CCSI

Carbon Capture Simulation Initiative

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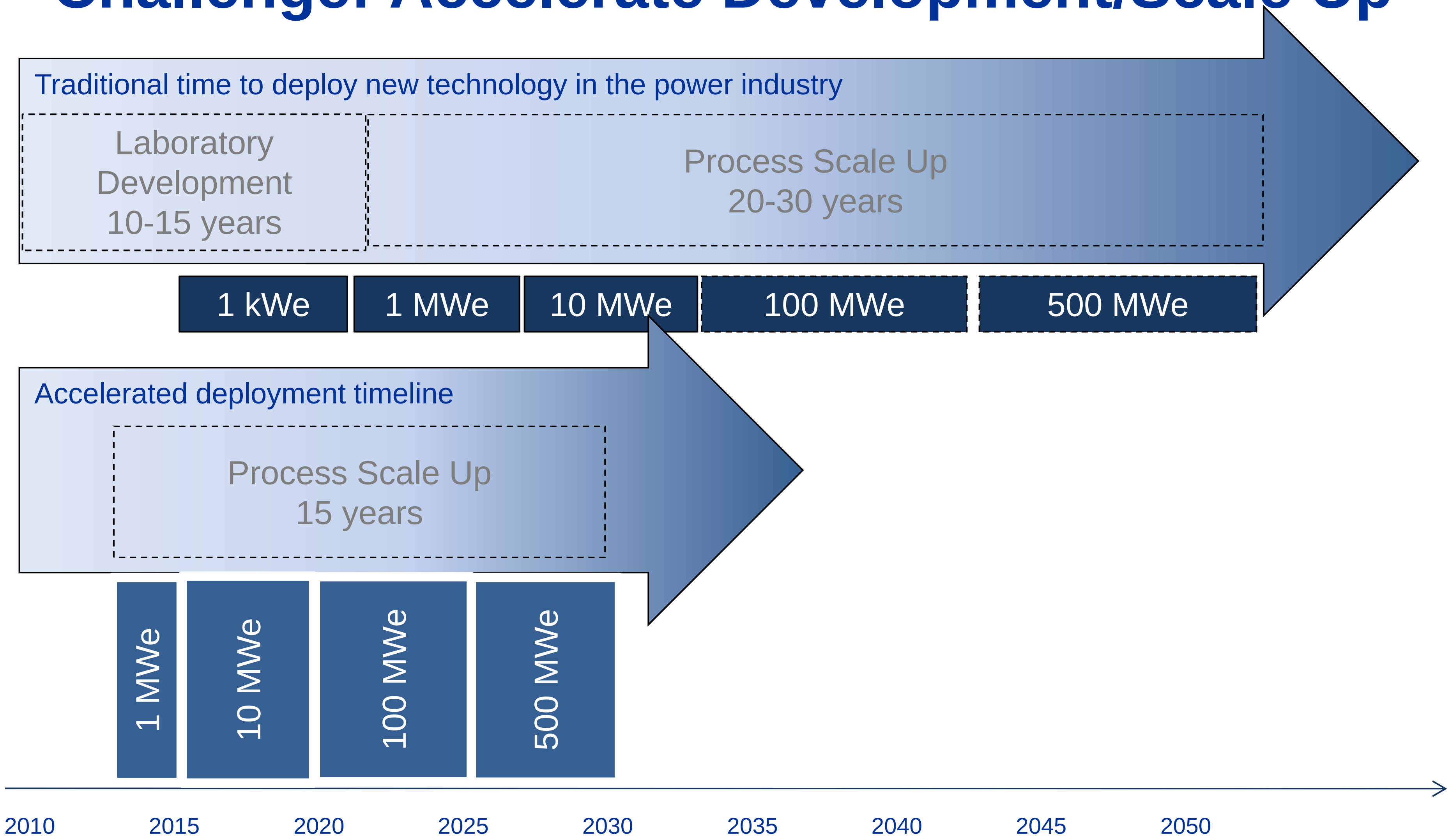
Challenge: Accelerate Development/Scale Up



