

CCSI

Carbon Capture Simulation Initiative

AspenTech Global Conference

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U.S. DOE/NETL

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U.S. DEPARTMENT OF
ENERGY

Outline

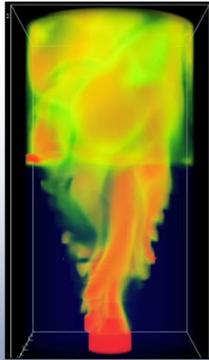
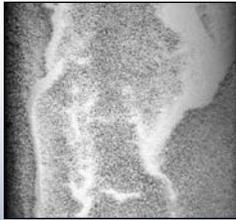
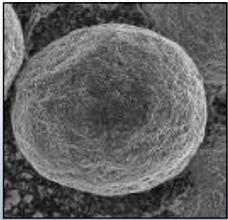
- **Overview**
- CCSI Toolset
- Technical Approach

Carbon Capture Challenge

- The pathway from discovery to commercialization of energy technologies can be quite long: 2-3 decades¹
 - Technology innovation (doing something different) increases the cost growth, schedule slippage, and the probability of operational problems²
- President's plan to overcome the barriers to the widespread, cost-effective deployment of CCS within 10 years³.
- **Need new approaches to take concepts from lab to power plant, quickly, at low cost**
- Opportunity for simulation initiative
 - **Physics-based simulations at multiple scales → screening concepts ... quantifying technical risk**

1. International Energy Agency Report: *Experience Curves for Energy Technology Policy*, 2000

2. RAND Report: *Understanding the Outcomes of Mega-Projects*, 1988; 3. <http://www.whitehouse.gov/the-press-office/presidentialmemorandum-a-comprehensive-federal-strategy-carbon-capture-and-storage>



