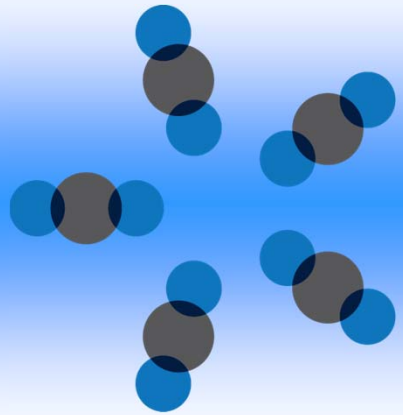

CCSI

Carbon Capture Simulation Initiative

Computational Toolset for Accelerating Carbon Capture Technology Development

Madhava Syamlal

U.S. Department of Energy

National Energy Technology Laboratory

7 September 2014

23rd International Symposium on Chemical Reaction Engineering, Bangkok, Thailand, 7-10 September 2014.

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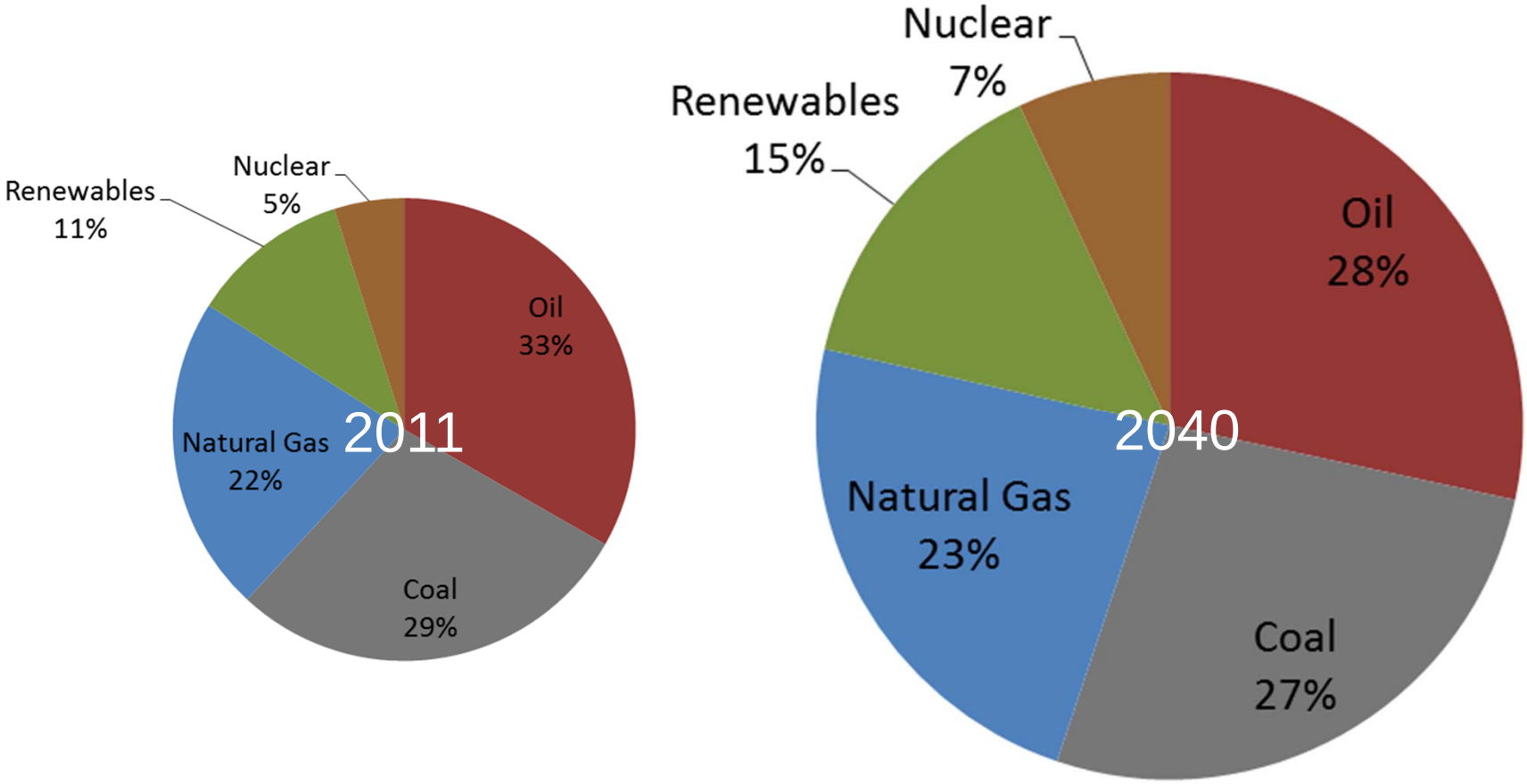
Fossil fuels helped build the modern world … will remain the major fuel for next 30 years



536 Quad

820 Quad

U.S. Energy Information Administration, International Energy Outlook 2012, DOE/EIA-0484(2012)

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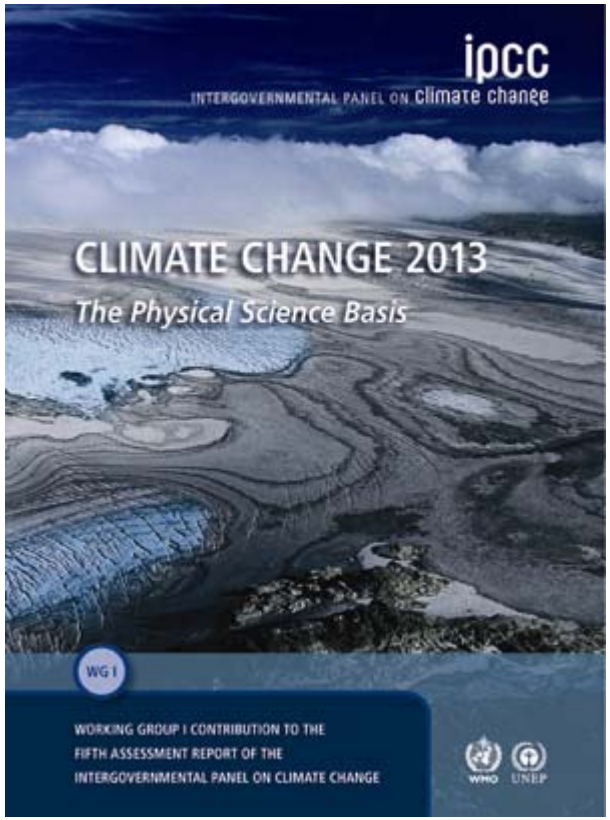
IPCC AR5: “Warming of the climate system is unequivocal”

Global surface temperature change is likely to exceed 1.5°C to 2°C by 2100.