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CCSI For Accelerating Technology Development

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Carbon Capture Simulation Initiative

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

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Boston University
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EPRI Electric Power Research Institute
FLUOR
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Southern California Edison
An Edison International Company
San Onofre Nuclear Generating Station
Southern Company
ExxonMobil
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Air Products
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ANSYS
Schneider Electric
PSE

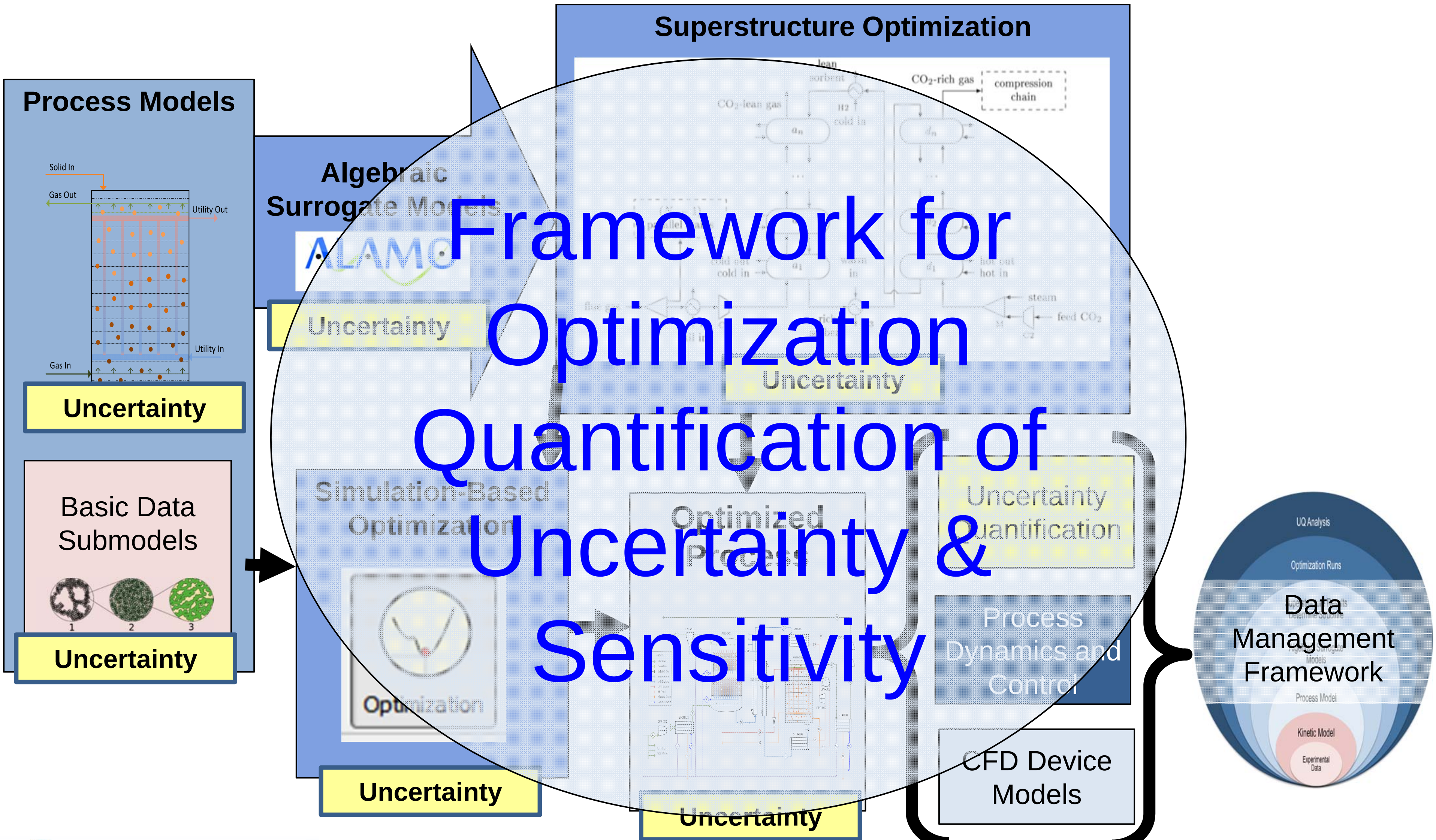
Goals & Objectives of CCSI

- **Develop** new computational tools and models to enable industry to more rapidly develop and deploy new advanced energy technologies
  - Base development on industry needs/constraints

- **Demonstrate** the capabilities of the CCSI Toolset on non-proprietary case studies
  - Examples of how new capabilities improve ability to develop capture technology

- **Deploy** the CCSI Toolset to industry
  - Initial licensees

CCSI Toolset Workflow and Connections



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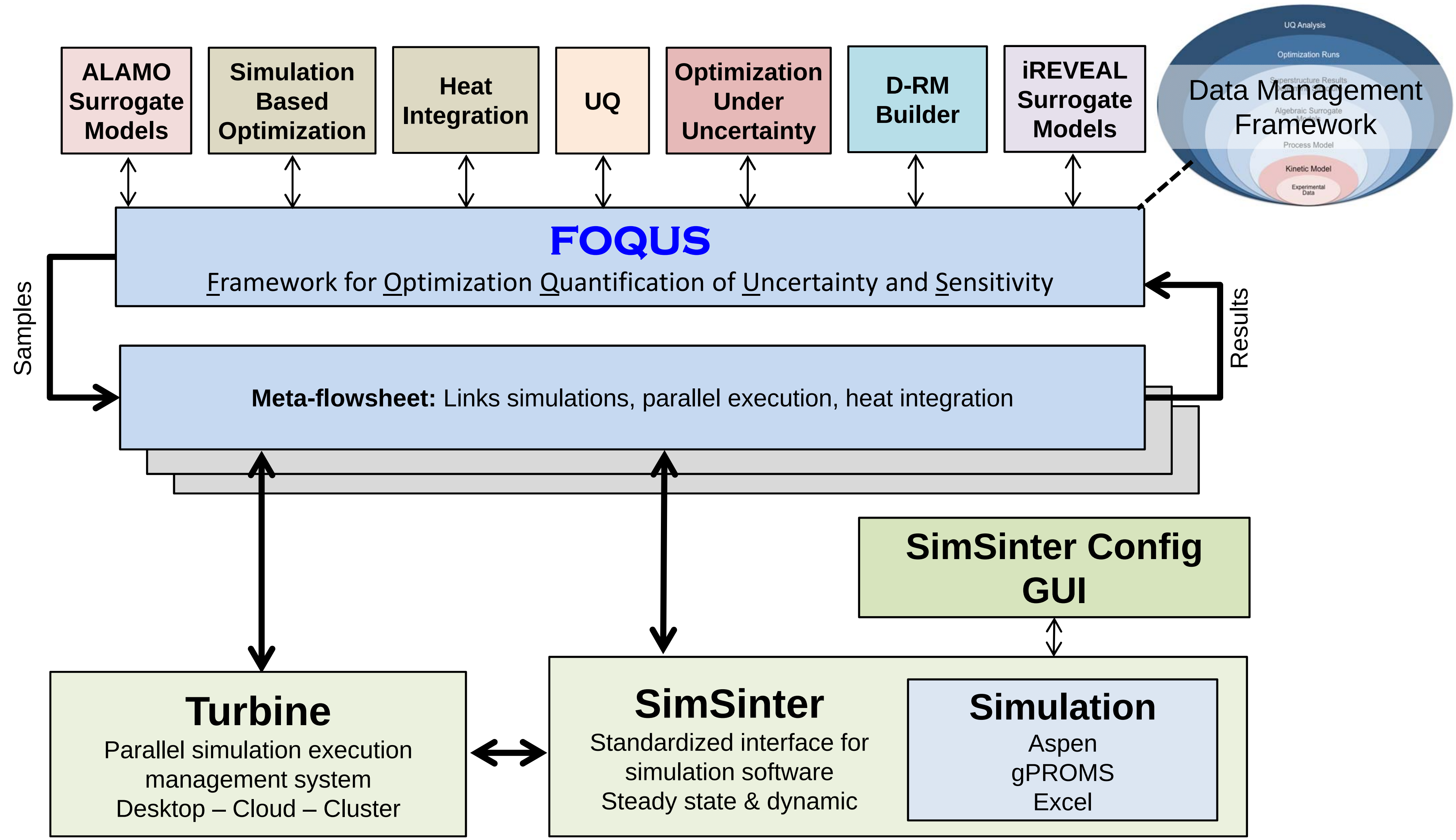
Framework for Optimization, Quantification of Uncertainty and Sensitivity