Identify promising concepts



Reduce the time for design & troubleshooting



Quantify the technical risk, to enable reaching larger scales, earlier

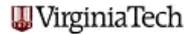


Stabilize the cost during commercial deployment

National Labs



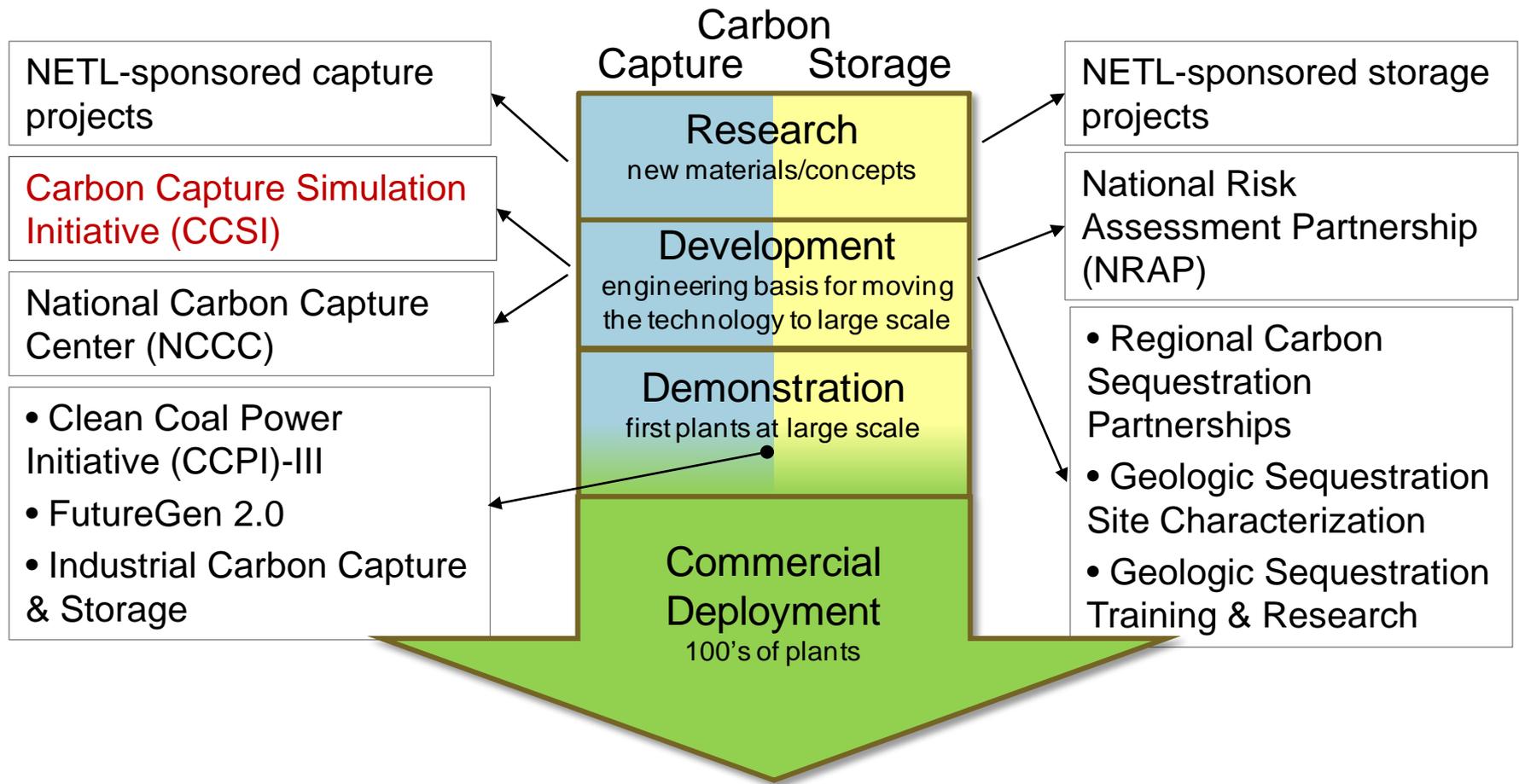
Academia



Industry



CCSI is a Pathway on DOE CCS RD&D Roadmap

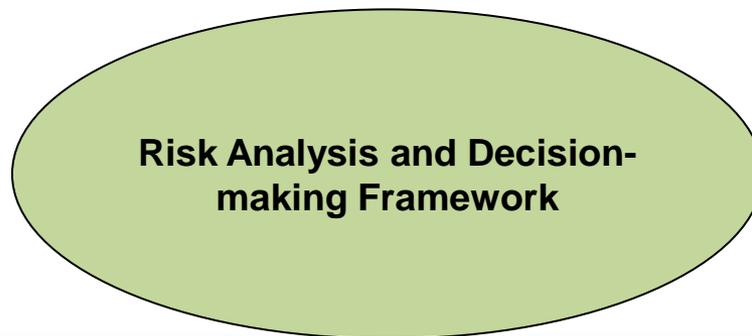
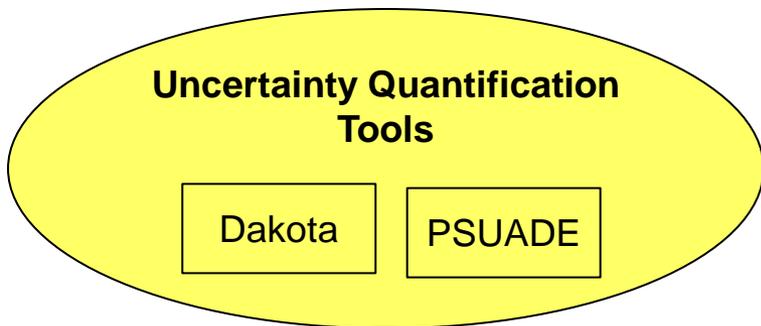
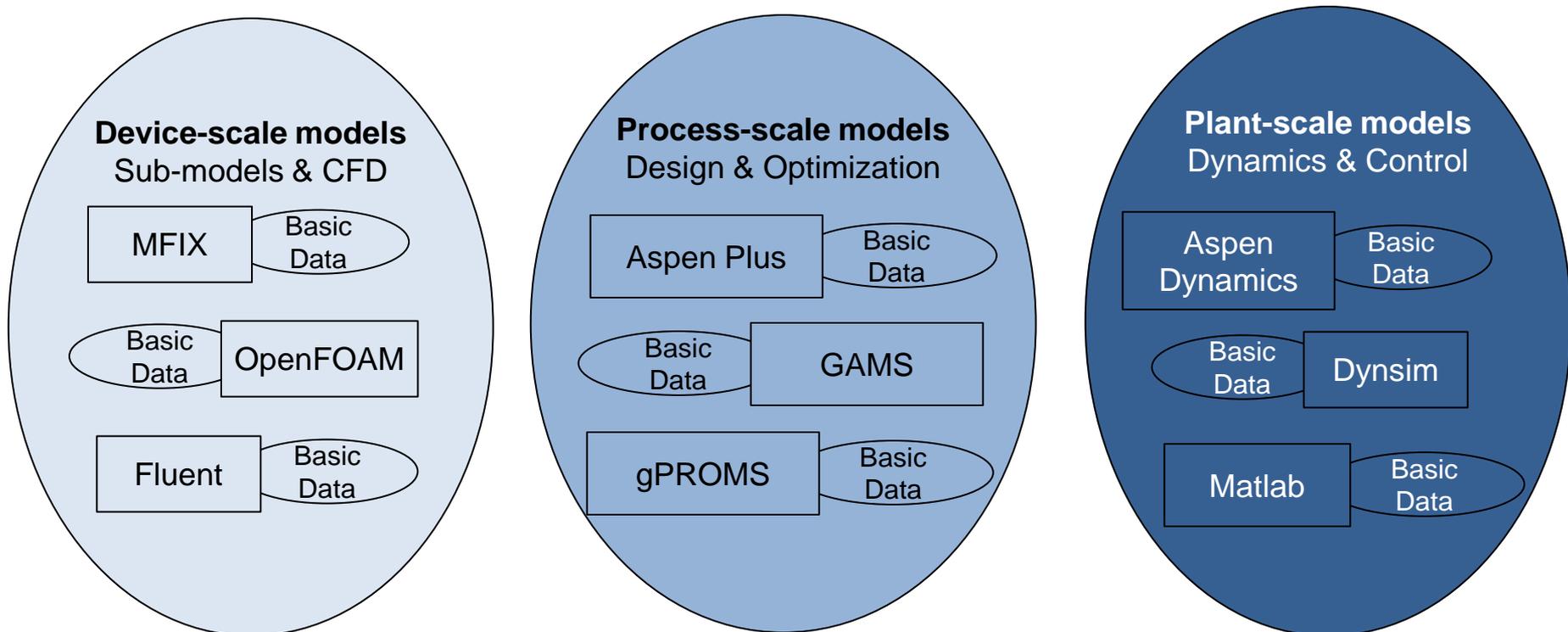