Human influence on the climate system is clear.



Climate Change 2013, The Physical Science Basis, Working Group I Contribution to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change, Summary for Policymakers

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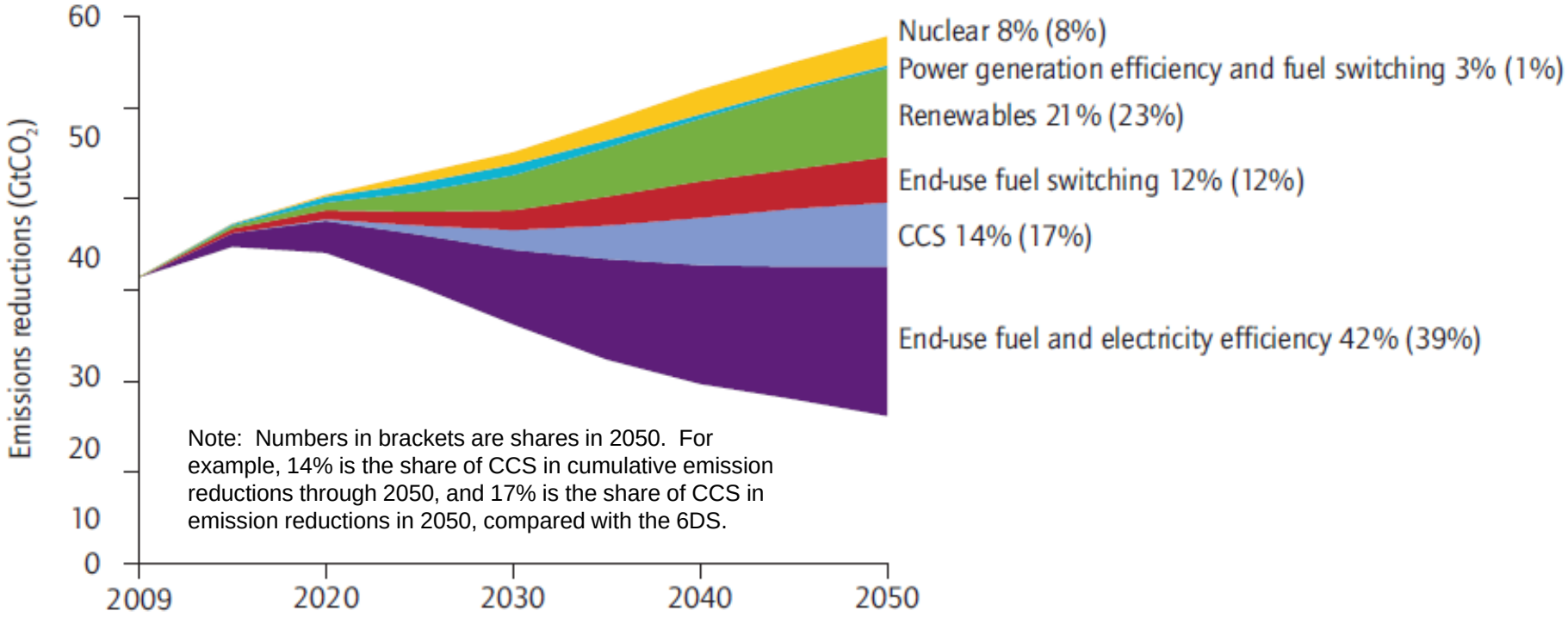
CCS is a key technology for reducing global CO_2 emissions



Most 2050 climate budgets require CCUS from NatGas power

Source: J. Friedmann, "A Decade of Projects: CCS to 2022," MIT 15th Carbon Sequestration Forum, 27 January 2014, Austin, TX.

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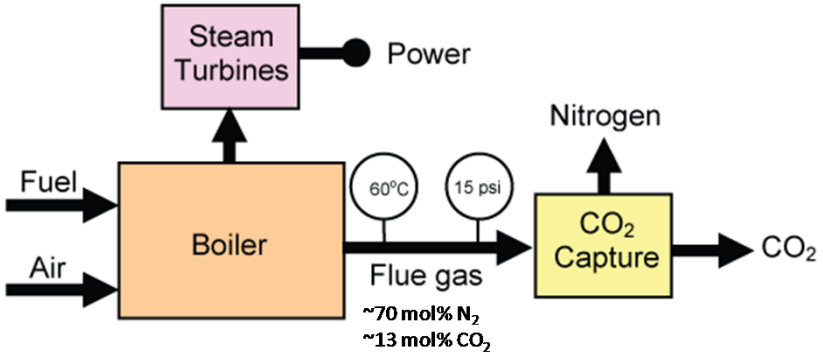
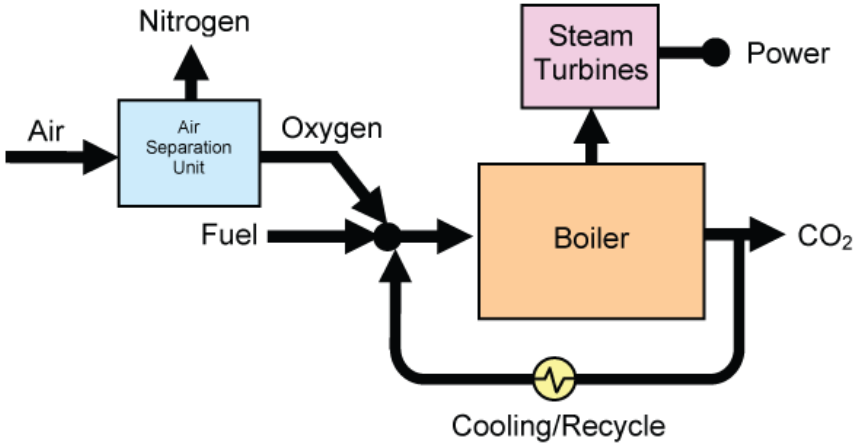
Three options for CO_2 capture in power plants

