CLEAN COAL RESEARCH PROGRAM

United States Department of Energy | Office of Fossil Energy

CROSSCUTTING RESEARCH
TECHNOLOGY PROGRAM PLAN

JANUARY 2013

OFFICE OF FOSSIL ENERGY

NETL

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CHAPTER 1: OVERVIEW

1.1 INTRODUCTION

The Department of Energy's (DOE) Crosscutting Research program is conducted under the Clean Coal Research Program (CCRP). DOE's overarching mission is to increase the energy independence of the United States and to advance U.S. national and economic security. The DOE Office of Fossil Energy (FE) is responsible for fostering developments that ensure the availability of ultraclean (near-zero emissions), abundant, low-cost domestic energy from coal in which to support economic prosperity, strengthen energy independence, and enhance environmental quality. As a component of the CCRP effort, the Office of Clean Coal and the National Energy Technology Laboratory (NETL) are engaged in research, development, and demonstration (RD&D) activities to create technology and technology-based options for public benefit. The CCRP is addressing environmental concerns related to coal use by developing a portfolio of innovative technologies, including those for carbon capture and storage (CCS). The CCRP comprises two major program areas: CCS and Power Systems and CCS Demonstrations. The CCS and Power Systems program area is a technology development program designed to resolve technological and economic barriers and reduce risk associated with new power generation and carbon capture technology by performing essential research and development (R&D) effort. The technology advancements resulting from the CCS and Power Systems program area are complemented by the CCS Demonstrations program area, which provides a platform to demonstrate advanced power generation and industrial technologies at commercial scale through cost-shared partnerships between the Government and industry.

Through R&D, the CCRP is gathering the data, building the knowledge base, and developing the advanced technology platforms that support CCS as viable strategies for reducing greenhouse gas (GHG) emissions. In concert with these efforts, there is work to identify approaches that strive to lower costs, increase efficiency, maintain preeminent safety, and support a revitalization of the power infrastructure. Through successful maturation of the technology, this R&D will culminate in an industry that offers affordable and reliable low-cost power with mitigation of any environment impact thus supporting long-term sustainability and growth of domestic resources. Program efforts have positioned the United States as the global leader in clean coal technologies.

This document serves as a program plan for NETL's Crosscutting Research effort, which is conducted under the CCRP's CCS and Power Systems program area. The program plan describes the R&D efforts in 2013 and beyond. The program plan describes the Technology Areas and how the program is allocated for CCRP's CCS and Power Systems program area. Strategic direction in each Technology Area is addressed along with goals, timelines, and risks. The relationship of the Crosscutting Research program to the CCS and Power Systems program area is outlined below.

1.2 CCS AND POWER SYSTEMS PROGRAM AREA

The CCS and Power Systems program area conducts and supports long-term, high-risk R&D to significantly reduce fossil fuel power-plant emissions—including carbon dioxide (CO_2)—and substantially improve efficiency and availability, leading to viable, near-zero-atmospheric-emissions fossil fuel energy systems. The success of NETL research and related program activities will enable CCS technologies to overcome economic, social, and technical challenges including cost-effective CO_2 capture, compression, transport, and storage through successful CCS integration with power-generation systems; effective CO_2 monitoring and verification; permanence of underground CO_2 storage; and public acceptance. The overall program consists of four subprograms: Advanced Energy Systems, Carbon Capture, Carbon Storage, and Crosscutting Research (see Figure 1-1). These four subprograms are further divided into numerous Technology Areas. In several instances, the individual Technology Areas are further subdivided into key technologies.

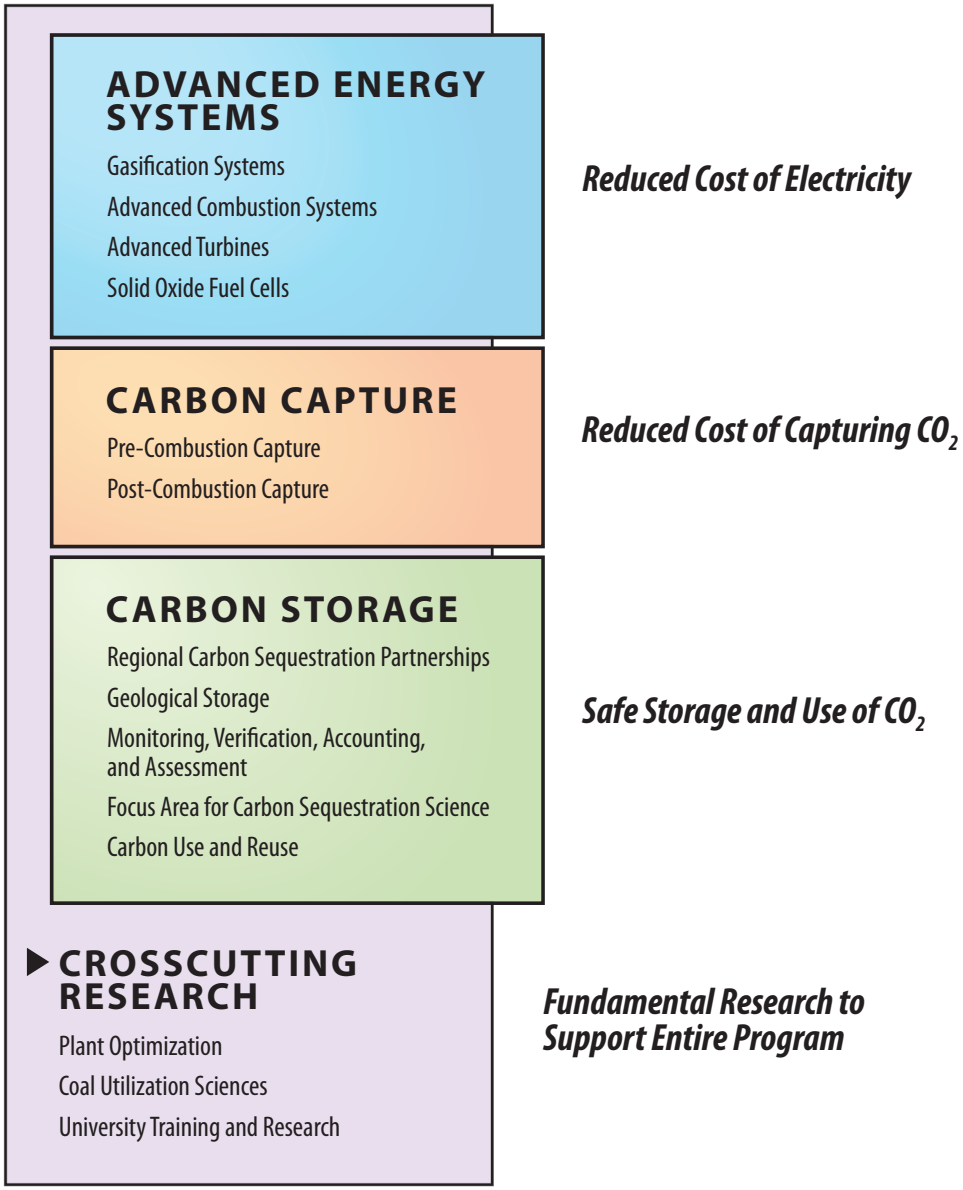

Figure 1-1. CCS and Power Systems Subprograms

These subprograms are described below including the primary activities within each subprogram.

The ***Advanced Energy Systems subprogram*** is developing a new generation of clean fossil fuel-based power systems capable of producing affordable electric power while significantly reducing CO_2 emissions. This new generation of technology will essentially be able to overcome potential environmental barriers and meet any projected environmental emission standards. A key aspect of the Advanced Energy Systems subprogram is targeted at improving overall thermal efficiency, including the capture system, which will be reflected in affordable CO_2 capture and reduced cost of electricity (COE). The Advanced Energy Systems subprogram consists of four Technology Areas as described below:

- ***Gasification Systems*** research to convert coal into clean high-hydrogen synthesis gas (syn-gas) that can in-turn be converted into electricity with over 90 percent CCS.
- ***Advanced Combustion Systems*** research that is focused on new high-temperature materials and the continued development of oxy-combustion technologies.

- ***Advanced Turbines*** research, focused on developing advanced technology for the integral electricity-generating component for both gasification and advanced combustion-based clean energy plants fueled with coal by providing advanced hydrogen (H_2)-fueled turbines, supercritical CO_2-based power cycles and advanced steam turbines.
- ***Solid Oxide Fuel Cells*** research is focused on developing low-cost, highly efficient solid oxide fuel cell power systems that are capable of simultaneously producing electric power from coal with carbon capture when integrated with coal gasification.

The ***Carbon Capture subprogram*** is focused on the development of post-combustion and pre-combustion CO_2 capture technologies for new and existing power plants. Post-combustion CO_2 capture technology is applicable to conventional combustion-based power plants, while pre-combustion CO_2 capture is applicable to gasification-based systems. In both cases, R&D is underway to develop solvent-, sorbent-, and membrane-based capture technologies.

The ***Carbon Storage subprogram*** advances safe, cost-effective, permanent geologic storage of CO_2. The technologies developed and large-volume injection tests conducted through this subprogram will be used to benefit the existing and future fleet of fossil fuel power-generating facilities by developing tools to increase our understanding of geologic reservoirs appropriate for CO_2 storage and the behavior of CO_2 in the subsurface.

The ***Crosscutting Research subprogram*** serves as a bridge between basic and applied research by fostering R&D in sensors and controls, modeling and simulation, and high-performance materials. These activities target enhanced availability and cost reduction for advanced power systems. The Crosscutting Research program facilitates its R&D efforts through collaboration with other Government agencies, large and small businesses, and universities. Figure 1-2 provides an overview of the Crosscutting Research program. This subprogram is focused primarily on the tools and techniques needed to realize the vision of the CCRP.

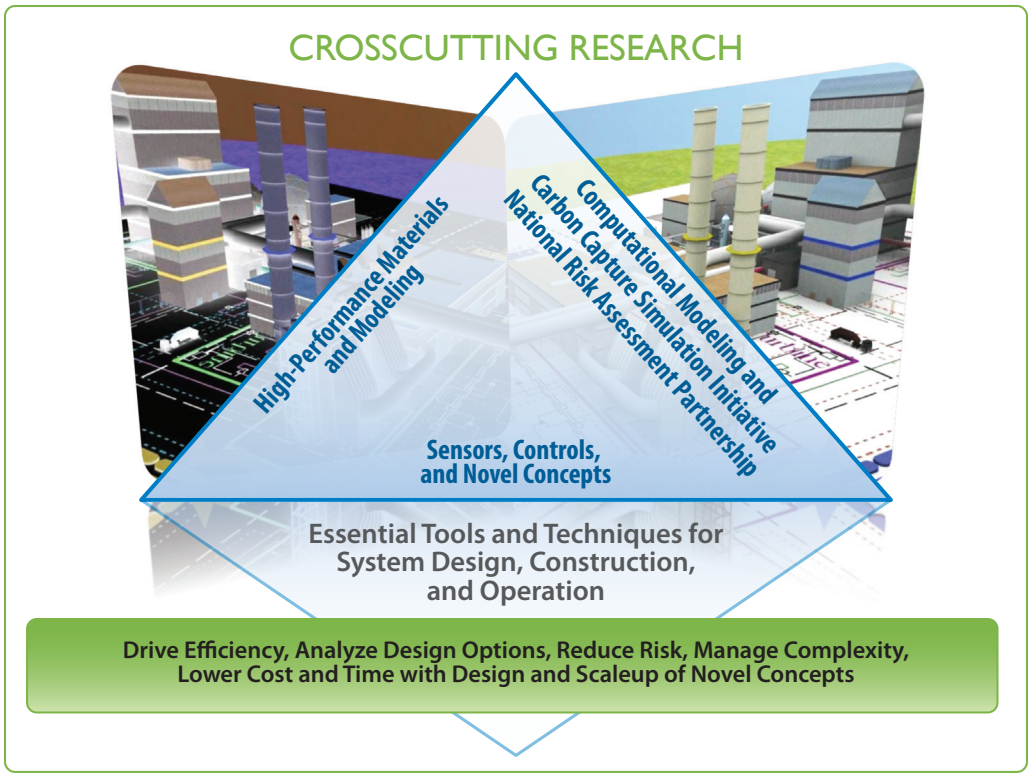

Figure 1-2. Key Activities and Targets within the Crosscutting Research Subprogram

These tools and techniques are viewed as essential technologies to reduce the design timeline, make components easier to construct, and improve the operational availability and reliability of advanced power plants with CCS. Utilization of the tools and techniques impact efficiency, reduce risk, manage complexity, enable rapid analysis of design options, and reduce time and cost associated with scaleup of new systems. Because of these essential functions, these activities reside in the Crosscutting Research program, and the individual plans for these areas are designed to benefit the Advanced Energy Systems, Carbon Capture, and Carbon Storage subprograms. The Crosscutting Research program provides support to each subprogram by conducting research to address technology issues to increase the efficiency of major components, including gasifiers, syngas coolers, advanced turbines, and boilers. Sensors and controls are being improved by enabling wireless installations to reduce capital costs and furthering research of sapphire technology to measure high temperatures inside the harsh environment of gasifiers. Materials research is conducted to improve the refractory linings of gasifiers to allow the linings to have an extended life to reduce the maintenance cost of shutting down integrated gasification combined cycle (IGCC) plants to perform inspections. Improved sensor systems are being explored to monitor refractory performance to increase the time between shutdowns required for inspection of the liner and replacement. Improved sensors and controls are being developed to extend the life of major equipment, such as pumps, with a concurrent increase in reliability and availability while eliminating the need for dual pumps in a system to reduce capital cost.

