CCSI

Carbon Capture Simulation Initiative

NETL CO$_2$ Capture Technology Meeting

David C. Miller

Technical Team Lead
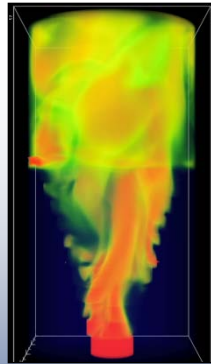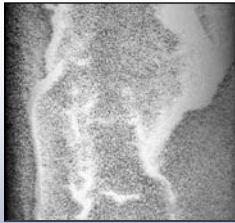
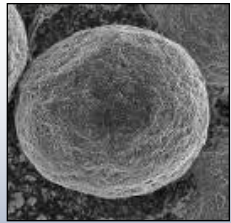National Energy Technology Laboratory

9 July 2012

The U.S. DOE's Carbon Capture Simulation Initiative for Accelerating Commercialization of CCS Technology

- CCSI Toolset
- 5 Year Development Plan
- Technical Accomplishments
  - How these computational tools can be used today

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

Berkeley Lab
Pacific Northwest NATIONAL LABORATORY
NETL
Los Alamos NATIONAL LABORATORY EST. 1943
Lawrence Livermore National Laboratory
CCSI Carbon Capture Simulation Initiative

Academia

Carnegie Mellon
PRINCETON UNIVERSITY
West Virginia University
BOSTON UNIVERSITY
Institute for CLEAN AND SECURE ENERGY THE UNIVERSITY OF UTAH

Industry

FLUOR
ADA ENVIRONMENTAL SOLUTIONS
B&W the babcock & wilcox company
GE
EPRI ELECTRIC POWER RESEARCH INSTITUTE
AIR PRODUCTS
Burns & McDonnell SINCE 1898
SOUTHERN CALIFORNIA EDISON An EDISON INTERNATIONAL Company San Onofre Nuclear Generating Station
ALSTOM
SOUTHERN COMPANY
Duke Energy
URS
BOEING
DUPONT
ExxonMobil
Chevron
PHILLIPS 66
WorleyParsons resources & energy
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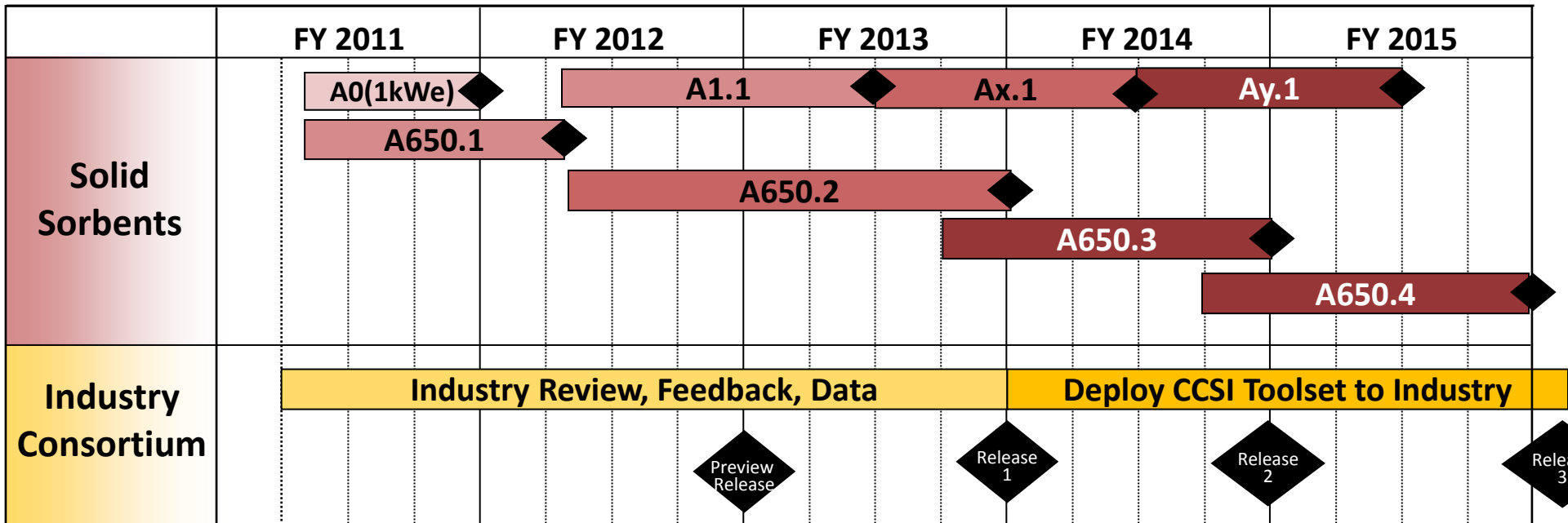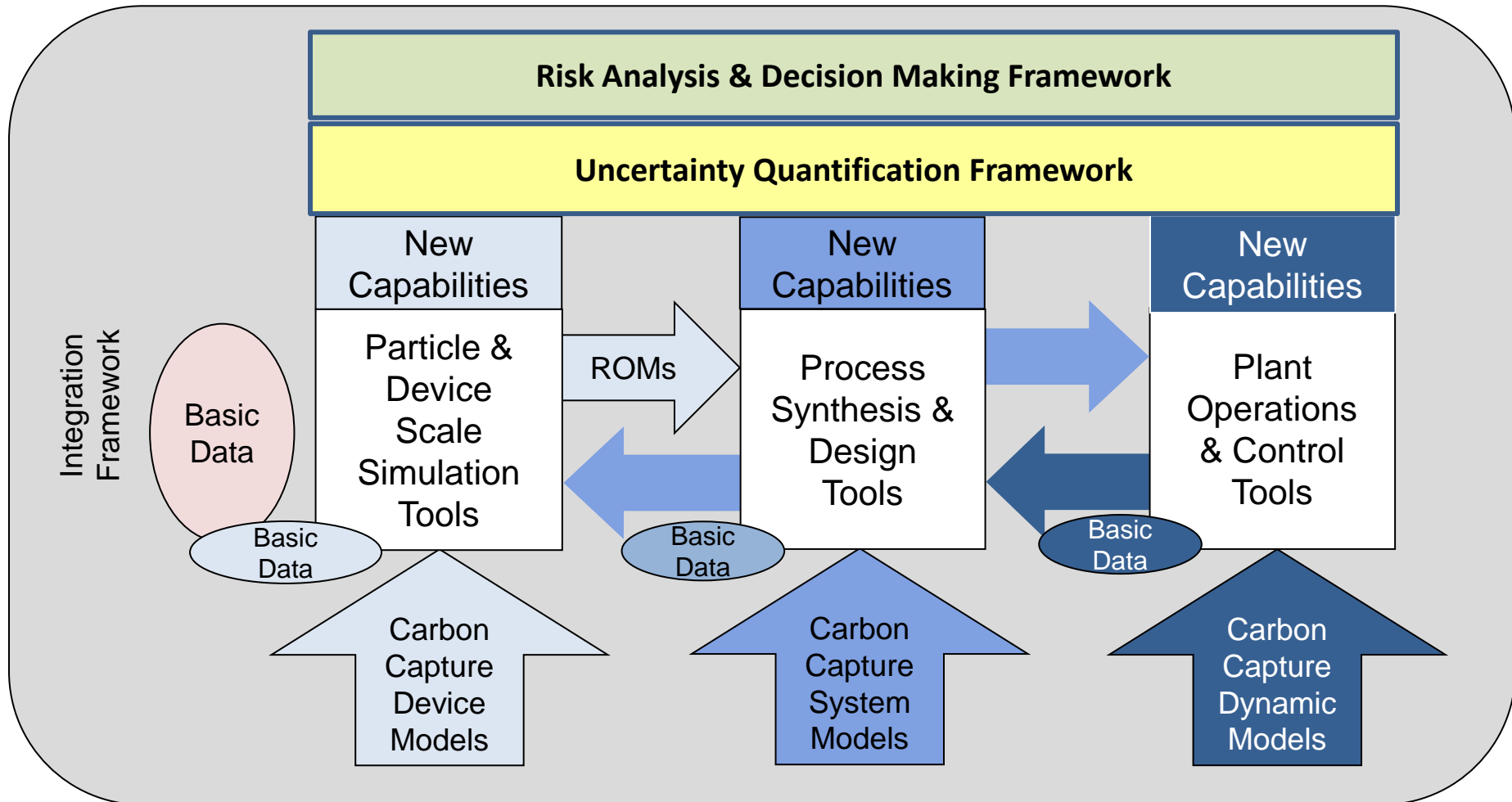Pacific Northwest NATIONAL LABORATORY
U.S. DEPARTMENT OF ENERGY