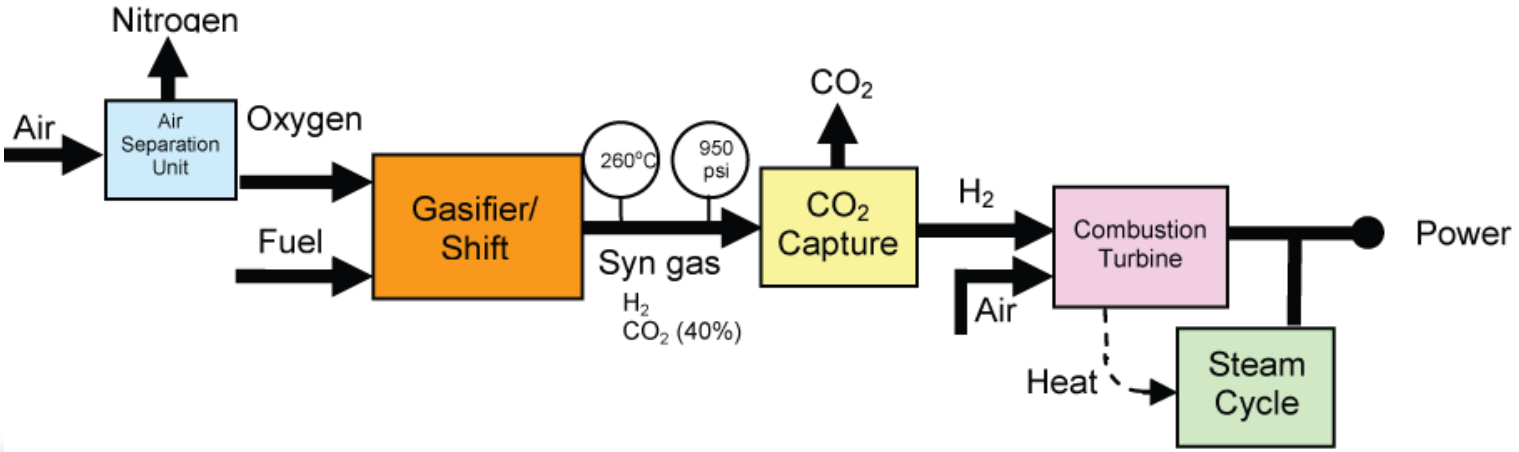
Post-combustion capture



Oxycombustion



Pre-combustion capture



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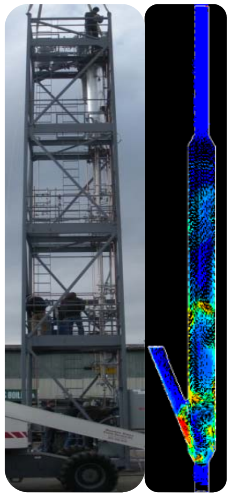
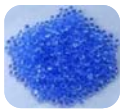
Accelerating capture technology development

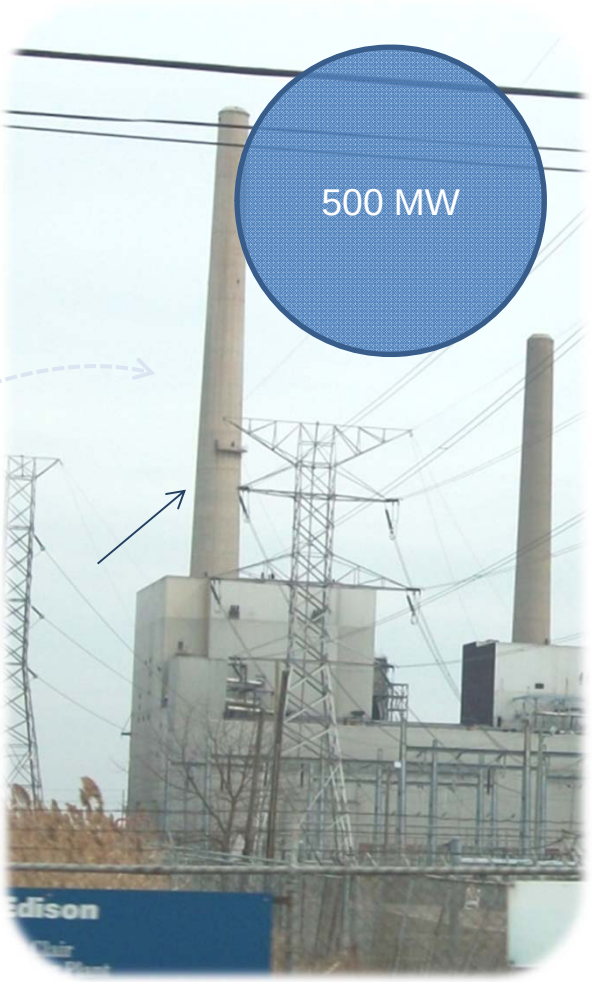


Scale up with greater confidence

Aided by predictions from physics-based simulations



1 kW → 1 MW → 5 MW → 20 MW → 100 MW → 500 MW



Solid-sorbent based CO_2 capture

Source of photo:
http://en.wikipedia.org/wiki/File:DTE_St_Clair.jpg

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Modeling & Simulation tools for accelerating the development of CO_2 capture technology

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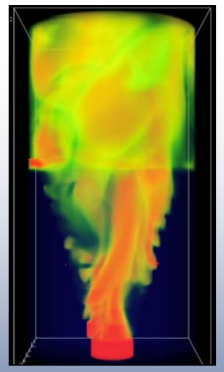
Carbon Capture Simulation Initiative






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

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Pacific Northwest National Laboratory
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Lawrence Livermore National Laboratory

Academia

Carnegie Mellon
Princeton University
West Virginia University
Boston University
The University of Texas at Austin

Industry

ADA Environmental Solutions
Alstom
B&W
GE
EPRI Electric Power Research Institute
Fluor
Southern California Edison
Southern Company
Phillips 66
AEP American Electric Power
Chevron
URS
ExxonMobil
Air Products
Eastman
ANSYS
aspentech
invensys
PSE

D.C. Miller et al., "Carbon Capture Simulation Initiative: A Case Study in Multiscale Modeling and New Challenges," *Annu. Rev. Chem. Biomol. Eng.,* 2014. 5:301–23

