CCSI™

Carbon Capture Simulation Initiative

Overview for CAPD ESI Meeting

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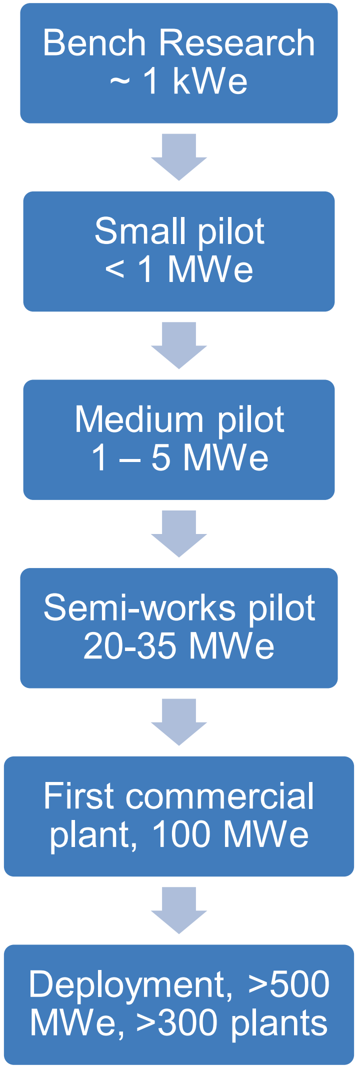
Technical Team Lead

11 March 2012

U.S. DEPARTMENT OF
ENERGY

Carbon Capture Challenge

- The traditional pathway from discovery to commercialization of energy technologies can be quite long, i.e., ~ 2-3 decades
- President's plan requires that barriers to the widespread, safe, and cost-effective deployment of CCS be overcome within 10 years
- To help realize the President's objectives, new approaches are needed for taking carbon capture concepts from lab to power plant, quickly, and at low cost and risk
- CCSI will accelerate the development of carbon capture technology, from discovery through deployment, with the help of science-based simulations



Bench Research
~ 1 kWe

Small pilot
< 1 MWe

Medium pilot
1 – 5 MWe

Semi-works pilot
20-35 MWe

First commercial plant, 100 MWe

Deployment, >500 MWe, >300 plants

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

Academia

Carnegie Mellon

Princeton University

West Virginia University

Boston University

Institute for Clean and Secure Energy
The University of Utah

Industry

B&W the babcock & wilcox company

ADA Environmental Solutions

Fluor

GE

EPRI Electric Power Research Institute

Air Products

Burns & McDonnell Since 1898

Duke Energy

URS

Alstom

Southern Company

Southern California Edison
An Edison International Company
San Onofre Nuclear Generating Station

Boeing

Chevron

ExxonMobil

WorleyParsons resources & energy

Eastman

1-31-2012

Essential for accelerating commercial deployment

CCSI™ Carbon Capture Simulation Initiative

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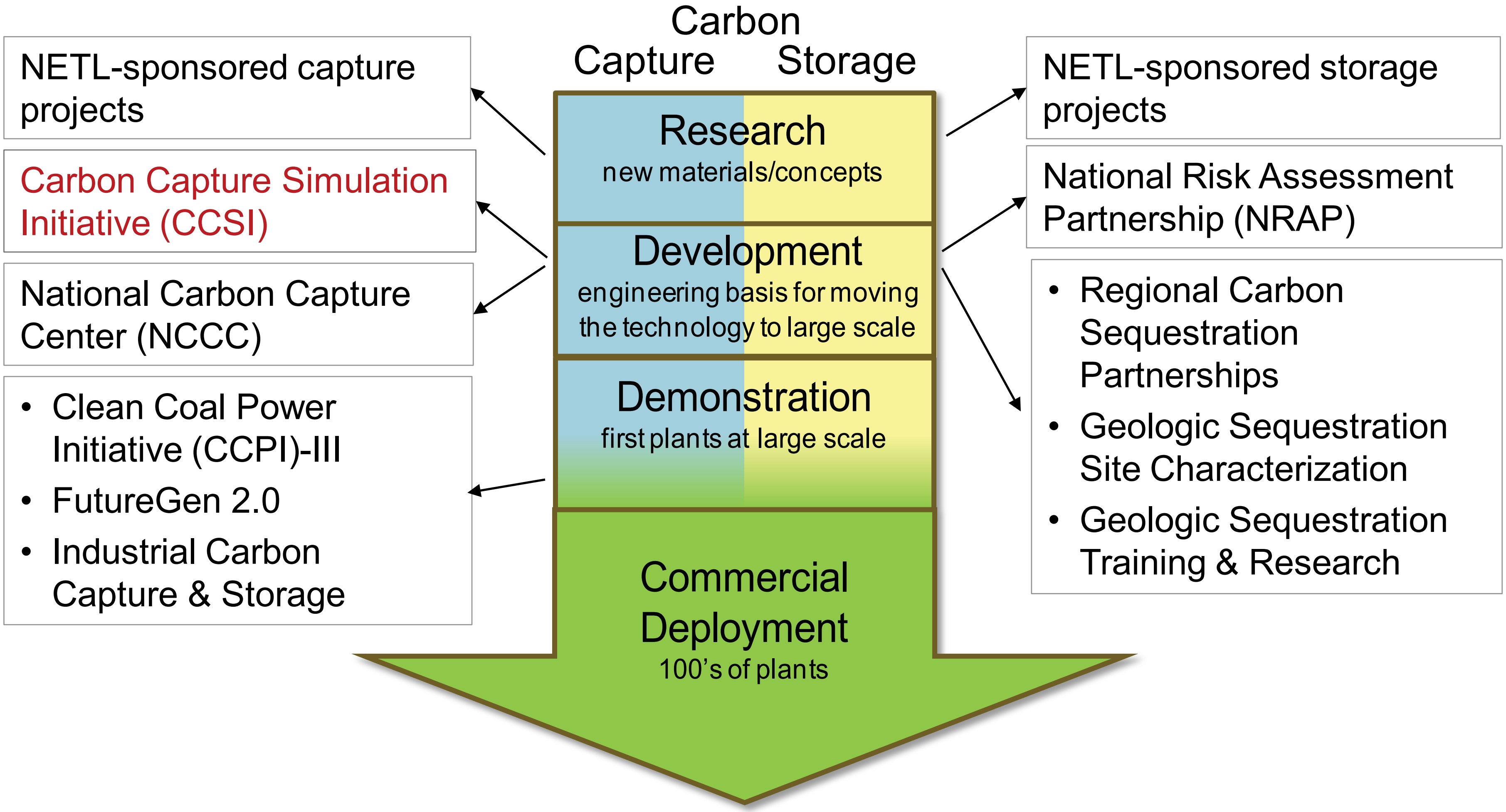
Pacific Northwest National Laboratory

U.S. Department of Energy

CCSI is part of the DOE CCS RD&D Roadmap



NETL-sponsored capture projects

Carbon Capture Simulation Initiative (CCSI)

National Carbon Capture Center (NCCC)

- Clean Coal Power Initiative (CCPI)-III
- FutureGen 2.0
- Industrial Carbon Capture & Storage

NETL-sponsored storage projects

National Risk Assessment Partnership (NRAP)

- Regional Carbon Sequestration Partnerships
- Geologic Sequestration Site Characterization
- Geologic Sequestration Training & Research

http://www.netl.doe.gov/publications/press/2011/110106-DOE-NETL_CO2_Capture_and_Storage_RDD_Roadmap.html

Industrial Challenge Problem (ICP) Underpin CCSI Toolset Development

Desirable ICP Attributes

- Provides relevant results to problems of current interest
- Develops CCSI capability that can be used for a wide range applications later
- Data available for validation

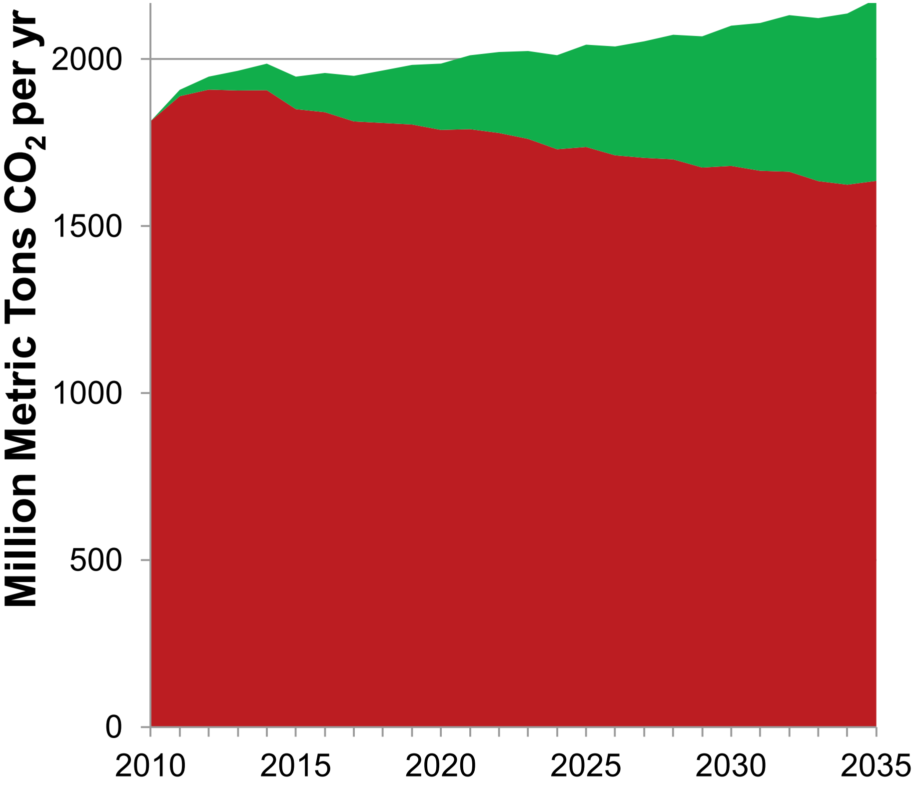
ICP priority: Pulverized coal plants

- 80% of emissions in 2030 will be from plants existing in 2010
- Approximately 280 U.S. pulverized coal plants are CCS candidates*

Initial focus: Solid Sorbents

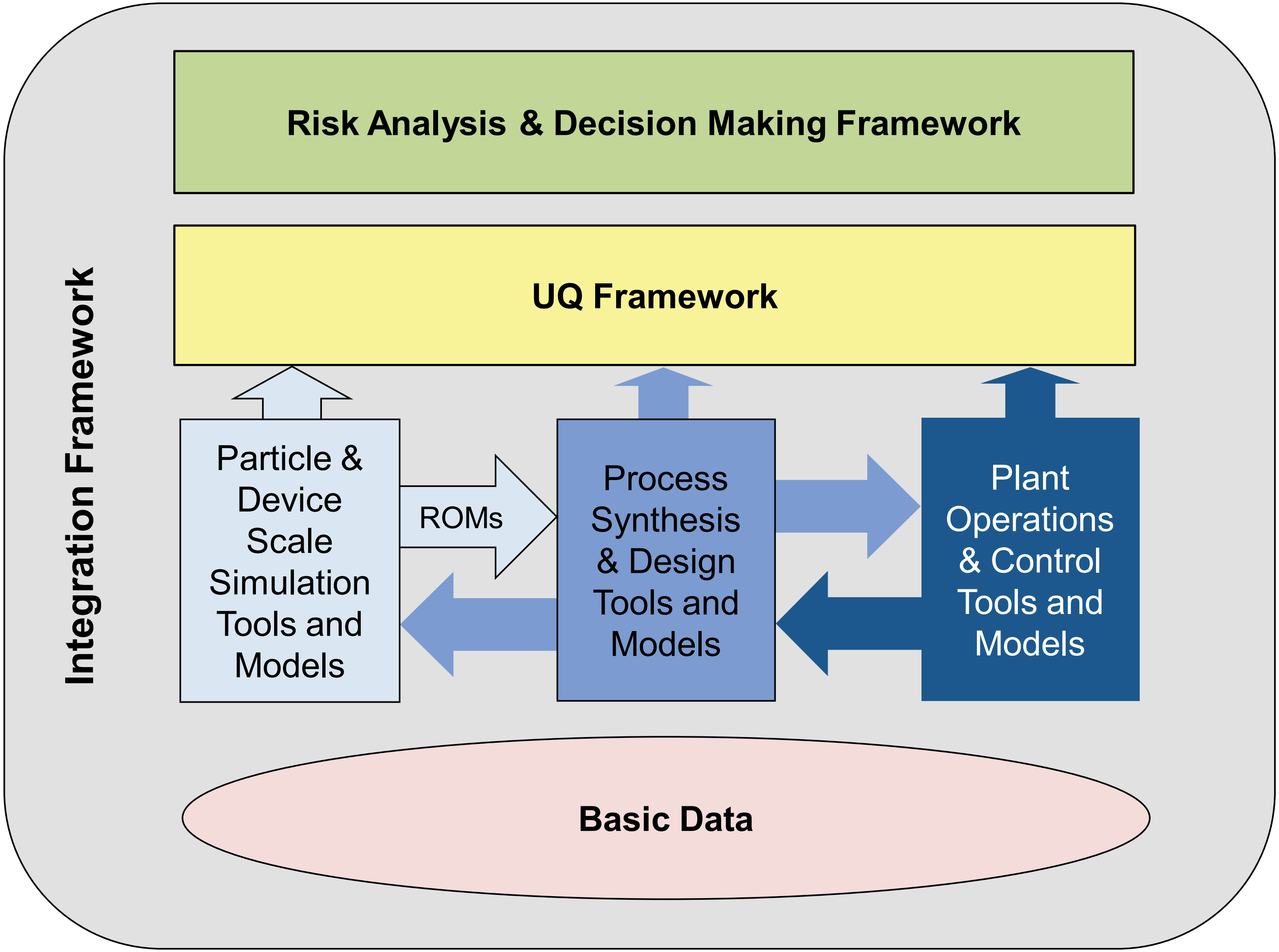
- Opportunity to impact reactor & system design

