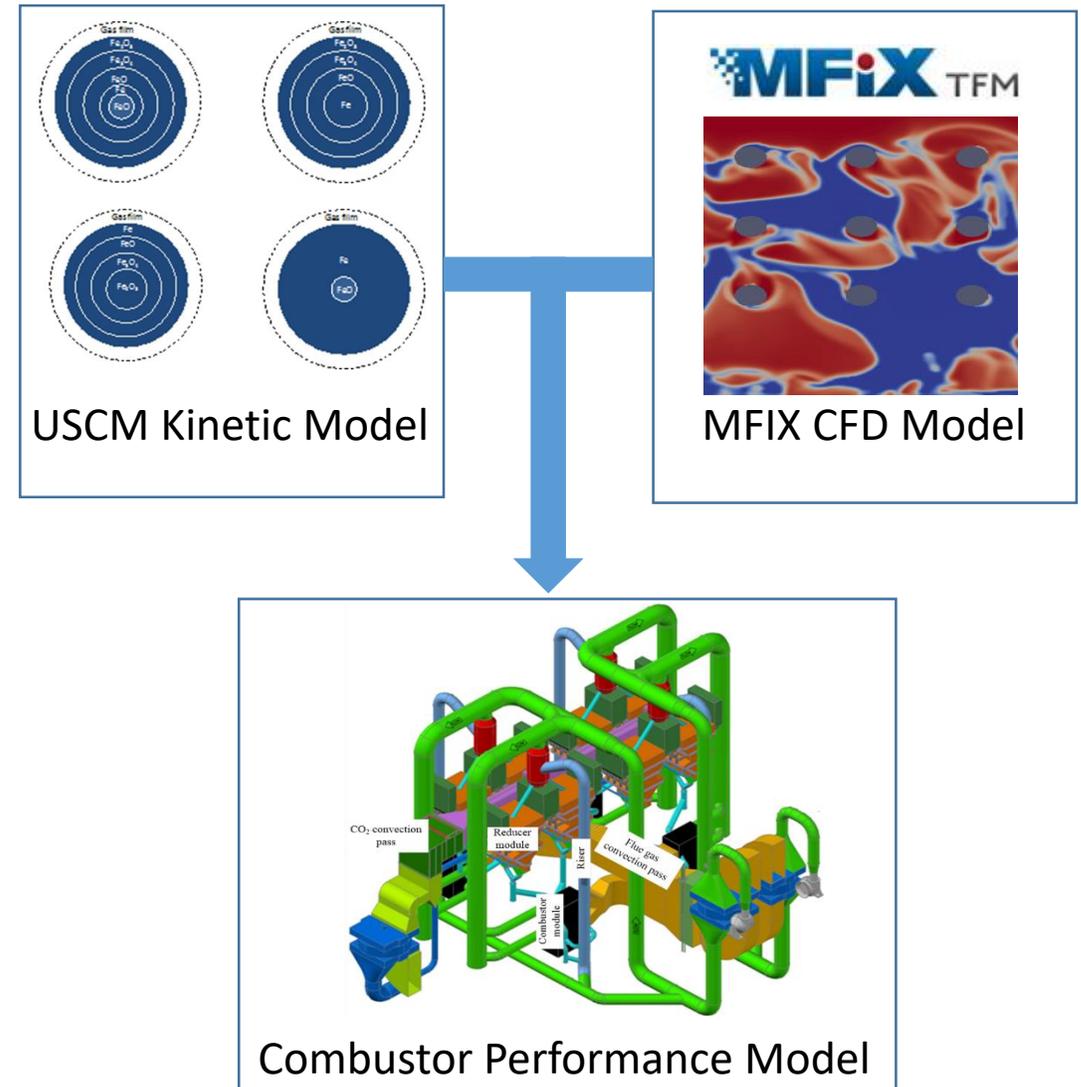
1. Enable Commercialization
2. Enable Scale-Up

Tasks/Milestones		BP1				BP2				BP3			
		1	2	3	4	1	2	3	4	1	2	3	4
<b>1</b>	<b>Project Management and Planning</b>												
	Quarterly Reports												
	Final Report Preparation												
<b>2</b>	<b>Chemical Looping Combustor Simulation</b>												
2.1	Bench Unit Combustor Apparatus Setup												
2.2	Oxygen Kinetic Model Development and Verification												
2.3	Modeling Scheme Including Coupling of Hydrodynamics, Heat Transfer and Reaction												
2.4	Pilot and Commercial Scale Combustor Analysis												
	Milestone 2.1: Combustor Apparatus Ready for Operation		◆										
	Milestone 2.2: Oxygen Carrier Kinetic Model Developed			◆									
	Milestone 2.3: Modeling Scheme Coupling of Hydrodynamics, Heat Transfer and Reaction Developed							◆					
<b>3</b>	<b>Heat Exchanger Network Integration and Optimization</b>												
3.1	CDCL Static Model Development												
3.2	HEN Design with Steam Cycle												
3.3	HEN Optimization												
3.4	Heat Exchanger Sizing and CDCL 550 MWe Cost Analysis Update												
	<i>Decision Point 1: Integrated CDCL Systems Analysis Model Developed</i>							◆					
	Milestone 3.2: HEN Design Developed for Cost Analysis											◆	
<b>4</b>	<b>Dynamic Modeling of Integrated CDCL-Steam Cycle System</b>												
4.1	CDCL Process Model Development												
4.2	Steam Cycle Model Development												
4.3	Integrated System Model Development												
4.4	System Operation Simulation												
	Milestone 4.1: Dynamic Model for 10 MWe CDCL Reactor Developed			◆									
	Milestone 4.2: Dynamic Model for 10 MWe Steam Cycle Developed								◆				
	<i>Decision Point 2: Integrated Dynamic Model for 10 MWe CDCL Process Developed</i>												◆
	<i>Decision Point 2: Integrated Dynamic Model for 10 MWe CDCL P</i>												◆