- ~\$2 billion effort FY11-FY15

Outline

- Overview
- **CCSI Toolset**
- Technical Approach

Current State of Simulation Tools is Disjointed



Limited Models Available for Carbon Capture

Device-scale models Sub-models & CFD

Limited models of specific configurations for specific technology

Very little validation of devices or sub-models

Process-scale models Design & Optimization

Limited capability for handling complex systems (i.e., solids)

Lack of models appropriate for process synthesis, optimization, heat integration

Plant-scale models Dynamics & Control

Minimal consideration of system dynamics and impacts on overall plant control strategies

Current models lack ability to predict solid flow dynamics

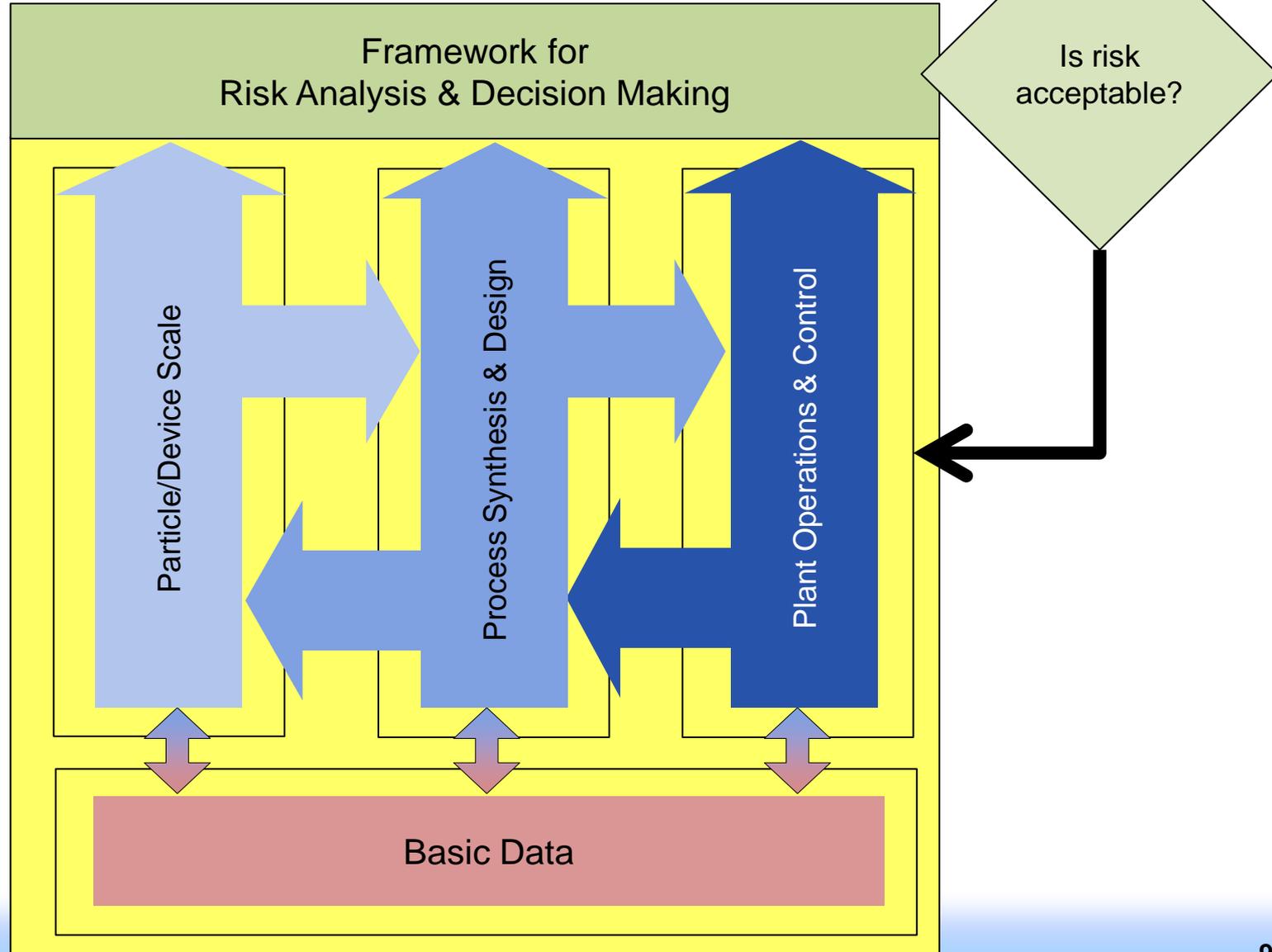
Uncertainty Quantification Tools

Not applied to current commercial simulation tools

Risk Analysis and Decision-making Framework

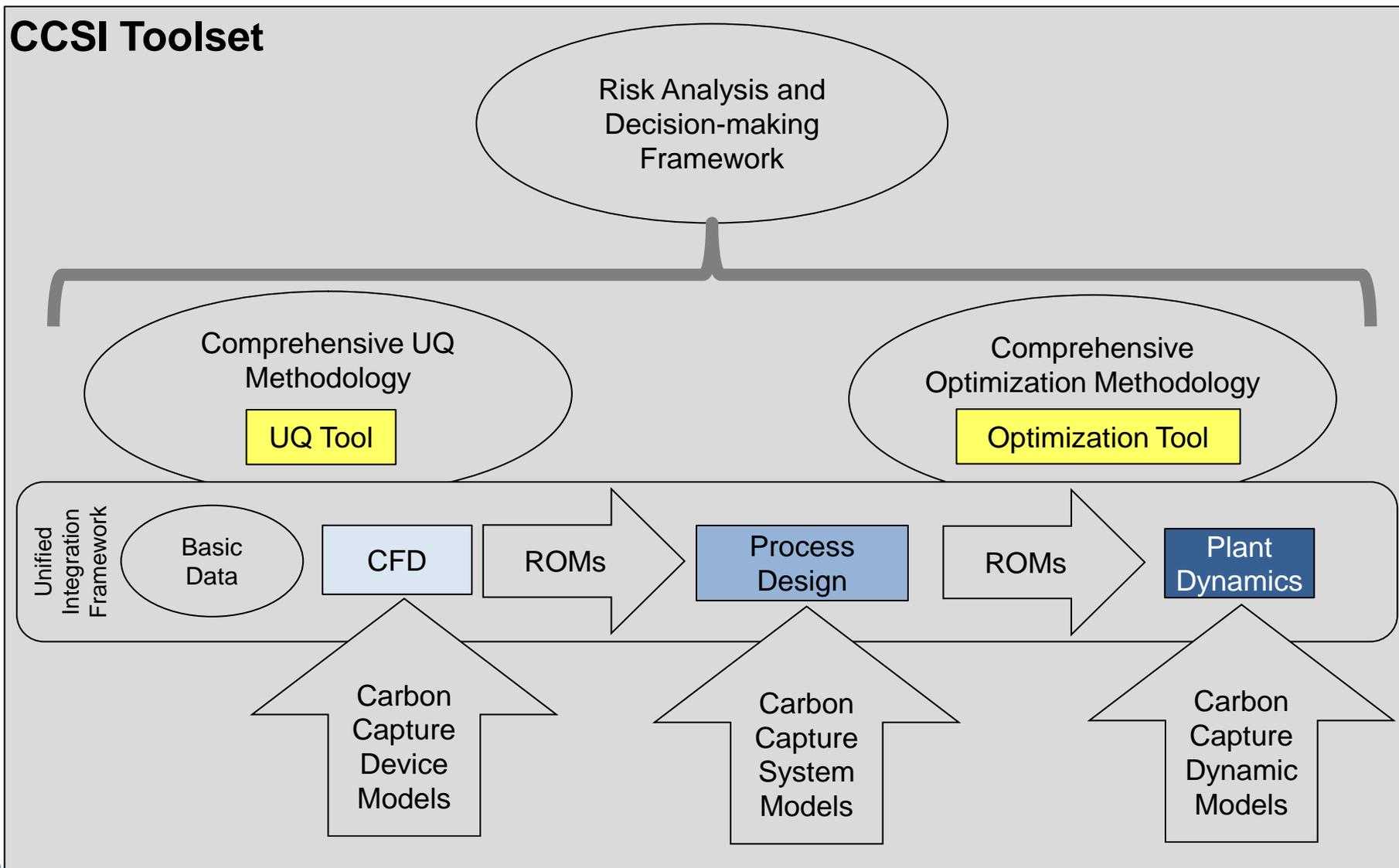
Not connected to technical simulation tools

Carbon Capture Development



CCSI will Integrate Toolset for Carbon Capture

CCSI Toolset



Outline

- Overview
- CCSI Toolset
- **Technical Approach**

Technical Scope – 3 Focus Areas

Physicochemical modeling and simulation

1. *Basic Data and Models*
2. *Particle and Device Scale Models*
3. *Process Synthesis & Design*
4. *Plant Operations and Control*

Analysis and software

5. *Integration Framework*
6. *Uncertainty Quantification and Optimization*
7. *Risk Analysis and Decision Making*
8. *Software Development Support*

Industrial applications

9. *Industrial Challenge Problems*
10. *Industrial Collaboration*

Industry Partnership

Essential to accelerate commercial deployment of capture technology

- Goals
 - Industry requirements, capabilities and knowledge flow into CCSI
 - Obtain industry knowledge of key issues affecting deployment
 - CCSI Toolset used to support capture development process
- Industry Advisory Board: Decision-makers with influence over deployment of capture technology
 - Steer the overall direction of CCSI to ensure effectiveness of CCSI products in supporting capture deployment decisions
- Industry Collaborators: Industry technical leaders
 - Engage with CCSI Technical Teams on a day-to-day basis
 - IAB and CCSI Leadership identify key individuals with supportive skills
 - CCSI Task Sets identify individuals within industry with key capabilities