Projected CO_2 Emissions from U.S. Coal-Fired Power Plants



Source: EIA, Annual Energy Outlook 2010 Early Release, Dec. 2009

Nichols, C., (2010). "Coal-Fired Power Plants in the United States: Examination of the Cost of Retrofitting with CO2 Capture Technology and the Potential for Improvements in Efficiency", DOE/NETL-402/102309



Integration Framework

Risk Analysis & Decision Making Framework

UQ Framework

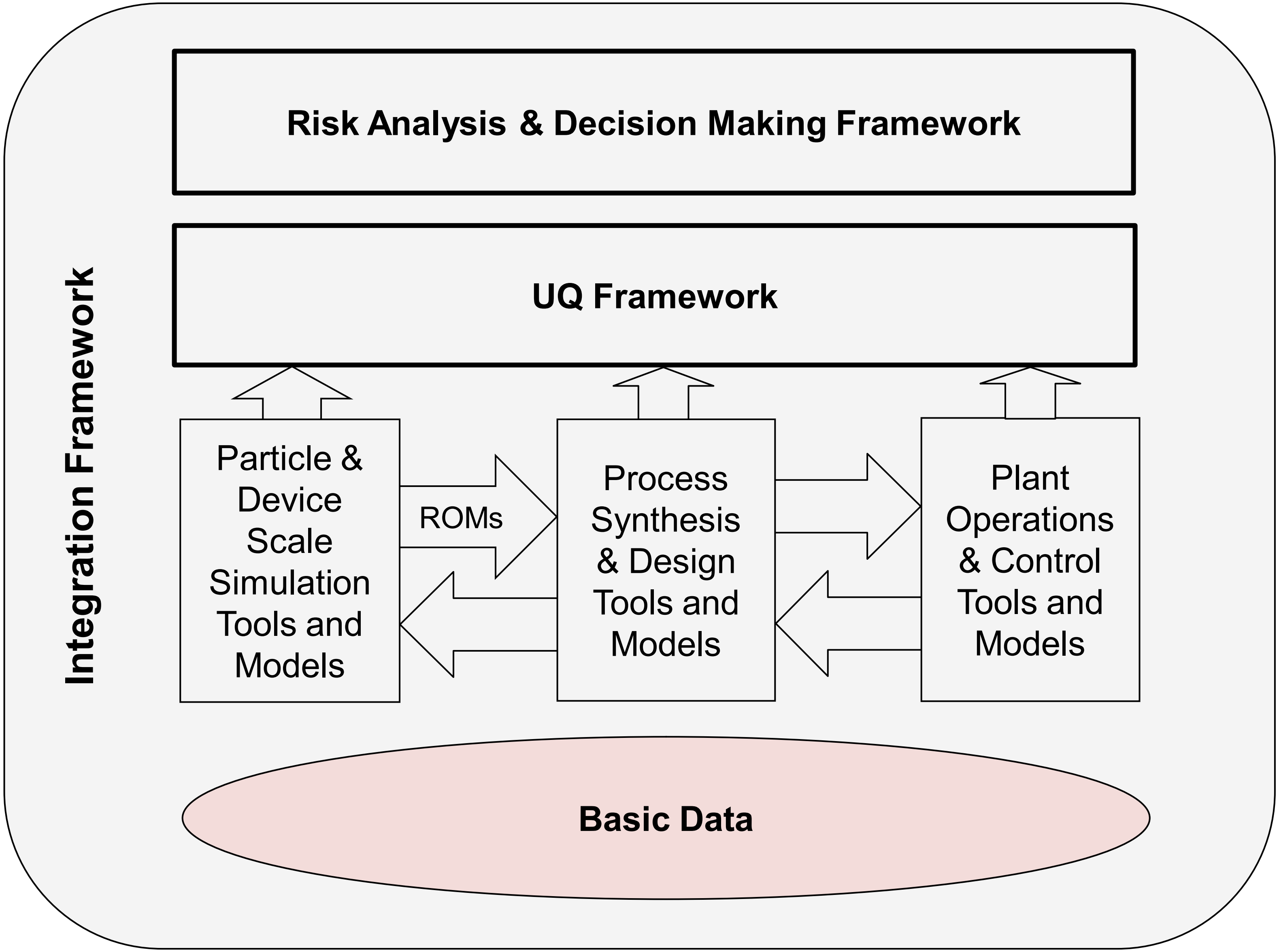
Particle & Device Scale Simulation Tools and Models

ROMs

Process Synthesis & Design Tools and Models

Plant Operations & Control Tools and Models

Basic Data



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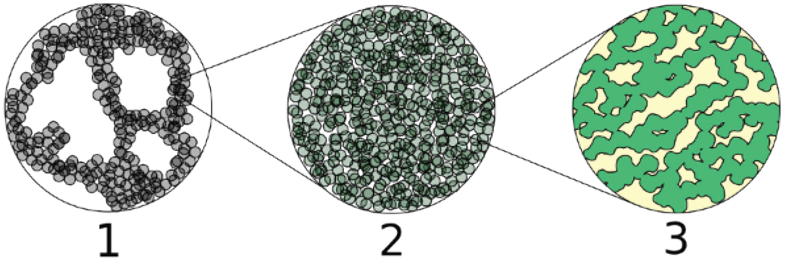
PEI-Impregnated Silica Sorbent Reaction Model

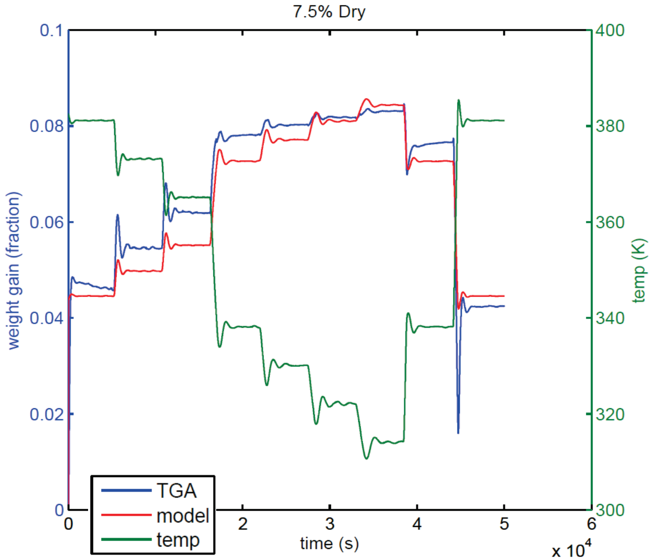
- A general lumped kinetic model, quantitatively fit to TDA data, needed for initial CFD and process simulations
- High-fidelity model:
  - Sorbent microstructure broken down into three length scales
  - Separate treatment of gas-phase and polymer-phase transport
  - Accurately describes TGA features arising from bulk CO_2 transport effects

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

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

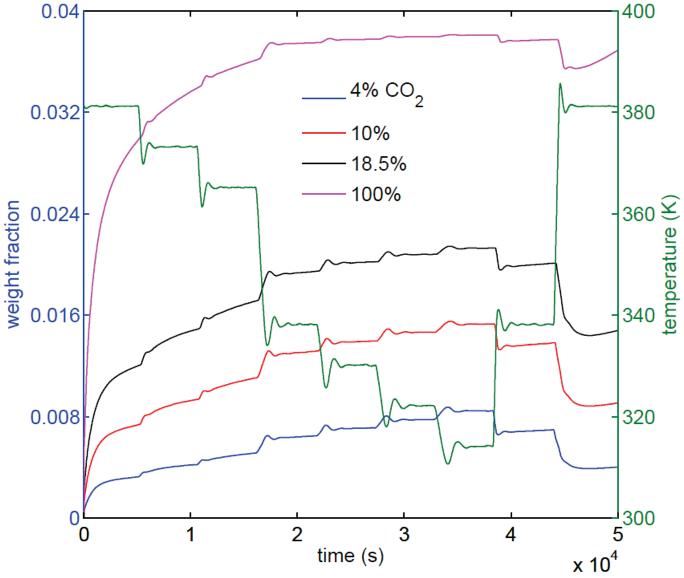
$$H_2O(gas) \rightleftharpoons H_2O(phys)$$





(left) lumped kinetic fit to experimental TGA for NETL-32D sorbent

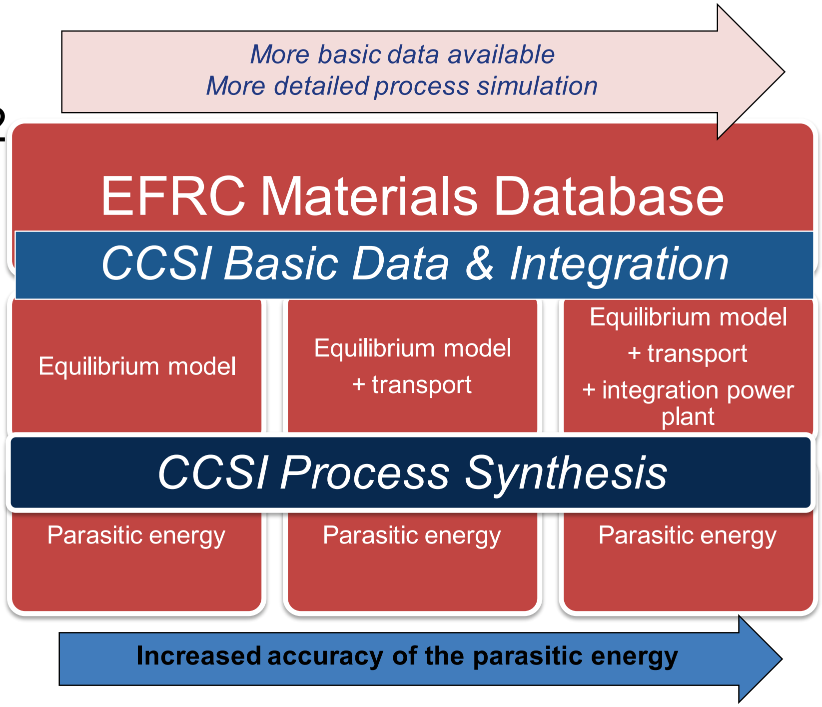
(right) simulated TGA (not fit to data) showing transport-influenced desorption behavior



Hierarchal Material Design

- Develop an API to enable access to the LBNL materials database.
    - Develop formats for exporting data.
    - Test with the microporous zeolite CO2 capture material.

- Providing new API functionality for adding new structures of solid sorbents to the LBNL materials database.
    - Automatic characterization using the available tools.
    - Test with PEI polymer-impregnated microporous silica.