# Task 2: Combustor Simulation

- CDCL Combustor Model
  - USCM Kinetic Model
  - MFiX CFD Model
- Design and Analysis of 10MW<sub>e</sub> Pilot and 550MW<sub>e</sub> Commercial Plant
  - Lateral Transport & Mixing
  - Oxygen Carrier Conversion
  - Heat Transfer



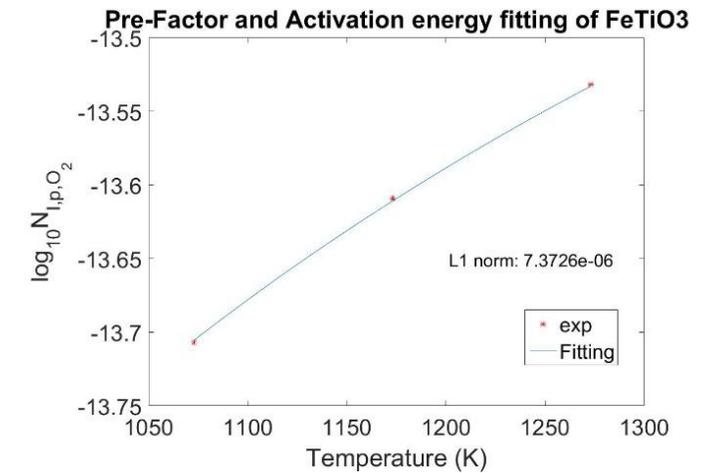
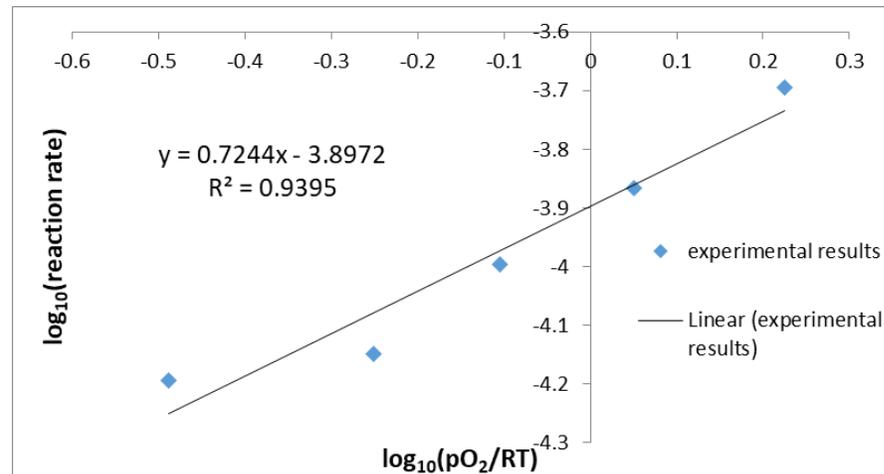
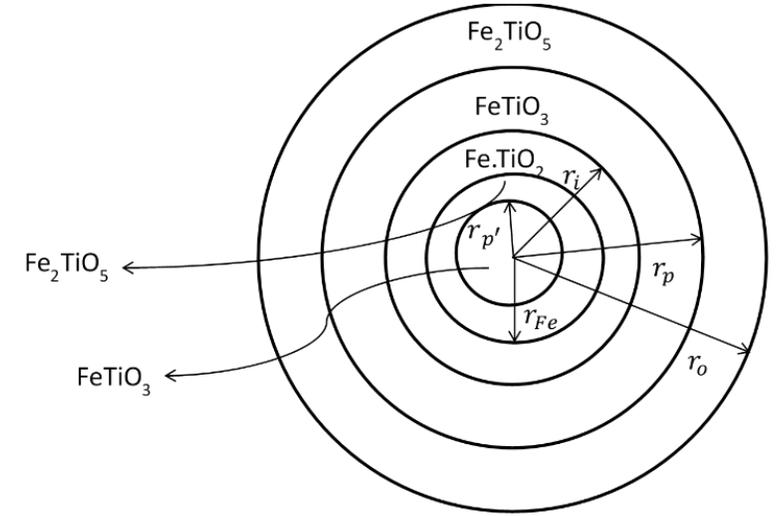
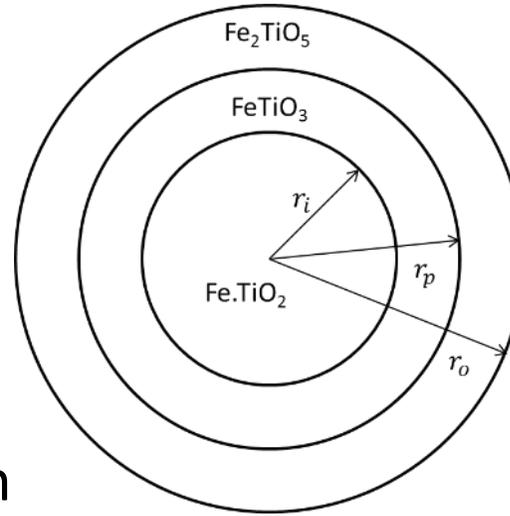
# Task 2: Combustor Simulation

URSM for Fully-reduced Particle

URSM for Partially-reduced Particle

## USCM Kinetic Model

- Extended model to consider partially-reduced particle
- Used TGA experiments to determine rate constants
- Model tested at different temperature and  $O_2$  concentration