D. C. Miller, B. Ng, J. C. Eslick, C. Tong and Y. Chen, 2014, Advanced Computational Tools for Optimization and Uncertainty Quantification of Carbon Capture Processes. In *Proceedings of the 8th Foundations of Computer Aided Process Design Conference – FOCAPD 2014*. M. R. Eden, J. D. Siirola and G. P. Towler Elsevier.

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Optimization with Heat Integration

	w/o heat integration	Sequential	Simultaneous
Net power efficiency (%)	31.0	32.7	35.7
Net power output (MW_e)	479.7	505.4	552.4
Electricity consumption [b] (MW_e)	67.0	67.0	80.4
IP steam withdrawn from power cycle (MW_{th})	0	0	0
LP steam withdrawn from power cycle (MW_{th})	336.3	304.5	138.3
Cooling water consumption [b] (MW_{th})	886.8	429.3	445.1
Heat addition to feed water (MW_{th})	0	125.3	164.9

Base case w/o CCS: 650 MW_e, **42.1 %**

Y. Chen, J. Eslick, I.E. Grossmann, D.C. Miller, "Simultaneous Process Optimization and Heat Integration Based on Rigorous Process Simulations", Computers & Chemical Engineering, Accepted, April 23, 2015.

Uncertainty Quantification for Prediction Confidence

- Now that we have
  - A chemical kinetics model with quantified uncertainty
  - A process model with other sources of uncertainty
  - Surrogates with approximation errors
  - An optimized process based on the above
- UQ questions
  - How do these errors and uncertainties affect our prediction confidence (e.g. operating cost) for the optimized process?
  - Can the optimized system maintain >= 90% CO_2 capture in the presence of these uncertainties?
  - Which sources of uncertainty have the most impact on our prediction uncertainty?
  - What additional experiments need to be performed to give acceptable uncertainty bounds?

CCSI UQ framework is designed to answer these questions

Optimization Under Uncertainty using a Two-Stage Approach

Design Phase

Uncertain parameters are characterized probabilistically

Optimize design variables while taking into account uncertainty of unknown parameters

Operating Phase

Uncertain parameters have been realized

Optimize operational variables in response to realized uncertain parameters

Bubbling Fluidized Bed (BFB) System

Design Variables:
- **Absorber/regenerator dimensions**
- **Heat exchanger areas and tube diameters**

Uncertain Parameters:
- **Flue gas flowrate (load-following)**
- **Flue gas composition (fuel type)**
- **Reaction kinetics**