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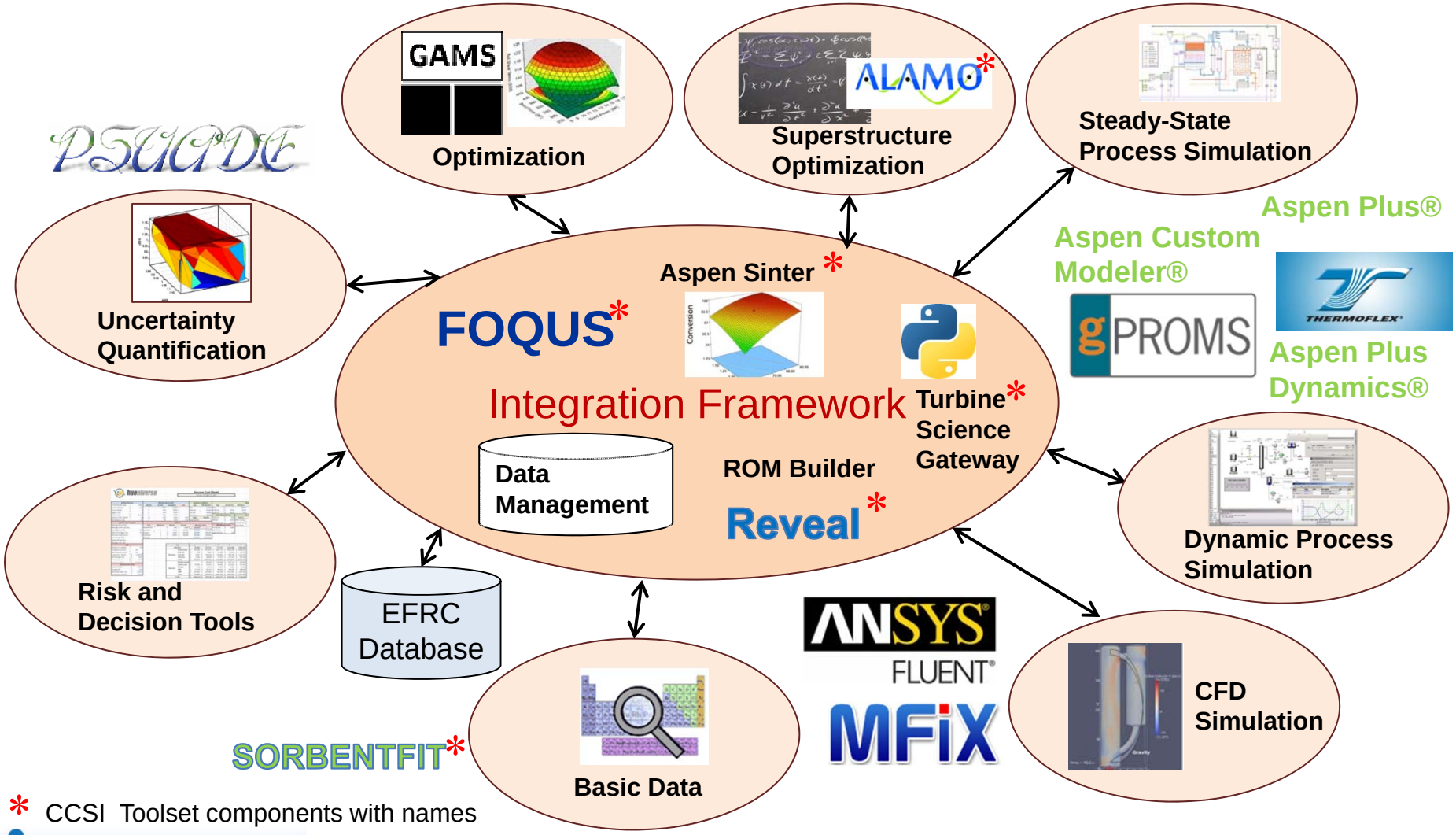
CCSI framework for integrating modeling and simulation tools



* CCSI Toolset components with names

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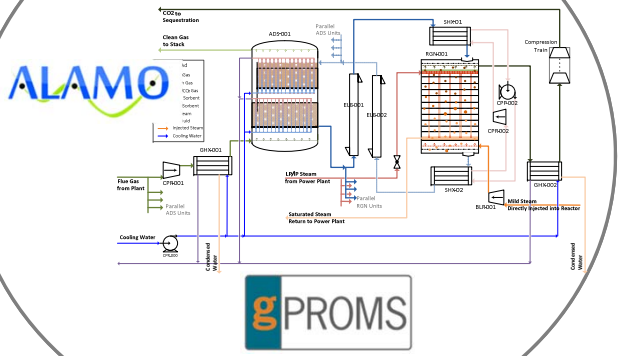
CCSI toolset enables the integration of models at multiple scales

FOQUS

D-RM Builder



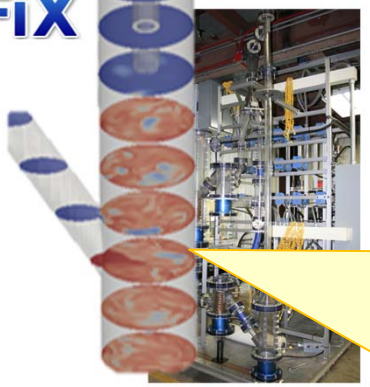
ALAMO

gPROMS

Aspen Plus®

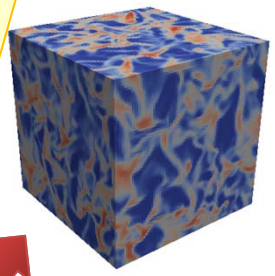
Process scale

MFiX

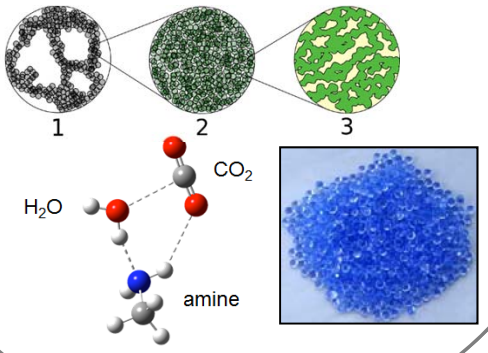


Device scale

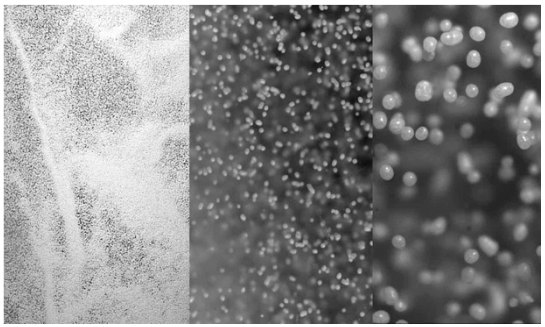
Filtered sub-models



SORBENTFIT



Particle scale



Gas-solids hydrodynamics

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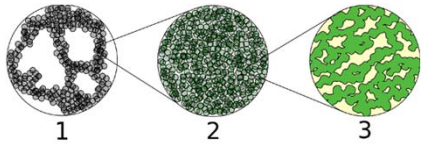
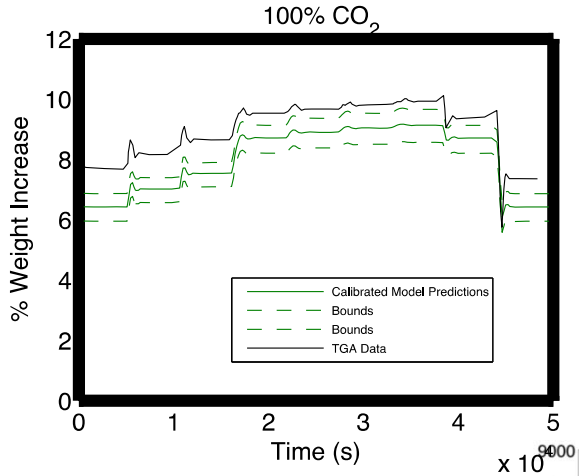
Particle-scale reaction kinetics model