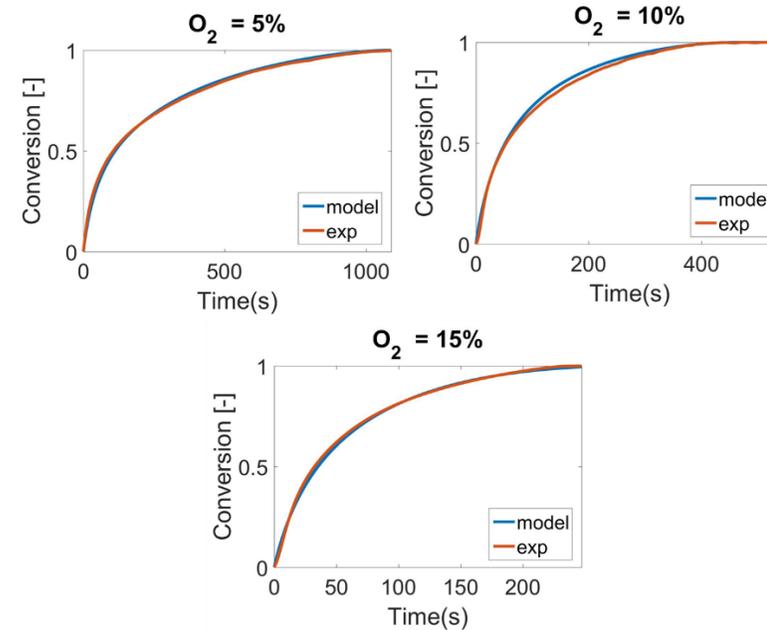


# Task 2: Combustor Simulation

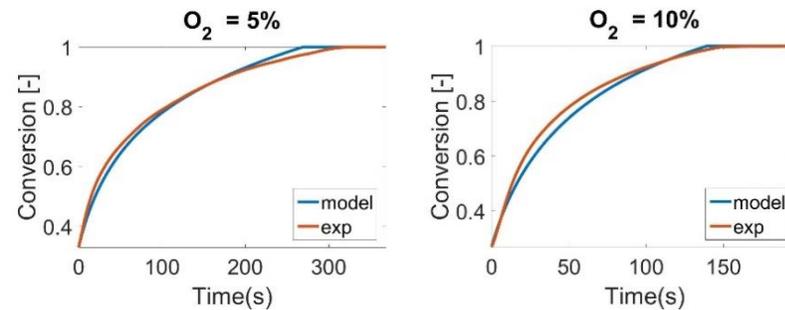
- USCM Kinetic Model
  - Extended model to consider partially-reduced particle
  - Used TGA experiments to determine rate constants
  - Model tested at different temperature and O<sub>2</sub>