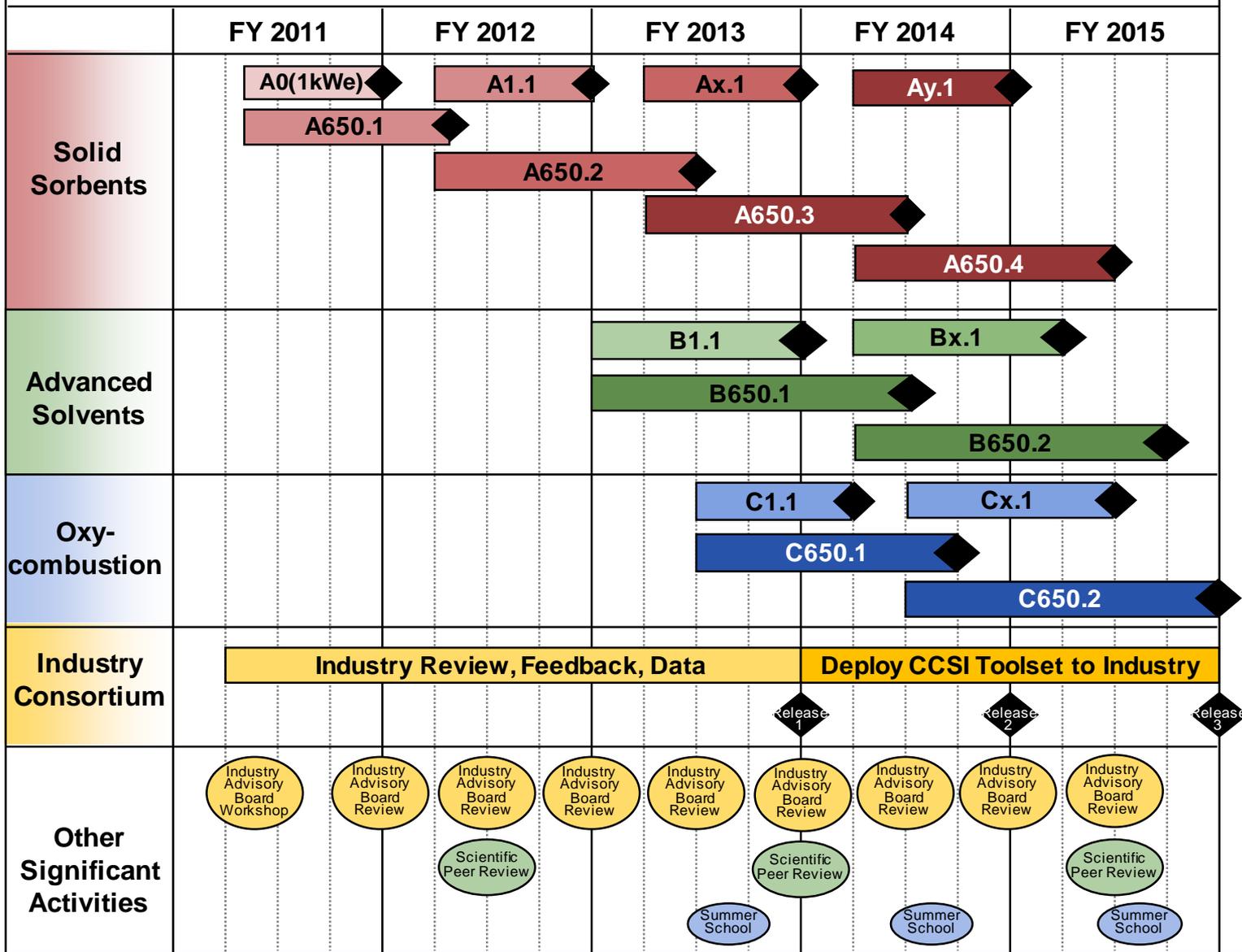
Industrial Challenge Problems (ICP) will Underpin CCSI Toolset Development

- **Desirable ICP Attributes**
 - Develops and uses CCSI capability for a wide range applications
 - IGCC, NGCC, or industrial
 - Provides relevant results to problems of current interest
 - Available process and validation data
- **ICP priority: Pulverized coal**
 - Approximately 280 U.S. pulverized coal plants are CCS candidates²

Capture Technology	Technology Status and Characteristics
Solid Sorbents	<ul style="list-style-type: none"> • Entering process development. • Pilot data/tests in progress. • System design/optimization need now.
Liquid Solvents	<ul style="list-style-type: none"> • Existing solvents currently in pilot and demonstration tests. • Established empirical approach for first generation scale up. • Optimization of new solvents/systems is a near-term CCSI opportunity.
Oxy-combustion	<ul style="list-style-type: none"> • Commercial designs exist for first generation systems, specific coals. • Dynamic operation, optimization, and new fuels is a near-term CCSI opportunity.