More basic data available
More detailed process simulation

EFRC Materials Database

CCSI Basic Data & Integration

Equilibrium model

Equilibrium model
+ transport

Equilibrium model
+ transport
+ integration power plant

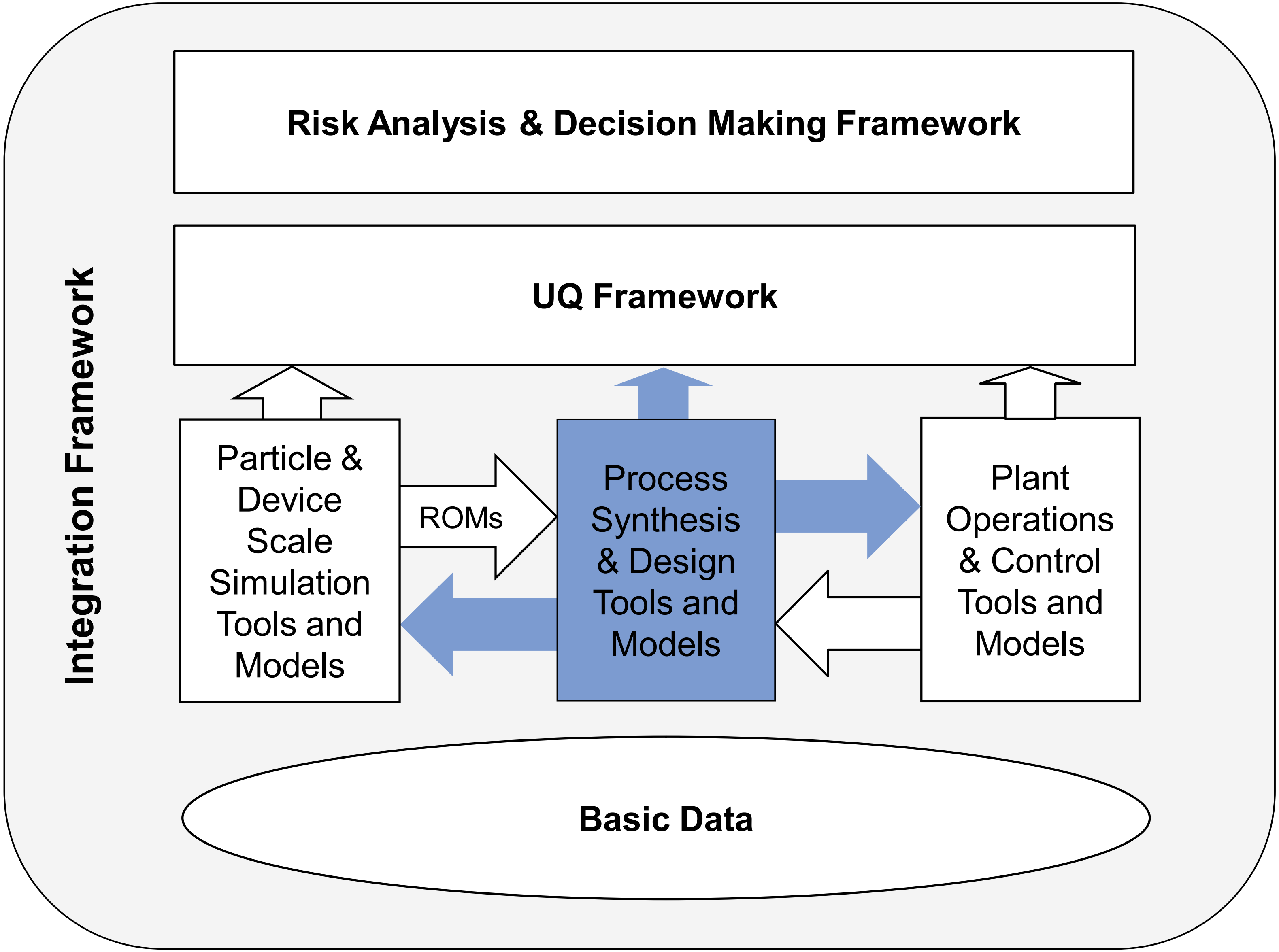
CCSI Process Synthesis

Parasitic energy

Parasitic energy

Parasitic energy

Increased accuracy of the parasitic energy



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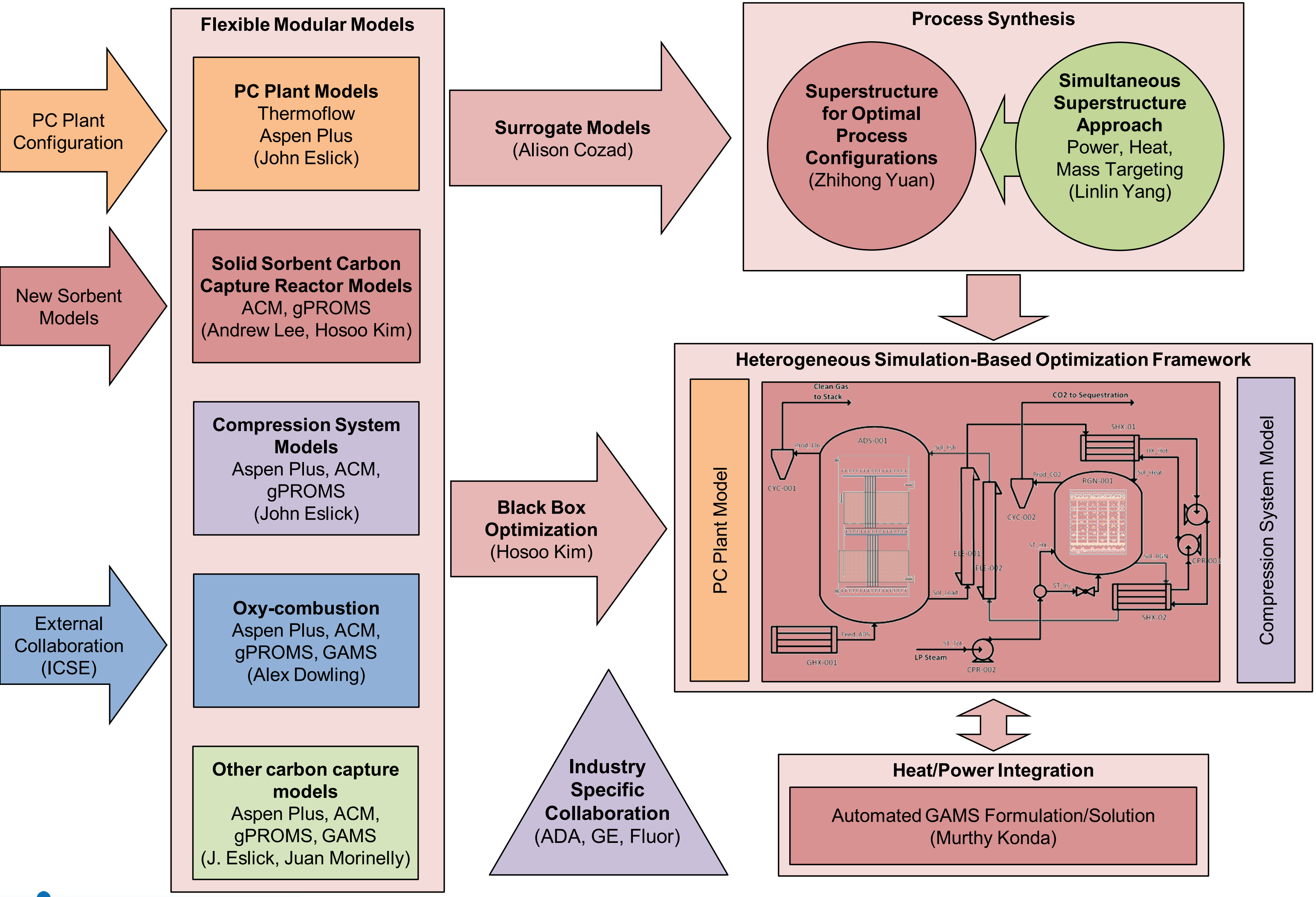

PC Plant Configuration

New Sorbent Models

External Collaboration (ICSE)

Flexible Modular Models

PC Plant Models
Thermoflow
Aspen Plus
(John Eslick)

Solid Sorbent Carbon Capture Reactor Models
ACM, gPROMS
(Andrew Lee, Hosoo Kim)

Compression System Models
Aspen Plus, ACM, gPROMS
(John Eslick)

Oxy-combustion
Aspen Plus, ACM, gPROMS, GAMS
(Alex Dowling)

Other carbon capture models
Aspen Plus, ACM, gPROMS, GAMS
(J. Eslick, Juan Morinelly)

Surrogate Models
(Alison Cozad)

Black Box Optimization
(Hosoo Kim)

Industry Specific Collaboration
(ADA, GE, Fluor)

Process Synthesis

Superstructure for Optimal Process Configurations
(Zhihong Yuan)

Simultaneous Superstructure Approach
Power, Heat, Mass Targeting
(Linlin Yang)

Heterogeneous Simulation-Based Optimization Framework

PC Plant Model

Compression System Model

Heat/Power Integration

Automated GAMS Formulation/Solution
(Murthy Konda)

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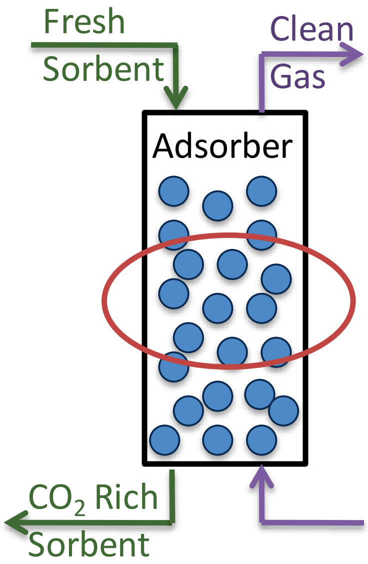
Methodology for Determining Optimal Process Configurations

Detailed model developed in commercial process simulation tool



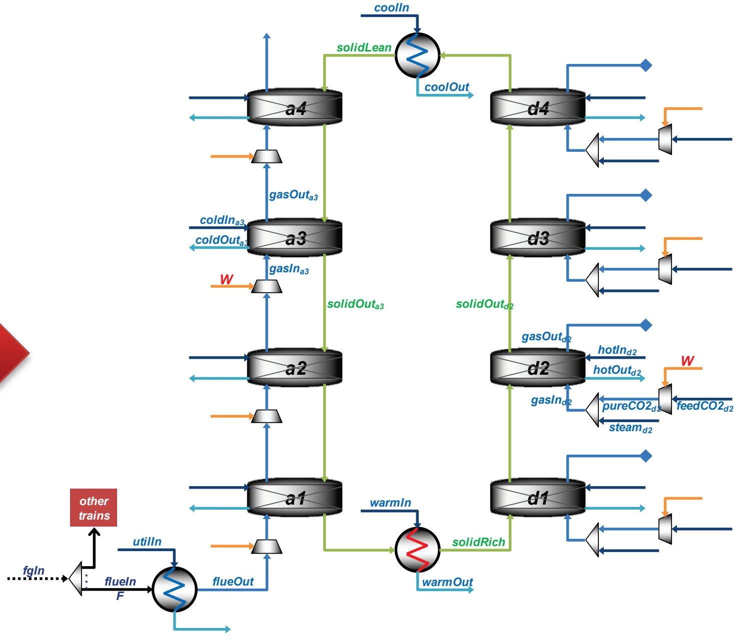
Develop algebraic model

ALAMO

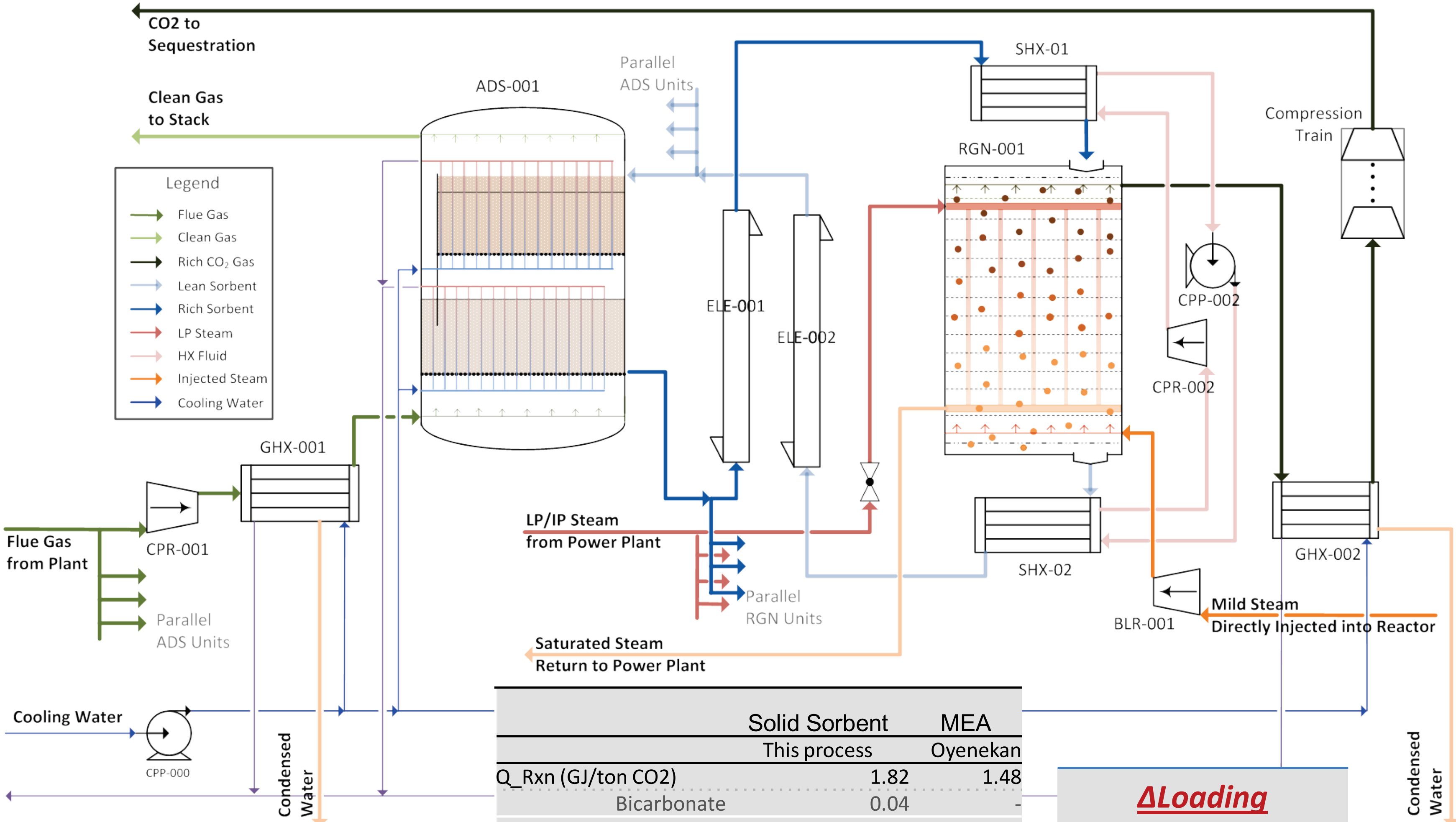
Automated Learning of Algebraic Models for Optimization