Operational Variables:
- **Steam flowrate**
- **Cooling water flowrate**
- **Recirculation gas split fraction**

$$\min_X \quad \cancel{COE(BFB, X)}$$

$$\text{subject to } CO_2 \text{ capture} \geq 90\%$$

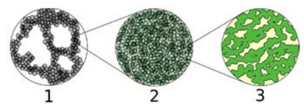
G() – some statistics, e.g. mean

Θ - uncertain parameters

$$G(COE(BFB, X, \Theta))$$

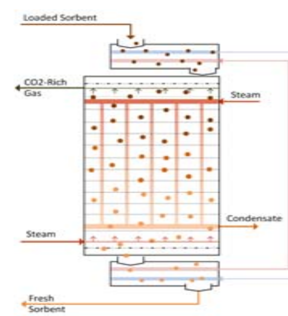
Solid Sorbents Models & Demonstration

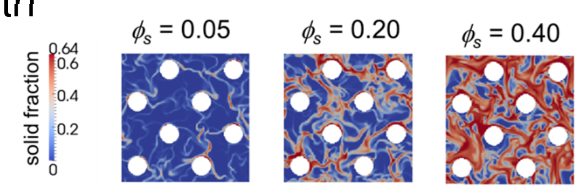
- **Basic data models**
  - SorbentFit (1st gen model)
  - SorbentFit extension for packed beds
  - 2nd generation sorbent model which accounts for diffusion and reaction separately



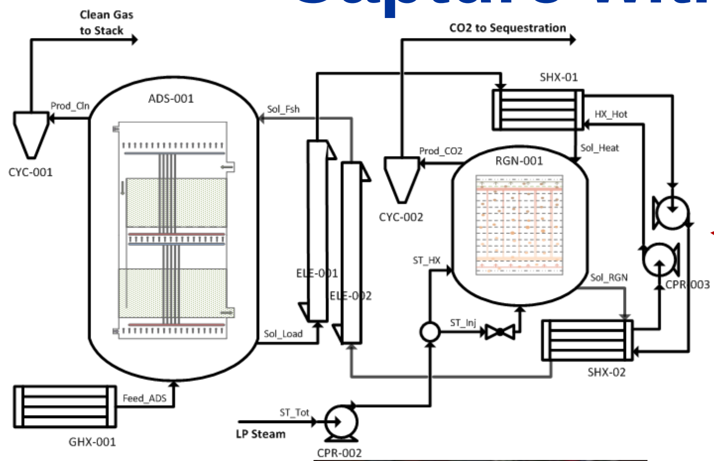
- **CFD models**
  - Attrition Model
  - 1 MW bubbling fluidized bed adsorber with quantified predictive confidence
  - High resolution filtered models for hydrodynamics and heat transfer considering horizontal tubes
  - Validation hierarchy
  - Comprehensive 1 MW solid sorbent validation case via CRADA
  - Coal particle breakage model with validation

- **Process models**
  - Bubbling Fluidized Bed Reactor Model
  - Dynamic Reduced Order BFB Model
  - Moving Bed Reactor Model
  - Multi-stage moving bed model
  - Multi-stage Centrifugal Compressor Model
  - Solids heat exchanger models
  - Comprehensive, integrated steady state solid sorbent process model
  - Comprehensive, integrated dynamic solid sorbent process model with control