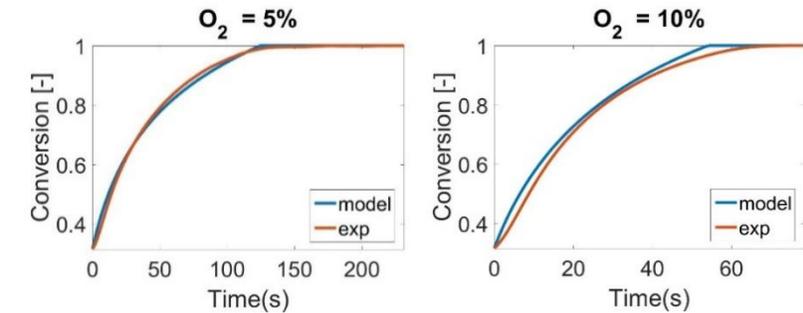
## 800°C, Fully-reduced Particle



## 800°C, Partially-reduced Particle



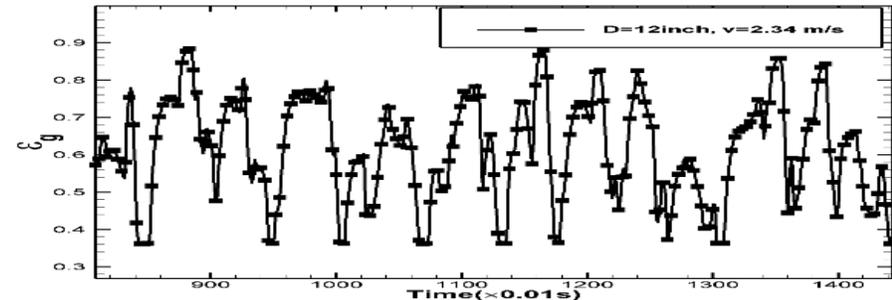
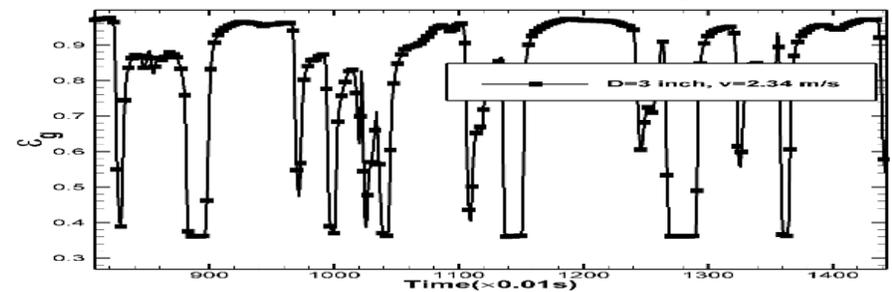
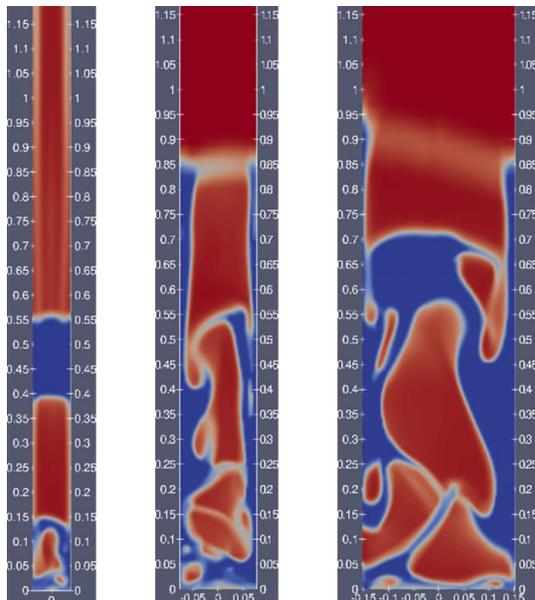
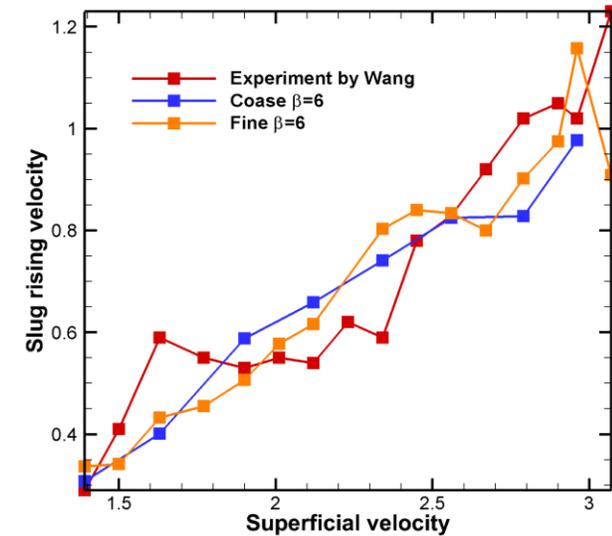
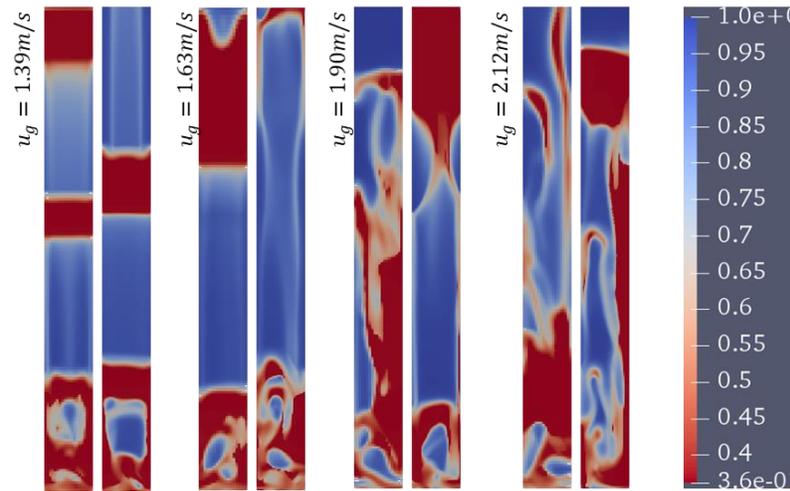
## 1000°C, Partially-reduced Particle





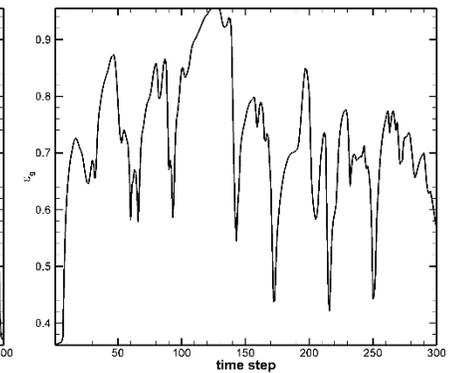
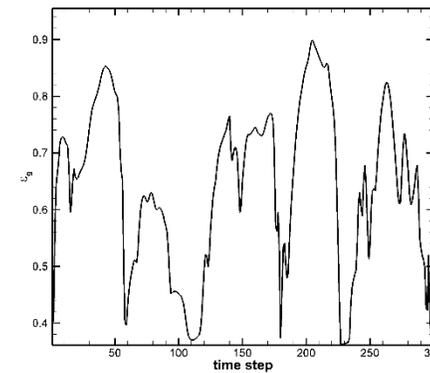
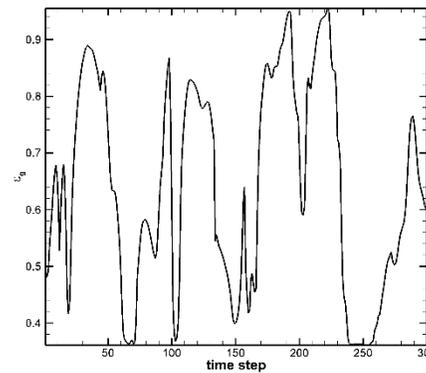
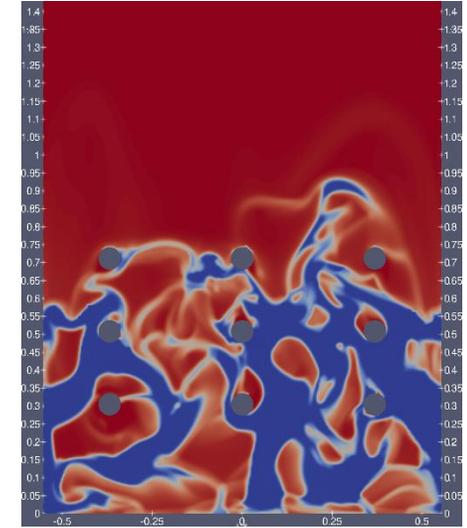
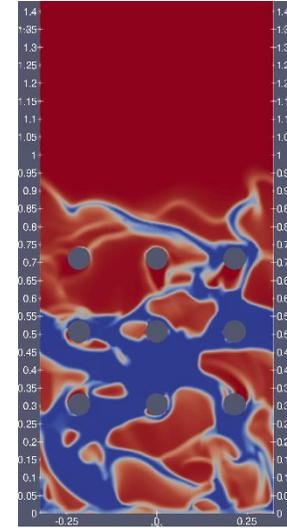
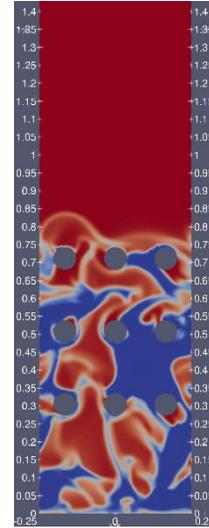
# Task 2 Hydrodynamic Modeling