For purposes of outlining the Crosscutting Research tools and techniques required to realize the vision of the CCRP, Figure 1-3 outlines the terms used to delineate the technologies within the CCS and Power Systems programs. These terms will be referenced when describing specific work and technology pathways for the Crosscutting Research subprogram.

1st-Generation Technologies—include technology components that are being demonstrated or that are commercially available.

2nd-Generation Technologies—include technology components currently in R&D that will be ready for demonstration in the 2020–2025 timeframe.

Transformational Technologies—include technology components that are in the early stage of development or are conceptual that offer the potential for improvements in cost and performance beyond those expected from 2nd-Generation technologies. The development and scaleup of these "Transformational" technologies are expected to occur in the 2016–2030 timeframe, and demonstration projects are expected to be initiated in the 2030–2035 time period.

Figure 1-3. CCS Technology Category Definitions

1.3 CROSSCUTTING RESEARCH PROGRAM

The Crosscutting Research program develops tools, supports research, and sponsors science and engineering education designed to contribute to, and encourage, greater synergy among disciplines and across each of the CCRP's core Technology Areas. Its mission space is bound by investments in innovative sensor and control technology; advanced materials; innovative, application-focused modeling and simulation tools; and university training and research that reinforce the education of students at U.S. universities and colleges with emphasis on longer term research in the area of fossil-energy science.

1.3.1 PROGRAM FUNDING STRUCTURE

The Crosscutting Research structure enables the program to foster technology advances to meet the requests and needs of all CCRP subprograms to assist them in reaching their challenging milestones and goals for the Gasification Systems; Advanced Combustion Systems; Advanced Turbines; Solid Oxide Fuel Cells; Pre- and Post-Combustion Capture; Geological Storage; Monitoring, Verification, Accounting, and Assessment; and Carbon Use and Reuse Technology Areas. The Crosscutting Research program funding structure is divided into three primary Technology Areas and five key technology disciplines (Figure 1-4).

Plant Optimization has research efforts that aim at developing:

- ***Sensors, Controls, and Other Novel Concepts:*** New classes of sensors and measurement technology to enable low-cost, robust monitoring of advanced power plants and employ novel control strategies. These strategies will manage complexity and enable real-time optimization of fully integrated, highly efficient power-generation systems including large-scale environmental and carbon control systems, and support fundamental advanced materials research applicable to a full range of power-generation technologies.
- ***High-Performance Materials and Modeling:*** Research also supports fundamental advanced materials development applicable to a full range of power-generation technologies. Computational techniques are being tested to design and develop optimal materials for use in advanced combustion and advanced ultra-supercritical fossil power systems.

Coal Utilization Sciences efforts target:

- ***Computational System Dynamics:*** Develop dynamic computation, simulation, and modeling tools aimed at the optimization of plant design and shortening of developmental timelines. A new multilaboratory mission-oriented CCS modeling effort, the National Risk Assessment Partnership (NRAP), is charged with developing a defensible, science-based quantitative methodology for determining risk profiles (and, hence, residual risk) at CO_2 storage sites.
- ***Computational Energy Sciences:*** Develop science-based models of the physical phenomena occurring in fossil fuel conversion processes and multiscale, multiphysics simulation capabilities that couple fluid flow, heat and mass transfer, and complex chemical reactions. These tools will facilitate optimization of the design and operation of critical unit processes in advanced power-generation systems. A new multilaboratory mission-oriented initiative, the Carbon Capture Simulation Initiative (CCSI), is charged with developing integrated multiscale physics-based simulations of post-combustion capture processes.

University Training and Research supports science and engineering education at major universities (University Coal Research) and in minority colleges (Historically Black Colleges and Universities and Other Minority Institutions):

- ***Historical Black Colleges and Universities (HBCU)/Other Minority Institutions (OMI):*** Education and training program awards research grants to HBCUs and OMIs that emphasize longer-term research for achieving FE's strategic objectives. The research focus is on sensors and controls in extreme environments, computational energy sciences, and advanced materials for power generation. Funding will be used to conduct fossil energy research activities at these institutions and to support an HBCU/OMI annual technology transfer symposium.
- ***University Coal Research (UCR):*** This program will continue to (1) improve DOE's understanding of the chemical and physical processes involved in the conversion and utilization of coal in an environmentally acceptable manner, (2) maintain and upgrade the coal

research capabilities and facilities of U.S. colleges and universities, and (3) support the education of students in the area of coal science through grants at U.S. colleges and universities that emphasize longer-term research for achieving FE's strategic objectives.

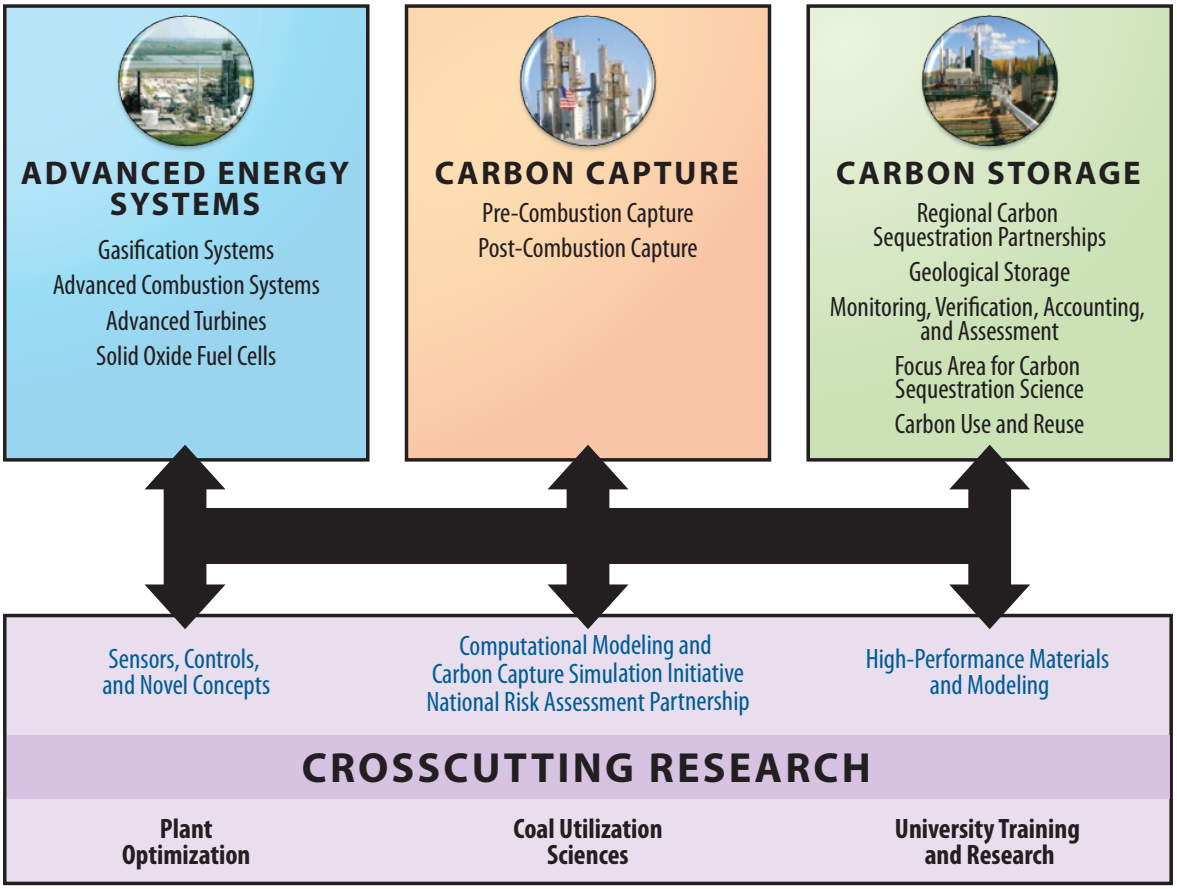

Figure 1-4. Crosscutting Research Technology Areas and Associated Key Technologies

1.3.2 PROGRAM TECHNOLOGY RESEARCH FOCUS

NETL's Crosscutting Research program is an applied research effort with a multidisciplinary approach aimed at addressing barriers to clean fossil energy-based power generation. The program fosters breakthrough concepts that offer the potential to result in a step-change improvement over current technology. Crosscutting Research invests in innovative sensor and control technology, advanced materials, revolutionary modeling and simulation tools, and university training and research that promote the education of students at U.S. universities and colleges.

Crosscutting Research is developing advanced technologies to reduce the cost and increase the efficiency of power-generation facilities with carbon capture in five key technologies and the research focus areas as shown in Figure 1-5.

- Sensors, Controls, and Novel Concepts (Plant Optimization and Advanced Combustion)
- Computational Modeling (Coal Utilization Sciences)
- Carbon Capture Simulation Initiative (Coal Utilization Sciences)
- National Risk Assessment Partnership (Coal Utilization Sciences)
- High-Performance Materials and Modeling

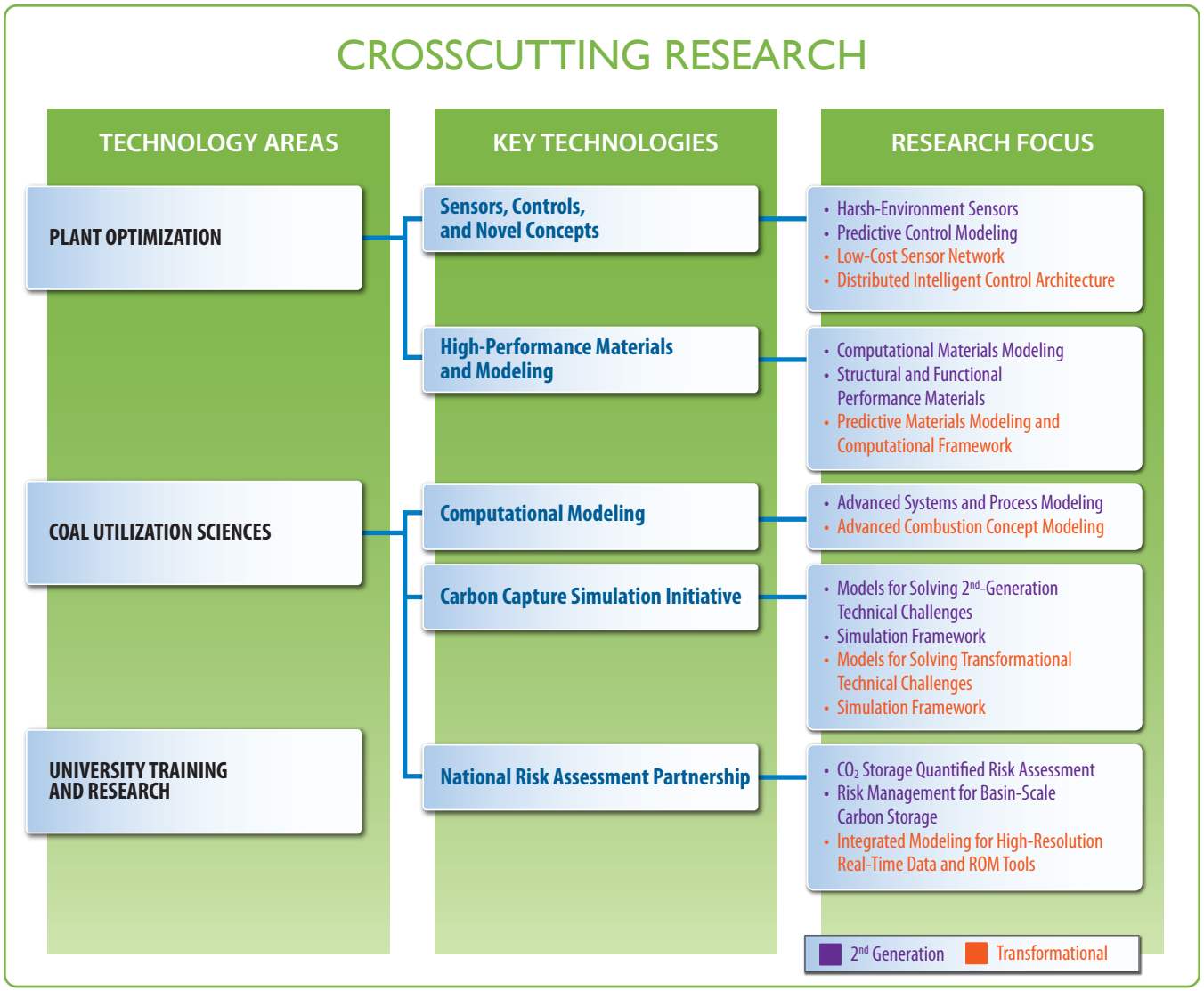

Figure 1-5. Key Technologies and Associated Research Focus in Crosscutting Research

The level of technology R&D conducted by program ranges from laboratory- to pilot-scale activities. Lists of active Crosscutting Research projects are presented in Appendix A. The issues for each of the technologies being supported are summarized as follows:

- **SENSORS, CONTROLS, AND NOVEL CONCEPTS**—The basis for this research focus area is to make available new classes of sensors and measurement tools that manage complexity, permit low-cost, robust monitoring, and enable real-time optimization of fully integrated, highly efficient power-generation systems. Research is focused on sensors capable of monitoring key parameters (temperature, pressure, and gas compositions) while operating in harsh environments and on analytical sensors capable of online, real-time evaluation and measurement. Controls development research centers around self-organizing information networks and distributed intelligence for process control and decision making, and includes investigating fundamental combustion and gasification chemistry to discern rates and mechanisms affecting emissions behavior under combustion and gasification conditions. Research in the area of additive manufacturing is being conducted to determine the feasibility of constructing embedded sensors into such devices as turbine blades, boiler walls, piping, and tubing.