- **Sample points**
- **Build model**
- **Adaptive sampling** and **Model validation**
- **Done**

Formulate and solve superstructure to determine optimal process configuration



Optimized Capture Process

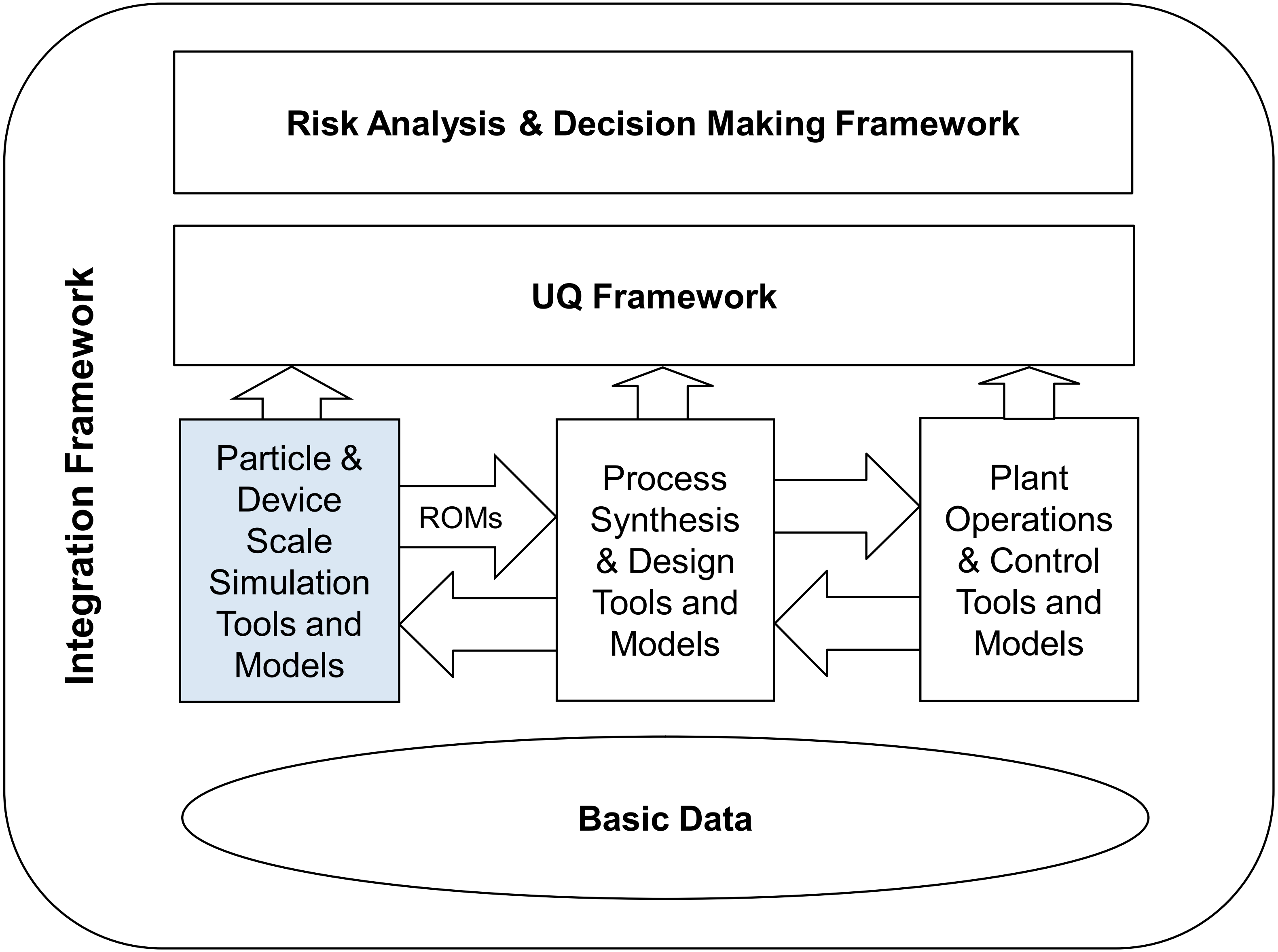


	Solid Sorbent This process	MEA Oyenekan
Q_Rxn (GJ/ton CO2)	1.82	1.48
Bicarbonate	0.04	-
Carbamate	1.41	-
Water	0.38	-
Q_Vap (GJ/ton CO2)	0.00	0.61
Q_Sen (GJ/ton CO2)	1.13	1.35
Total Q	2.95	3.44

ΔLoading

1.8 mol CO2/kg

0.66 mol H2O/kg



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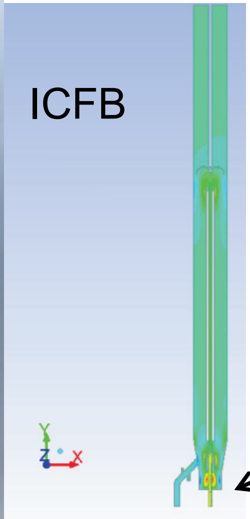
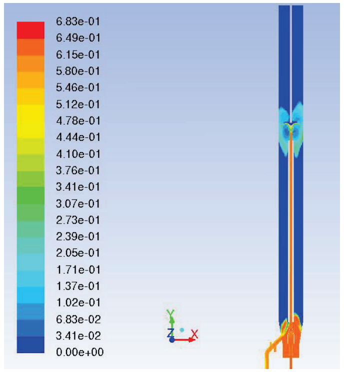
Device Scale Simulations of 1kWe ADA System

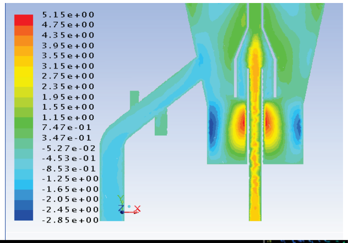
- Developed a simplified CFD model geometry for performing numerical flow simulations from the original ADA-ES CAD model
- Reduced the complexity of the geometry by dividing the reactor into simpler components:
    - 3D Riser bottom section
    - 2D Riser top section
    - ICFB
    - Regenerator
- Generated various meshes and performed computational analysis using ANSYS FLUENT® :
    - Eulerian-Eulerian (E-E)
    - Dense discrete particle method (DDPM)
- Compared the computational efficiency and predicted solutions of the EE and DDPM methods
- Incorporated reaction chemistry and thermodynamics in Fluent simulations

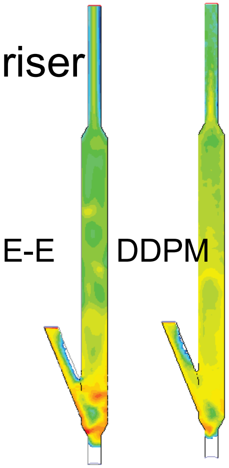


city of particles

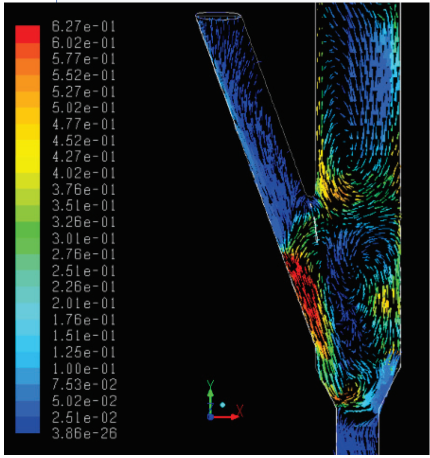


Distribution of solid volume fraction





Predicted y solid volume fraction

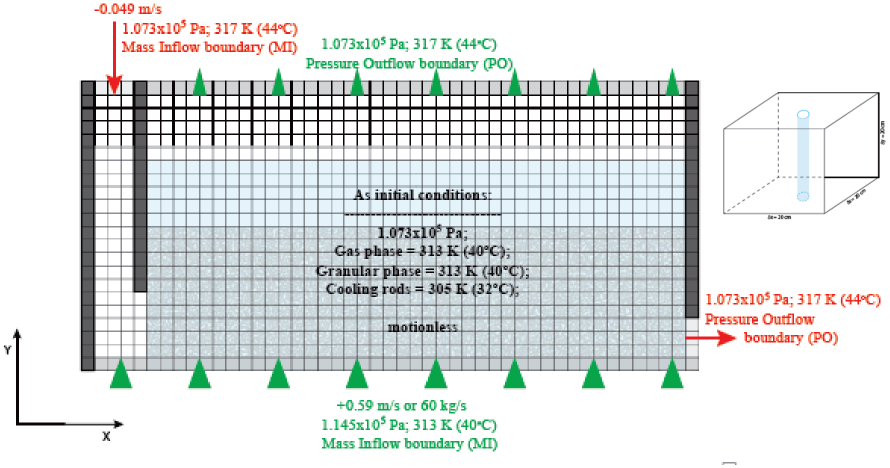


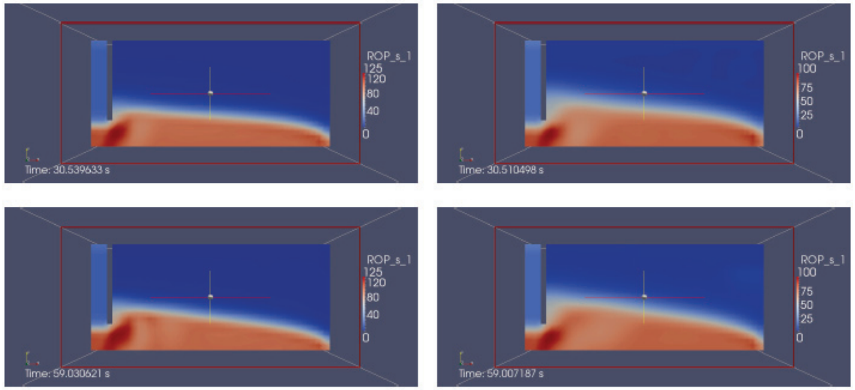
Predicted y solid velocity vector

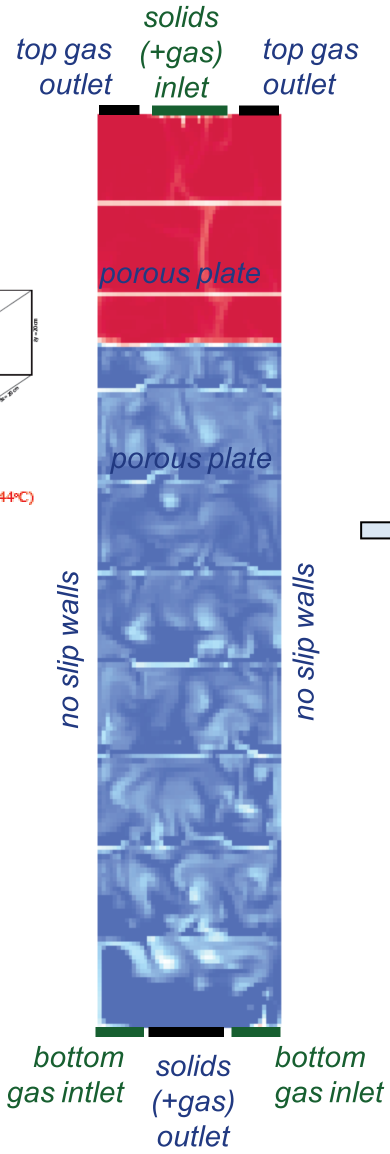
Full Scale CFD of Adsorber & Regenerator

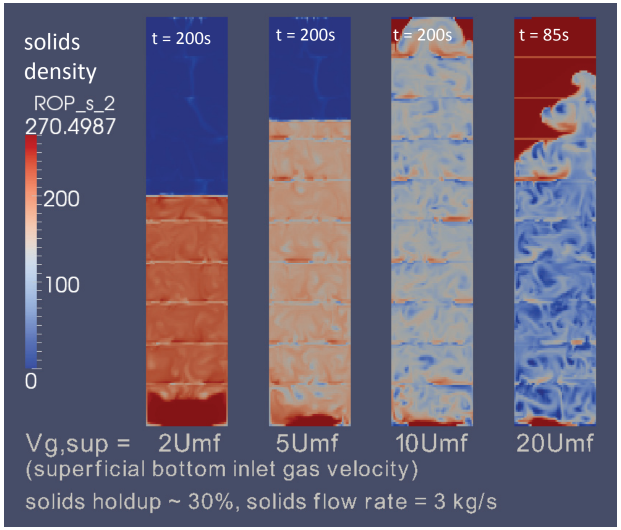
- 3D a coarse grid model of bubbling bed adsorber
- 2D strip for moving bed regenerator
- Parametric studies