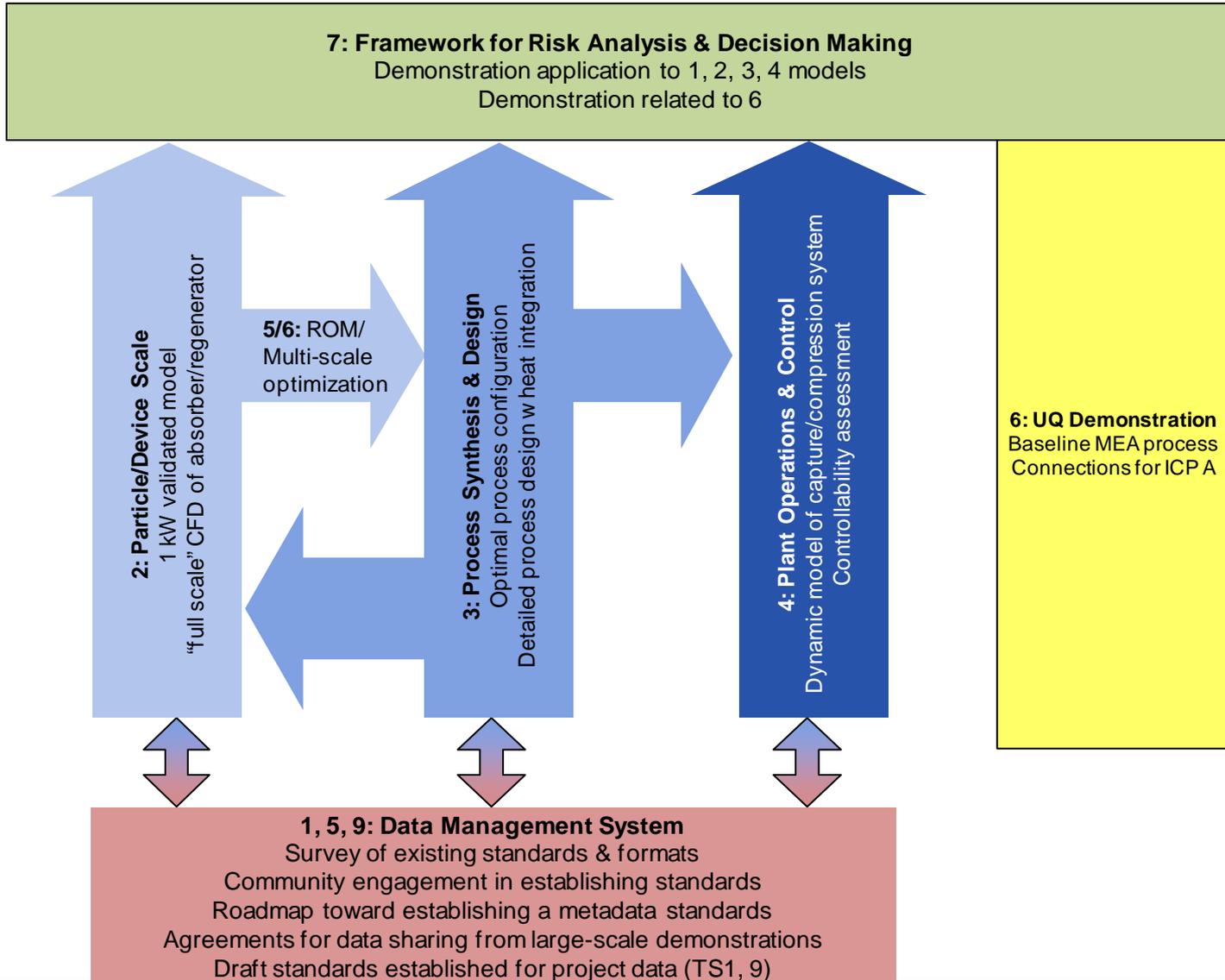
1. *Clean Coal Technology & The Clean Coal Power Initiative (2010). details available at <http://fossil.energy.gov/programs/powersystems/cleancoal/index.html>*
2. *Nichols, C., (2010). "Coal-Fired Power Plants in the United States: Examination of the Cost of Retrofitting with CO2 Capture Technology and the Potential for Improvements in Efficiency", DOE/NETL-402/102309*

Carbon Capture Simulation Initiative (CCSI) Five-Year Plan Overview

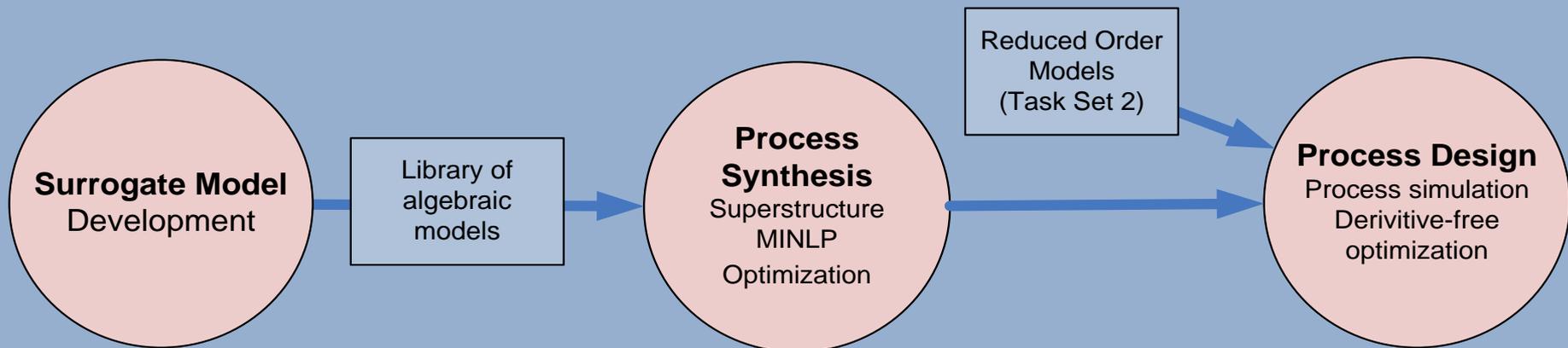


Schedule and scope subject to change.