- **COMPUTATIONAL MODELING**—Simulating the complex processes that occur inside a coal gasifier, or across an entire chemical or power plant, requires a powerful tool made possible by today's supercomputers and advanced simulation software. The Computational System Dynamics focus area provides such tools to the Coal Utilization Sciences Technology Area. The goal is to help scientists and engineers better understand the fundamental steps in this complex process so they can optimize the equipment needed to run it. This not only costs less, but also provides more information than a long series of experiments performed under varying conditions to try to isolate important variables. Of course, the data are only as good as the computer model; some of today's computer models have proven to be excellent when measured against as-built configurations.

- **CARBON CAPTURE SIMULATION INITIATIVE**—The CCSI will develop and deploy state-of-the-art computational modeling and simulation tools to accelerate the commercialization of carbon capture technologies from discovery to development, demonstration, and ultimately the widespread deployment to hundreds of power plants. By developing the CCSI Toolset—a comprehensive, integrated suite of validated science-based computational models—the CCSI will provide simulation tools that will increase confidence in designs, thereby reducing the risk associated with incorporating multiple innovative technologies into new carbon capture solutions. The scientific underpinnings encoded into the suite of models will also ensure that learning will be maximized for successive technology generations.

- **NATIONAL RISK ASSESSMENT PARTNERSHIP**—A multilaboratory, multiyear CCS modeling effort, termed the NRAP was formed and designed to harness scientific capabilities across the DOE national laboratory system. Through 2020, efforts within the NRAP project will focus on developing a quantitative understanding of risk-related phenomena as needed for key decisions related to the long-term storage of CO_2. These issues include both site-related and basin-related aspects, as well as near-term and long-term phenomena. The decisions tie to a broad spectrum of stakeholders, including governmental agencies, the business community, and the public.

- **HIGH-PERFORMANCE MATERIALS AND MODELING**—The research cuts across many scientific and technological disciplines to address materials requirements for all fossil-energy systems, including innovative advanced power systems. The goal is to bridge the gap between basic and applied research, often by pursuing "breakthrough" concepts based on mechanistic understanding from any discipline to develop materials with unique thermal, chemical, and mechanical capabilities.

1.4 THE RD&D PROCESS

The research, development, and demonstration of advanced fossil fuel power-generation technologies follows a sequential progression of steps toward making the technology available for commercial deployment, from early analytic study through pre-commercial demonstration. Planning the RD&D includes estimating when funding opportunity announcements (FOAs) will be required, assessing the progress of ongoing projects, and estimating the costs to determine budget requirements.

1.4.1 TECHNOLOGY READINESS LEVELS

The Technology Readiness Level (TRL) concept was adopted by the National Aeronautics and Space Administration (NASA) to help guide the RD&D process. TRLs provide an assessment of technology development progress on the path to meet the final performance specifications. The typical technology development process spans multiple years and incrementally increases scale and system integration until final-scale testing is successfully completed. The TRL methodology is defined as a "systematic metric/measurement system that supports assessments of the maturity of a particular technology and the consistent comparison of maturity between different types of technology."[1] Appendix B includes a table of TRLs as defined by DOE Office of Fossil Energy.

1 Mankins, J., Technology Readiness Level White Paper, 1995, rev. 2004, Accessed September 2010. http://www.artemisinnovation.com/images/TRL_White_Paper_2004-Edited.pdf

The TRL score for a technology is established based upon the scale, degree of system integration, and test environment in which the technology has been successfully demonstrated. Figure 1-6 provides a schematic outlining the relationship of those characteristics to the nine TRLs.

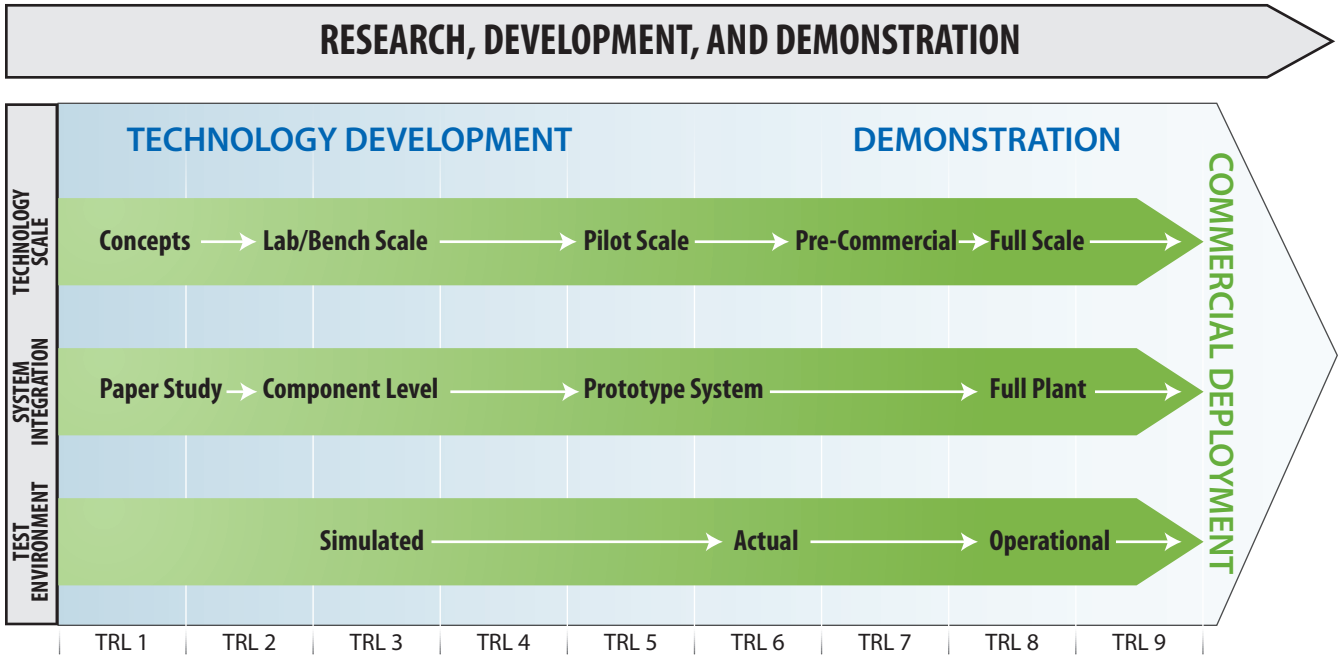

Figure 1-6. Technology Readiness Level—Relationship to Scale, Degree of Integration, and Test Environment

The scale of a technology is the size of the system relative to the final scale of the application, which in this case is a full-scale commercial power-production facility. As RD&D progresses, the scale of the tests increases incrementally from lab/bench scale, to pilot scale, to pre-commercial scale, to full-commercial scale. The degree of system integration considers the scope of the technology under development within a particular research effort. Early research is performed on components of the final system, a prototype system integrates multiple components for testing, and a demonstration test of the technology is fully integrated into a plant environment. The test environment considers the nature of the inputs and outputs to any component or system under development. At small scales in a laboratory setting it is necessary to be able to simulate a relevant test environment by using simulated heat and materials streams, such as simulated flue gas or electric heaters. As RD&D progresses in scale and system integration, it is necessary to move from simulated inputs and outputs to the actual environment (e.g., actual flue gas, actual syngas, and actual heat integration) to validate the technology. At full scale and full plant integration, the test environment must also include the full range of operational conditions (e.g., startup and turndown).

With the Crosscutting Research program, full-scale components may be developed and tested before being integrated into the system development in the other CCRP program areas. These components may be applied in existing systems separately while being evaluated for integration into either emerging or transitional energy systems. The TRLs for Crosscutting Research projects range from TRL 2 to 6.

1.4.2 RD&D RISK AND COST PROGRESSION

As the test scale increases, the duration and cost of the projects increase, but the probability of technical success also tends to increase. Given the high technical risk at smaller scales, there will often be several similar projects that are simultaneously supported by the program. On the other hand, due to cost considerations, the largest projects are typically limited to one or two that are best-in-class. Figure 1-7 provides an overview of the scope of laboratory/bench-, pilot-, and demonstration-scale testing in terms of test length, cost, risk, and test conditions. In the TRL construct, "applied research" is considered to be equivalent to lab/bench-scale testing, "development" is carried out via pilot-scale field testing, and "large-scale testing" is the equivalent of demonstration-scale testing. The CCS and Power Systems program area encompasses the lab/bench-scale and pilot-scale field testing stages and readies the technologies for demonstration-scale testing.

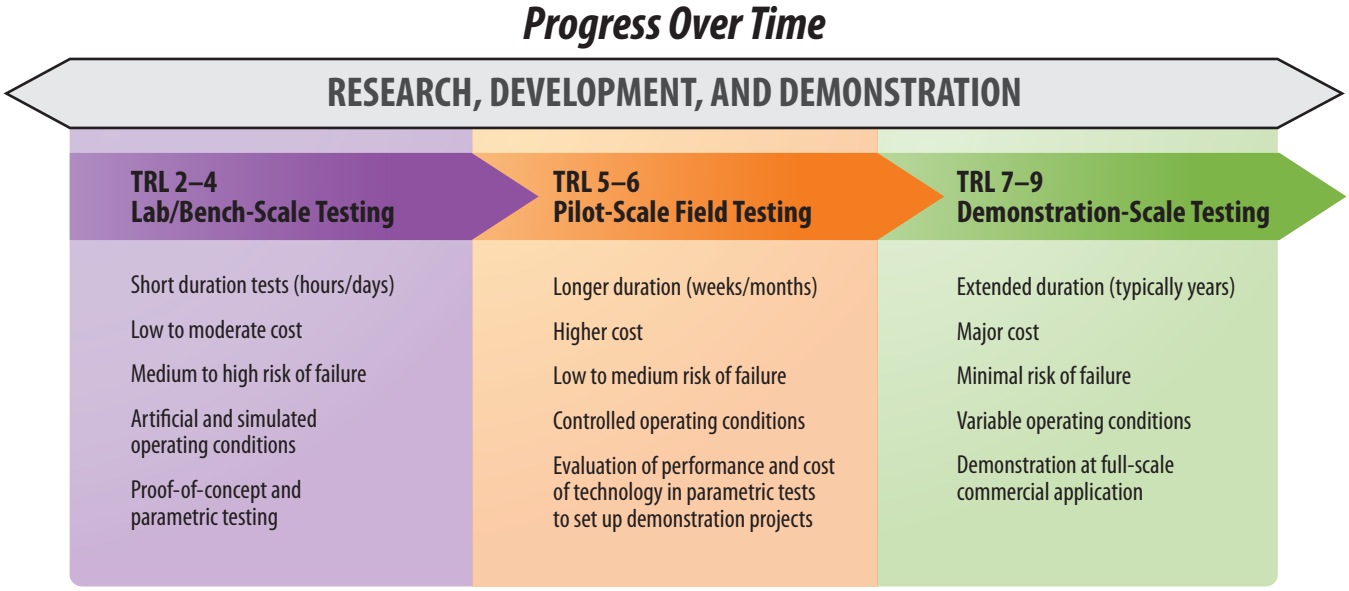

Figure 1-7. Summary of Characteristics at Different Development Scales

1.5 BARRIERS/RISKS AND MITIGATION STRATEGIES

The overarching challenge to be addressed by the CCS and Power Systems program area is to economically generate clean energy using fossil fuels. Table 1-1 provides a summary of issues/barriers, risks, and mitigation strategies for accomplishing the goals.