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CCSI Timeline

- Organizational Meetings
  - March 2010 - October 2010
- HQ organized Scientific Peer Review
  - Jan 25, 2011
- Technical work initiated
  - Feb. 1, 2011
- Industry Advisory Board Workshops
  - Feb. 2011
  - Sept. 2011
  - April 2012
- Board of Directors Review
  - January 2012
- SCC Merit Review (ASME)
  - April 2012
- Preliminary Release of CCSI Toolset
  - September 2012
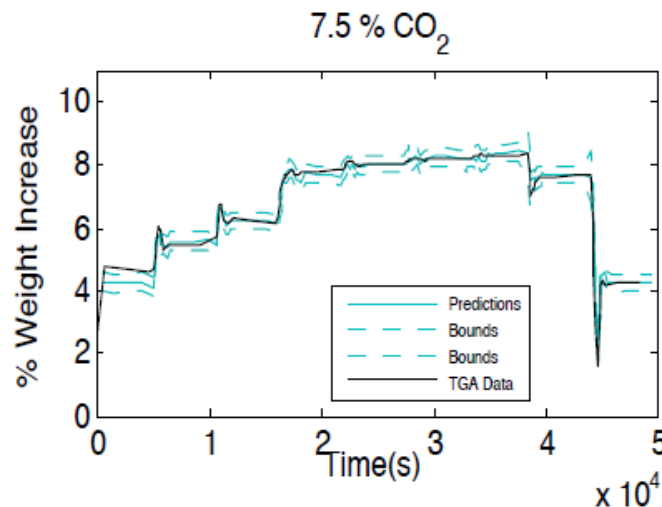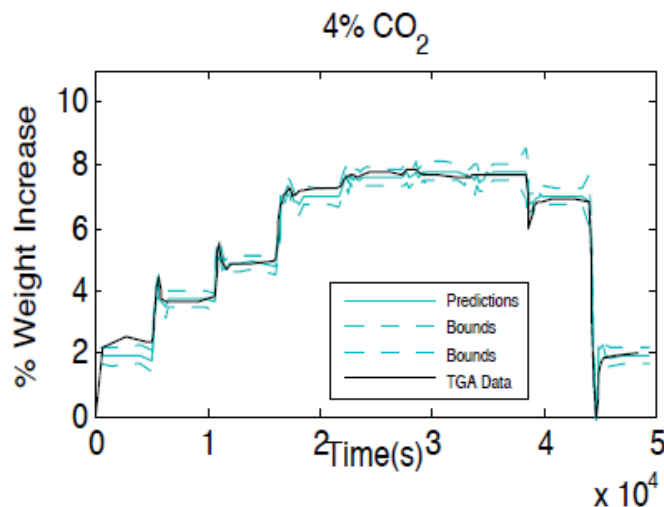
5 Year Plan for Demonstrating CCSI Toolset