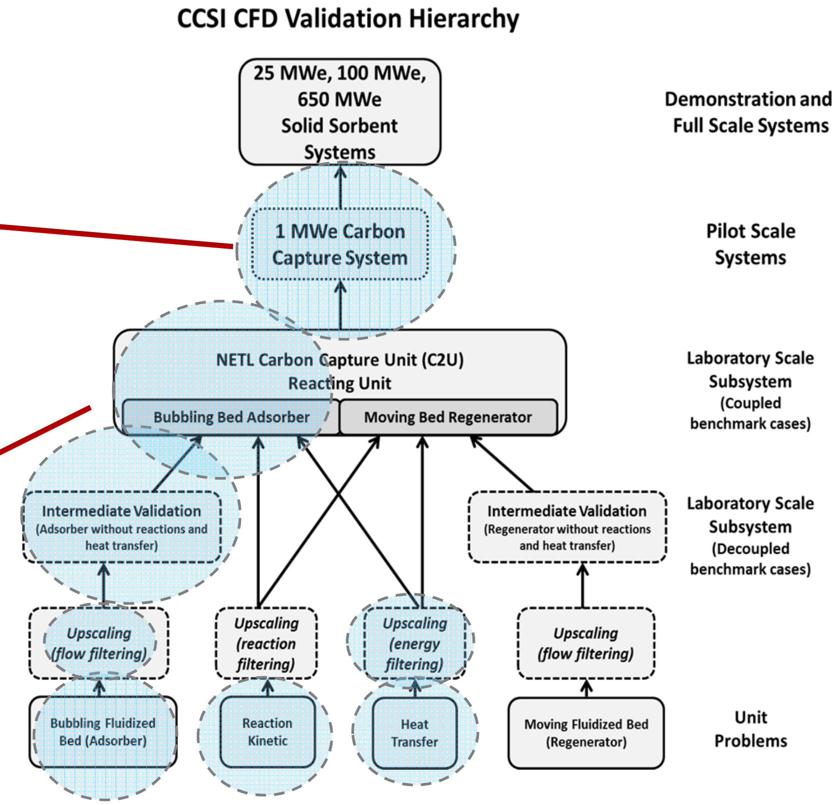


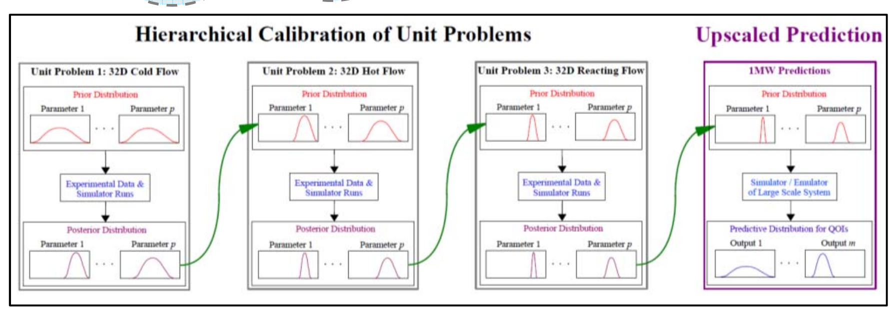


Building Predictive Confidence for Device-scale CO_2 Capture with Multiphase CFD Models



C2U Batch Unit





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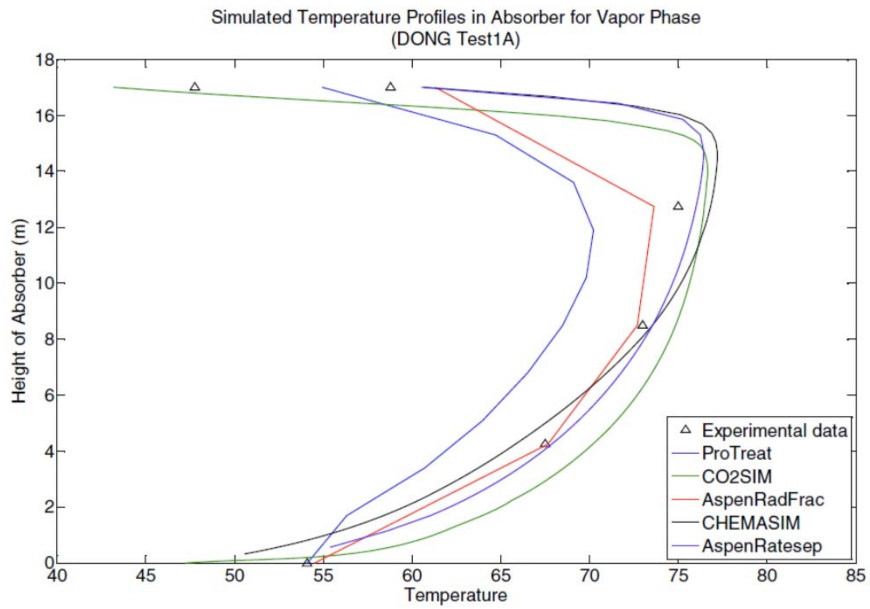
Solvent System Models & Demonstration