Table 1-1. **Issues/Barriers and Mitigation Strategies**

Issue/Barriers	Risks	Mitigation Strategy	Mitigation Strategy Risks	Program Plan Basis
U.S. need for low-cost power to maintain global industrial competitiveness	A resurgent economy will have greater energy needs than planned	Reduce the cost as much as possible	• Low R&D funding: - DOE - Cost share due to low industry interest • Unsuccessful R&D • GHG control legislation may not be enacted	• Develop technologies designed to support the Advanced Energy Systems goals for clean power production and show progress to demonstrate program value • Develop technologies in concert with industry input and needs, including support of multiple products via coal gasification • Ensure R&D pathways allow for creative solutions in early TRL phases • Ensure technologies have potential to meet programmatic targets, with thorough review at each phase of project development • Develop highly efficient, low-cost technologies that will be useful to the U.S. industrial base even if GHG legislation is not enacted
GHG emissions are increasing due to global increase in coal use	The environment may become unstable, and less able to support life as we know it	90% CCS		
Use of fossil fuels must have minimal environmental impact in terms of water and contaminant emissions	Air and water pollution may increase if current technologies are used to convert coal into power, chemicals, or liquid fuels	Near-zero emissions and reduced water use		
Natural gas prices historically unpredictable and unstable U.S. economy is dependent on foreign oil supply and price	Natural gas prices may not stay as low an anticipated under heavy demand scenarios Oil prices may rise to unacceptable levels or become unstable	Reduce the cost of gasification technologies to enable creation of chemicals and liquids from coal to reduce the need for imports and increase export potential		

CHAPTER 2: GOALS AND BENEFITS

2.1 GOALS

The goals of the Crosscutting Research program support the energy goals established by the Administration, DOE, FE, and the CCRP. The priorities, mission, goals, and targets of each of these entities are summarized in Appendix C.

2.1.1 CCRP GOALS

Currently, the CCRP is pursuing the demonstration of 1st-Generation CCS technologies with existing and new power plants and industrial facilities using a range of capture alternatives and storing CO_2 in a variety of geologic formations. In parallel, to drive down the costs of implementing CCS, the CCRP is pursuing RD&D to decrease the COE and capture costs and increase base power-plant efficiency, thereby reducing the amount of CO_2 that has to be captured and stored per unit of electricity generated. FE is developing a portfolio of technology options to enable this country to continue to benefit from using our secure and affordable coal resources. The challenge is to help position the economy to remain competitive, while reducing carbon emissions.

There are a number of technical and economic challenges that must be overcome before cost-effective CCS technologies can be implemented. The experience gained from the sponsored demonstration projects focused on state-of-the-art (1st Generation) CCS systems and technologies will be a critical step toward advancing the technical, economic, and environmental performance of 2nd-Generation and Transformational systems and technologies for future deployment. In addition, the core RD&D projects being pursued by the CCRP leverage public and private partnerships to support the goal of broad, cost-effective CCS deployment. The following long-term performance goals have been established for the CCRP:

- Develop 2nd-Generation technologies that:
  - Are ready for demonstration in the 2020–2025 timeframe (with commercial deployment beginning in 2025)
  - Cost less than $40/tonne of CO_2 captured
- Develop Transformational technologies that:
  - Are ready for demonstration in the 2030–2035 timeframe (with commercial deployment beginning in 2035)
  - Cost less than $10/tonne of CO_2 captured

The planning necessary to implement the above goals and targets is well underway and the pace of activities is increasing. The path ahead with respect to advancing CCS technologies, particularly at scale, is very challenging given today's economic risk-averse climate and that no regulatory framework is envisioned in the near term for supporting carbon management. These conditions have caused DOE/FE to explore a strategy with increased focus on carbon utilization as a means of reducing financial risk. This strategy benefits from FE's investment in the beneficial utilization of CO_2 for commercial purposes, particularly through the development of next-generation CO_2 injection/enhanced oil recovery (EOR) technology, with the objective of creating jobs and increasing energy independence. Carbon dioxide injection/enhanced oil recovery is a specific market-based utilization strategy that will positively impact domestic oil production and economical CO_2 capture and storage.

2.1.2 CROSSCUTTING RESEARCH STRATEGIC GOALS

The Crosscutting Research program supports the achievement of the CCRP goals described above. In support of those overall goals are the specific cost and performance goals for 2025 and 2035 described in the following sections and summarized Table 2-1.

Table 2-1. **Market-Based R&D Goals for Advanced Coal Power Systems**

	Goals (for nth-of-a-kind plants)		Performance Combinations that Meet Goals	
R&D Portfolio Pathway	*Cost of Captured CO_2, $/tonne*[1]	*COE Reduction*[2]	*Efficiency (HHV)*	*Capital/O&M Reduction*[3]
2nd-Geneneration R&D Goals for Commercial Deployment of Coal Power in 2025[4]				
In 2025, EOR revenues will be required for 2nd-Generation coal power to compete with natural gas combined cycle and nuclear in absence of a regulation-based cost for carbon emissions.				
Greenfield Advanced Ultra-Supercritical (A-USC) Pulverized Coal (PC) with CCS	40	20%	37%	13%
Greenfield Oxy-Combustion PC with CCS	40	20%	35%	18%
Greenfield Advanced IGCC with CCS	≤40	≥20%	40%	18%
Retrofit of Existing PC with CCS	45	n/a		
Transformational R&D Goals for Commercial Deployment of Coal Power in 2035[4]				
Beyond 2035, Transformational R&D and a regulation-based cost for carbon emissions will enable coal power to compete with natural gas combined cycle and nuclear without EOR revenues.				
New Plant with CCS—Higher Efficiency Path	<10[5]	40%	56%	0%
New Plant with CCS—Lower Cost Path	<10[5]	40%	43%	27%
Retrofit of Existing PC with CCS	30	≥40%	n/a	
Transformational pathways could feature advanced gasifiers, advanced CO_2 capture, 3,100 °F gas turbines, supercritical CO_2 cycles, pulse combustion, direct power extraction, pressurized oxy-combustion, chemical looping, and solid oxide fuel cells.				

NOTES:

(1) Assumes 90 percent carbon capture. First-year costs expressed in 2011 dollars, including compression to 2,215 pounds per square inch absolute (psia) but excluding CO_2 transport and storage (T&S) costs. The listed values do not reflect a cost for carbon emissions, which would make them lower. For greenfield (new) plants, the cost is relative to a 2nd-Generation ultra-supercritical PC plant without carbon capture. For comparison, the nth-of-a-kind cost of capturing CO_2 from today's IGCC plant, compared to today's supercritical PC without carbon capture, is about $60/tonne. For retrofits, the cost is relative to the existing plant without capture, represented here as a 2011 state-of-the-art subcritical PC plant with flue gas desulfurization and selective catalytic reduction. The cost of capturing CO_2 via retrofits will vary widely based on the characteristics of the existing plant such as its capacity, heat rate, and emissions control equipment. The nth-of-a-kind cost of capture for retrofitting the representative PC plant described above (a favorable retrofit target) using today's CO_2 capture technology would be about $60/tonne. (In contrast, today's first-of-a-kind cost of CO_2 capture for a new or existing coal plant is estimated to be $100–$140/tonne.)

(2) Relative to the first-year COE of today's state-of-the-art IGCC plant with 90 percent carbon capture operating on bituminous coal, which is currently estimated at $133/MWh. For comparison, the first-year COE of today's supercritical PC with carbon capture is estimated to be $137/MWh. Values are expressed in 2011 dollars. They include compression to 2,215 psia but exclude CO_2 T&S costs and CO_2 EOR revenues. However, CO_2 T&S costs were considered, as appropriate, when competing against other power-generation options in the market-based goals analysis.

(3) Cost reduction is relative to today's IGCC with carbon capture. Total reduction is comprised of reductions in capital charges, fixed operating and maintenance (O&M) and non-fuel variable O&M costs per million British thermal unit (Btu) (higher heating value [HHV]) of fuel input. Cost reductions accrue from lower equipment and operational costs, availability improvements, and a transition from high-risk to conventional financing. The ability to secure a conventional finance structure is assumed to result from lowering technical risk via commercial demonstrations.

(4) 2nd-Generation technologies will be ready for large-scale testing in 2020, leading to commercial deployment by 2025 and attainment of nth-of-a-kind performance consistent with R&D goals by 2030. Transformational technologies will be ready for large-scale testing in 2030, leading to initial commercial deployment in 2035 and attainment of nth-of-a-kind performance consistent with R&D goals by 2040.

(5) Cost of captured CO_2 ranges from $5 to $7/tonne for the cost reductions and efficiencies noted.

2ND-GENERATION R&D GOALS

Complete the R&D needed to prepare 2nd-Generation gasification and advanced combustion technologies—that show the ability to produce low-cost, ultraclean energy with near-zero emissions—for demonstration-scale testing (leading to commercial deployment beginning in 2025). These technologies will reduce the cost to produce energy—power with carbon capture, fuels/chemicals, or multiple products (i.e., polygeneration). Cost and performance improvements will be driven by advancements in technologies being developed in the Gasification Systems, Advanced Combustion Systems, Advanced Turbines, Crosscutting Research, and Carbon Capture R&D programs. As shown in Table 2-1, integrating the 2nd-Generation technologies has the potential to produce near-zero-emissions power with reductions in capital and O&M costs of 13–18 percent and plant efficiency of 35–40 percent. This is equivalent to a COE reduction of greater than 20 percent and a capture cost of less than $40/tonne of CO_2.

TRANSFORMATIONAL R&D GOALS

Successfully develop Transformational technologies with CCS that produce low-cost, near-zero-emissions energy generation and are ready for demonstration-scale testing leading to commercial deployment in 2035. These technologies will reduce the cost to produce energy—power with carbon capture, fuels/chemicals, or multiple products (i.e., polygeneration). For power production, maturing technologies continue to show anticipated cost and per-

formance improvements that will be driven by advancements in technologies being developed in the Gasification Systems, Advanced Combustion Systems, Advanced Turbines, Solid Oxide Fuel Cells, Crosscutting Research, and Carbon Capture R&D programs, which will result in near-zero-emissions power production with capital and O&M cost reductions of 0–27 percent and plant efficiency of 43–56 percent. This is equivalent to a COE reduction of greater than 40 percent and a capture cost of less than $10/tonne of CO_2.

2.2.3 CROSSCUTTING RESEARCH KEY TECHNOLOGY GOALS

The targets for Crosscutting Research directly support the CCRP strategic goals. These have been established in alignment with five categories—Sensors, Controls, and Novel Concepts; Computational Modeling; Carbon Capture Simulation Initiative; National Risk Assessment Partnership; and High-Performance Materials and Modeling. The goals are summarized in Table 2-2.

Table 2-2. **Crosscutting Research Program Goals**

Key Technologies	2nd-Generation	Transformational
Sensors, Controls, and Novel Concepts	• Demonstrate potential cost savings in existing and new plants through field testing of full-scale sensors. Validate benefits.*	• Develop integrated operation and optimization of the whole plant through dense wireless sensor networks coupled to advanced "smart parts" to manage complex power systems.
Computational Modeling	• Reduce system model validation uncertainty by 20%, and reduce the model time-to-solution by a factor of 2. • Determine system model improvements in accuracy of solutions and reductions in computational time.	• Reduce system model validation uncertainty by 40% and time-to-solution by a factor of 5. • Validate overall reduction in solution speeds and accuracy of solutions. Evaluate reduction in downtime and potential increase in revenue.
Carbon Capture Simulation Initiative	• Reduce carbon storage model validation uncertainty by 20%, and reduce the model time-to-solution by a factor of 2. • Determine improvements in accuracy of solutions and reductions in computational time.	• Reduce carbon storage validation uncertainty by 40% and time-to-solution by a factor of 5. • Validate overall reduction in solution speeds and accuracy of solutions. Evaluate reduction in downtime and potential increase in revenue.
National Risk Assessment Partnership	• Deploy tools to assess and verify 99% storage permanence for a variety of sites and basins. • Demonstrate 25% reduction in uncertainty for risk management.	• Demonstrate 75% uncertainty reduction for risk management based on real-time high-resolution data. • Validate modeling tools and verify storage permanence.
High-Performance Materials and Modeling	• Develop materials capable of withstanding rapid ramping of PC plant startups. • Verify materials capable of operating under advanced steam cycle conditions (1,400 °F/5,000 psi), and gas turbine performance to 2,650 °F. Assess increased plant efficiency and availability.	• Validate improved plant component performance due to computationally designed materials. • Develop materials with enhanced durability and lifetime under extreme conditions. Assess boost to efficiency.

NOTE:
* If installed at a 500-MW plant—for every 1% efficiency improvement, 22 thousand tonnes of CO_2 per year removed and for every 1% availability improvement, 35 million kWh per year in added generation.

2.2 BENEFITS[1]

The Crosscutting Research program assists in achieving the CCRP's 2nd-Generation and Transformational goals by contributing novel and innovative sensor and control technology, advanced materials, and sophisticated computational tools to each of the core combustion, gasification, turbine, and advanced carbon capture programs. Crosscutting Research develops technologies that support new and existing power plants to provide significant benefits for the U.S. energy market. Installation of improved sensors and controls will produce savings and enable lower costs for industrial, commercial, and residential power customers with significant operational and performance gains. Re-

1 Outage Data—NERC GADS Database July 28, 2010. Accessed April 18, 2011.

Average Wholesale Price Data—EIA http://www.eia.doe.gov/cneaf/electricity/wholesale/wholesale.html.