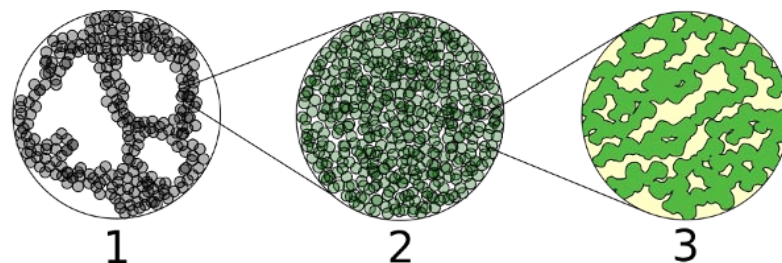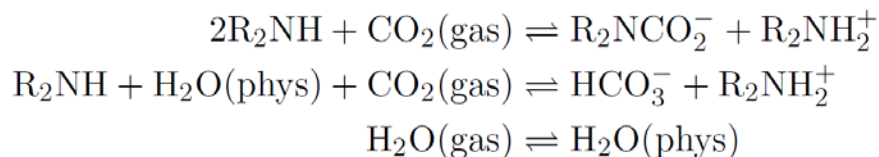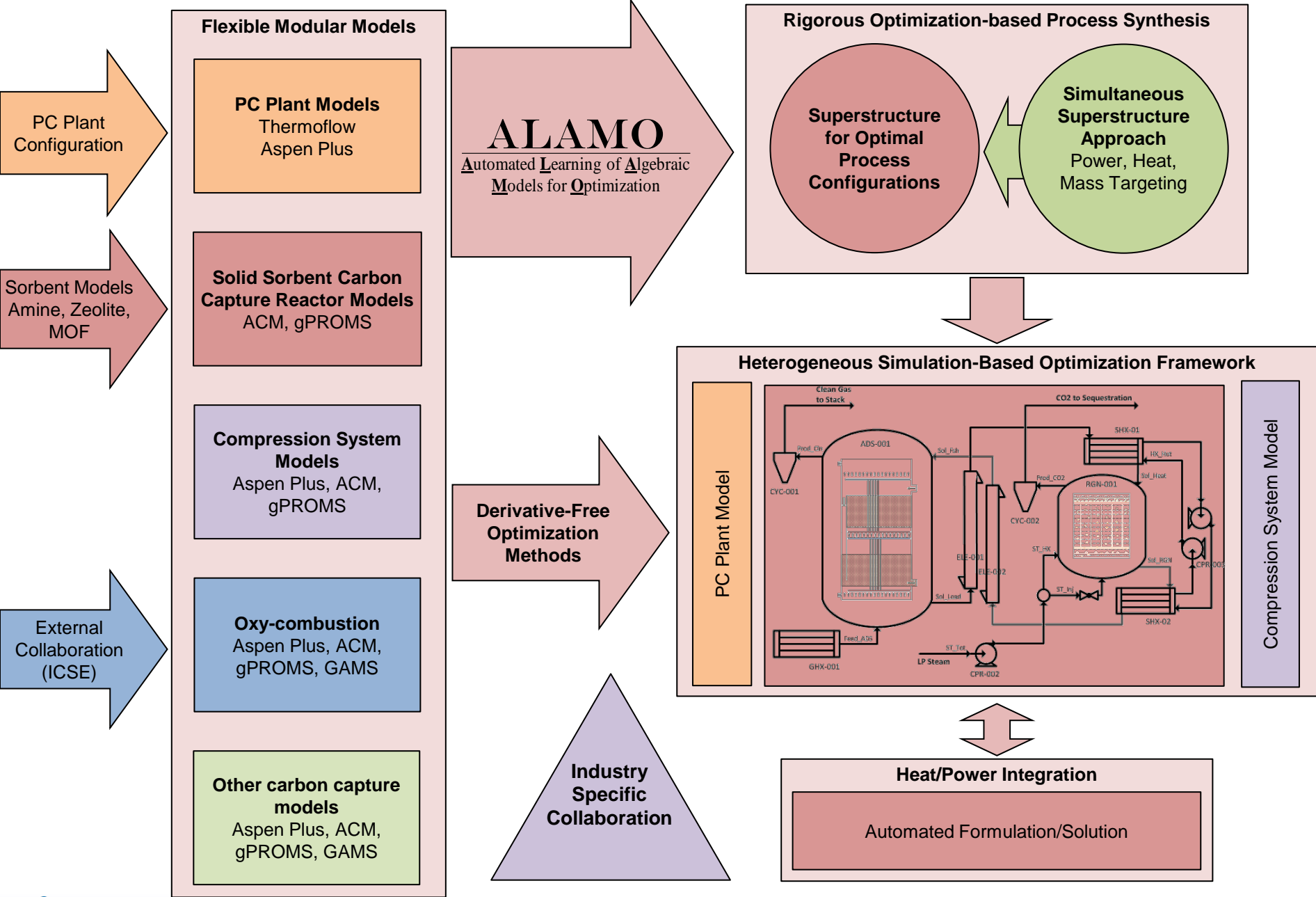|	FY 2011	FY 2012	FY 2013	FY 2014	FY 2015
Solid Sorbents	A0(1kWe) ◆	A1.1 ◆	Ax.1 ◆	Ay.1 ◆	
	A650.1 ◆				
		A650.2 ◆			
			A650.3 ◆		
				A650.4 ◆	
Industry Consortium	Industry Review, Feedback, Data			Deploy CCSI Toolset to Industry	
		Preview Release ◆	Release 1 ◆	Release 2 ◆	Rele 3 ◆

CCSI Toolset Overview

Sorbent Reaction Model with Bayesian-based UQ

- A general lumped kinetic model, quantitatively fit to TDA data, needed for initial CFD and process simulations

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

- 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

KS Bhat, DS Mebane, H Kim, et al., submitted.

