

CCSI² Brief: Computational Support for the Carbon Capture Program

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Carbon Capture Review Meeting
October 6th, 2020

CCSI Toolset: New Capabilities for Modeling & Simulation

Maximize the learning at each stage of technology development
and integrate development stages- moving away from linear path of development

- **Early stage R&D**

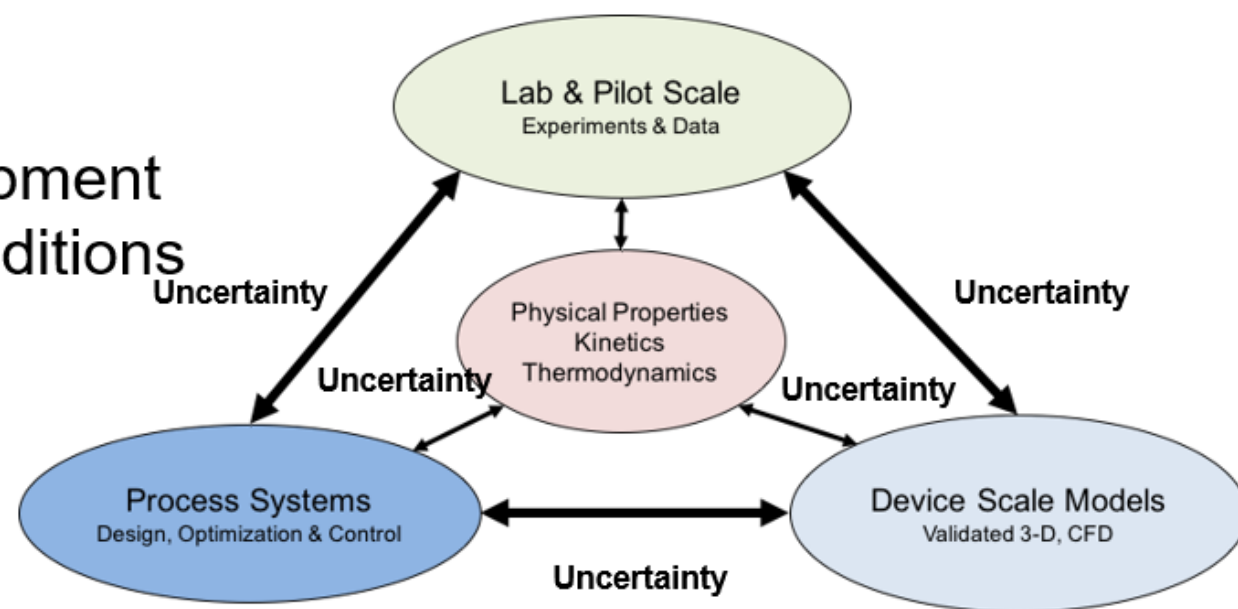
- Screening concepts
- Identify conditions to focus development
- Prioritize data collection & test conditions

- **Pilot scale**

- Ensure the right data is collected
- Support scale-up design

- **Demo scale**

- Design the right process
- Support deployment with reduced risk



CCSI² Project Summary and Updates

- **Industrial Collaborations**

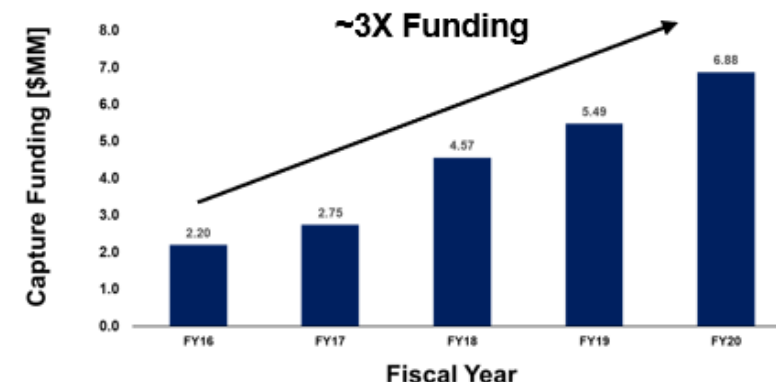
- 11 CO₂ Capture Program projects **\$80MM+** in total project value (TRL 3-7)

- **Four New CCSI² Project Partners**

- Oak Ridge National Lab (ORNL), University of Notre Dame, University of Pittsburgh, University of Toledo

- **Equipment and Process Modeling, Optimization and Control Frameworks**

- **Fundamental** characterization of material, device and system
- Solvent, sorbent, membrane **modeling frameworks for CCS**
- **Steady state and dynamic** modeling
- Parametric **uncertainty quantification**
- **Optimization** (under uncertainty) of process configuration and operation
- Advanced **process control**
- **Machine learning** for surrogate model development, black box optimization
- **Neural networks** for CFD model reduction
- Unifying Framework for Optimization and Quantification of Uncertainty and Surrogates (**FOQUS**)



- **Optimal Design of Experiments**

- Improves model while optimizing lab- or pilot-scale experimental data generation
 - NCCC and TCM MEA pilot models accurate on CO₂ Capture percentage within **3-6% with 95% confidence**

- **Computational Toolset Maintenance**

- Software updates and revision management – **open source**

Complete CCSI Toolset Publically Available



CCSI Toolset

The Carbon Capture Simulation Initiative (CCSI) Toolset is a suite of computational models for carbon capture processes.