Wholesale Market Data—PJM West, NEPOOL, ERCOT Weighted Average.

Boiler Repair Costs—Personal Communication with WorleyParsons Group, Inc.

fractory materials research will extend the life of linings in gasifiers to increase commercial operation time between outages now required to inspect linings for degradation to prevent overheating and potential breach of the gasifier's steel pressure boundary. Materials modeling research is being performed to develop software capable of identifying novel alloys for application in higher pressure and higher temperature A-USC plants, which operate with higher efficiency, less fuel consumption, and lower emissions.

Preliminary results from a systems study shows that an average 1 percent improvement in heat rate across the United States for just the 500-MW net capacity units can have a fuel cost savings of up to $300 million per year. Also, an average 1 percent increase in unit availability can produce an additional 35 billion kWh of electricity per year. These improvements are easily achievable by installing new technology in both new power systems and as a retrofit to existing power systems. Figure 2-1 estimates the benefit of a 1 percent increase in heat rate and availability as a result of Crosscutting Research technology upgrades to an existing 500-MW coal-fired power plant.

Crosscutting Research addresses a wide array of technologies that support improved plant efficiencies and operational availability.

1% HEAT RATE IMPROVEMENT	1% INCREASE IN AVAILABILITY
• Single 500-MW net capacity unit - $780,000/year coal cost savings - 1 percent reduction in gaseous and solid emissions • Entire coal-fired fleet - $340 million/year coal cost savings - Reduction of 13.8 million tonnes of CO_2/year	• Single 500-MW net capacity unit - 44 million kWh/year in added generation - Approximately $2.6 million/year in sales (at 6 cents/kWh) • Entire coal-fired fleet - More than 2 GW of additional power from existing fleet

Figure 2-1. Contributions from Crosscutting Research—Value Derived for an Existing Coal-Fired Power Plant

The potential technology developments of the Crosscutting Research program can be economically installed on 150–300 GW of the existing coal power-generation fleet. The net efficiency improvements will reduce emissions by the same percentage. Studies show a 1 percent gain of efficiency over the current 32 percent average would reduce coal-fired power-plant CO_2 emissions by up to 13.8 million tonnes per year for the entire coal fleet with respect to the proposed Crosscutting Research-based refurbishments.

Economic studies have been performed that determined the impact of upgrading the current power-generation fleet. Figure 2-2 and Figure 2-3 show the limited deployment potential to the fleet based on a 2-year return on investment while assuming a modest 2 percent improvement in efficiency. Figure 2-2 shows that about 250 GW of existing plants could be upgraded for an investment of $1 million per unit when considering the benefits of efficiency improvements alone. Figure 2-3 shows that about 150 GW of existing plants could be upgraded for an investment of $5 million per unit.

Through the use of Crosscutting Research technologies, a successful retrofit can produce an additional 75 hours of runtime. This amounts to about 300 GW of the current fleet with an investment of $1 million per unit using a payback period of 2 years. Figure 2-4 shows potential annual revenue increases and amount of avoided annual maintenance costs that can be expected for various size power plants.

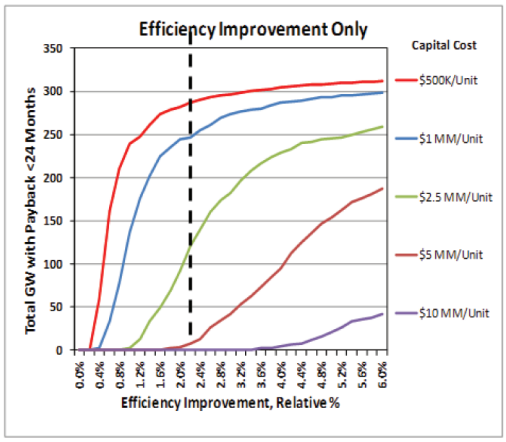

Figure 2-2. Advanced Sensors and Controls Technology, Potential Efficiency Improvement Only

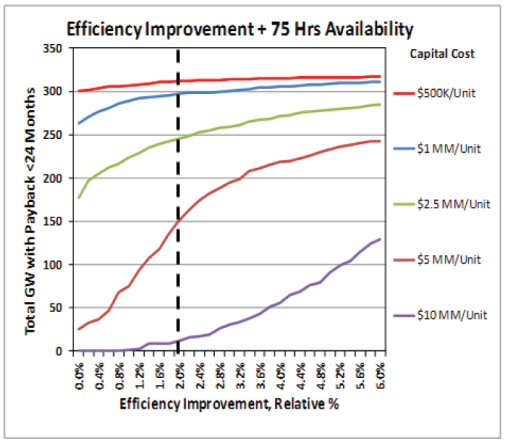

Figure 2-3. Advanced Sensors and Controls Technology, Potential Combined Efficiency and Availability Improvement

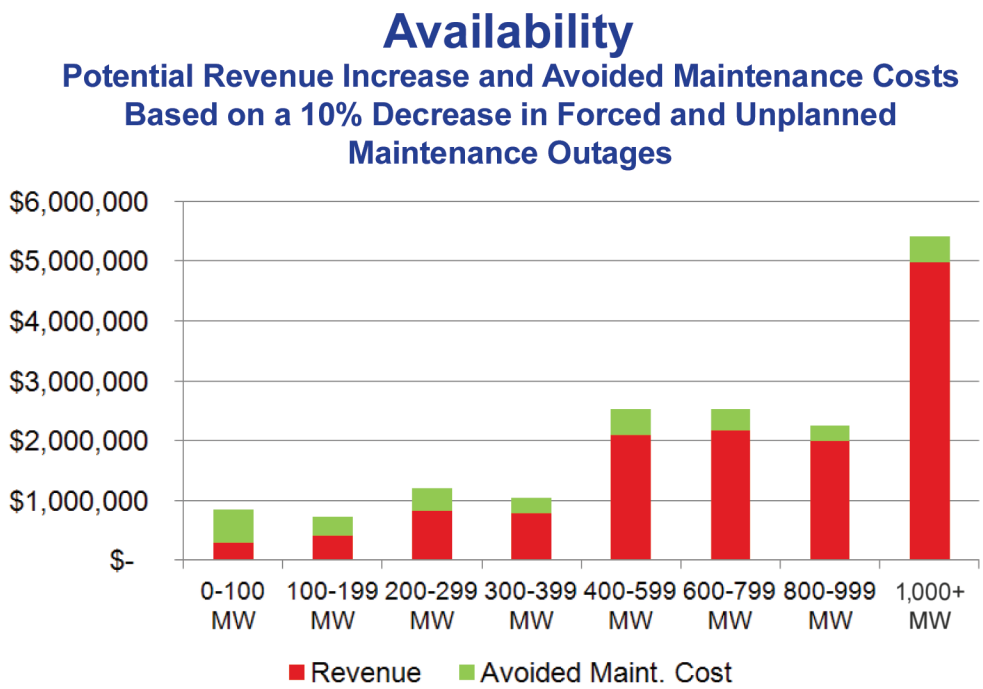

Figure 2-4. Potential Contribution Due to Plant Availability Improvements

Table 2-3 outlines the key technology research initiatives for achieving these goals.

Table 2-3. **Crosscutting Research Initiatives**

Key Technologies	2nd-Generation Technologies	Transformational Technologies
Sensors, Controls, and Novel Concepts	Improve plant efficiency and availability through (1) new classes of sensors, integration for distributed sensing, and placement and (2) advanced process controls	Develop Transformational intelligence embedded control strategies for advanced complex power systems, using advanced imaging and communication frameworks
Computational Modeling	Increase the confidence in the scaleup and design of complex multiphase reactors used in fossil-energy technology through MFIX modeling and toolset development	Demonstrate advanced combustion concept modeling, validation, and uncertainty quantification of multiphase fluid flow models for simulation of advanced concept power systems
Carbon Capture Simulation Initiative	Develop validated suite of models and simulation tools (CCSI Toolset) to reduce the cost and time of taking carbon capture concepts from lab to commercial deployment	Expand use of Transformational CCSI tools and simulation framework to evaluate/accelerate advanced power-generation concepts
National Risk Assessment Partnership	Develop of risk assessment and management tools for CO_2 to quantify risks and reduce uncertainty associated with long-term liability of geologic carbon storage	Demonstrate use of risk management tools—integrated modeling for high-resolution real-time data for validation and management of carbon storage systems
High-Performance Materials and Modeling	Improve efficiency and availability of power generation through use of A-USC materials/power plants Develop computational materials modeling to reduce the time to create advanced materials	Use predictive computational framework for rapid development of new materials critical for next-generation advanced power technologies

The following is a summary of the objectives of the Crosscutting Research key technologies.

SENSORS, CONTROLS, AND NOVEL CONCEPTS

The goal of the Sensors, Controls, and Novel Concepts effort is focused on developing new classes of sensors and measurement technology to enable robust low-cost monitoring of advanced power plants and on employing Transformational control strategies to manage real-time optimization of highly efficient carbon capture-ready systems. These new technologies are designed to benefit both existing and advanced power system such that meaningful improvements can be made to efficiency and availability. As 2nd-Generation and Transformational systems mature, sensors and controls will serve as an essential and enabling technology to operate these systems under conditions where optimal performance is balanced with reliability. New computational tools emerging from this effort will enable real-time decision making to occur in the plant so that the performance goals of advanced power systems can be realized in practice.

COMPUTATIONAL MODELING SCIENCES

The goal of Computational Modeling Science is to predict the behavior of complex multiphase flow reactors used in fossil-energy technologies. This effort combines theory, computational modeling, experiments, and industrial input. Physics-based computational models and tools will be developed to support the development and deployment of advanced fossil-fuel energy devices such as gasifiers and carbon capture reactors. It is critical to develop a practical framework to quantify the various types of uncertainties and assess the impact of their propagation in the computer models of the physical system. This will provide quantitative error-bars on the simulation data to help the designers, decision makers, and operators of reactors. A hierarchy of models is required to balance the needs of solution accuracy and time-to-solution. The benefit of the integrated model is that it is both consistent and complete. Such an integrated model with uncertainty quantification would provide a predictive capability, ensuring that the design decisions at each scale lead to feasible decisions at other scales and that globally optimal designs are achieved. Accomplishing this goal should provide for significantly faster and less costly R&D for the development of high-efficiency, zero-emission energy systems.

CARBON CAPTURE SIMULATION INITIATIVE

The goal of the CCSI is to provide technology developers and plant operators with a validated suite of models and simulation tools that enable the rapid development and deployment of new carbon capture technologies. The total cost savings that could be realized by using the CCSI Toolset to scale up and widely deploy just one carbon capture technology is estimated to be approximately $500 million on a net present value basis. With the help of the CCSI Toolset, industry will be able to reduce the time and expense of new technology development, from discovery to demonstration to widespread deployment, by a minimum of 5 years. The CCSI Toolset will include validated models of carbon capture equipment and processes, as well as new design and analysis tools and methodologies. This toolset will be made widely available by the team working within the CCSI through the auspices of a user center.

NATIONAL RISK ASSESSMENT PARTNERSHIP

The expected results for the NRAP include: (1) a platform—and associated computational tools—and robust methodology for quantifying potential risks—and associated uncertainties—for long-term CO_2 storage at a site over time, which provides a technical basis for quantifying potential long-term liability; (2) a protocol for integrating risk-based strategic monitoring and mitigation to reduce uncertainties and risk at a site; and (3) a science-based ability to identify safe operational envelopes to minimize potential risks.

As has been noted by many others, while costs are the main barrier to wide-scale implementation of carbon capture, the perception of risk and long-term liability are the greatest barriers to the widespread implementation of carbon storage. The NRAP toolset will improve our ability to evaluate risk at specific carbon sequestration sites. Successful development of this capability will help the Carbon Storage program achieve its goal of developing the ability to demonstrate 99 percent storage containment. Additionally, the tools and improved science base generated by NRAP will aid operators in the design and application of monitoring and mitigation strategies, potentially saving more than $100 million (net present value basis). The tools can also be used by regulators or their agents to help identify and quantify risks associated with geologic carbon sequestration and perform appropriate cost-benefit analysis for specific sequestration projects. Costs of long-term liability can be more easily estimated with less uncertainty, allowing greater confidence by potential investors in CCS projects.

HIGH-PERFORMANCE MATERIALS AND MODELING

Fundamental R&D on new materials will lower the cost and improve the performance (or efficiency) of next-generation fossil-fueled power-generation systems, such as A-USC combustion, oxygen (O_2)-fired combustion, gasification, and advanced turbines. In addition, research on improving predictive modeling capabilities—for both structural characteristics and fundamental properties—and computational techniques will optimize material design, reduce R&D costs, and shorten the time-to-market. These advances are required to significantly improve performance and reduce the costs of existing fossil energy power-generation systems or to enable the development of new systems and capabilities. The program is concerned with materials operating in the harsh conditions created when fossil fuels are converted to energy. These conditions include high temperatures, elevated pressures, and corrosive environments (e.g., reducing and oxidizing conditions, molten salts, and gaseous alkali compounds). The goal of the program is to ensure that the materials are available for FE to meet its technology performance requirements at a cost that is viable for market penetration.