- MFiX CFD Model of Combustor
  - Based on MFiX Two Fluid Model
  - Study the effect of reactor geometry and in-bed heat exchanger on combustor performance
- Validation by cold flow model with heat exchanger tubes



# Task 2 Hydrodynamic Modeling

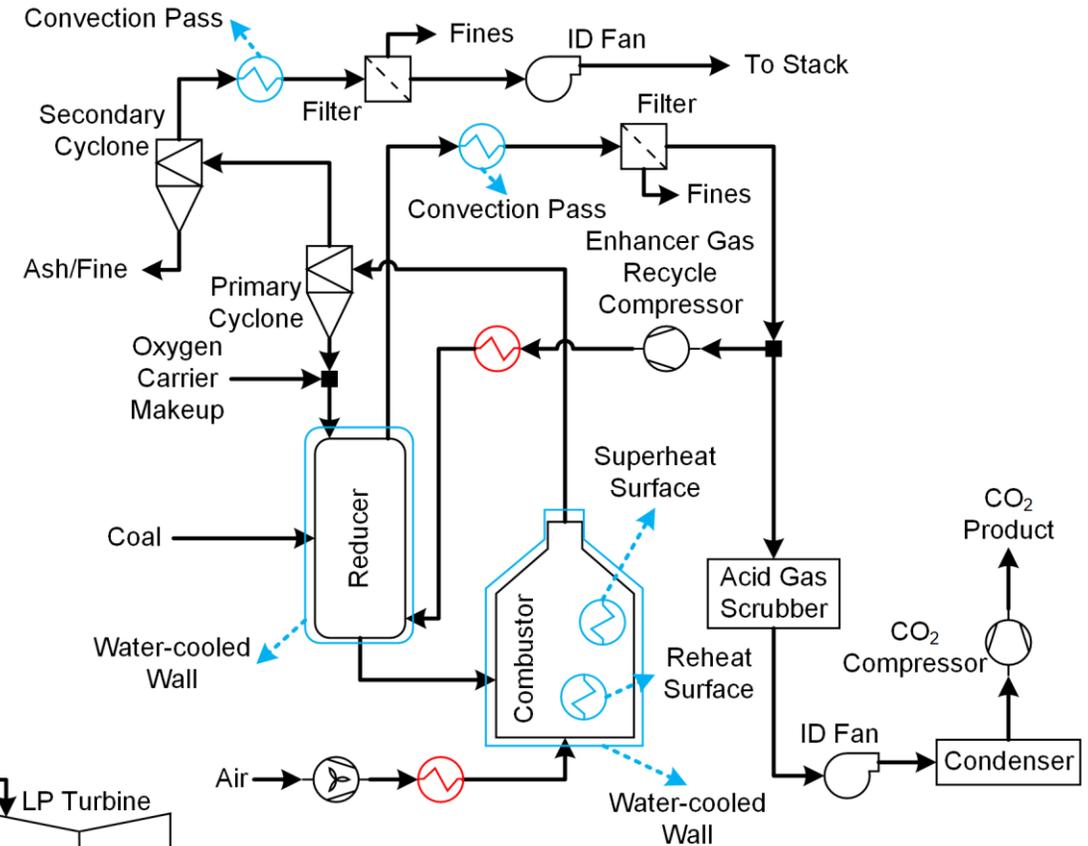
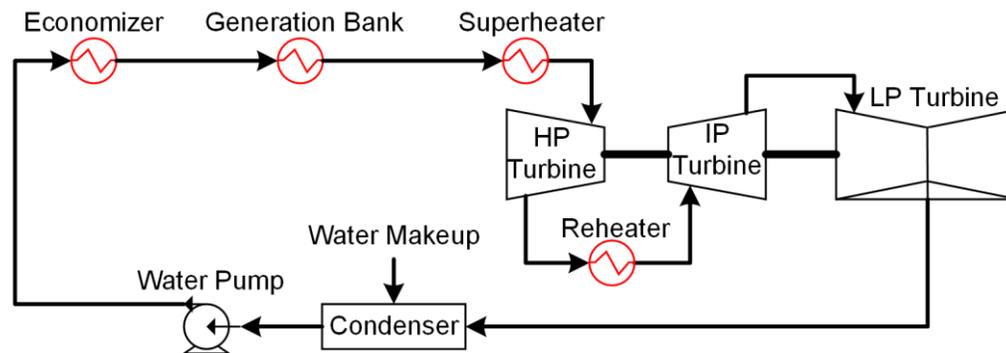
- MFiX CFD Model of Combustor
  - Based on MFiX Two Fluid Model
  - Study the effect of reactor geometry and in-bed heat exchanger on combustor performance
- Validation by cold flow model with heat exchanger tubes