<https://www.acceleratecarboncapture.org/> ccsi-support@acceleratecarboncapture.org

github.com/CCSI-Toolset



Repositories 30 **People** 26 **Teams** 6 **Projects** 1 **Settings**

Pinned repositories

FOQUS

FOQUS: Framework for Optimization and Quantification of Uncertainty and Surrogates

Python ★ 1 🍴 8

ProcessModels_bundle

A suite of process models implemented in both Aspen Custom Modeler and gPROMS Model Builder, as well as models implemented within Aspen Plus and Aspen Plus Dynamics.

Makefile ★ 1

CFDModels_bundle

High fidelity device scale Computational Fluid Dynamics (CFD) models

Makefile

Oxy-CombustionModels_bundle

The Oxy-Combustion Models package consists of two primary components: A detailed boiler model and a suite of equation-based models of the other components of a complete oxycombustion power generati...

Makefile

APCFramework

Unified framework in MATLAB for application and testing of advanced control algorithms towards efficient process operation and control

Matlab

iRevealLite

Automated reduced order model generation for improved computational time

Java 🍴 3

Project Focus

Execution year 2020

Task 2: DOCCSS Support

- 2.1: LBNL - MOF 11:30 Oct 6th
- 2.2: PNNL - CO₂BOL 3:15 Oct 5th
- 2.3: LLNL – Advanced Absorber Design

Task 3: Capture Program Support

- 3.1: Sequential Design Of Experiments (SDoE)
- 3.2: Dynamic MEA Modeling and TEA
- 3.3: Advanced Solvent Configurations
- 3.4: Advanced Process Control
- 3.5: CO₂ Absorber Intensification 3:45 Oct 5th
- 3.6: Industrial Capture (cement)

Task 4: CCSI Toolset Support

Task 5: Pilot Support

- 5.1 RTI NAS 10:00 Oct 7th
- 5.2 SRI Mixed Salt
- 5.3 MTR Membrane 10:30 Oct 7th
- 5.4 TDA Sorbent 11:00 Oct 7th

Execution year 2021

Task 2: DOCCSS Support

Task 3: Capture Program Support

Task 4: CCSI Toolset Support

Task 5: Pilot Support

Potential New EY21 Projects

- 1: DAC Modeling Framework
- 2: Hydrogen Process and CO₂ Separation Optimization
- 3: Reactive Capture
- 4: Dynamic Design Of Experiments with Data Reconciliation Tools
- 5: Modular Capture to Support Coal FIRST
- 6: BECCSS Modeling and Pilot Support
- 7: Optimized Capture with NGCC Systems

Machine Learning to
accelerate CFD analysis
1:05, Oct 6th

MTR Pilot Support: Modeling
Framework Capturing Non-
Idealities in Membrane Module
Performance 1:30pm Oct 6th

Points of Interest

Joint IDAES and CCSI² Stakeholder Meeting



Register: https://lbnl.zoom.us/webinar/register/WN_T9X0KwA5RkGSPYUbkVVGQWg

Thursday, Oct. 1st

11:00	Welcome and Meeting Overview David Miller
11:15	Plenary Talk Angelos Kokkinos, Associate Deputy Assistant Secretary, Clean Coal and Carbon Management, Office of Fossil Energy, U.S. Department of Energy
11:45	Overview: Carbon Capture Simulation for Industry Impact (CCSI ²) Michael Matuszewski
12:15	CCSI ² Success: Improving Knowledge Gain from Pilot Testing Debangsu Bhattacharyya
12:45	Break
1:00	Overview: Institute for the Design of Advanced Energy Systems (IDAES) David Miller
1:30	IDAES Partnership Successes Tony Burgard
2:00	Discussion
2:30	Adjourn for the day

Thursday, Oct. 8th

11:00	Welcome and Meeting Overview John Shinn
11:10	Advanced Models for System Optimization: Carbon Capture Example Debangsu Bhattacharyya
11:35	Process Optimization of Advanced CO ₂ Binding Organic Liquid (CO ₂ BOL) Solvent System Joshua Morgan
12:00	Break
12:10	Sequential Design of Experiments for Optimizing Investment in Technology Development Christine Anderson-Cook
12:35	Robust Design and Uncertainty in IDAES Chrysanthos Gounaris
1:00	Discussion
1:30	Adjourn for the day

Thursday, Oct. 15th

11:00	Welcome and Meeting Overview John Shinn
11:10	Framework for Optimization and Quantification of Uncertainty and Surrogates (FOQUS) Anuja Deshpande
11:35	Equation Oriented Modeling: Enabling Optimization of Large-Scale Dynamic Systems Larry Biegler
12:00	Break
12:10	Grid and Market Integration via Multi-Scale Approaches John Sirola and Alex Dowling
12:35	Discussion
1:00	Stakeholder Applications and Panel Discussion John Shinn
1:50	Adjourn for the day

Thursday, Oct. 22nd Live Toolset Demonstration

	CCSI ² FOQUS Toolset Tutorial Demonstration Duration: 4 hours
11:00	Comprehensive Example Anuja Deshpande
12:30	Solvent based carbon capture system analysis Break
12:45	Flowsheet Set-Up and Analysis Anuja Deshpande and Joshua Morgan
1:15	Surrogate Modeling and Optimization Anuja Deshpande and Joshua Morgan
1:45	Break
2:00	Uncertainty Quantification and Optimization Under Uncertainty Brenda Ng and Pedro Sotorrio
2:30	Sequential Design of Experiments Abby Nachtsheim





For more information

<https://www.acceleratecarboncapture.org/>

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