

### **Overview of Carbon Capture Simulation for Industry Impact** (CCSI<sup>2</sup>) Project

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## **CCSI<sup>2</sup> Mission: Accelerate CO<sub>2</sub> Capture RD&D**







Rapidly synthesize optimized processes to identify promising concepts



Better understand internal behavior to reduce time for troubleshooting







Quantify sources and effects of uncertainty to guide testing & reach larger scales faster

Stabilize the cost during commercial deployment



# **CCSI<sup>2</sup> Summary, Capabilities, Highlights**



### • Industrial Collaborations – Actively Seeking External Collaborators

- 11 CO<sub>2</sub> Capture Program projects \$80MM+ in total project value (TRL 3-7)
- FLECCS: Dynamic, Intensified NGCC + CCS RTI
- ACT: Sustainable OPEration of post-combustion Capture plants (SCOPE) SINTEF
- ACT Alternate: Capture Operation with Generic Engineering for Net-zero Targets (COGENT) U. Sheffield
- · Computational efforts limited to CCS and related improvements

### Sequential Design of Experiments for lab-, bench-, or pilot-testing

- Improves model while optimizing lab- or pilot-scale experimental data generation can save years off of pilot test schedule
  - NCCC and TCM MEA pilot models accurate on CO<sub>2</sub> Capture percentage within 3-6% with 95% confidence

#### Process Optimization

Rigorously ensures proper balance of cost and performance. Minimize captured cost of 1. PNNL CO<sub>2</sub>BOL Process (>10% improvement over baseline), 2. Advanced Solvent Flash Stripper Process (optimization performed for multiple solvents)

### Process Intensification/Equipment Design

- Intensified solvent absorber design can improve capture rates by >10%
- Machine Learning
  - Increased speed of CFD based hydrodynamic simulations by 4000x for 13-22% accuracy (or 14x with better accuracy)

#### Computational Toolset Maintenance

• Regular software updates and revision management - open source



# **Capture Support for CCSI<sup>2</sup>**

### Capture Funding Remains Healthy





**Fiscal Year** 



#### NATIONAL **Complete CCSI Toolset Publically Available** TECHNOLOGY github.com/CCSI-Toolset CCSI Toolset The Carbon Capture Simulation Initiative (CCSI) Toolset is a suite of computational models for carbon capture processes. https://www.acceleratecarboncapture.org/ Second Contemport@acceleratecarboncapture.o... 2016 R&D 100 Awards Repositories 30 L People 26 Teams 6 Projects 1 C Settings Pinned repositories ≡ FOQUS ≡ ProcessModels bundle ≡ CFDModels bundle FOQUS: Framework for Optimization and A suite of process models implemented in both High fidelity device scale Computational Fluid Main website: https://www.acceleratecarboncapture.org/ Quantification of Uncertainty and Surrogates Aspen Custom Modeler and gPROMS Model Dynamics (CFD) models Builder, as well as models implemented within Support/Contact Us email: Aspen Plus and Aspen Plus Dynamics. ccsi-support@acceleratecarboncapture.org Pvthon ¥ 8 Makefile \* Makefile FOQUS User Documentation: https://fogus.readthedocs.io **≡** APCFramework ≡ Oxy-CombustionModels bundle ≡ iRevealLite YouTube Channel - tutorials: https://www.voutube.com/channel/UCBViFnxrs The Oxy-Combustion Models package consists of Unified framework in MATLAB for application and Automated reduced order model generation for WpNIcnDvh0 GzQ/ two primary components: A detailed boiler model testing of advanced control algorithms towards improved computational time and a suite of equation-based models of the other efficient process operation and control FOQUS GitHub repo - development: components of a complete oxycombustion power https://github.com/CCSI-Toolset/FOQUS generati... ¥ 3 Makefile Matlab Java

## **CCSI<sup>2</sup> FOQUS Framework**

NATIONAL ENERGY TECHNOLOGY TORY

FOQUS -- [not saved yet]





Surrogates

## For More Information: CCSI<sup>2</sup> Presentations Today

FOQUS -- [not saved yet]





## **CCSI<sup>2</sup> Offers Services to CCUS Stakeholders**



FOQUS -- [not saved yet]





# **Collaborating with CCSI<sup>2</sup>**

### Ask Us – How to Help Accelerate and De-Risk CCS R&D



#### **External Funding Opportunities** •

- Partner on eligible FOAs: e.g. FLECCS, ACT, etc. •
- Broad PSE modeling, optimization, CFD capabilities available at NETL
- Complementary expertise provided by CCSI<sup>2</sup> lab/university consortium, as needed
- Approval must be granted by NETL Program Management
- Proposal process coordinated through NETL Partnerships program
- Agreements for IP protection coordinated by NETL partnerships program

### **Provide Computational Services to Capture Program Stakeholders**

- As part of Capture funded project, or other as desired by stakeholder
- Approval must be granted by NETL and HQ Program management
- CRADA agreement usually executed to protect exchanged/created IP
- Expert Application of CCSI<sup>2</sup> Framework for Optimization and Quantification of Uncertainty and Surrogates (FOQUS)







For more information <u>https://www.acceleratecarboncapture.org/</u>

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