Year 1 Activities/Milestones



Task Set 3: Process Synthesis & Design (Modular Approach)



Existing Plants Modules

- Combustion system
- Feed water heater
- Boiler
- Economizer
- Superheater
- Steam turbines
- Condensers
- FGD

Solid Sorbent Reactor Modules

- Bubbling fluidized bed
- Fast fluidized beds
- Fixed bed
- Moving bed
- Solids heat exchange

Advanced Solvent Modules

- Ionic liquids
- Absorbers
- Strippers
- Rate-based models
- Intercoolers

Oxy-combustion Modules

- ASU
- Boiler models
- Gas cleanup

Compression System Modules

- Centrifugal
- Inline machines
- Ramgen technology
- Intercooling
- Heat integration

Process Models within Optimization Framework

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Variable	Value	Unit	Description
steam	387790	lb/hr	main steam flow rate
coal	431770	lb/hr	coal feed rate
Hcomb	13126	Btu/lb	heat of combustion of coal (dry)
air	4597962	lb/hr	total air feed rate to the boiler
T_comb_p01	9411.5	F	temperature of combustion products in stream COMB-P01
T_comb_p05	499.5	F	temperature of combustion products in stream COMB-P05
T_comb_p06	347.2	F	temperature of combustion products in stream COMB-P06
T_heater	480.9	F	temperature of feed water
T_hear	246.9	F	temperature of heated feed air
Qreheat	6.9794E+08	Btu/hr	reheater heat transfer
Qsuper	1.4440E+09	Btu/hr	superheater heat transfer
Qdum	2.3318E+09	Btu/hr	steam generator heat transfer
Qecon	2.9887E+08	Btu/hr	economizer heat transfer
power	-786487.9	hp	electrical power output

Excel

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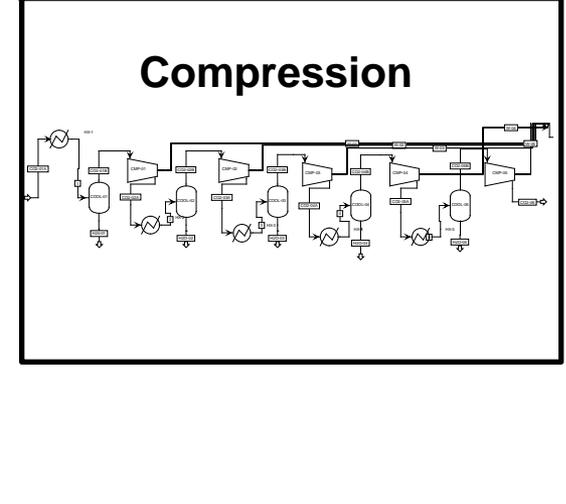
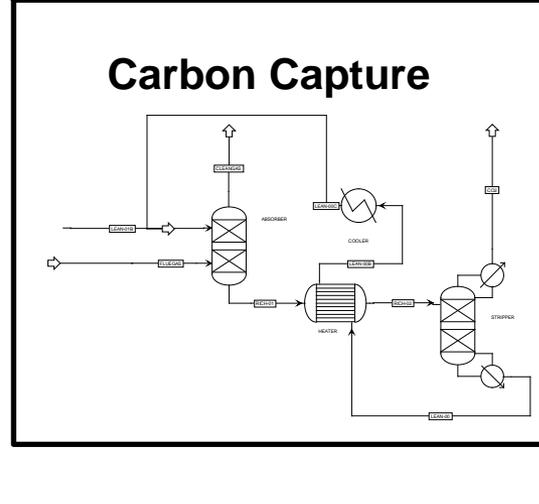
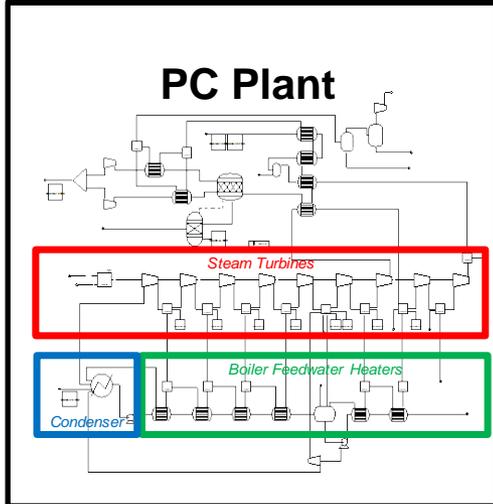
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Excel