Flexible Modular Models

- **PC Plant Models**
  Thermoflow
  Aspen Plus

- **Solid Sorbent Carbon Capture Reactor Models**
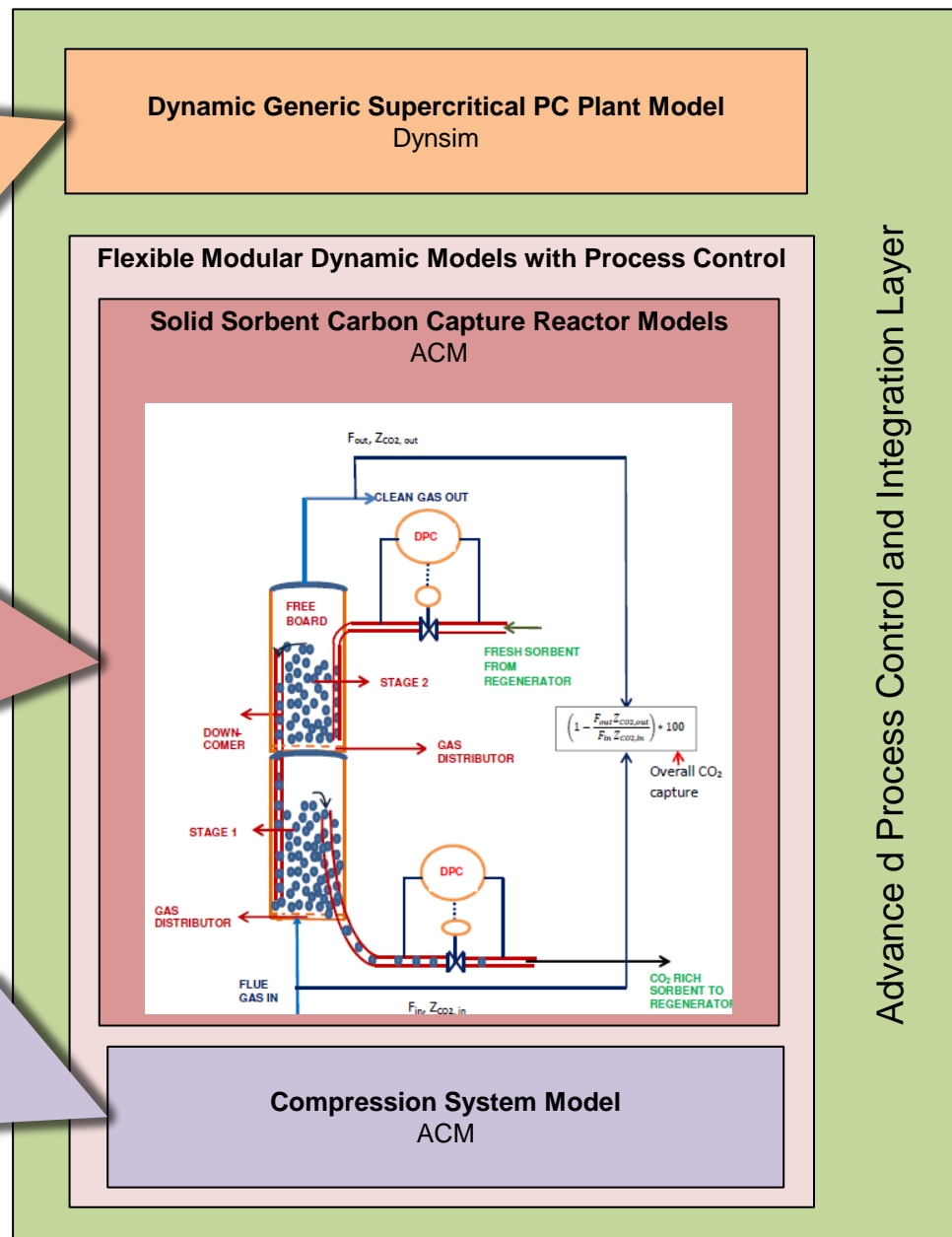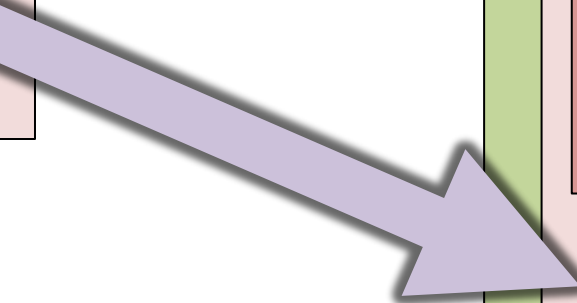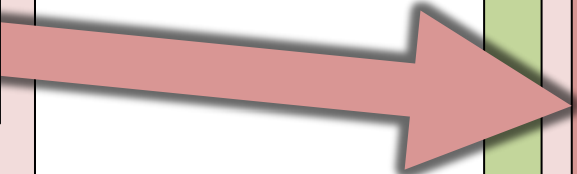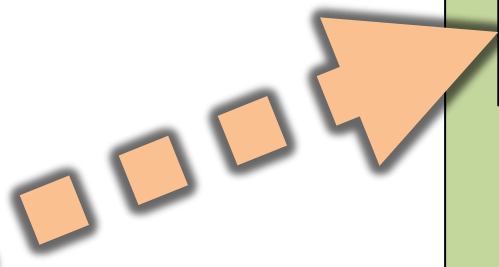 ACM, gPROMS

- **Compression System Models**
  Aspen Plus, ACM, gPROMS

- **Oxy-combustion**
  Aspen Plus, ACM, gPROMS, GAMS

- **Other carbon capture models**
  Aspen Plus, ACM, gPROMS, GAMS

PC Plant Configuration

Sorbent Models Amine, Zeolite, MOF

External Collaboration (ICSE)