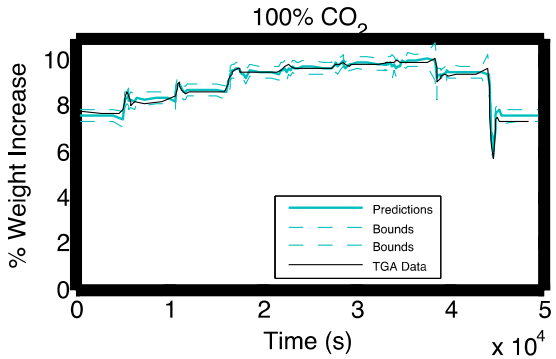


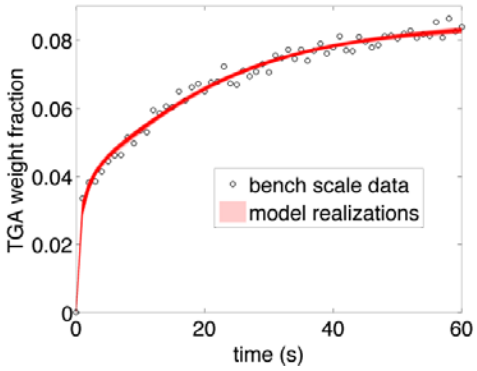
PEI-impregnated silica sorbent

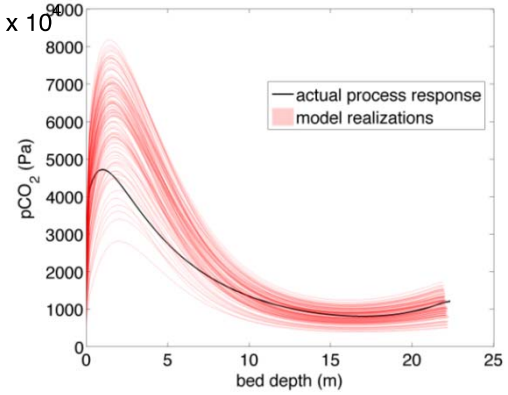
$$2R_2NH + CO_2(gas) \rightleftharpoons R_2NCO_2^- + R_2NH_2^+$$
$$R_2NH + H_2O(phys) + CO_2(gas) \rightleftharpoons HCO_3^- + R_2NH_2^+$$
$$H_2O(gas) \rightleftharpoons H_2O(phys)$$

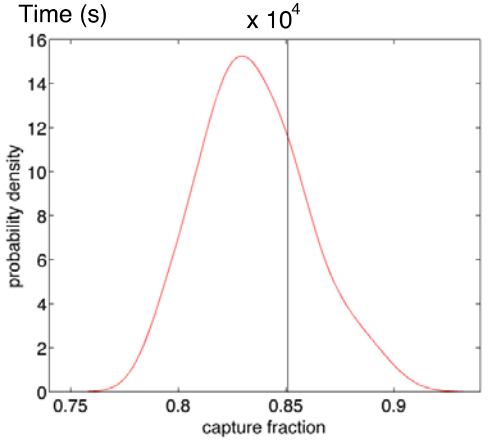


With Discrepancy









1. K.S. Bhat, D.S. Mebane, H. Kim, J. Eslick, J.R. Wendelberger, D.C. Miller, LANL Tech. Rep. LA-UR-12-21855, 2012.
2. D.S. Mebane, J.D. Kress, C.B. Storlie, D.J. Fauth, M.L. Gray, K. Li, *J. Phys. Chem. C* 117 (2013) 26617.
3. K.S. Bhat, D.S. Mebane, C.B. Storlie and P. Mahapatra, *J. Am. Stat. Association* , 2014 submitted.

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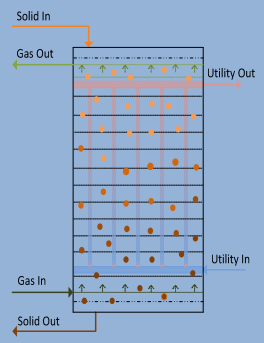
Optimization tools enable rigorous screening and design of new processes

Process Models

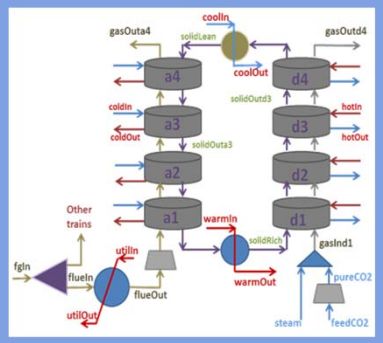


Basic Data Submodels

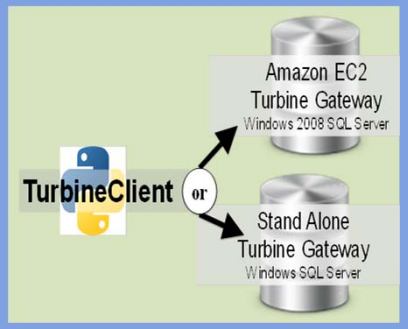
Algebraic Surrogate Models

ALAMO

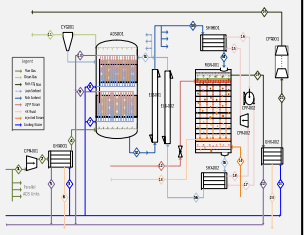
Superstructure Optimization (Determine Configuration)



