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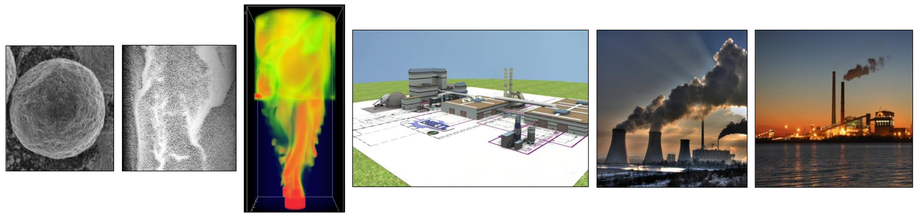
AMERICAN INDUSTRY AND AMERICA'S NATIONAL LABS

MODELING AND SIMULATION

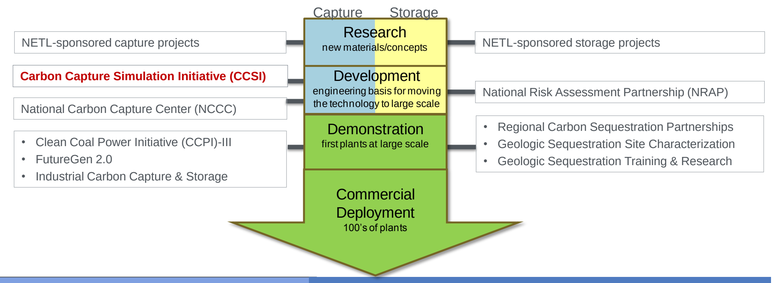
CARBON CAPTURE SIMULATION INITIATIVE FOR ACCELERATING COMMERCIAL TECHNOLOGY DEVELOPMENT

Overview

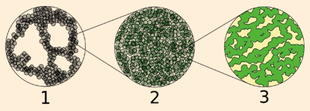
The U.S. Department of Energy's Carbon Capture Simulation Initiative (CCSI) brings together the National Energy Technology Laboratory (NETL), Los Alamos National Laboratory (LANL), Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), and Pacific Northwest National Laboratory (PNNL) in partnership with academic and industrial institutions to develop and deploy state-of-the-art computational modeling and simulation tools to accelerate the commercialization of carbon capture technologies from discovery to development, demonstration, and widespread deployment. The CCSI Toolset will be used during the scale-up of carbon capture processes to assess and mitigate technical and financial risks, to improve designs, and to shorten the design cycle.



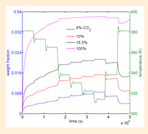
CCSI is part of the DOE CCS RD&D Roadmap



Basic Data and Models



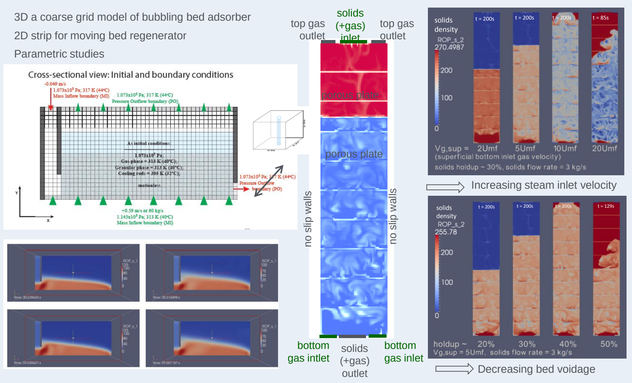
High-fidelity model:
- Sorbent microstructure broken down into three length scales
- Separate treatment of gas-phase and polymer-phase transport
- Accurately describes TGA features arising from bulk CO_2 transport effects



Parameter estimation (calibration) for 5 parameter **ideal equilibrium model**-probability dist. using Bayesian methods and expert priors.

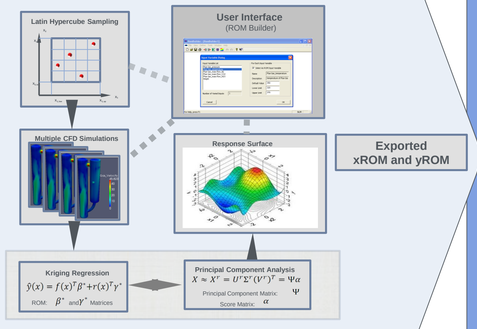
Particle & Device Scale Simulation Tools and Models

3D a coarse grid model of bubbling bed adsorber
2D strip for moving bed regenerator
Parametric studies

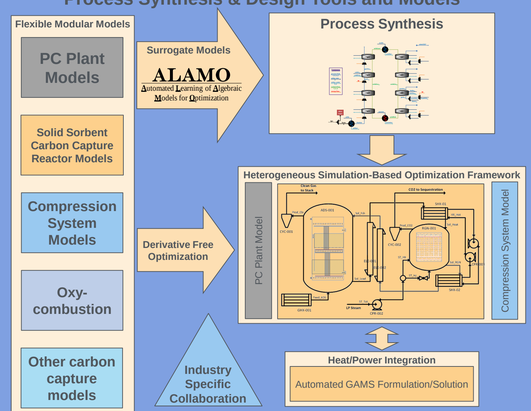


Simulation results from NETL's open source multiphase CFD software MFIX

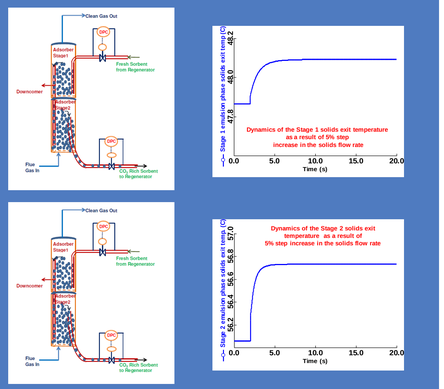
Reduced Order Model Development



Process Synthesis & Design Tools and Models

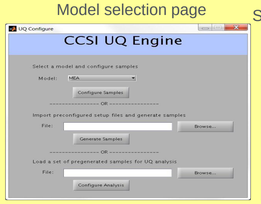


Plant Operations & Control Tools and Models

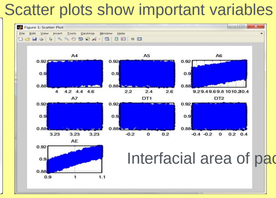


Uncertainty Quantification Framework

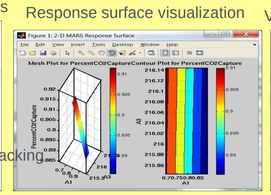
Model selection page



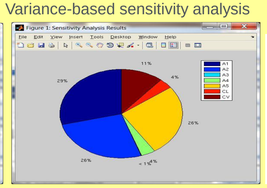
Scatter plots show important variables



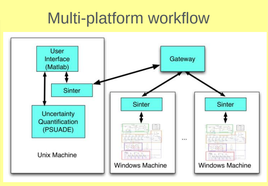
Response surface visualization



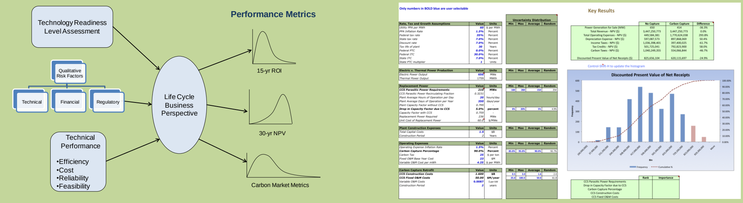
Variance-based sensitivity analysis



Multi-platform workflow



Risk Analysis & Decision Making Framework



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