The benefits of the Crosscutting Research program will provide achievable performance gains across all the NETL fossil-energy system programs toward achieving their program goals. Table 2-4 summarizes the Crosscutting Research technology drivers and the anticipated benefit of the R&D effort.

Table 2-4. **Crosscutting Research Key Technology Benefits**
Improving Plant Efficiency and Availability
• Availability is a key driver for unit refurbishment that includes advanced sensors and controls. - Advanced sensors and controls could reduce forced outages by 10%, making it economical for the coal fleet to refurbish sensors and controls at capital cost under $1 million. - Coal-fired units could produce an additional 35 million kWh per year in added generation for each 1% improvement in availability, resulting in ≈$2 million per year in sales (at 6 cents per kWh). • Increased unit efficiency from use of advanced sensors and controls can reduce CO_2 emissions. - Refurbishing a coal-fired unit with advanced sensors and controls could reduce CO_2 emissions by 20 million tonnes per year for every 1% efficiency improvement. - Low cost per tonne of CO_2 avoided, $2–$10 per tonne of CO_2.
Gasifier Enhanced Technology Research
• Software tools for sensor placement and life-cycle asset management could enhance overall gasifier performance by realizing: - 1–2% improvement in gasifier availability over 3 years of refractory life in an entrained flow gasifier - $5 million increase in revenue due to improved availability - 1% improvement in efficiency through better management of refractory degradation and other fouling issues • Integrated model-based control algorithm and associated sensors can: - Increase gasifier ramping rate by 20–25% compared to current approaches - Save significant O_2 with 7–10% savings at partial load of the gasifier - Achieve 1–2% improvement in unit capacity via improved operation
Advanced Technology Modeling and Prototyping
• Advanced model-based tools may shorten power-system component development cycles and improve assessment of uncertainties and risks. Enhanced knowledge sharing with industry may reduce capital cost by 5% during commercialization and yield cost savings for the power industry on the order of $3 billion. - Achieving the CCSI goal could allow development cycle to skip over one intermediate-scale plant (e.g., 120 MWe) while improving risk assessment. Reaching larger scale demonstration 5 years earlier could result in estimated cost savings of ≈$100 million. - Achieving the NRAP goal can create science-based tools that will raise confidence in defined storage-security metrics and identify safe operational envelopes to ensure 99% permanent storage. - The NRAP, working with industry and insurance companies, aims to remove a key barrier to the business case for long-term CO_2 storage.
Increasing Power Systems Efficiency
• Evaluate and develop materials technologies that allow use of advanced steam cycles in coal-based power plants operating at steam conditions of up to 760 °C (1,400 °F) and 5,000 psi. • Novel materials can allow for increased temperature and pressure, resulting in power-plant efficiencies of 45–47% and CO_2 emissions reduction of 15–20%. • Developing materials to enable an oxygen-fired A-USC plant would lower the balance-of-plant cost due to less coal handling and smaller pollution control components for the same net plant output. • Computational methods applied to the design, development, and optimization of materials to accelerate creation of cost-effective, functional materials deployable with less repetitive testing; and for assisting advanced plant designs to go operational more rapidly.

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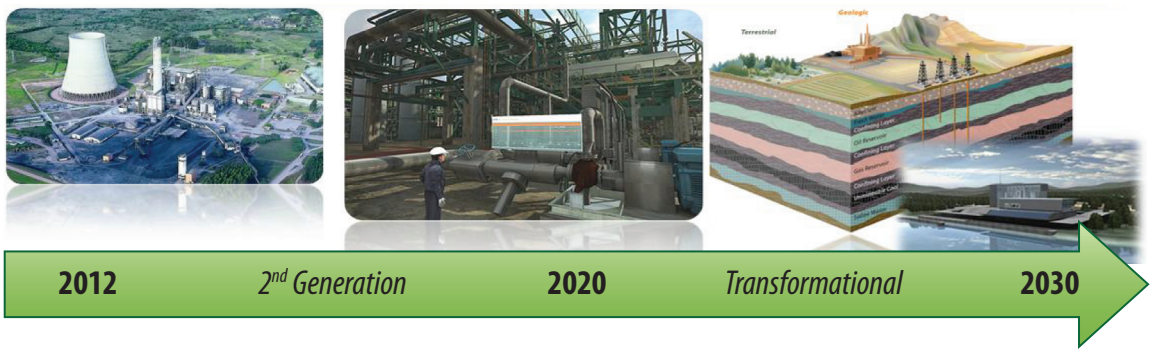
CHAPTER 3: TECHNICAL PLAN

3.1 SENSORS, CONTROLS, AND NOVEL CONCEPTS

The goal for this key technology is to make available new classes of sensors and measurement devices to increase the efficiency and accuracy that manage complexity; permit low-cost, robust monitoring; and enable real-time optimization of fully integrated, highly efficient power-generation systems. Pathways toward this goal include development of sensors capable of monitoring key parameters (temperature, pressure, and gas compositions) while operating in harsh environments, with real-time online analytical evaluation and measurement capabilities. A complementary pathway is focused on the development of advanced process control including research in self-organizing information networks and distributed intelligence for process control and decision making. Research in the area of advanced sensor manufacturing is being conducted to determine the feasibility of constructing embedded sensors into such devices as turbine blades, boiler walls, piping, and tubing. Together these pathways provide a holistic approach that can bring about value and derive benefits for existing systems leading to important contributions toward realizing the goals of Transformational systems. Figure 3-1 presents the planned evolution of sensor and control technology from the current state toward a unified and highly integrated system concept. This approach provides measurable benefit for existing systems and serves as an essential and enabling technology for 2nd-Generation and Transformational power systems.

WHOLE SYSTEM APPROACH IN R&D –

Seeking Breakthrough Concepts That Target Stakeholder Needs



Low-Cost High-Benefit Technology for Existing Power System's Performance and Efficiency Goals

Enabling System for Emerging Plants

- Essentail for managing complexity
- Link to supply infrastructures
- Link carbon capture to unit operations
- Link to Smart Grid management

Fully-Immersive and Intelligent Control for Transformational Power-Generation Technology

- Dynamic control via multiscale networks
- Predictive capability with self-diagnosing "smart parts" and virtual management capability
- Self organization of information networks to distribute intelligence and enable real-time optimization
- Fully interactive simulation to evaluate changes, perform troubleshooting, and optimize system performance near real-time

Figure 3-1. Targeted Evolution of 2nd-Generation and Transformational Technologies Within Advanced Energy Systems and Carbon Capture

3.1.1 BACKGROUND

The Sensors, Controls, and Novel Concepts key technology addresses barriers and challenges associated with operation existing power plants and advanced energy systems. The motivation for conducting R&D in the Sensors, Controls, and Novel Concepts key technology is based on the following technical drivers:

- Explores system upgrades using low-cost, high-benefit technologies that enhance large equipment performance and reliability.
- Explores existing sensor technology potential for operations under harsh-environmental conditions associated with current and future energy conversion processes.
- Boosts efficiency of existing facilities and contributes to high reliability of emerging systems
- Supports other power-generation technologies and related infrastructures by providing the foundation for actionable information, intercommunication across infrastructures, and intracommunciation within a highly integrated, large-scale power plant.
- Makes operation of future ultraclean energy plants possible by providing novel architectures for operational control that is designed to manage a nonlinear dynamic system with high levels of system integration and rapid response to system changes.
- Enables new paradigms in plant and asset management beyond traditional process control by offering a novel sensor and control system that can embed intelligent sensors at various levels to monitor, in real time, asset condition, system performance, and plant operation through a computational architecture that self-organizes data and information and takes action at a time scale faster than that of the current capability.

Implementation of the Sensors, Controls, and Novel Concepts key technology has been shown to increase efficiency and lower emissions of existing coal-fired power plants. The implementation of improved monitoring technology also affords better insight into the condition of equipment and process upsets and therefore contributes to an increase in the reliability, availability, and maintainability of operating systems. Additionally, the Sensors, Controls, and Novel Concepts key technology directly impacts CO_2 emissions from large-scale plants to increase efficiency, heat rate, and fuel utilization—thus reducing the amount of CO_2 produced per unit of power generated. For each 1 percent increase in heat rate for a 500-MW coal-fired power plant, over 30 tonnes of CO_2 can be avoided without any significant retrofit to plant equipment or components. These improvements can be implemented on existing power plants to derive immediate benefit for the nation. While these contributions may only have an incremental impact relative to capture technologies, these changes are significantly less expensive and are easily maintained over long-term operation of the power system.

The 2nd Generation of the Sensors, Controls, and Novel Concepts key technology is centered on the measurement systems and approaches suitable for harsh environments. The utilization of fossil fuels in an environmentally benign manner drives the conversion of the fuel and the generation of steam to occur at high temperatures and elevated pressures with specific control over the conditions at which to attain the targeted performance goals. These conditions can include temperatures that extend up to 1,600 °C and pressures up to 1,000 psi on the fuel side and up to 760 °C and 5,000 psi on the steam side. Harsh conditions also include highly corrosive and erosive conditions leading to significant failure of commercially available instrumentation.

Given the harsh conditions, the primary driver was a science-based approach to improve measurement technology, which included consideration of new materials, novel sensor designs, and sensor packaging that addressed practical implementation issues.

As an example, R&D led to the development of sapphire-based fiber sensors enabling temperature measurement beyond 1,600 °C, along with packaging that enabled extended measurement capability in a full-scale coal gasifier. Other measurement technologies successfully developed for harsh environments included a simple dual-sensor

design to detect flashback in lean premix gas turbines. This combustion control and diagnostics sensor was designed to survive turbine combustion conditions and was successfully patented and licensed to industry by NETL. Another simple sensor design employed a complex materials matrix on an optical fiber to enable high-temperature gas detection for real-time monitoring of hydrogen and carbon monoxide. A simple optical fiber was coated with a nanocrystalline doped-ceramic mixture to measure the primary species in syngas and was successfully tested in the outlet stream of a pilot-scale gasifier. In addition to these technologies, other types of measurement technologies have sparked a range of new ideas and breakthrough concepts that are currently under development.

The progression from 2nd-Generation through Transformational technologies and the important contribution the technologies can make toward realizing design, construction, and operation of clean energy power systems is shown Table 3-1.

Table 3-1. **Sensors, Controls, and Novel Concepts Technology Development Summary**

Key Technology	1st-Generation Technologies	2nd-Generation Technologies	Transformational Technologies
Sensors, Controls, and Novel Concepts	• Fiber-based sensors • Laser-based and microsensors for online detection • Harsh-environment sensor packaging	• Extreme-environment sensors • Sensor placement and networking • Self-organizing systems control	• Energy harvesting • Wireless sensors • Advanced manufacturing technology for embedded sensors • Integrated, autonomous control—highly distributed sensor monitoring systems • Smart sensor networks

3.1.2 TECHNICAL DISCUSSION

The technologies for the 2nd-Generation systems include extreme-environment sensors, predictive control capabilities, and networked sensors with self-organizing capability. Technologies supporting this approach include noncontact optical sensors, fiber-optic sensors, microsensors, imaging techniques, self-powered wireless sensing devices, and model-based control of core energy processes (e.g., gasification, chemical looping).

Other efforts serving as a basis for support of the Transformational power systems include integration of advanced sensor concepts into a smart sensor network. Rapid prototyping and production of sensors via advanced manufacturing techniques and computational developments that build from process models, simulations, and visualizations will be needed to realize the concept of fully immersive intelligent control architectures. The development of distributed intelligent control architecture encompasses advanced sensing smart actuation and process control algorithms that enable dynamic control at multiple scales within a unified architecture. The concept will allow "smart" sensors to create "smart" parts to enable self-diagnostic capability that will lead to the system being capable of predicting maintenance. Algorithm development, in concert with sensor networks, will enable self-organization capability to allow for real-time optimization in conjunction with changing objectives for the operating plant. These approaches, when integrated into an interactive immersive environment, will enable the complexity of a Transformational type system (integrated carbon capture) to be managed for optimal performance and in balance with expectations for high availability and reliability of the plant.

The technologies to be developed supporting the Sensors, Controls, and Novel Concepts program plan for advanced sensors and control systems are shown with a timeline by research focus area in Figure 3-2.