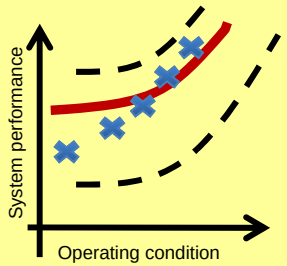
Simulation-Based Optimization



Optimized Process



Predictions with uncertainty quantified



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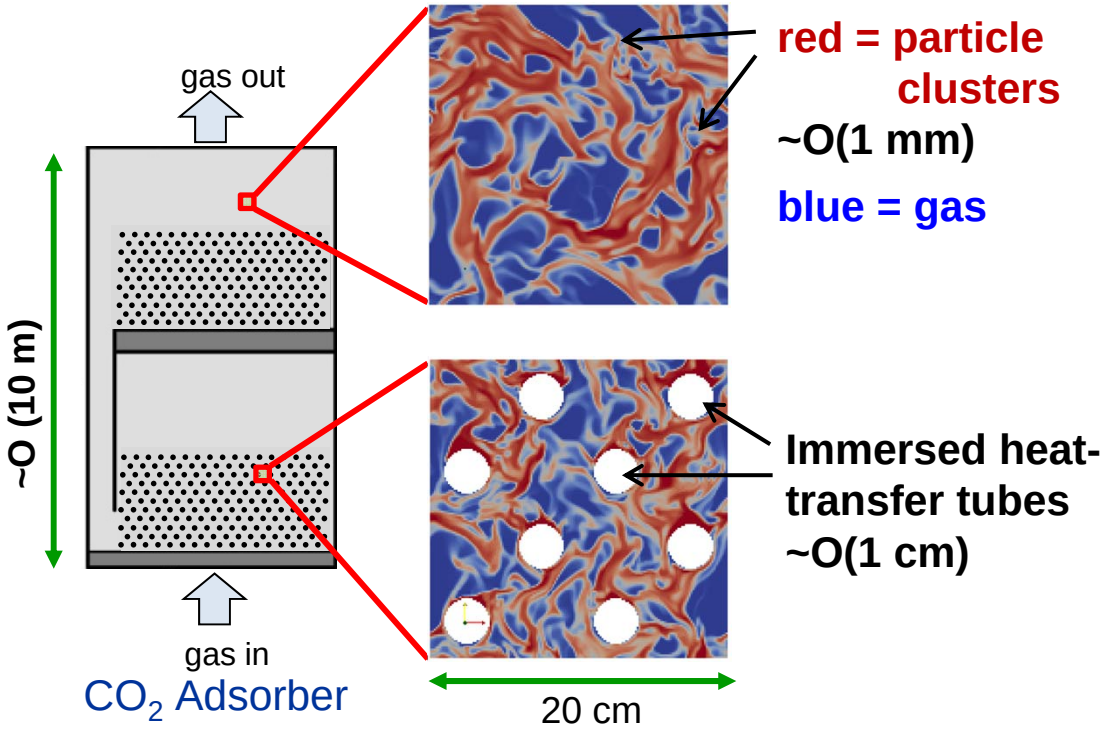
Device-scale models must account for meso-scale structures in fluidized beds



CFD grid size must be ~O(1 mm).

- **Millions of cells in 2D,**
- **Billions of cells in 3D!**

COMPUTATIONALLY INTRACTIBLE!

Approach: Probe meso-scale structures and develop effective coarse-grained **"filtered" constitutive models**.

Developed for fluidized beds with and without immersed tubes.

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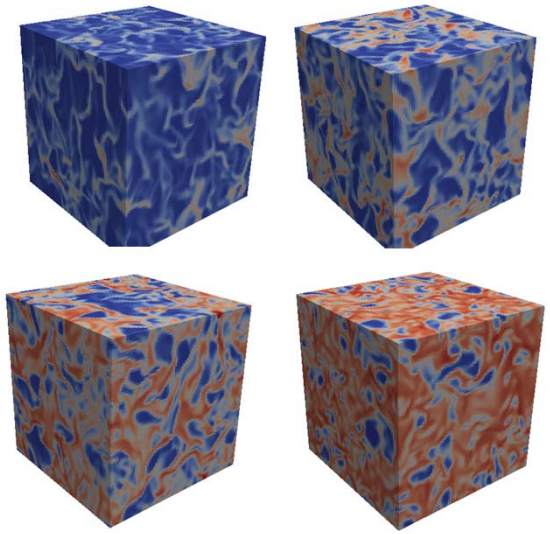
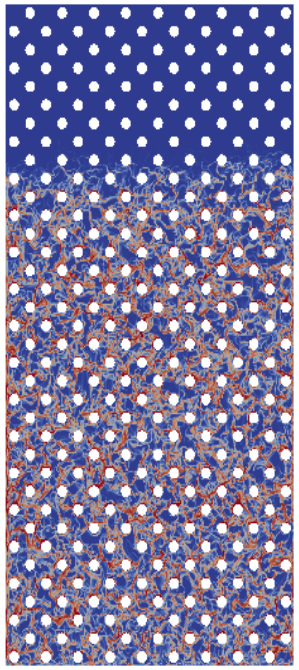
Filtered constitutive models

Higly-resolved periodic cell simulations used to construct filtered models.

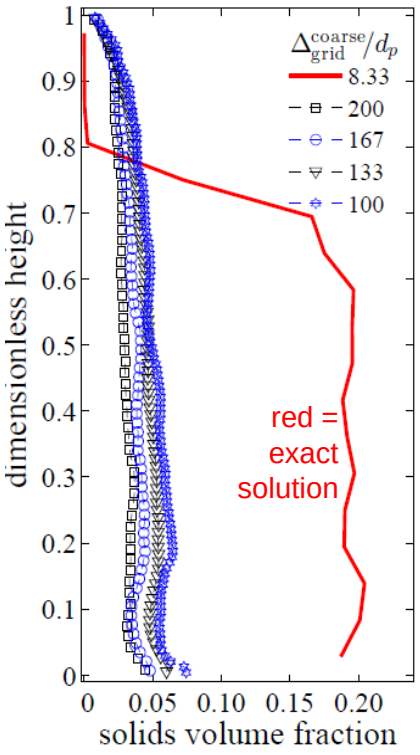


These filtered models yield **accurate predictions** using **affordable CFD simulations** with coarse-grids.

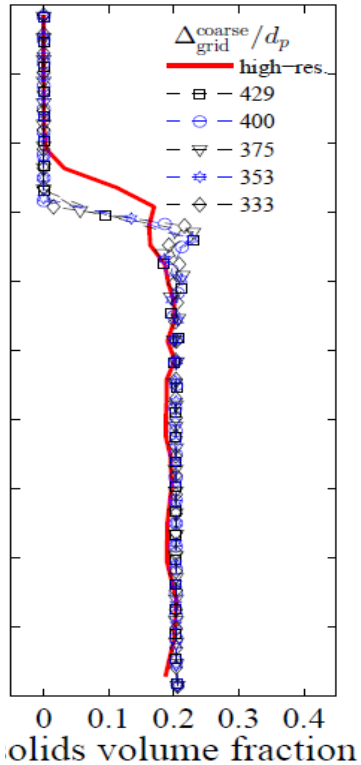
Fine-grid **"exact solution"**



Coarse-grid **WITHOUT filtered models**



Coarse-grid **WITH filtered models**



$$\beta_{gs}^{filt} = \left[1 - H\left(\Phi_s\right)\right]\beta_{gs}^{micro}$$

filtered coarse-grid drag coefficient

filtered correction when using coarse grids

unfiltered drag coefficient

Sarkar A, Sun X, Sundaresan S. Verification of sub-grid filtered drag models for gas-particle fluidized beds with immersed cylinder arrays. *Chem. Eng. Sci.*, 2014.