Cross-sectional view: Initial and boundary conditions

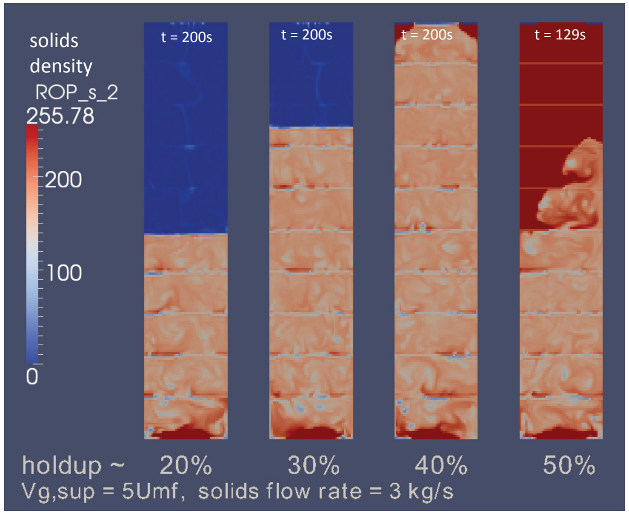






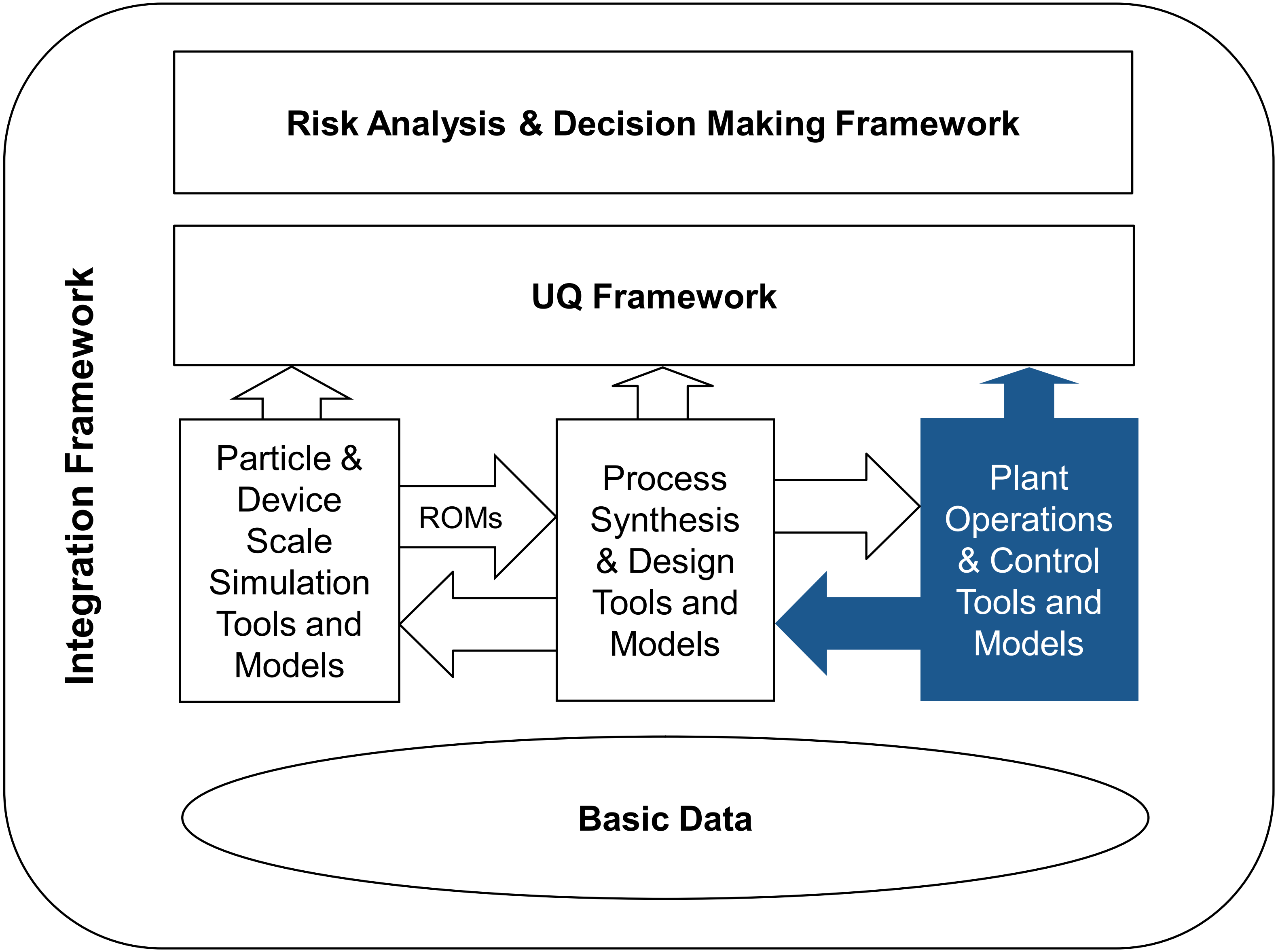


Increasing steam inlet velocity



Decreasing bed voidage

CCSI™ Carbon Capture Simulation Initiative



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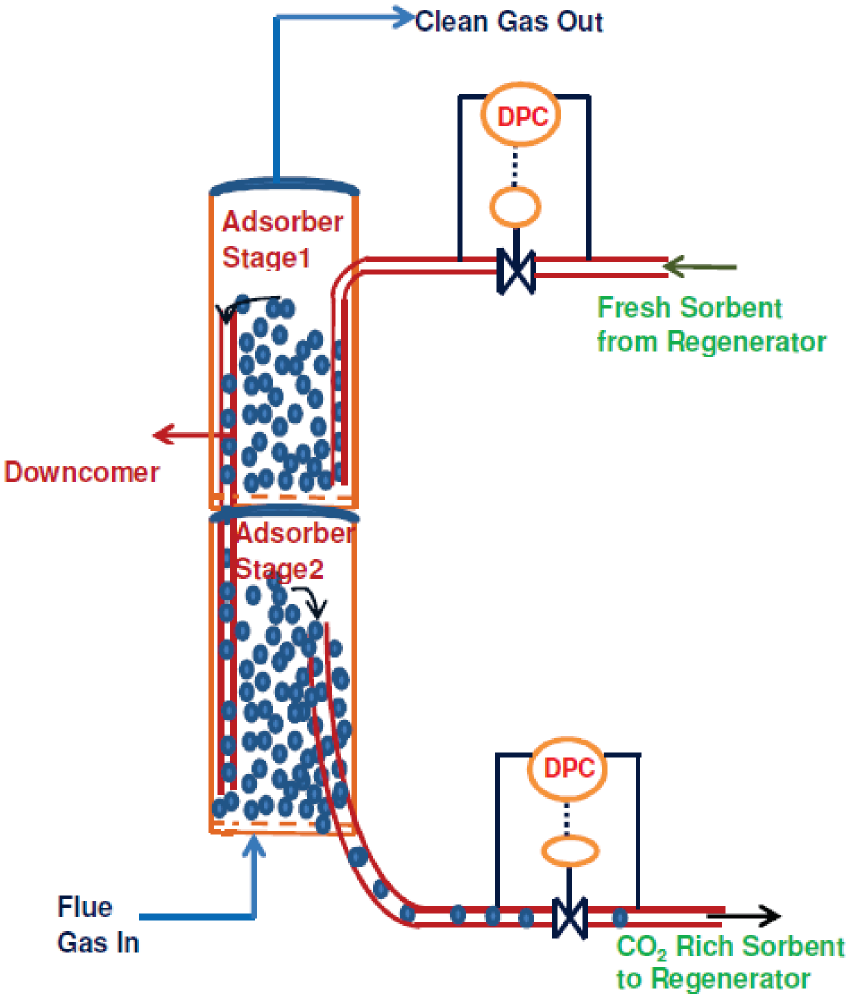
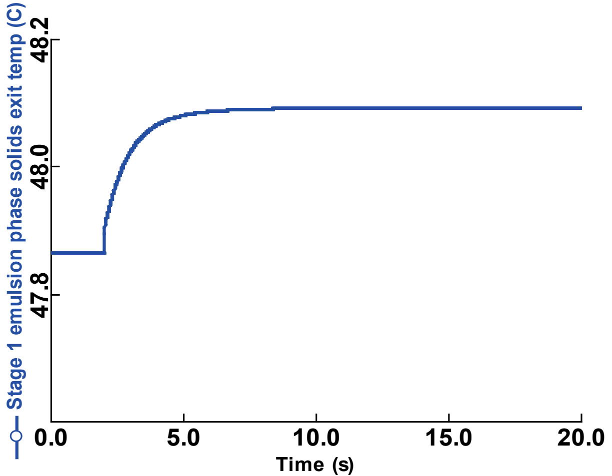
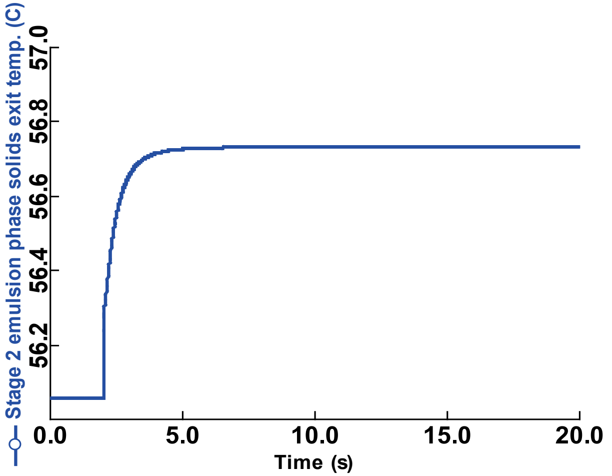
Dynamic Response of Solid Sorbent Adsorber

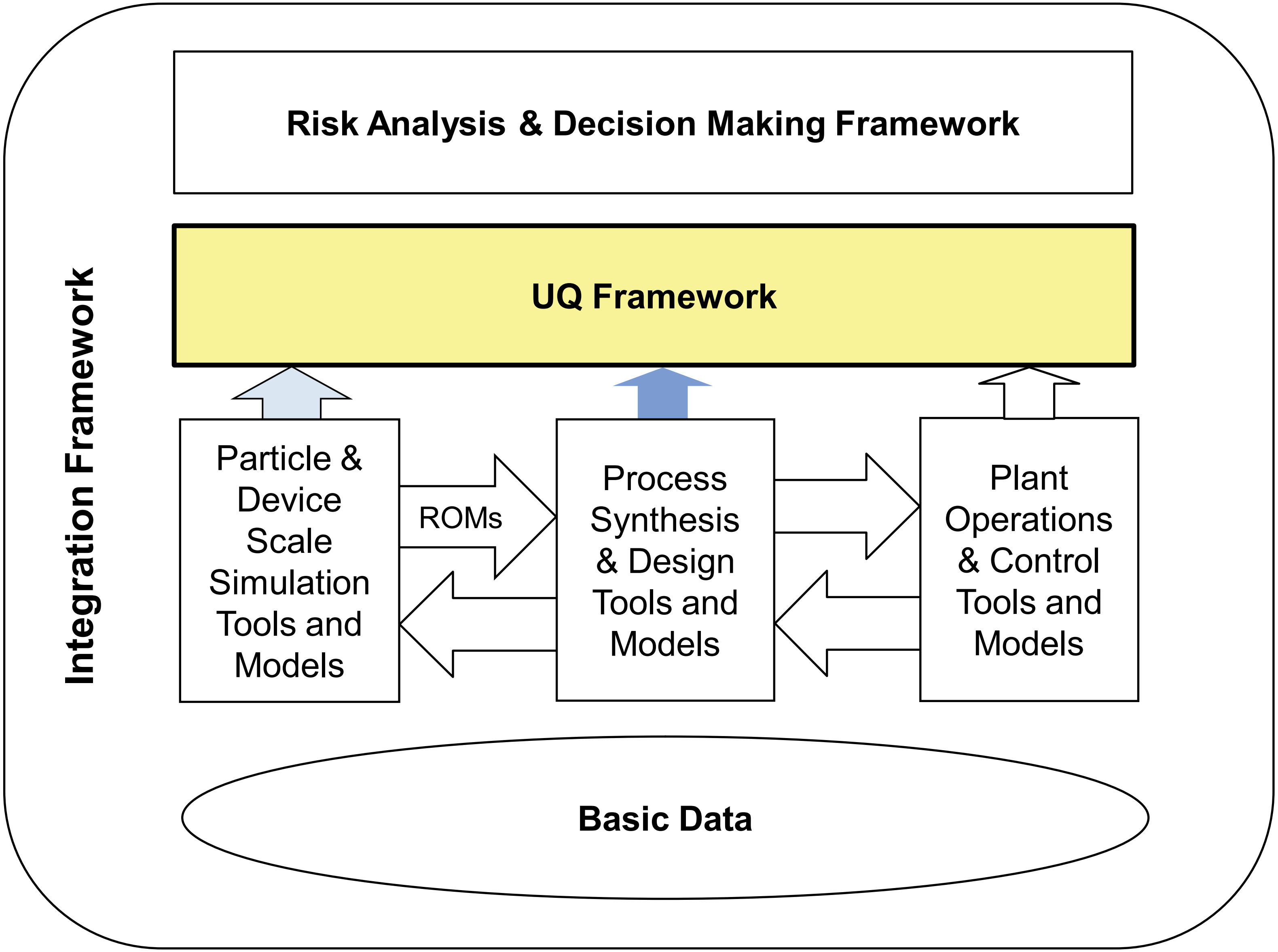




Dynamics of the Stage 1 solids exit temperature as a result of 5% step increase in the solids flow rate