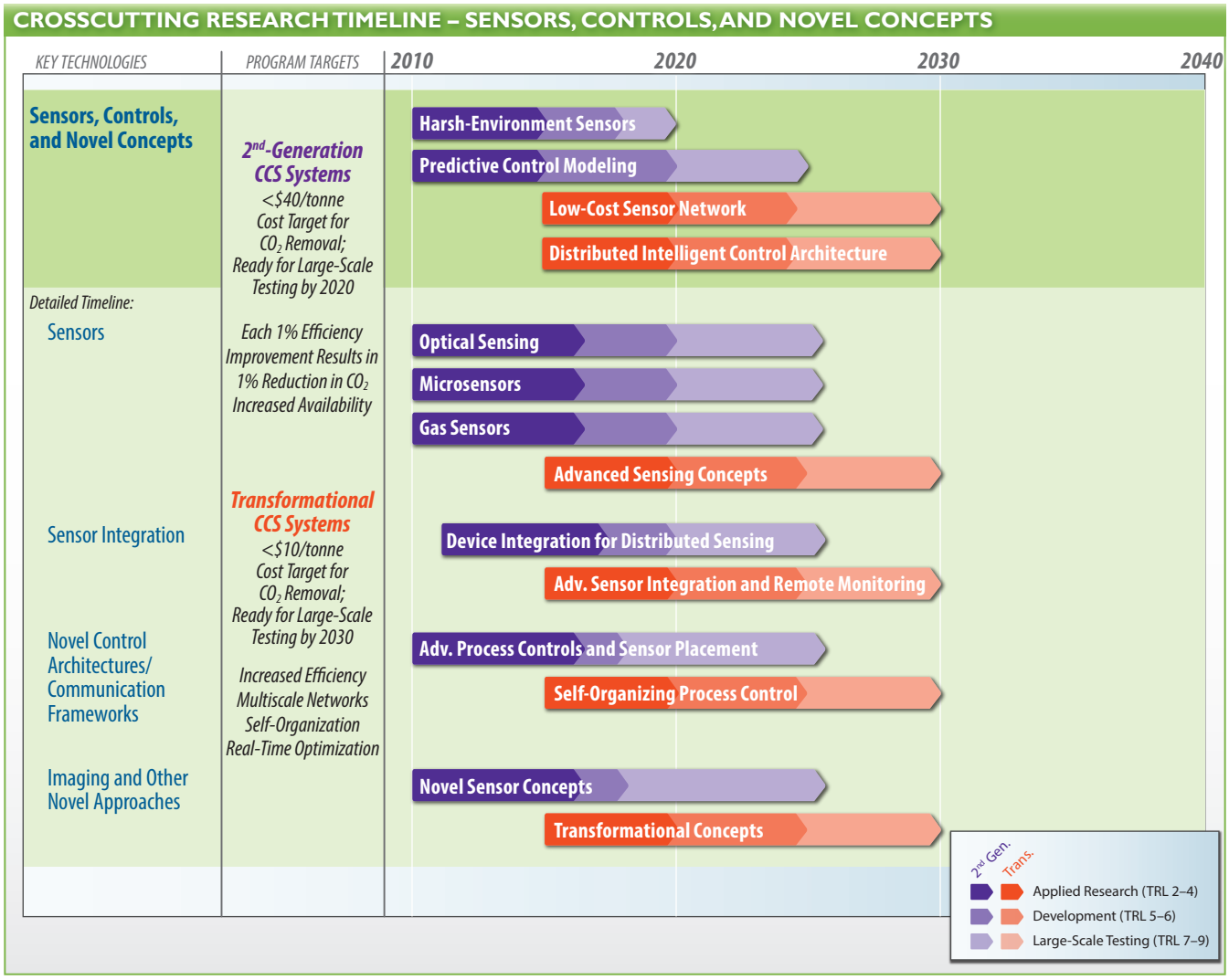


Figure 3-2. Sensors, Controls, and Novel Concepts—2nd-Generation and Transformational Technologies Development Timeline

2ND GENERATION TECHNOLOGIES

The 2nd-Generation Crosscutting Research technologies build from 1st-Generation technologies with specific focus on bridging technology that will enable the vision to be realized for the Transformational power systems. It is within the 2nd-Generation technologies that the synergy between the Crosscutting Research technologies (sensors, controls, novel concepts, advanced modeling and simulation, and high-performance materials) is most evident and value of the work is significant. The technology is poised to make important contributions toward the goals of the 2nd-Generation power systems by reducing cost and time for design, offering viable materials construction, and contributing to measurement control technology required to operate the new systems. This research not only buys down the risk for the individual technologies but also brings realistic insight into which power-generation technologies should move forward.

Crosscutting Research for sensors and controls is pursuing multiple research focus areas of sensor technology for measurement approaches that can offer superior performance in harsh environments as well as enable low-cost and dense distribution of measurements within a unit or plant to improve the understanding of operational performance. Research focus areas include optical sensing, microsensors, novel sensor wireless, and energy harvesting technologies. Within each research focus area, the ability to perform multiple types of measurements (e.g., temperature pressure, gas species) and measurement distribution are being researched. In concert with making measurements

is the ability to take action on the information collected from the sensors. Traditional process control has evolved as computational capability has grown; however, the basis for process control has not changed since the mid-20th century. The research in advanced process control takes advantage of the computational capability to generate actionable information by employing model-based control and inserting cognitive capability at low levels with the sensor and control architectures such that power systems can respond in real time for optimization performance. This overall approach is based on 2nd-Generation technology, but growth of the concepts and application of the new control architectures target Transformational systems so that the inherent complexity of the Transformational power systems is not a barrier to deployment.

TRANSFORMATIONAL TECHNOLOGIES

Crosscutting Research efforts will continue to focus on maximizing the efficiency and environmental performance of advanced coal technologies while minimizing development and deployment costs. Crosscutting Research's approach emphasizes new technology development that has the capability to be commercialized and applied toward the efficient, economical solutions of Transformational power systems and the availability of CCS technology.

Transformational research in the sensor and control area is focused on development of a unifying sensor and control architecture that employs a variety of heterogeneous sensor networks and an appropriate distribution of computational intelligence to enable a fully immersive real-time process control with the following capabilities:

- Dynamic control via multiscale networks
- Predictive capability with self-diagnosing "smart parts" and virtual management capability
- Self organization of information networks to distribute intelligence and enable real-time optimization
- Fully interactive simulation to evaluate changes, perform troubleshooting, and optimize online

Sensor networks will afford more flexibility in the operation of a power plant. This network will allow greater integration of individual systems to optimize overall plant performance through acquisition of additional data from more system locations. Computational intelligence capability development is necessary to support a new generation of intelligent power systems. It will enhance system performance and be supported by low-cost sensors that can be freely distributed in all desired system monitoring locations, which can simultaneously provide data to optimize operations and transmit component health conditions prior to failure.

3.1.3 R&D APPROACH—PERFORMANCE TARGETS AND MEASURES

This section provides details on the performance measures and milestones for the categories identified within the overall timeline (Figure 3-2). Projects being conducted within these areas to achieve the targets are also provided. A portfolio of projects is managed within each category to address stakeholder needs, but to also accelerate development timelines for approaches that are viable and down-select those deemed not viable for commercialization.

HARSH-ENVIRONMENT SENSORS

Includes R&D in fiber-optic sensors, noncontact optical approach, high-temperature microsensors, distributed sensor designs, coaxial cable sensors, and associated sensor packaging for harsh environments. Within advanced power systems, the harsh conditions can include temperatures that extend up to 1,600 °C and pressures up to 1,000 psi on the fuel side and up to 760 °C and 5,000 psi on the steam side. Harsh conditions also include highly corrosive and erosive conditions leading to significant failure of commercially available instrumentation. Other types of harsh environments include subsurface conditions for injection or storage of CO_2. These conditions can experience temperatures up to 250 °C and extreme pressures (up to 10,000 psi at depths down to 12,000 feet) with high salinity (250,000 ppm) and pH effects from the presence of dissolved and liquefied CO_2.

Performance targets in this area include materials, sensor designs, and packaging that are robust and enable accurate sensing for extended periods of time. For each application, the survival and sensor life is different. For gasification applications, the survival and sensor device is targeted to be 1 year before replacement. For subsurface applications, the goal is to permit long-term monitoring capability with survival times in the 10–20-year timeframe. Because survivability is a key parameter, the construction and sensing materials are key measures within a project to assess if the approach is viable. The ability to design a sensor for a specific application that is robust is the most common point where viability can be ascertained. As such, sensor testing in representative conditions is the key measure for each project. Because these measures occur for a portfolio of projects, these measures are established and tracked on an annual basis for each project.

PREDICTIVE CONTROL MODELING

Encompasses computational efforts to represent physical systems and processes in a dynamic manner by developing and using high-fidelity models. For the purposes of control, these high-fidelity models are reduced and configured to run in real time (second time scales) to represent the dynamics of the operating system. Using reduced and fast models in conjunction with estimation algorithms and other types of predictive algorithms, an overall control solution can be derived to enable model-based control to be used for real-time process control. This general approach is well understood for linear and steady-state systems. Research within the Sensors, Controls, and Novel Concepts key technology adopts these approaches but incorporates new approaches that have the ability to develop control systems with fast dynamics for nonsteady-state and incorporate controls that are capable of handling systems that are inherently nonlinear. Accomplishing these developments, with real system validation, provides significantly increased control compared with that of traditional proportional-integral-derivative control and is more robust than linear model predictive control algorithms.

LOW-COST SENSOR NETWORK

Includes a variety of sensor technologies and approaches that will enable the manufacturing cost of individual sensors to be low and allow many sensors to be installed at a low cost and with ease. This Transformational research focus area also includes research to enable dense distribution of sensors within a single device, via a single port for in situ monitoring or embedding as part of a component. Specific tracks of R&D include:

- Multimeasurement microdevices
- Distributed sensing element along a fiber or cable sensor
- Multiplexing of cable- or fiber-based sensors
- Wireless sensors with energy harvesting capability
- Advanced manufacturing of sensors including approach for embedding sensor into components

Measures for these diverse approaches are based on individual projects with preestablished milestones. In general the measure for this research focus area is the significant increase in usable information generated by a large number of highly distributed sensors. The balance between manufacturing, installation, placement, and value of the measurement needs to be established through the testing and tracking of value.

DISTRIBUTED INTELLIGENT CONTROL ARCHITECTURE

This research focus area is a Transformational effort that attempts to unify and apply a wide range of novel computational and measurement approaches to derive value and improve operation and control of complex systems. This research focus area encompasses novel computational approaches to optimize sensor placement for various objectives (e.g., performance, fault management, cost) and to enable cognitive capability within sensing and actuation components such that intelligence can be distributed within a control architecture. This distribution of intelligence, coupled with self organization of actuation and sensing devices, is anticipated to offer a robust approach to

managing fast dynamics and large amounts of data/information; and it addresses the need to make many decisions in millisecond time scales for a large and highly integrated power system with carbon capture. Measures for this area include the correct identification of algorithms and architecture to permit novel approaches to be combined and operated as a unified system. NETL has developed simulation tools and a hardware-based test bed to evaluate concepts and to provide a platform to assess the value of these breakthrough concepts.

The expected benefits and deliverables of each of the research focus areas for the Sensors, Controls, and Novel Concepts technologies are summarized in Figure 3-3 and Figure 3-4.