- **Basic data models**
  - Unified SorbentFIT tool to calibrate solvent data
  - High Viscosity Solvent Model, 2-MPZ
  - Properties model for Pz/2-MPz Blends (Aspen)
- **CFD models**
  - VOF Prediction on Wetted Surface
  - Prediction of mass transfer coefficients by calibration of fully coupled wetted wall column model
  - Preliminary CFD simulation of a solvent based capture unit
  - Validation hierarchy
- **Process models**
  - "Gold standard reference" process model, both steady-state and dynamic
  - Methodology for calibration/validation of solvent-based process models to support scale up

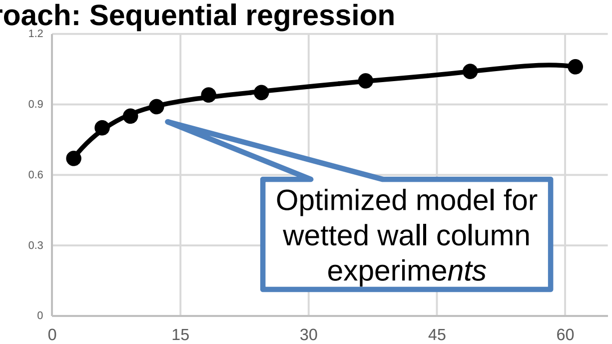


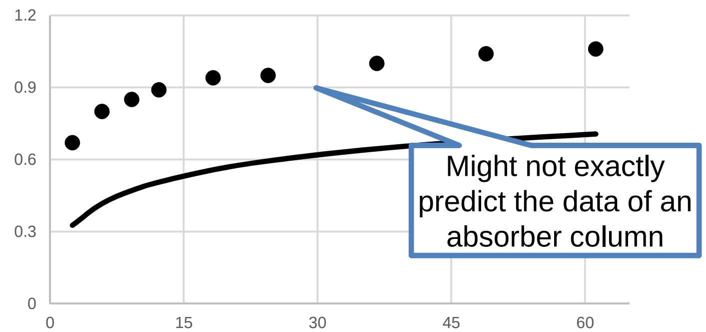
Luo et al., "Comparison and validation of simulation codes against sixteen sets of data from four different pilot plants", Energy Procedia, 1249-1256, 2009

Integrated Mass Transfer Model Development

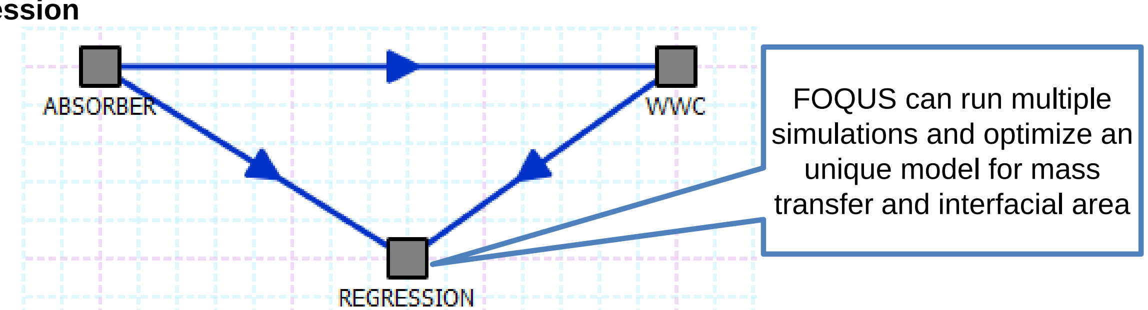
- Diffusivity, viscosity, surface tension, interfacial area, and mass transfer coefficients all important
- Data from both wetted wall column and packed column considered
- Simultaneous regression of these models not previously possible in Aspen
- FOQUS has the capability of simultaneous regression