ALAMO

Automated **L**earning of **A**lgebraic **M**odels for **O**ptimization

Rigorous Optimization-based Process Synthesis

Superstructure for Optimal Process Configurations

Simultaneous Superstructure Approach
Power, Heat, Mass Targeting

Derivative-Free Optimization Methods

Industry Specific Collaboration

Heterogeneous Simulation-Based Optimization Framework

PC Plant Model

Compression System Model

Clean Gas to Stack

CO2 to Sequestration

ADS-001

CYC-001

Prod_Cln

Sol_Fsh

Sol_Hot

Prod_CO2

CYC-002

RGN-001

SHX-01

HX_Hot

Sol_Heat

ELE-001

ELE-002

ST_HX

ST_Inj

Sol_RGN

CPR-001

Sol_Lean

Feed_ADS

GHX-001

LP Steam

ST_Tot

CPR-002

SHX-02

Heat/Power Integration

Automated Formulation/Solution

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Optimized Capture Process

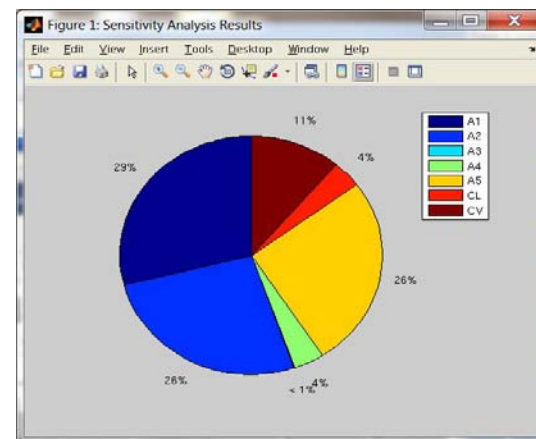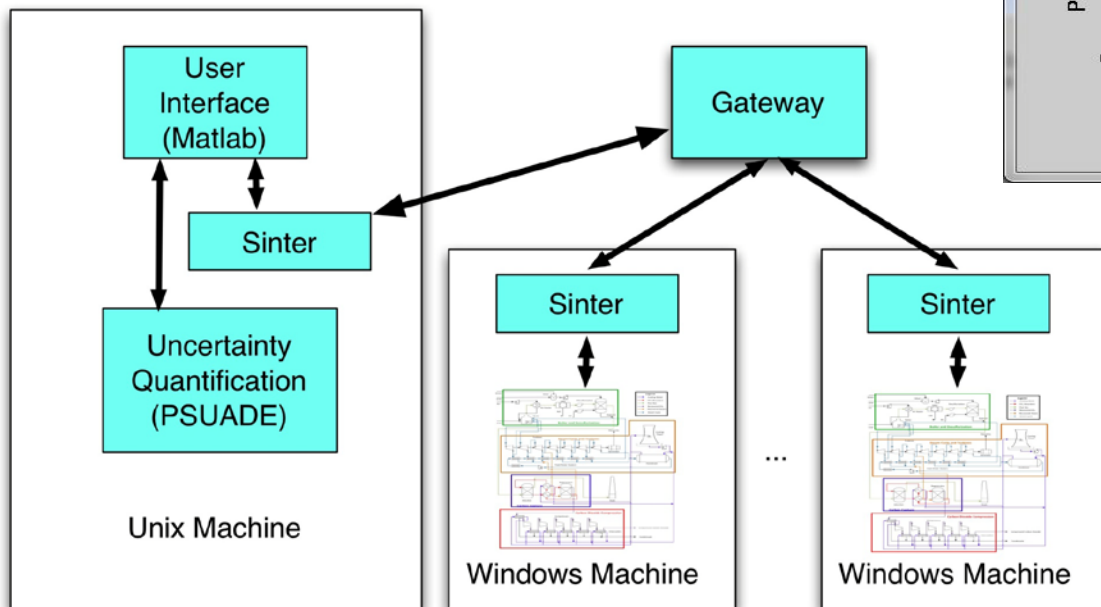|	Solid Sorbent	MEA
	This process	Oyenekan
Q_Rxn (GJ/ton CO2)	1.82	1.48
Bicarbonate	0.04	-
Carbamate	1.41	-
Water	0.38	-
Q_Vap (GJ/ton CO2)	0.00	0.61
Q_Sen (GJ/ton CO2)	1.13	1.35
Total Q	2.95	3.44

ΔLoading
1.8 mol CO2/kg
0.66 mol H2O/kg

Advance d Process Control and Integration Layer

Flexible Modular Models

PC Plant Models
Thermoflow
Aspen Plus

Solid Sorbent Carbon Capture Reactor Models
ACM, gPROMS

Compression System Models
Aspen Plus, ACM, gPROMS

Dynamic Generic Supercritical PC Plant Model
Dynsim

Flexible Modular Dynamic Models with Process Control

Solid Sorbent Carbon Capture Reactor Models
ACM

$F_{out}, Z_{CO2, out}$

CLEAN GAS OUT

DPC

FREE BOARD

STAGE 2

FRESH SORBENT FROM REGENERATOR

DOWN-COMER

GAS DISTRIBUTOR

$$\left(1 - \frac{F_{out} \cdot Z_{CO2, out}}{F_{in} \cdot Z_{CO2, in}}\right) * 100$$

Overall CO_2 capture

STAGE 1

DPC

GAS DISTRIBUTOR

FLUE GAS IN

$F_{in}, Z_{CO2, in}$

CO_2 RICH SORBENT TO REGENERATOR
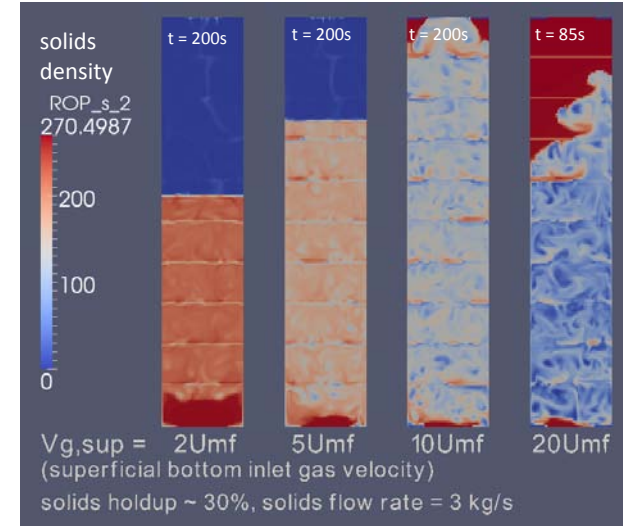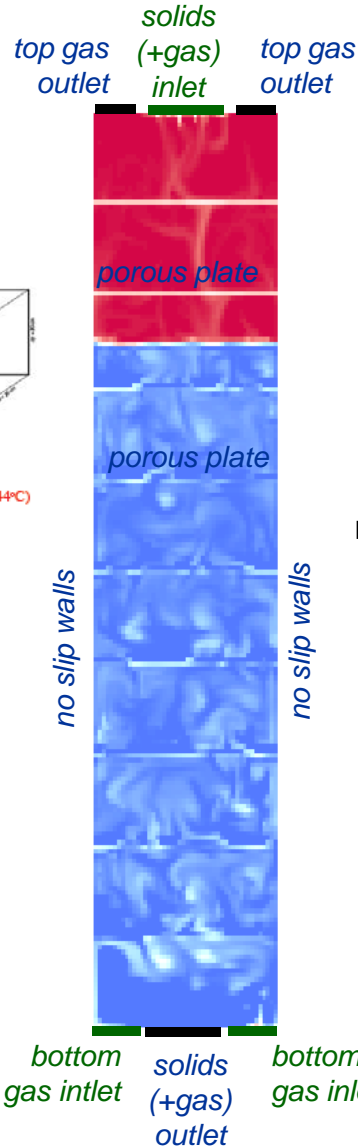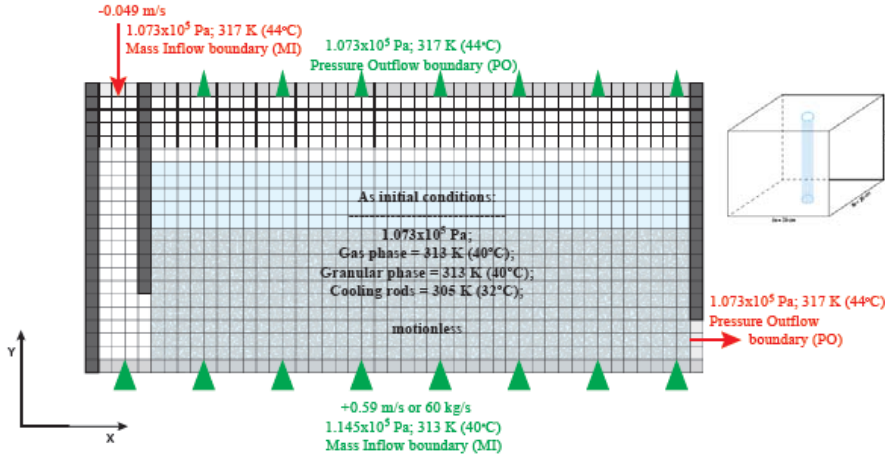
Compression System Model
ACM

