Advanced Computational Tools to Accelerate the Development of Next Generation Technologies

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For Accelerating Technology Development

- Identify promising concepts
- Reduce the time for design & troubleshooting
- Quantify the technical risk, to enable reaching larger scales, earlier
- Stabilize the cost during commercial deployment

National Labs
- Berkeley Lab
- Pacific Northwest National Laboratory
- NETL
- Los Alamos National Laboratory
- Lawrence Livermore National Laboratory

Academia
- Carnegie Mellon University
- Princeton University
- West Virginia University
- Boston University
- University of Texas at Austin
- University of Utah

Industry
- Fluor
- ADA
- B&W
- GE
- EPRI
- Electric Power Research Institute
- Burns & McDonnell
- AEP
- American Electric Power
- Duke Energy
- URS
- Boeing
- Dupont
- WorleyParsons
- ExxonMobil
- Eastman
- Chevron
- Phillips 66

U.S. Department of Energy
Advanced Computational Tools to Accelerate Next Generation Technology Development

Risk Analysis (Technical Risk, Financial Risk) & Decision Making

- Validated High-Fidelity CFD & UQ
  - Uncertainty Quantification
- Process Design & Optimization
  - Uncertainty Quantification
- Advanced Process Control & Dynamics
  - Uncertainty Quantification

- High Resolution Filtered Sub-models
- Process Models
  - Uncertainty Quantification

- Basic Data Sub-models

Cross-Cutting Integration Tools
- Data Management, Remote Execution Gateway, GUI, Build & Test Environment, Release Management

CCSI Carbon Capture Simulation Initiative
Advanced Process Systems Engineering Approaches

Basic Data Models

Process Models

Algebraic Surrogate Models

Superstructure Optimization

Optimal Process

Simulation Gateway

Simulation-Based DFO Framework

Uncertainty Quantification with Bayesian Calibration

SORBENTFIT

alamo

GAMS

CCSI

Carbon Capture Simulation Initiative

U.S. DEPARTMENT OF ENERGY
CFD models to reduce time for troubleshooting

Heat-transfer-tube-scale hydrodynamics

\[ f_{drag}^* = \beta^* \left( -v_s^* |v_s^*| \right) + \gamma^* \]
Dynamic Reduced Models & APC Framework
Risk analysis and decision making framework

Combine technical risk and financial risk factors into an integrated decision analysis framework that naturally handles propagation of uncertainties into a variety of decision metrics.
Deploys Initial Computational Toolset

- Released 21 Toolset components Sept. 2012
  - Reaction kinetics model of solid sorbents
  - CFD models of 1 MW adsorber & regenerator
  - Process models of solid-sorbent capture, membrane, and compression systems
  - New optimization tools (ALAMO, superstructure, framework)
  - Advanced dynamic & control models (adsorber, compression
  - New integration tools (REVEAL, Turbine, Sinter)
  - Uncertainty Quantification Framework
  - Financial Risk Tool
Thank you!

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