Dynamics of the Stage 2 solids exit temperature as a result of 5% step increase in the solids flow rate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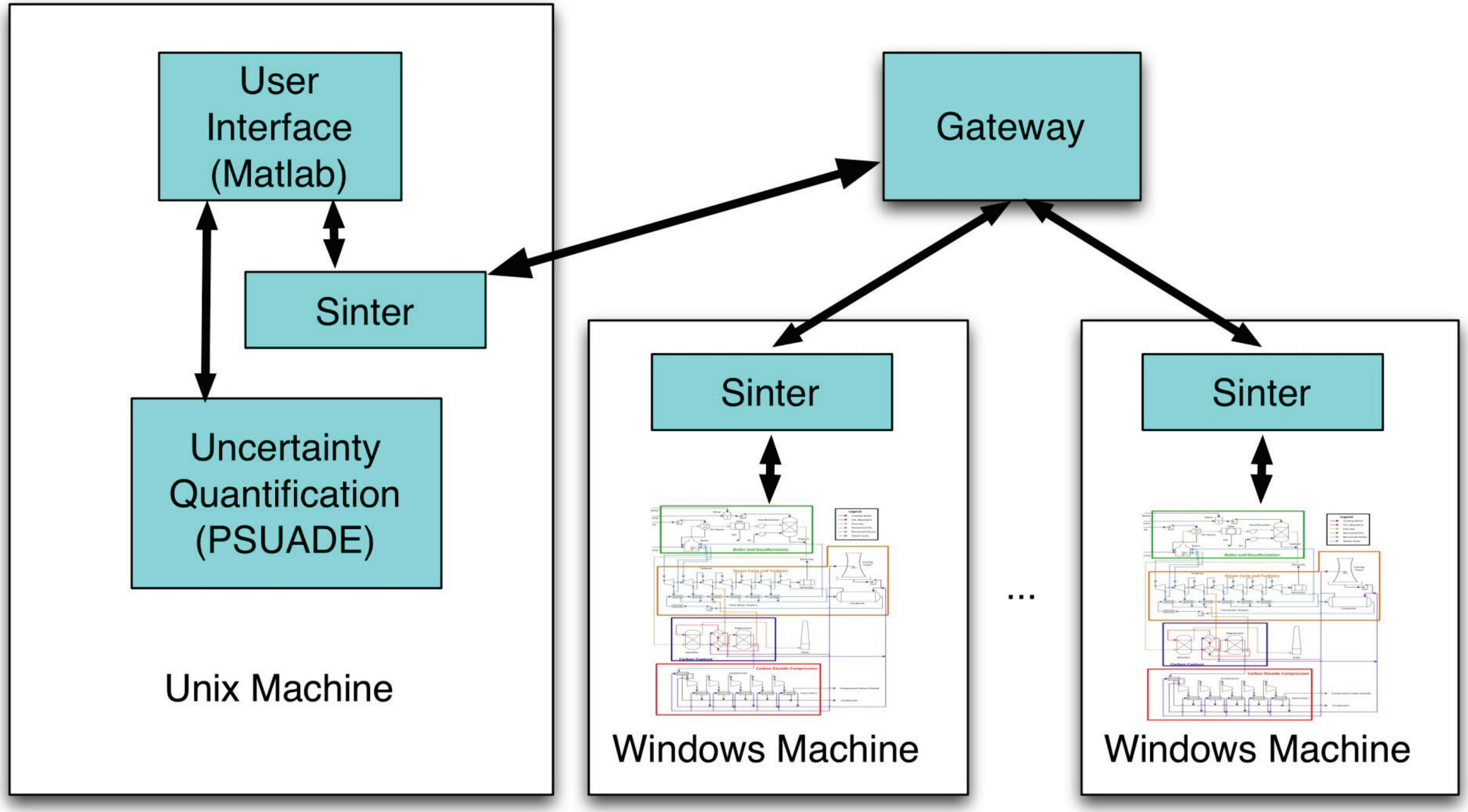
UQ Link to Process Simulation



User Interface (Matlab)

Sinter

Uncertainty Quantification (PSUADE)

Unix Machine

Gateway

Sinter

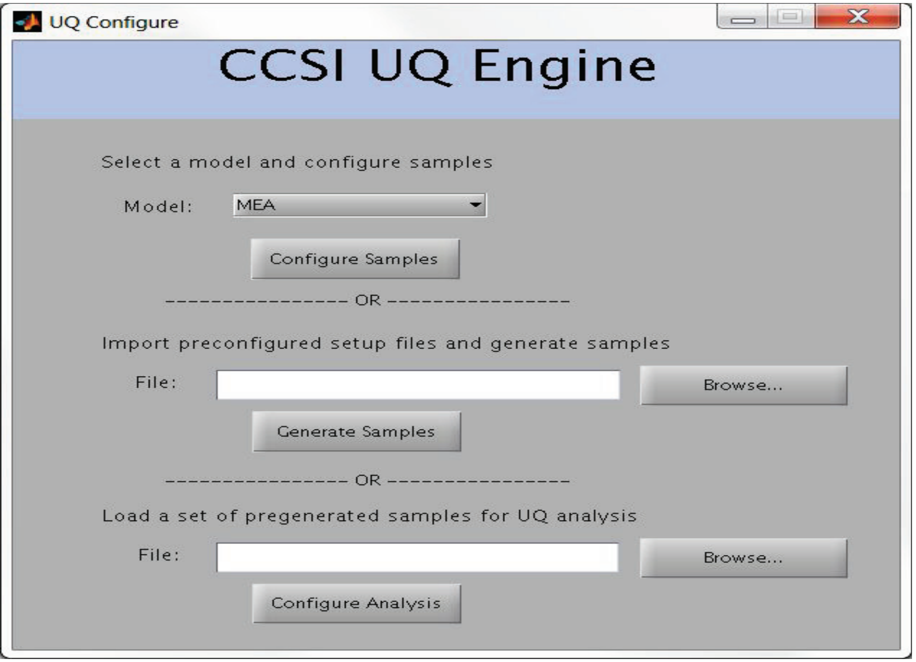
Windows Machine

...

Sinter

Windows Machine

Model selection page



CCSI UQ Engine

Select a model and configure samples

Model: MEA

---------------- OR ----------------

Import preconfigured setup files and generate samples

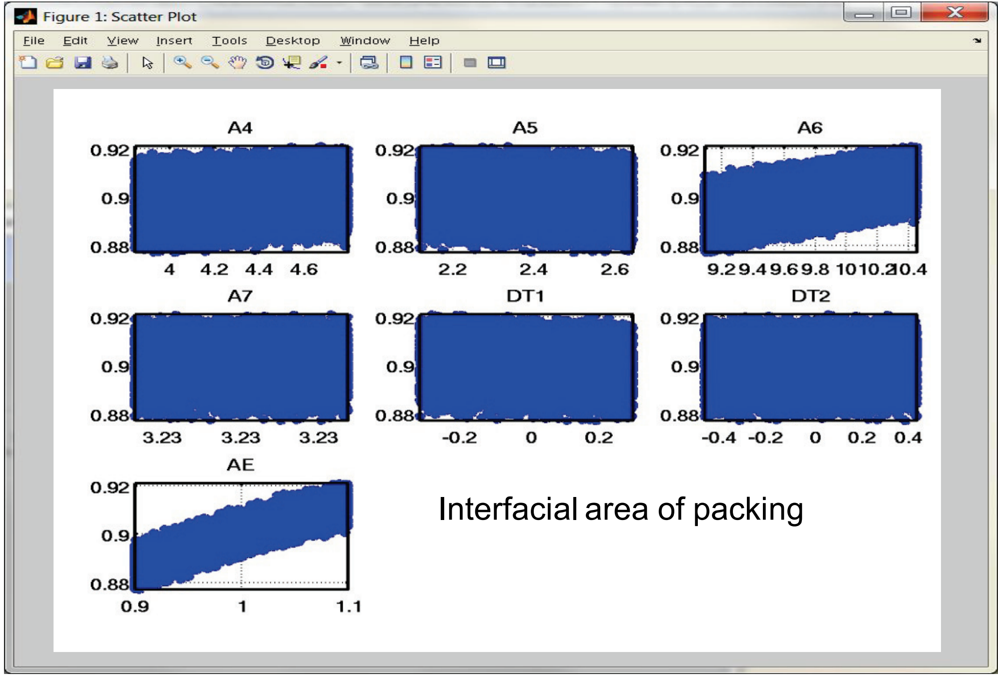
File:

---------------- OR ----------------

Load a set of pregenerated samples for UQ analysis

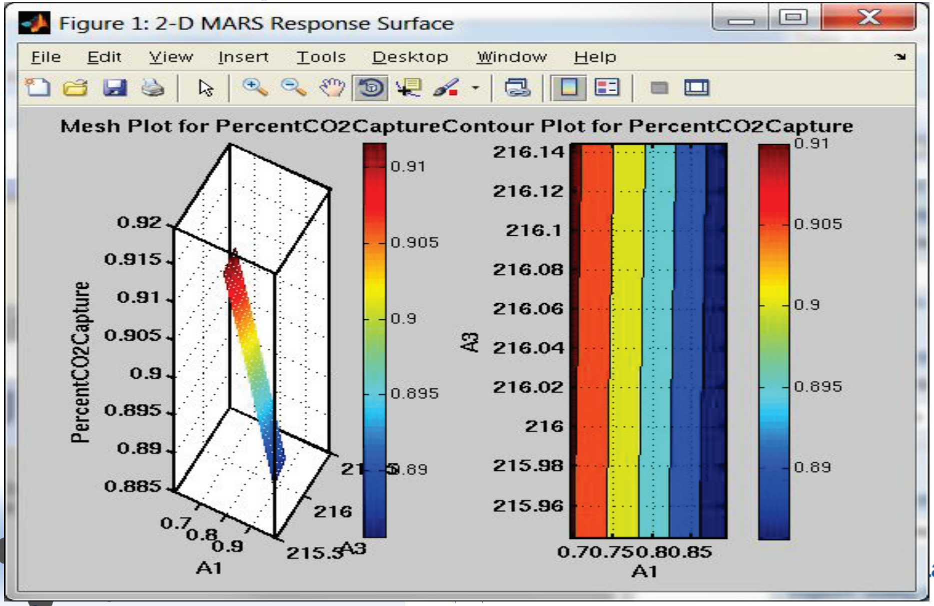
File:

Scatter plots show important variables

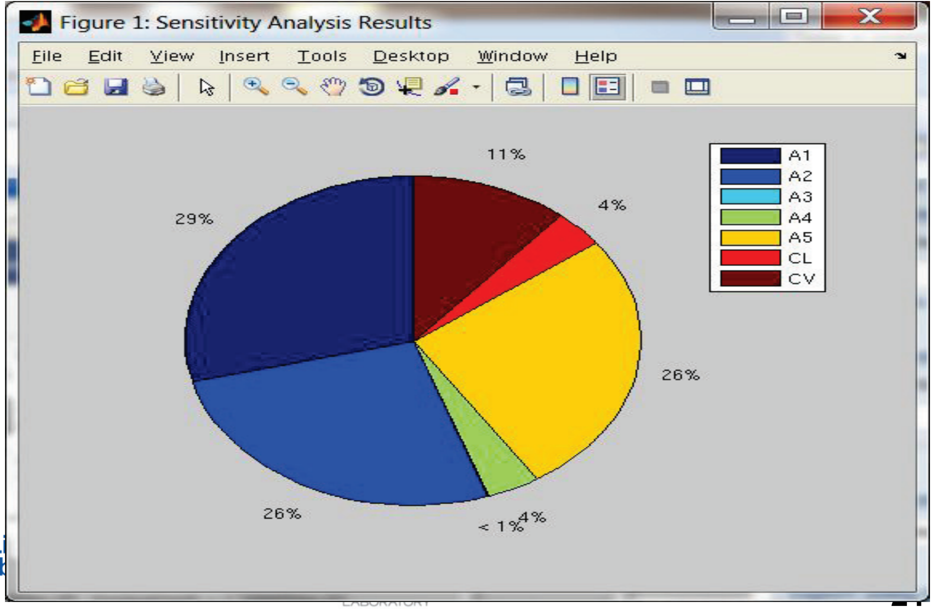


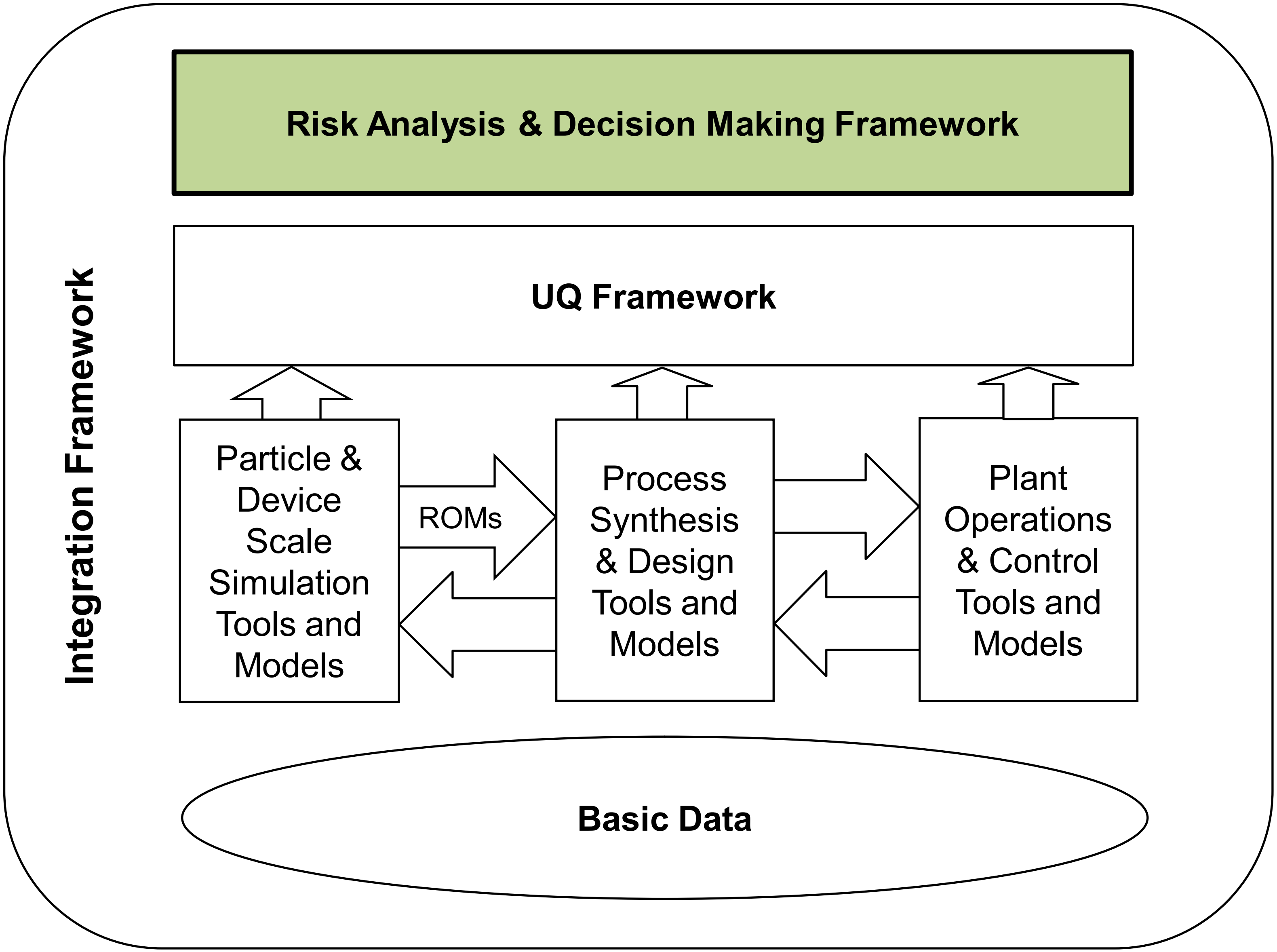
Interfacial area of packing

Response surface visualization



Variance-based sensitivity analysis





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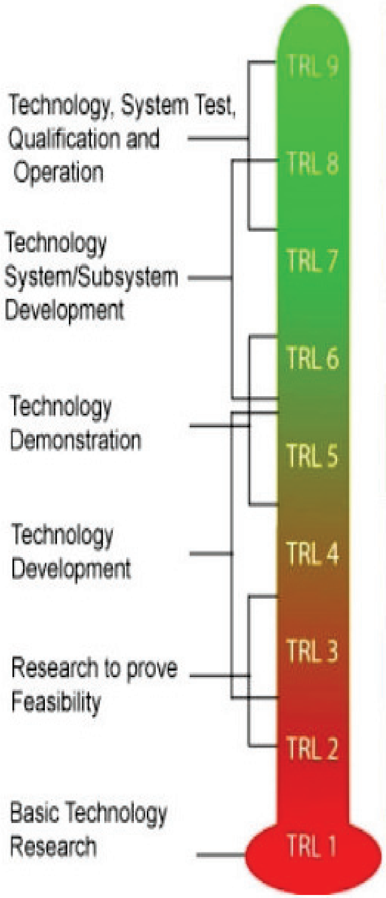
Formalize Risk Metrics as Flexible Tools (Risk Analysis, TRL)

Technology Readiness Level Definitions



Actual application of the technology in its final form and under mission conditions, such as those encountered in operational test and evaluation.

Technology has been proven to work in its final form and under expected conditions. In almost all cases, this TRL represents the end of true system development.

Prototype near, or at, planned operational system. Represents a major step up from TRL 6, requiring demonstration of an actual system prototype in an operational environment such as an aircraft, vehicle, or space.

Representative mod
that of TRL 5, is tes
major step up in a te

Fidelity of breadboa
technological compo
supporting elements

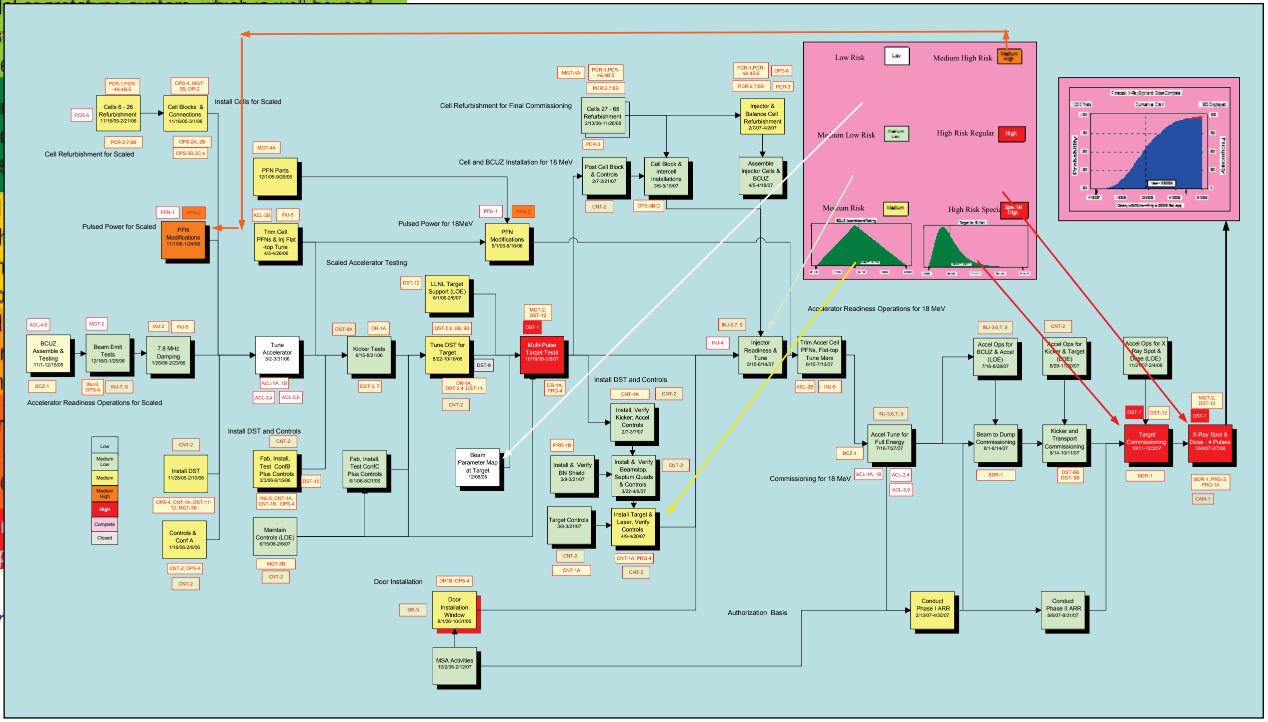
Basic technological
they will work togeth
the eventual system
hardware in the labo

Active research and
analytical studies ar
analytical prediction

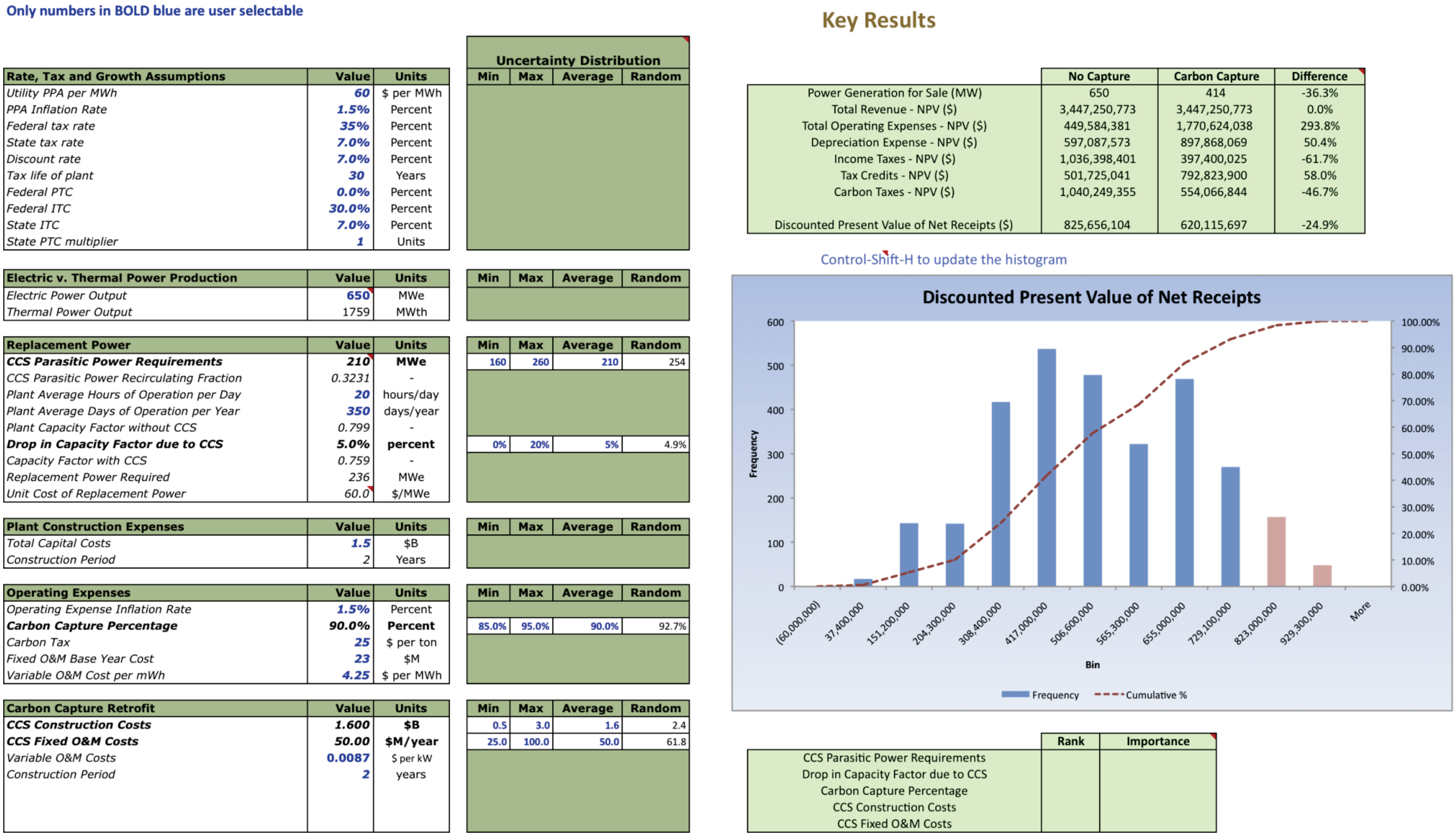
Invention begins. Or
applications can be
may be no proof or

Lowest level of techn
be translated into ap

Proceedings of the World Congress on En
WCECS 2009, October 20-22, 2009, San



Financial Risk Model



Only numbers in BOLD blue are user selectable

Rate, Tax and Growth Assumptions	Value	Units	Uncertainty Distribution			
			Min	Max	Average	Random
Utility PPA per MWh	***60***	$ per MWh				
PPA Inflation Rate	***1.5%***	Percent				
Federal tax rate	***35%***	Percent				
State tax rate	***7.0%***	Percent				
Discount rate	***7.0%***	Percent				
Tax life of plant	***30***	Years				
Federal PTC	***0.0%***	Percent				
Federal ITC	***30.0%***	Percent				
State ITC	***7.0%***	Percent				
State PTC multiplier	***1***	Units				