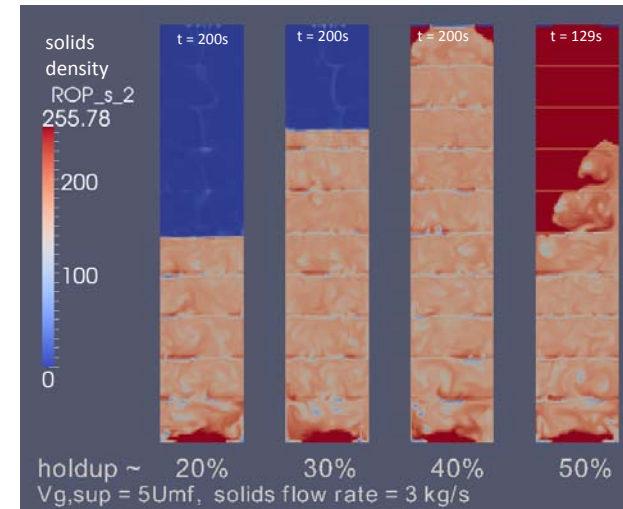# Link to Process Simulation for UQ Analysis

CFD of Adsorber & Regenerator (full scale, 1 MW)

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

Cross-sectional view: Initial and boundary conditions

top gas outlet   *solids (+gas) inlet*   *top gas outlet*

porous plate

porous plate

no slip walls   *no slip walls*

bottom gas intlet   *solids (+gas) outlet*   *bottom gas inlet*

solids density ROP_s_2
270.4987

t = 200s   t = 200s   t = 200s   t = 85s

Vg,sup = 2Umf   5Umf   10Umf   20Umf
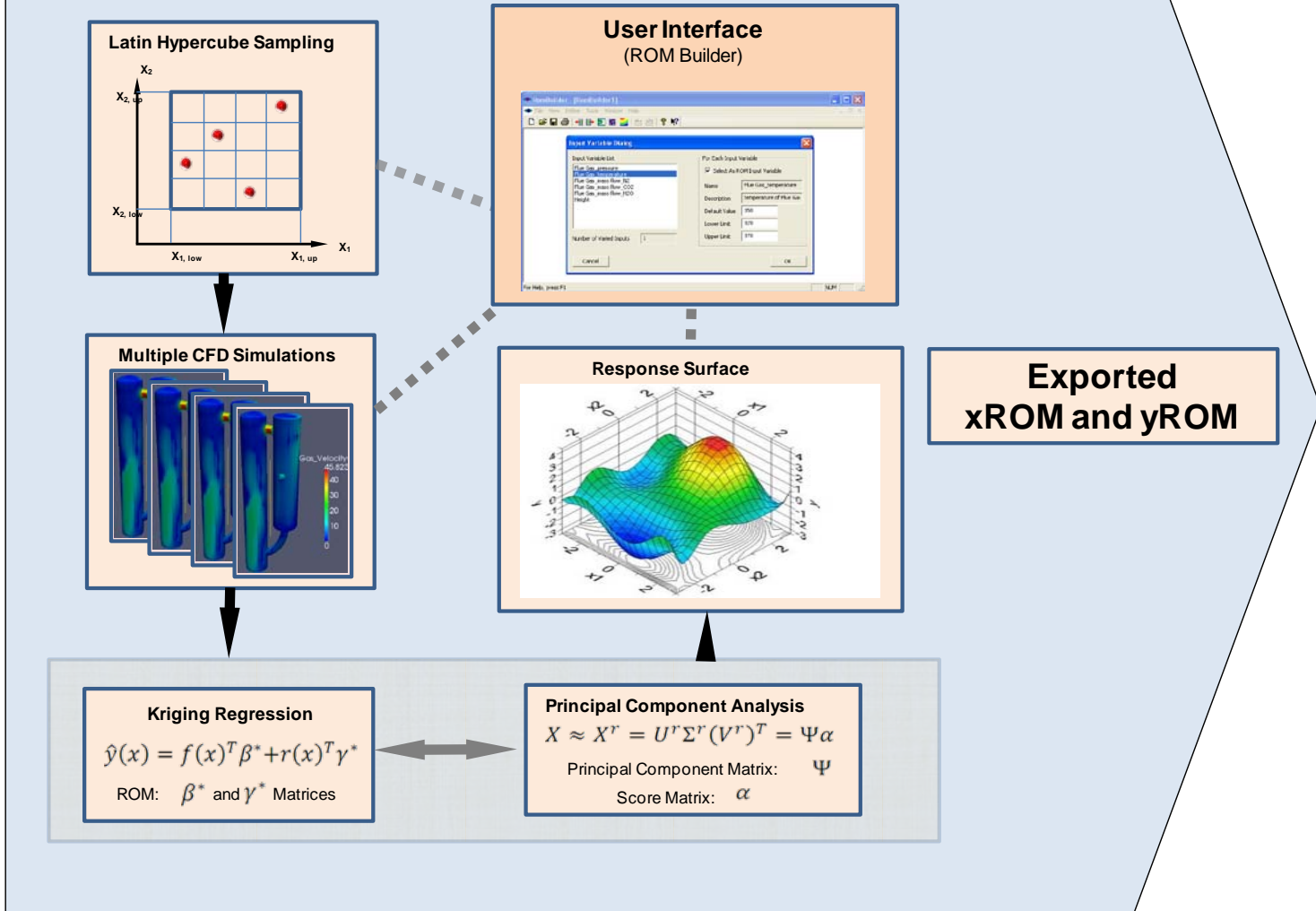(superficial bottom inlet gas velocity)
solids holdup ~ 30%, solids flow rate = 3 kg/s