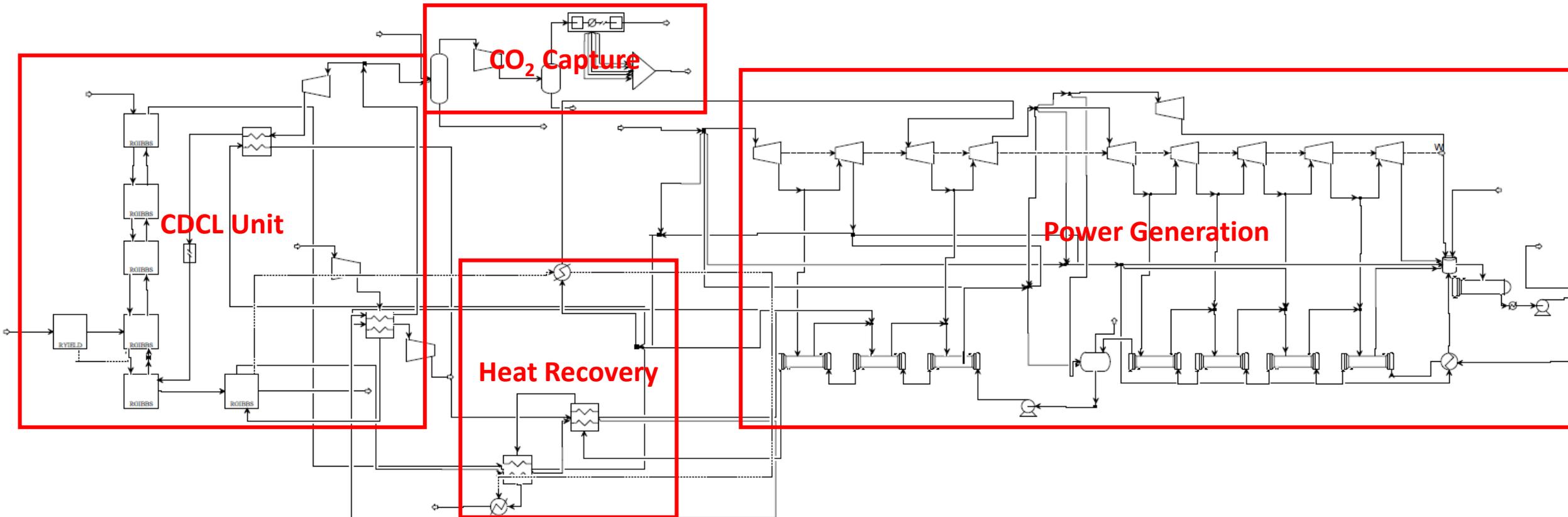


# Task 3: HEN Integration and Optimization

- CDCL Process Simulation
  - In-bed heat exchanger
  - Industrial relevant constrains
- Integration with Steam-Cycle
  - Multiple heat exchanging surfaces
- HEN Optimization
- Cost Estimation



# Task 3: HEN Integration and Optimization



# Task 3: HEN Integration and Optimization

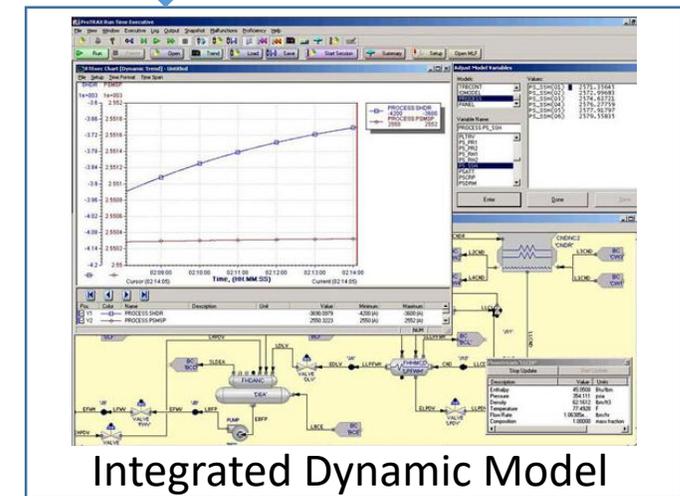
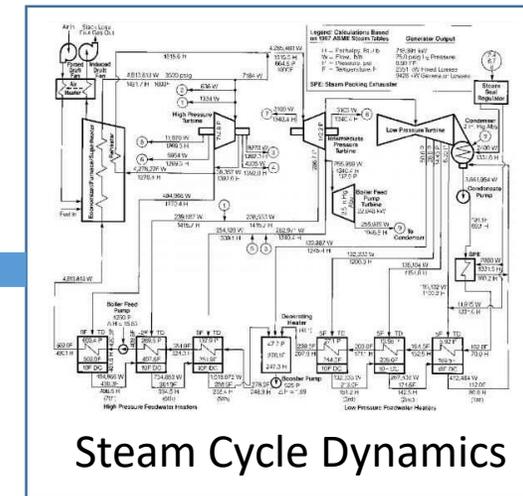
- Simulation settings
  - Coal: Illinois #6
  - Steam cycle
    - Supercritical cycle
    - 24.1 MPa/593 °C/593 °C
    - Adapted based on prior studies from B&W
- Preliminary results of HHV efficiency
  - Baseline: 32.5%
  - CDCL process: 37.6%

	CDCL Preliminary Design
Total Gross Power, MW <sub>e</sub>	643
Total Auxiliaries, MW <sub>e</sub>	93
Net Power, MW <sub>e</sub>	550
HHV Thermal Input, MW <sub>t</sub>	1462
HHV Net Plant Efficiency (%)	37.6
As- Received Coal Feed, kg/hr	194,110