Uncertainty Quantification

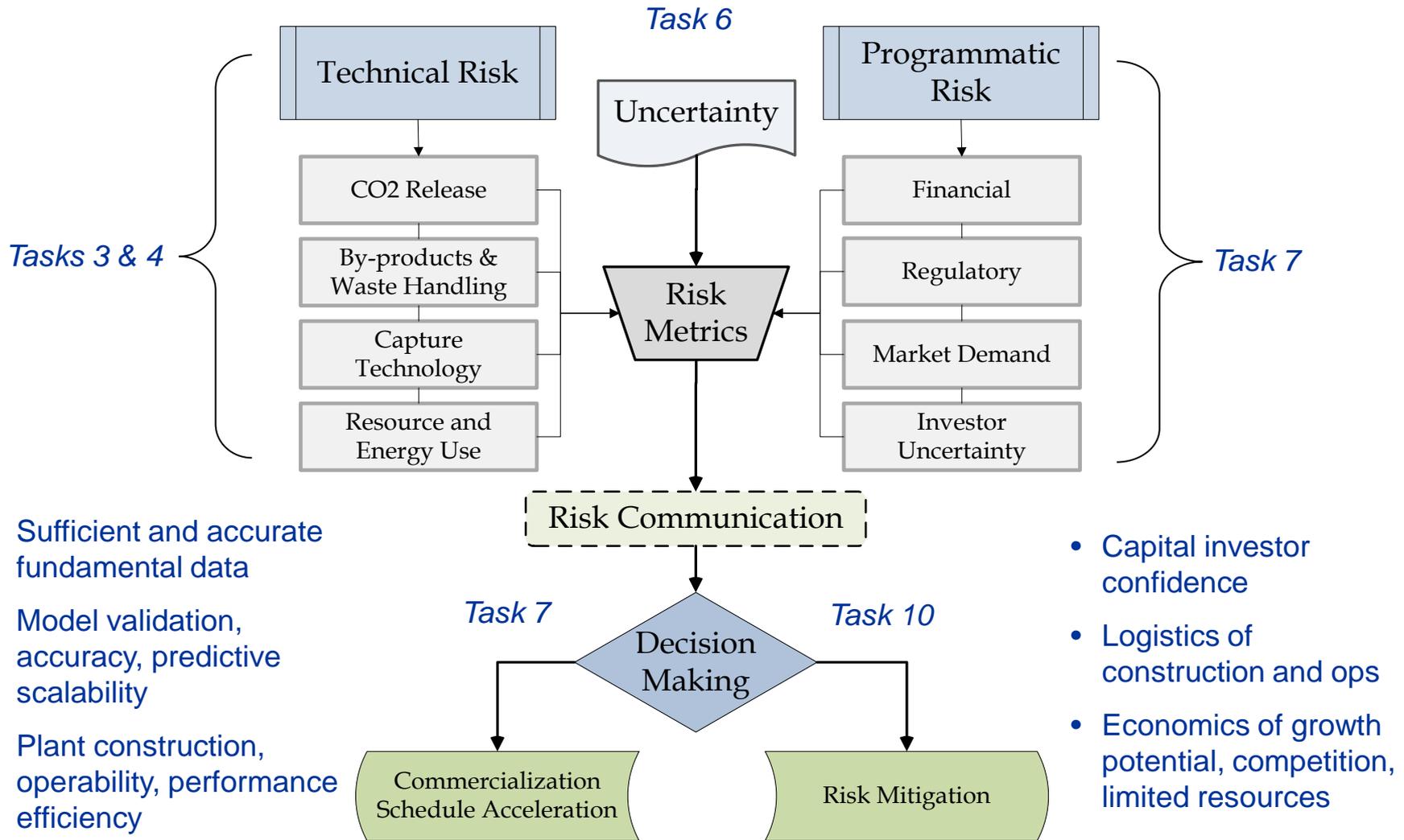
UQ Objectives

- Input to industry risk acceptance metrics & decision processes
- Identify major sources of uncertainty in models
 - Provide feedback to model development to reduce uncertainty

Approach

- Identify, adapt, and extend existing UQ methods/tools
 - Output sensitivity analysis w.r.t. uncertain inputs (identify major drivers)
 - Model calibration and validation (based on data)
 - Forward propagation of quantified input uncertainty
- Progress from UQ at the device/component level to system-level
 - Develop methods and tools for multi-scale/multi-model UQ
- Refine UQ methods/tools throughout the design cycle
- Progressively develop CCSI end-to-end UQ framework

Risk Analysis and Decision Making Framework



- Sufficient and accurate fundamental data
- Model validation, accuracy, predictive scalability
- Plant construction, operability, performance efficiency

- Capital investor confidence
- Logistics of construction and ops
- Economics of growth potential, competition, limited resources

Acknowledgements

- CCSI Leadership Team:
 - M. Syamlal, NETL; J. Meza, LBNL; D. Brown, LLNL; M. Fox, LANL; M. Khaleel, PNNL; R. Cottrell, URS/NETL; J. Kress, LANL; X. Sun, PNNL; S. Sundaresan, Princeton University; N. Sahinidis, Carnegie Mellon University; S. Zitney, NETL; D. Agarwal, LBNL; C. Tong, LLNL; G. Lin, PNNL; B. Letellier, LANL; D. Engel, PNNL; P. Calafiura, LBNL; G. Richards, NETL; J. Shinn, Chevron
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