⟹ Increasing steam inlet velocity

solids density ROP_s_2
255.78

t = 200s   t = 200s   t = 200s   t = 129s

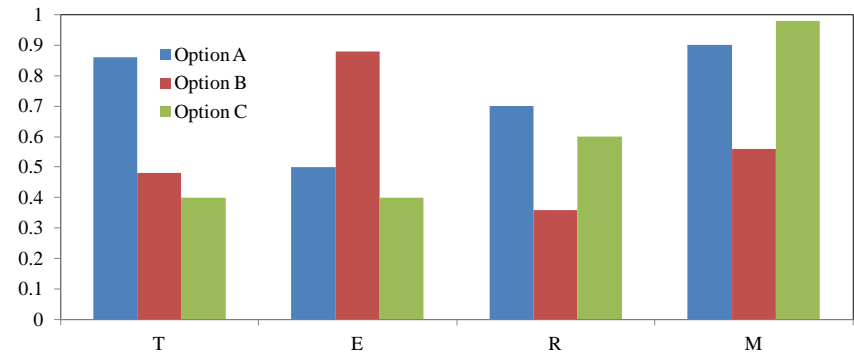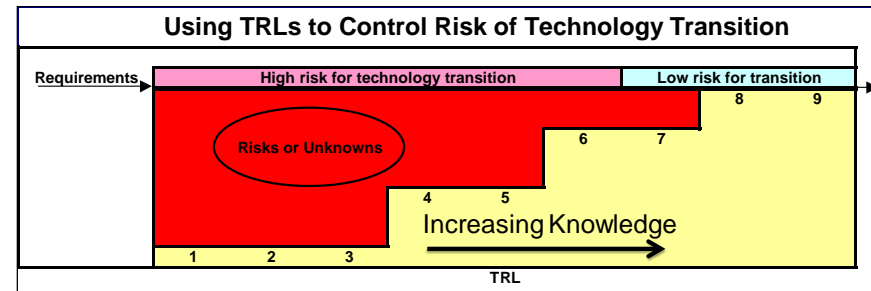holdup ~ 20%   30%   40%   50%
Vg,sup = 5Umf, solids flow rate = 3 kg/s

⟹ Decreasing bed voidage

Reduced Order Model Development

Latin Hypercube Sampling

User Interface
(ROM Builder)

Multiple CFD Simulations

Response Surface

**Exported
xROM and yROM**

Kriging Regression

$$\hat{y}(x) = f(x)^T \beta^* + r(x)^T \gamma^*$$

ROM: β^* and γ^* Matrices

Principal Component Analysis

$$X \approx X^r = U^r \Sigma^r (V^r)^T = \Psi \alpha$$

Principal Component Matrix: Ψ

Score Matrix: α

Formal Risk Metrics as Flexible Tools for Risk Analysis

Project Progression

| Component Validation in relevant environment TRL=5 | Mini-Plant Design and Development (small-scale pilot in relevant environment) TRL=6 | Pilot-Plant Design and Development (large-scale demonstration in operational environment) TRL=7 | Production Plant Design and Construction TRL=8 |

2   4   7   12

Using TRLs to Control Risk of Technology Transition

Requirements → High risk for technology transition | Low risk for transition

8   9

Risks or Unknowns

6   7

4   5

Increasing Knowledge

1   2   3

TRL

- Risk Mitigation
- Risk Prioriti-zation
- Decision Process

Models — Risk — Data

Option A
Option B
Option C
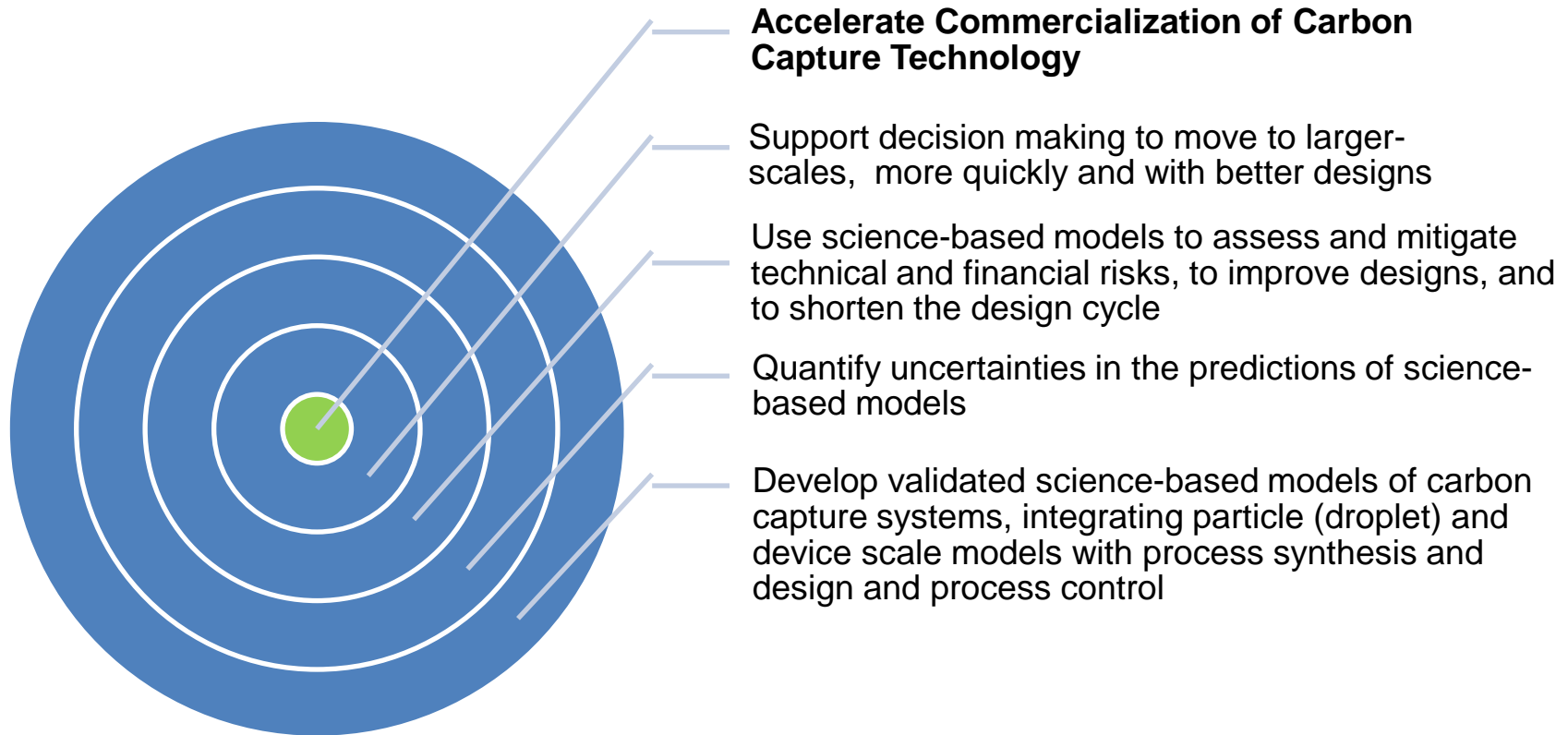
T   E   R   M