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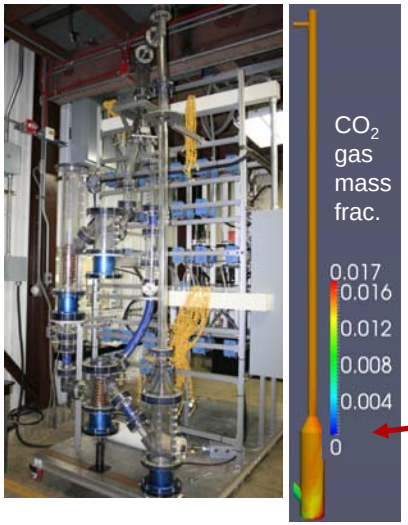
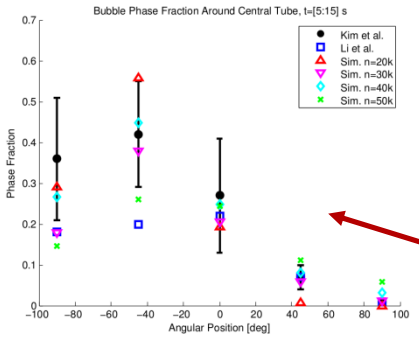
A validation hierarchy generates confidence in predictive simulations

Need to predict the performance of devices yet to be built.





25 MWe, 100 MWe, 650 MWe solid-sorbent systems

1 MWe carbon capture system

NETL carbon capture unit (C2U) reacting unit

Bubbling bed adsorber | Moving bed regenerator

Intermediate validation (adsorber without reactions and heat transfer)

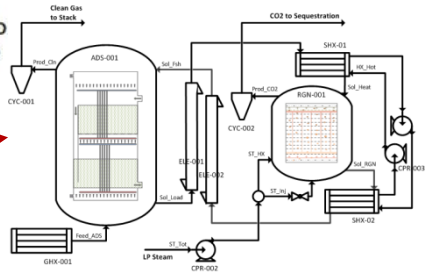
Intermediate validation (regenerator without reactions and heat transfer)

Upscaling (flow filtering) | *Upscaling (reaction filtering)* | *Upscaling (energy filtering)* | *Upscaling (flow filtering)*

Bubbling fluidized bed (adsorber) | Reaction kinetic | Heat transfer | Moving fluidized bed (regenerator)

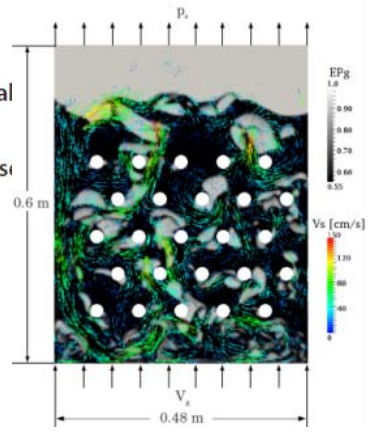
Demonstration and full-scale systems

Pilot-scale systems



Laboratory-scale subsystem (coupled benchmark cases)

Laboratory-scale subsystem (decoupled benchmark cases)



Unit problems

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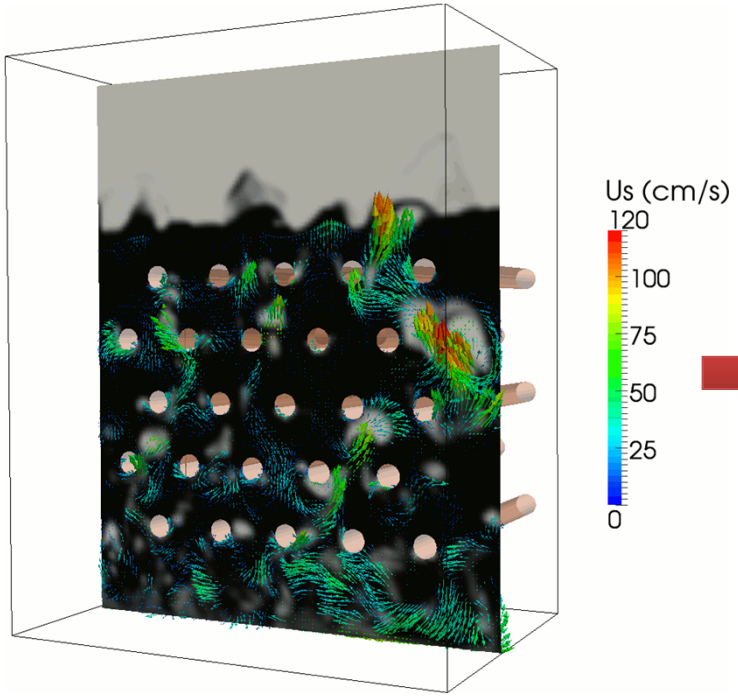
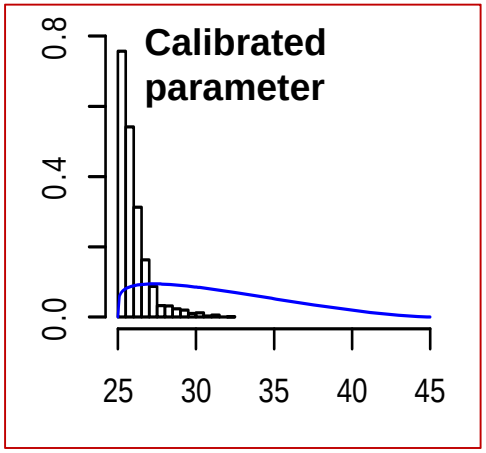
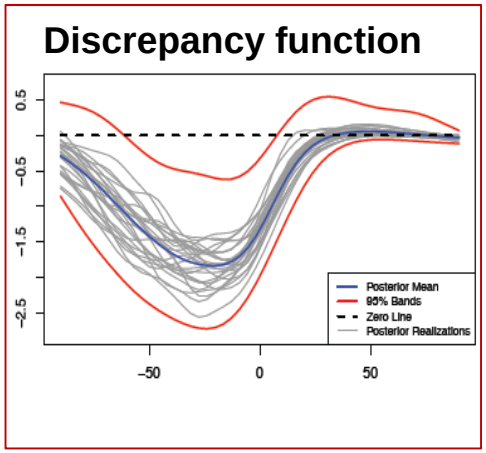
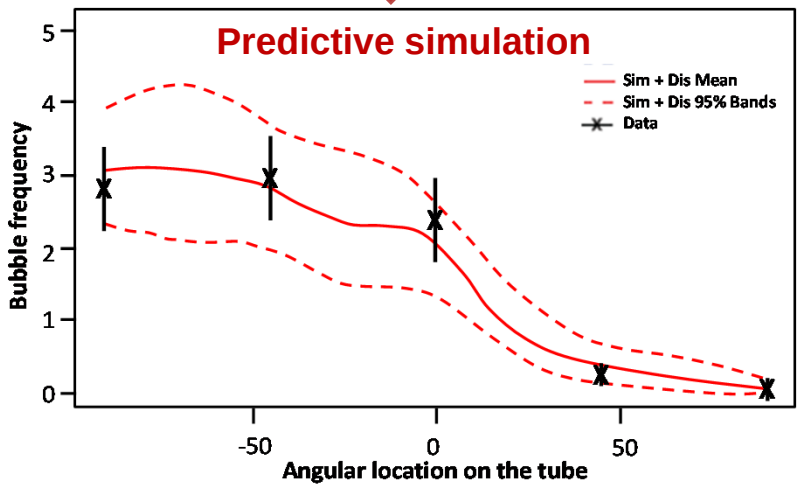
Uncertainty quantification enables the determination of confidence bands in predictions