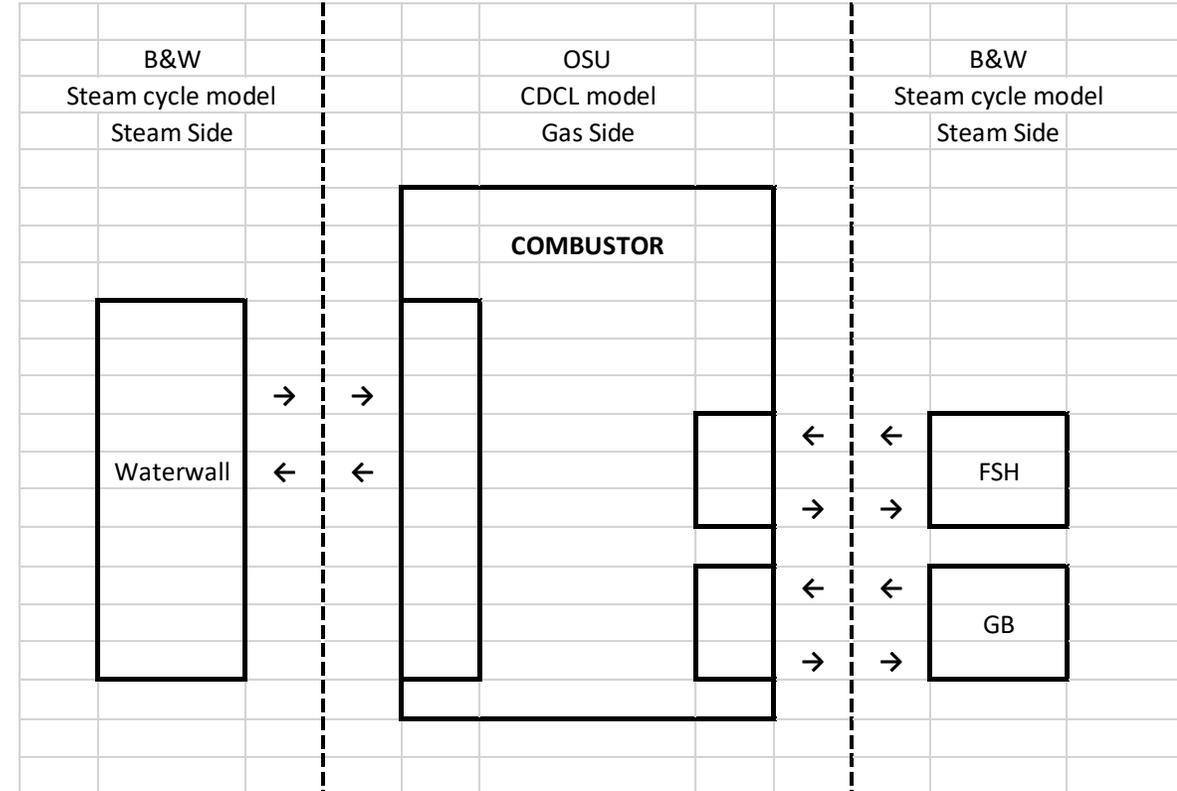
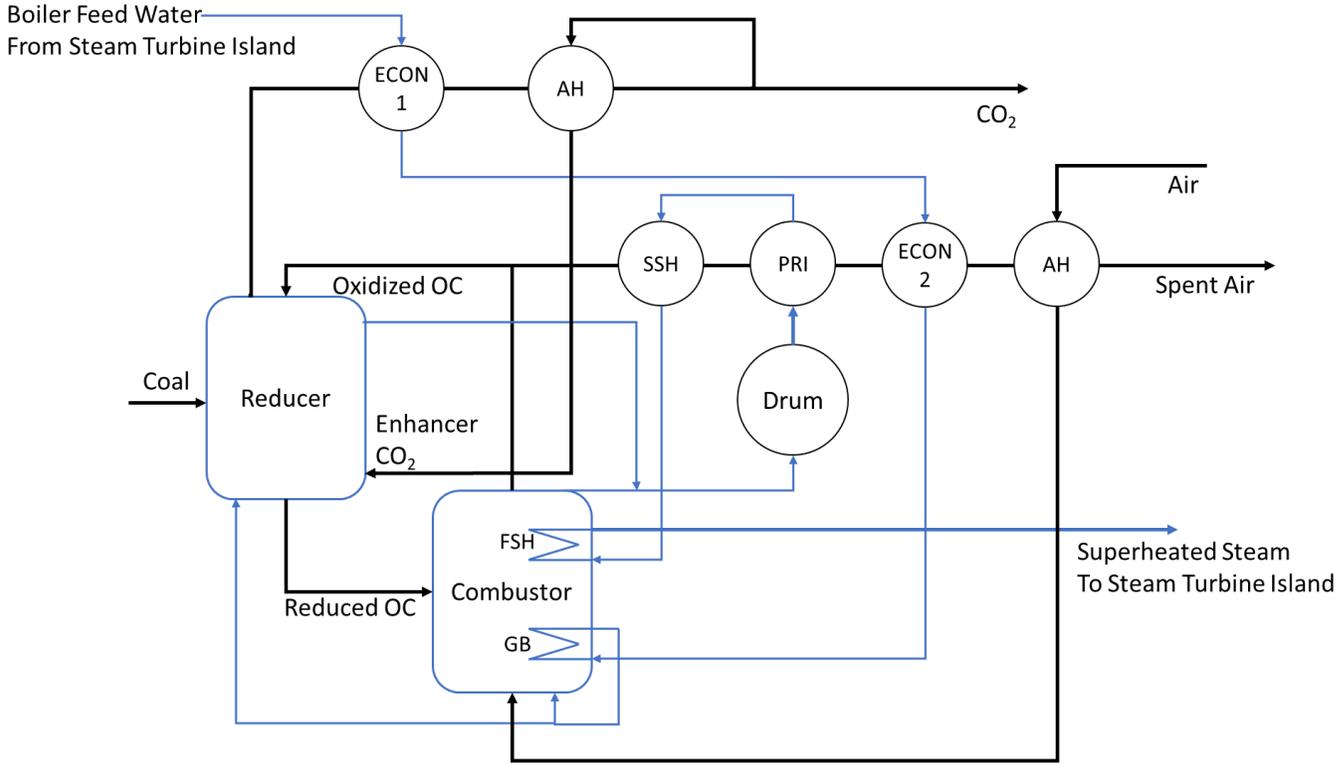