Usual approach: Sequential regression





FOQUS capability: Simultaneous regression



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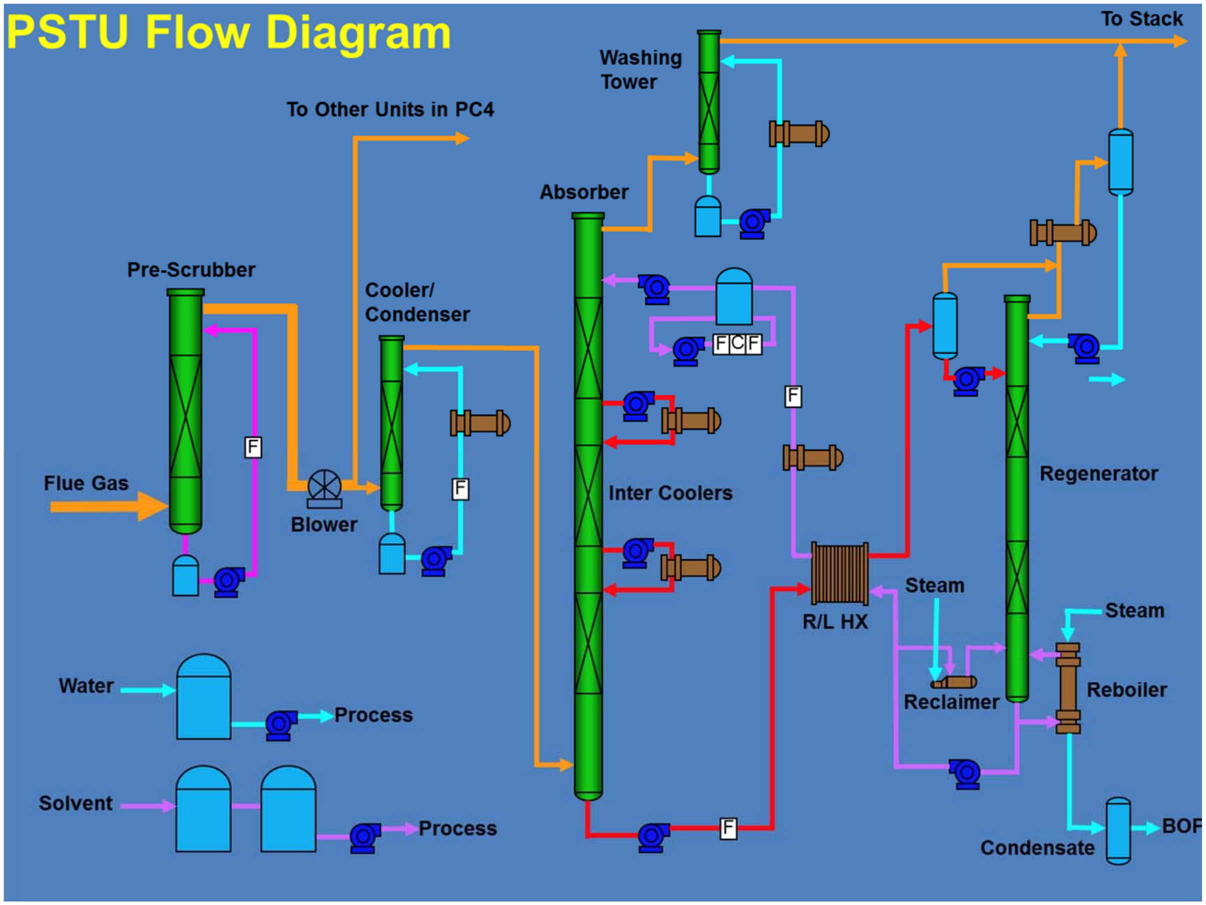
CCSI Team Conducted Tests at NCCC



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Acknowledgements

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Carbon Capture Simulation for Industry Impact

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