Electric v. Thermal Power Production	Value	Units	Min	Max	Average	Random
Electric Power Output	***650***	MWe				
Thermal Power Output	*1759*	MWth				

Replacement Power	Value	Units	Min	Max	Average	Random
CCS Parasitic Power Requirements	***210***	**MWe**	**160**	**260**	**210**	254
CCS Parasitic Power Recirculating Fraction	*0.3231*	-				
Plant Average Hours of Operation per Day	***20***	hours/day				
Plant Average Days of Operation per Year	***350***	days/year				
Plant Capacity Factor without CCS	*0.799*	-				
Drop in Capacity Factor due to CCS	***5.0%***	**percent**	**0%**	**20%**	**5%**	4.9%
Capacity Factor with CCS	*0.759*	-				
Replacement Power Required	*236*	MWe				
Unit Cost of Replacement Power	*60.0*	$/MWe				

Plant Construction Expenses	Value	Units	Min	Max	Average	Random
Total Capital Costs	***1.5***	$B				
Construction Period	*2*	Years				

Operating Expenses	Value	Units	Min	Max	Average	Random
Operating Expense Inflation Rate	***1.5%***	Percent				
Carbon Capture Percentage	***90.0%***	**Percent**	**85.0%**	**95.0%**	**90.0%**	92.7%
Carbon Tax	***25***	$ per ton				
Fixed O&M Base Year Cost	***23***	$M				
Variable O&M Cost per mWh	***4.25***	$ per MWh				

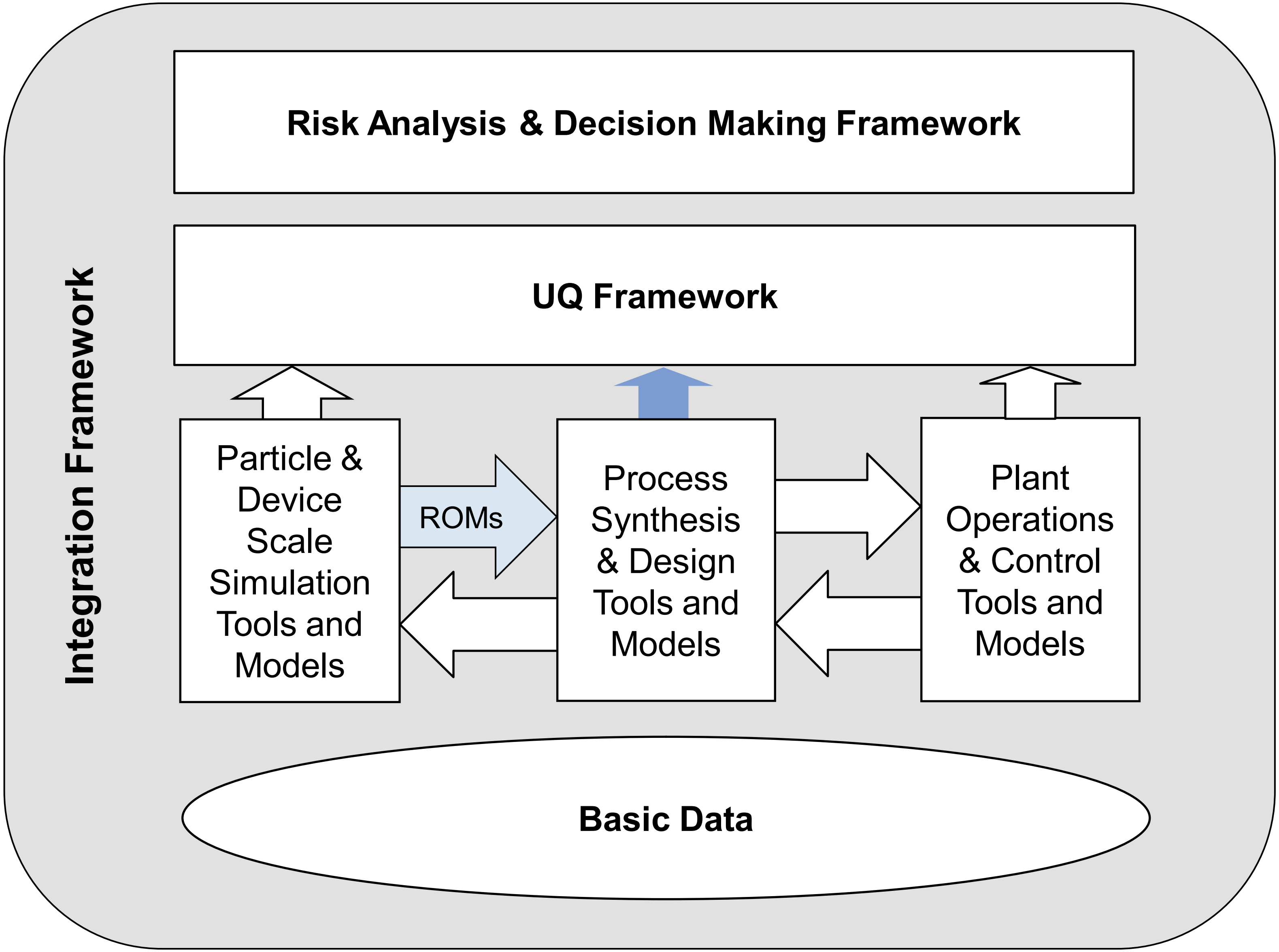
Carbon Capture Retrofit	Value	Units	Min	Max	Average	Random
CCS Construction Costs	***1.600***	**$B**	**0.5**	**3.0**	**1.6**	2.4
CCS Fixed O&M Costs	***50.00***	**$M/year**	**25.0**	**100.0**	**50.0**	61.8
Variable O&M Costs	**0.0087**	$ per kW				
Construction Period	**2**	years				

Key Results

	No Capture	Carbon Capture	Difference
Power Generation for Sale (MW)	650	414	-36.3%
Total Revenue - NPV ($)	3,447,250,773	3,447,250,773	0.0%
Total Operating Expenses - NPV ($)	449,584,381	1,770,624,038	293.8%
Depreciation Expense - NPV ($)	597,087,573	897,868,069	50.4%
Income Taxes - NPV ($)	1,036,398,401	397,400,025	-61.7%
Tax Credits - NPV ($)	501,725,041	792,823,900	58.0%
Carbon Taxes - NPV ($)	1,040,249,355	554,066,844	-46.7%
Discounted Present Value of Net Receipts ($)	825,656,104	620,115,697	-24.9%

Control-Shift-H to update the histogram

	Rank	Importance
CCS Parasitic Power Requirements		
Drop in Capacity Factor due to CCS		
Carbon Capture Percentage		
CCS Construction Costs		
CCS Fixed O&M Costs		



Integration Framework

Risk Analysis & Decision Making Framework

UQ Framework

Particle & Device Scale Simulation Tools and Models

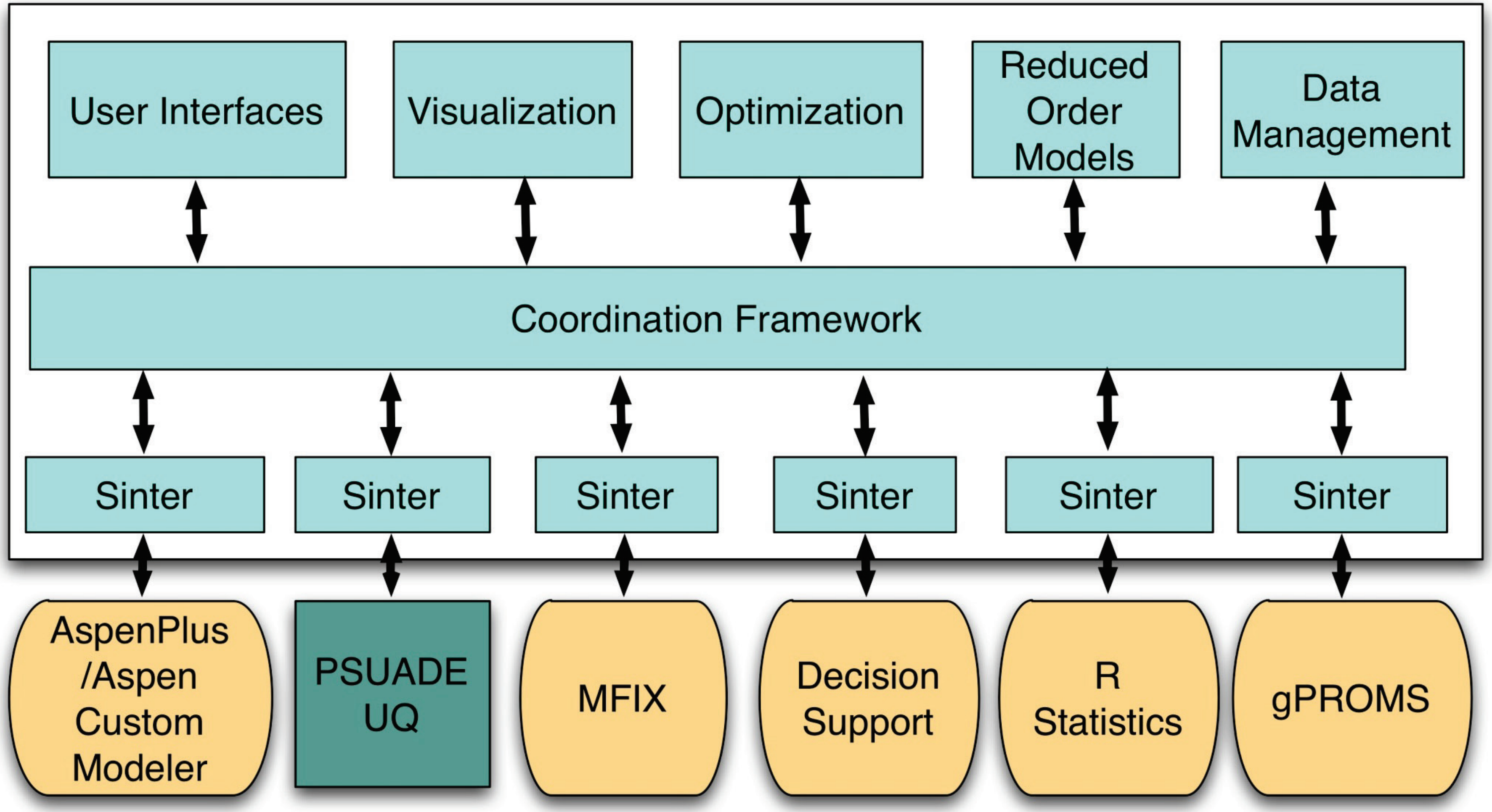
ROMs

Process Synthesis & Design Tools and Models

Plant Operations & Control Tools and Models

Basic Data

Integration Framework Technical Approach



User Interfaces

Visualization

Optimization

Reduced Order Models

Data Management

Coordination Framework

Sinter

Sinter

Sinter

Sinter

Sinter

Sinter

AspenPlus /Aspen Custom Modeler

PSUADE UQ

MFIX

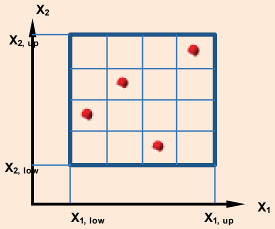
Decision Support

R Statistics

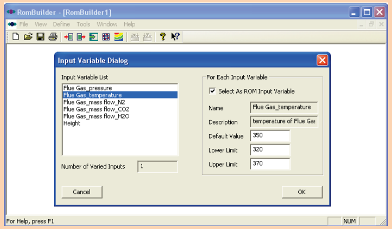
gPROMS

Reduced Order Model Development

Latin Hypercube Sampling



User Interface
(ROM Builder)



Input Variable List
- Flue Gas_pressure
- Flue Gas_temperature
- Flue Gas_mass flow_N2
- Flue Gas_mass flow_CO2
- Flue Gas_mass flow_H2O
- Height

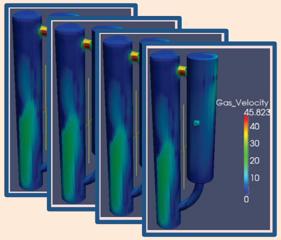
Number of Varied Inputs: 1

For Each Input Variable

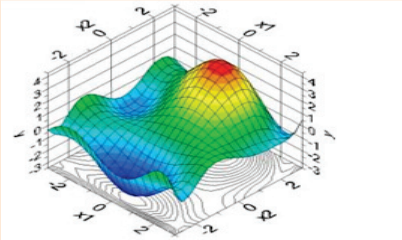
☑ Select As ROM Input Variable

Name: Flue Gas_temperature
Description: temperature of Flue Gas
Default Value: 350
Lower Limit: 320
Upper Limit: 370

Multiple CFD Simulations



Response Surface



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

Exported xROM and yROM

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