# Task 4: Dynamic Modeling of Integrated Power Plant

- Dynamic Modeling in ProTRAX
- 10 MW<sub>e</sub> CDCL pilot plant
  - Preliminary design from DE-FE0027654
- Existing 20 MW<sub>e</sub> steam cycle at Dover, OH
  - Based on data obtained from Dover Light & Power
- Startup and operation simulation

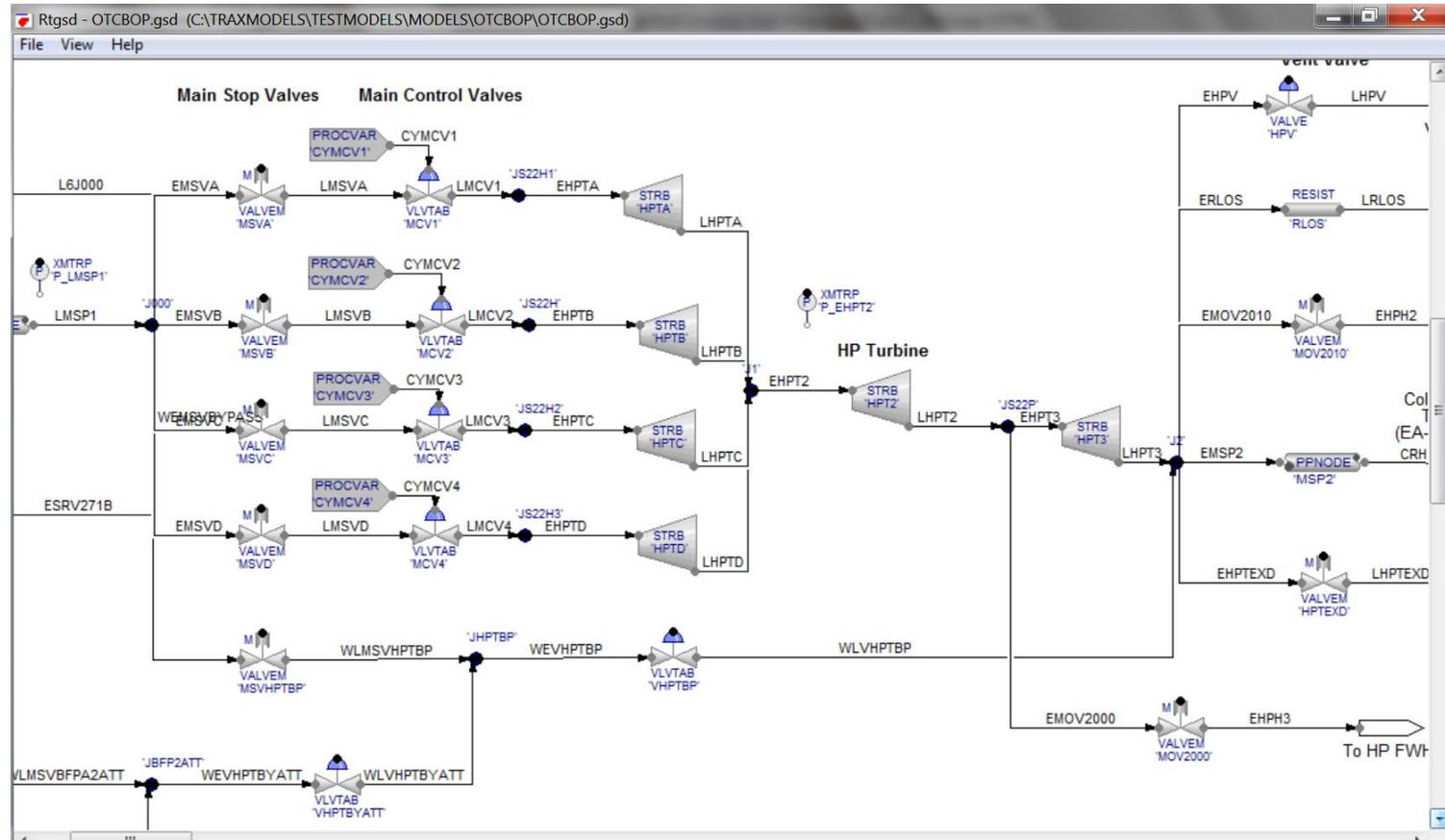


# Task 4: Dynamic Modeling of Integrated Power Plant



# Task 4: Dynamic Modeling of Integrated Power Plant

- Dynamic Model for CDCL
  - Mass and Energy Balance
  - Hydrodynamic Correlation
  - Chemical Reactions
- Dynamic Model for Steam Cycle
  - Obtained steam cycle design and parameter from Dover Light & Power



# Conclusion

- Combustor performance model will be developed in this project to support HEN integration and system dynamic studies
- HEN integration and optimization will be performed to enable the commercialization of the CDCL process
- Dynamic modeling will be performed to enable the scale-up of the CDCL process
- Kinetic model for oxygen carrier oxidation in CDCL combustor is developed to simulate the oxidation of fully- and partially- reduced oxygen carrier particles
- MFiX CFD model is being developed to study the effect of bed geometry and in-bed heat exchanger on fluidization properties of the combustor reactor
- ASPEN Plus model of 550 MW<sub>e</sub> integrated CDCL-steam cycle plant is developed for HEN optimization
- ProTRAX dynamic model is being developed for 10 MW<sub>e</sub> CDCL pilot plant at Dover



# Thank You

## Disclaimer

This presentation was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