T : Technical performance against objective

E : Economic

R : Risk (includes uncertainty in T, E, M, etc.)

M : Maturity (TRL-based)

Computational Tools to Accelerate Technology Development & Scale up
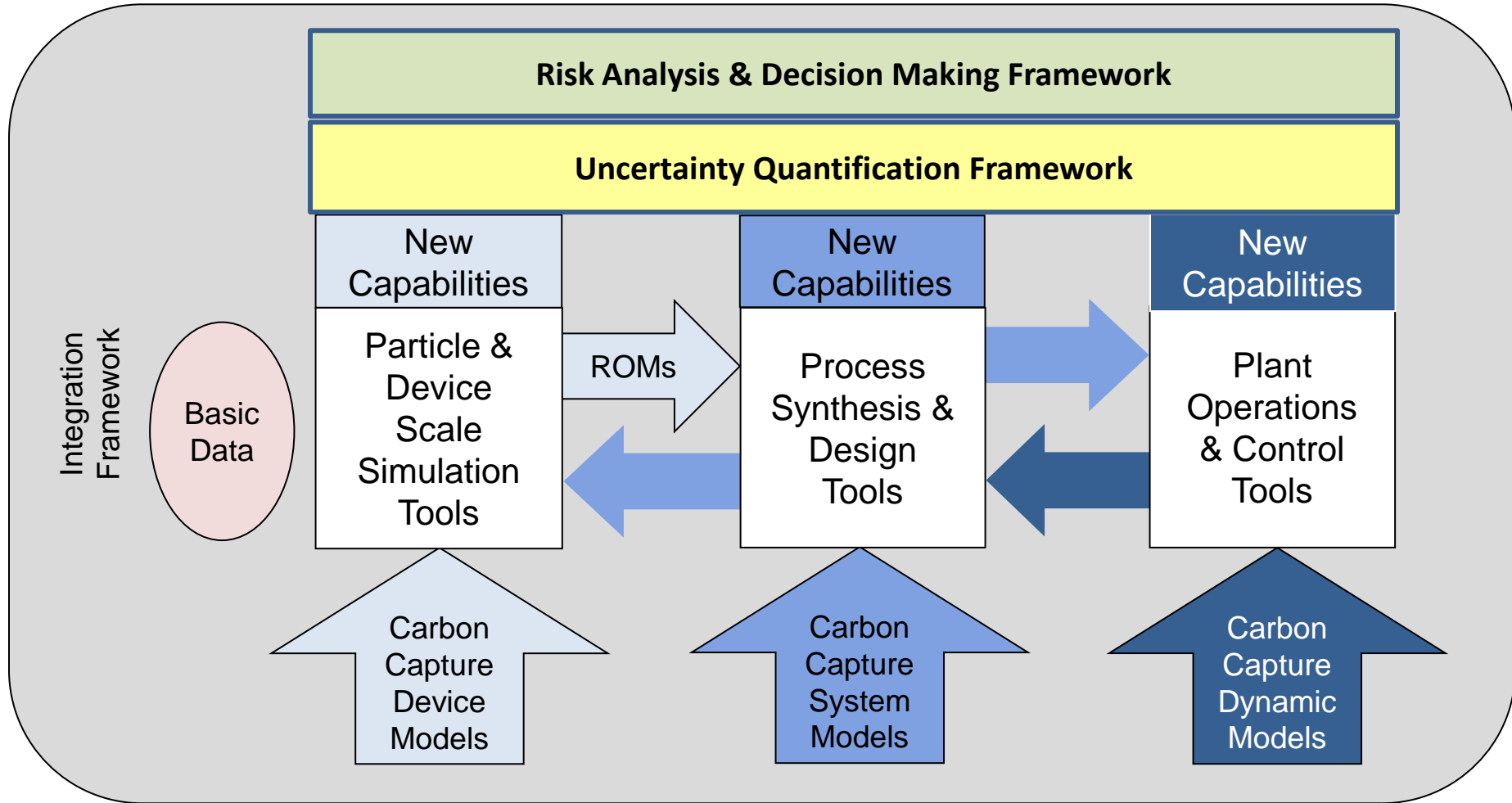
Potential Benefits to Program

Accelerate Commercialization of Carbon Capture Technology

Support decision making to move to larger-scales, more quickly and with better designs

Use science-based models to assess and mitigate technical and financial risks, to improve designs, and to shorten the design cycle

Quantify uncertainties in the predictions of science-based models

Develop validated science-based models of carbon capture systems, integrating particle (droplet) and device scale models with process synthesis and design and process control

CCSI Collaboration Opportunities Roundtable - Woodlawn I

This evening @ 5 PM

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