Courtesy: Tingwen Li, NETL







Storlie, C.B., Lane, W.A., and Ryan, E.M., "Calibration of Computational Models with Categorical Parameters and Correlated Outputs via Bayesian Smoothing Spline ANOVA," submitted to the *J. of Am. Stat. Association*, 2013.

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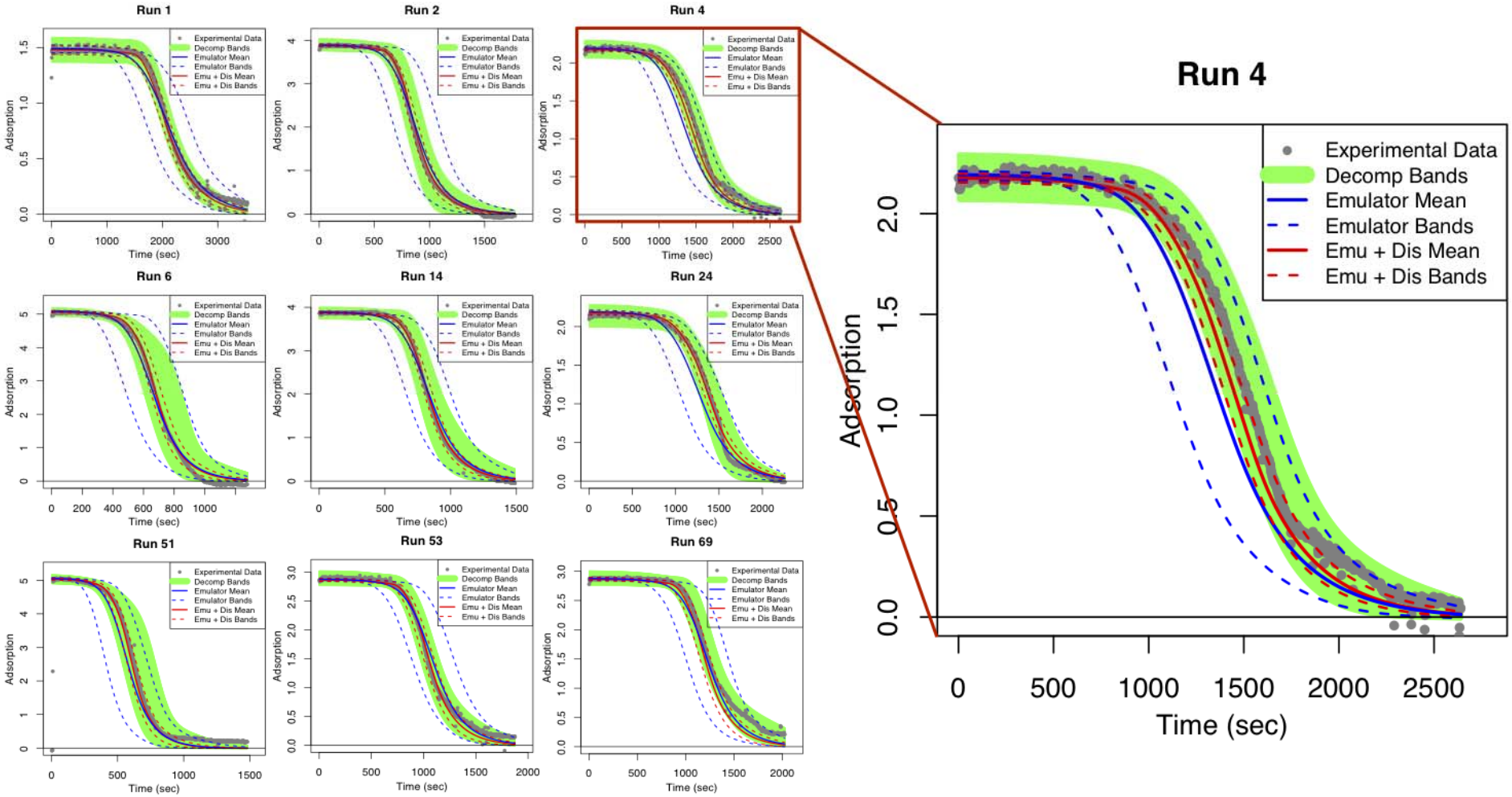
“The emulator prediction bands are within observation error in all cases”



K. Lai, Z. Xu, W. Pan, L. Shadle, C. Storlie, J. Dietiker, T. Li, S. Dartevelle, X. Sun, “Hierarchical Calibration and Validation of High-fidelity CFD Models with C2U Experiments ,” Milestone Report, 2014.

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Summary

The usual path from discovery to commercialization is too slow for developing urgently needed CO_2 capture technologies.

CCSI – a partnership among U.S. national laboratories, industry and universities – is developing a modeling and simulation toolset for accelerating CO_2 capture technology development.

The CCSI Toolset uses a multi-scale approach, including models of particle/film-scale reaction kinetics, CFD models of capture reactors, and steady and dynamic models of capture processes.

- Reduced order models transfer information between scales.
- Optimization tools enable rigorous screening and design of new processes.
- Filtered models speed up device-scale computations.
- A validation hierarchy generates confidence in predictive simulations.
- Uncertainty quantification enables the determination of confidence bands in predictions.

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