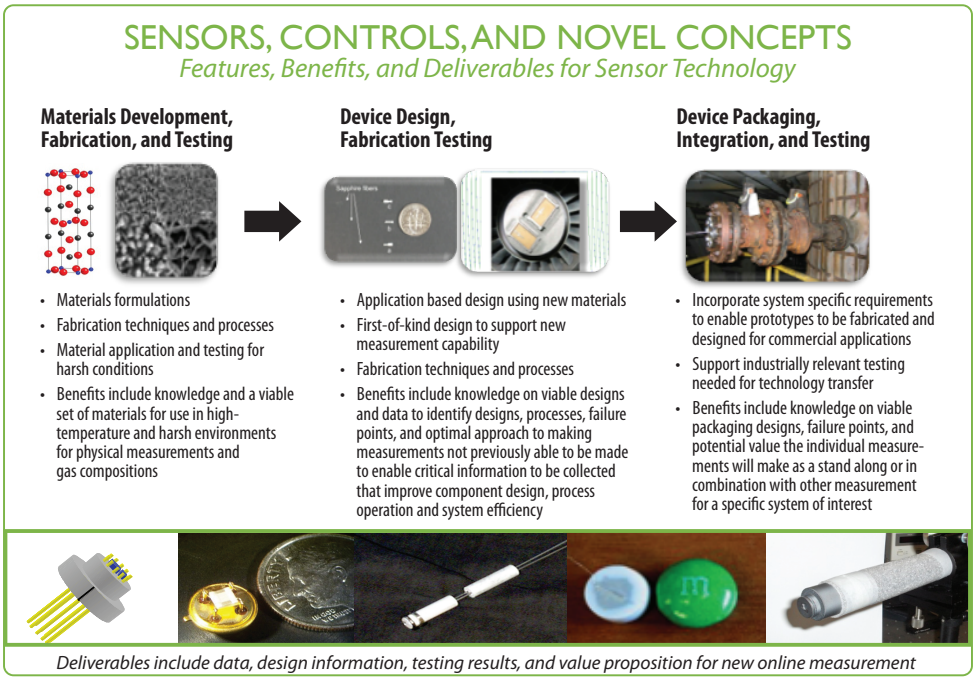


Figure 3-3. Features, Benefits, and Deliverables for Sensor Technology

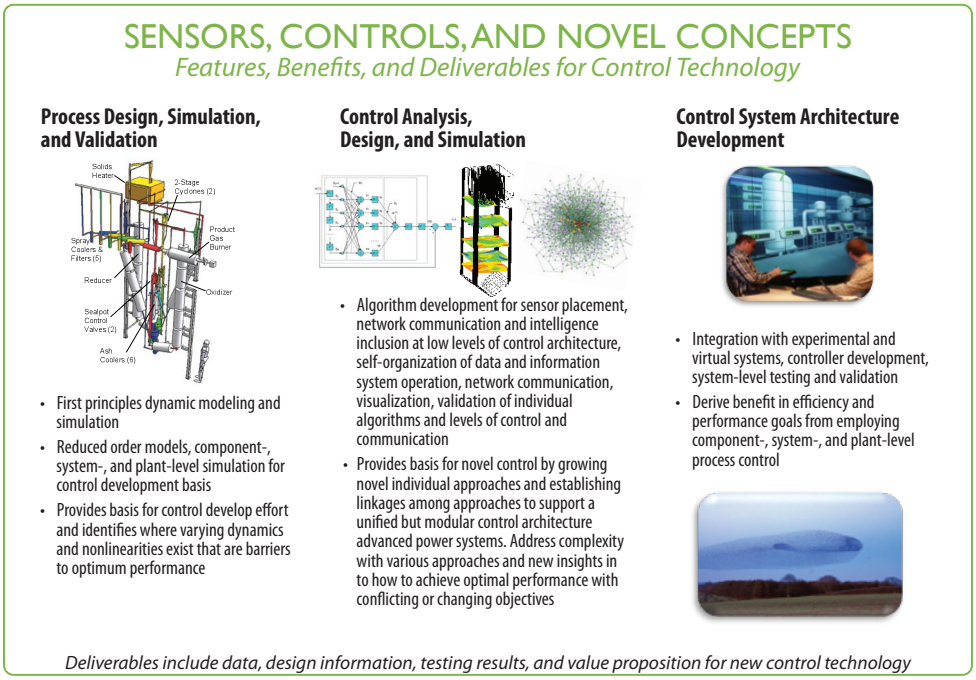
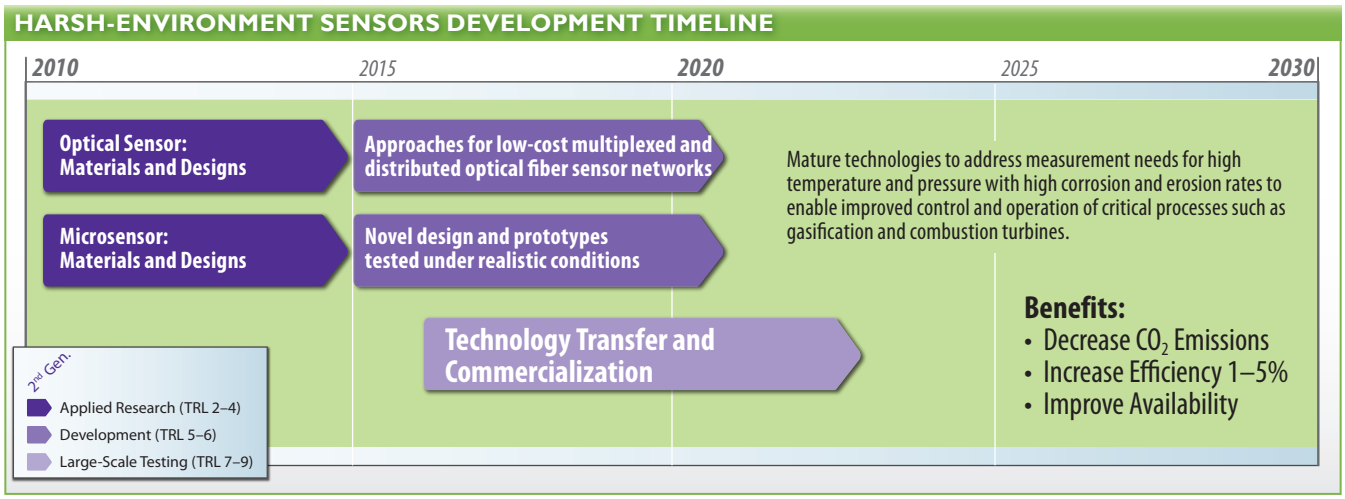


Figure 3-4. Features, Benefits, and Deliverables for Control Technology

3.1.4 PROGRAM PLAN TIMELINE

The Sensors, Controls, and Novel Concepts key technology comprises multiple research focus areas of sensor development and a variety of approaches for novel control development. As individual projects progress in their respective research, some approaches are determined to be viable, others require rescoping, and some projects are concluded due to the fact that the approach is not viable relative to programmatic goals. A rolling portfolio management approach is taken for each subarea so that advancements in each area can be fostered in a timely fashion and new ideas can be introduced. This approach helps to progress the timeline for sensors and controls, promote an accelerated development path for individual projects, and increase the probability that goals and milestones will be met in this key technology. Detailed timelines for the 2nd-Generation Sensors, Controls, and Novel Concepts technologies are shown in Figure 3-5 and Figure 3-6.



Project	Development Effort
Sapphire-Based Optical Sensor	Develop optical sensors using sapphire and ceramics to measure temperature (up to 1,600 °C) in coal gasifiers.
High-Temperature Ceramic Microgas Sensors	Target optimal design and packaging of integrated sensor probe for in situ measurement of O_2, NO_x, and carbon monoxide in high-temperature environments.
Nanocoated Fiber-Optic Sensors for Synthesis Gas Detection	Develop materials, synthesis techniques, and device fabrication methods to produce highly selective gas sensors by coating fiber optics with nanoscale materials for real-time detection of synthesis gas.
Polymer Derived Ceramic Microsensors for Extreme Environments	Enhance material performance, fabrication techniques, and sensor packaging designs to enable temperature and pressure measurement in high-temperature (up to 1,800 °C) dynamic system operation.

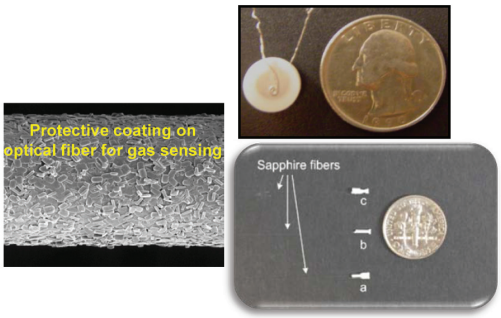
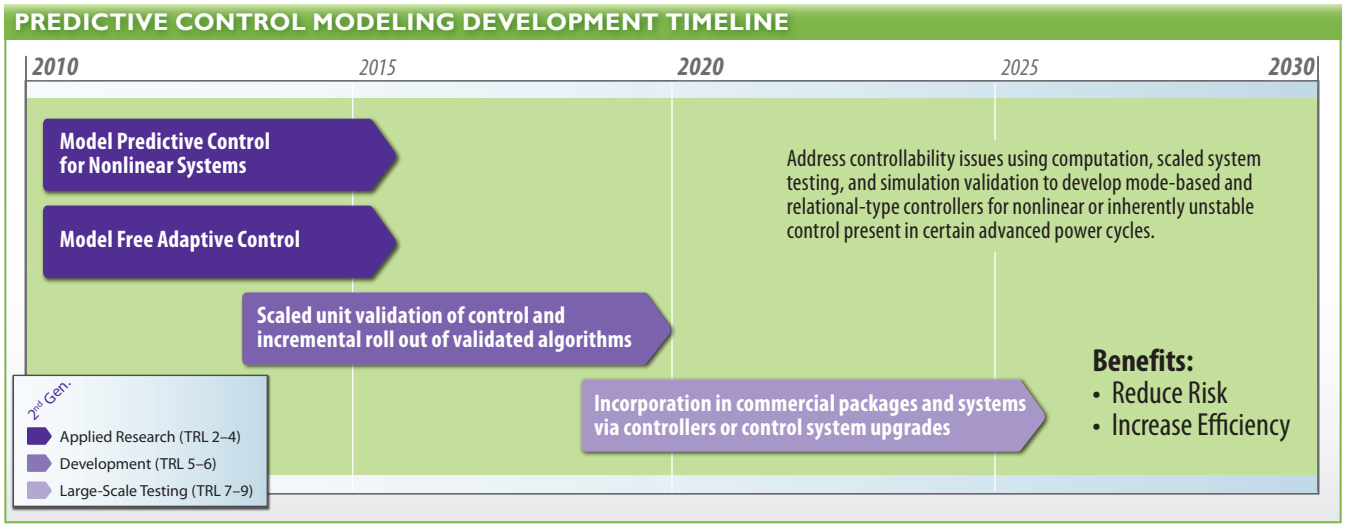


Figure 3-5. Sensors, Controls, and Novel Concepts—2nd-Generation Harsh-Environment Technologies Development Timeline



Project	Development Effort
Model-Based Control for Entrained Flow Gasifiers	First principles models and reduced order models based on a full-scale validated system to develop controller for fast nonlinear dynamics and improve operation during transient conditions.
Modeling and Control of Hybrid Combustion-Gasification Chemical Looping Systems	Fundamental process study and simulation to develop flow-loop control during multiloop reaction and operation of a 4-loop chemical looping system. Use model-based control to enhance loop stability and autothermal operation.
Model Free Adaptive Control for Actuation Control and Loop Stability	Develop neural and relational networks to support improved actuation control and greater stability in proportional-integral-derivative loops where oscillation leads to unstable and nonsteady control of combustion and other power cycles.

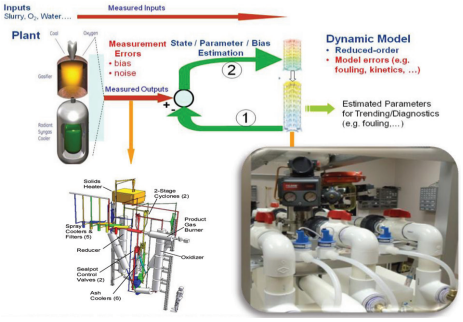
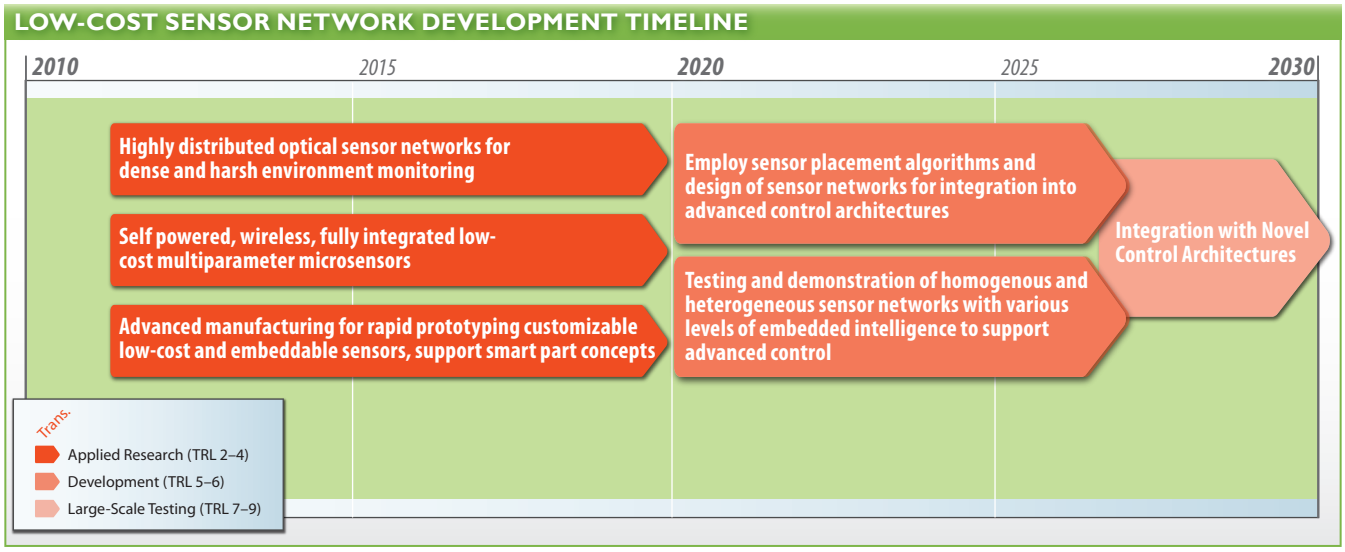
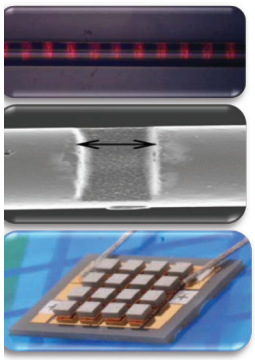


Figure 3-6. Sensors, Controls, and Novel Concepts—2nd-Generation Predictive Control Modeling Technologies Development Timeline

Detailed timelines for the Transformational Sensors, Controls, and Novel Concepts technologies are shown in Figure 3-7 and Figure 3-8.

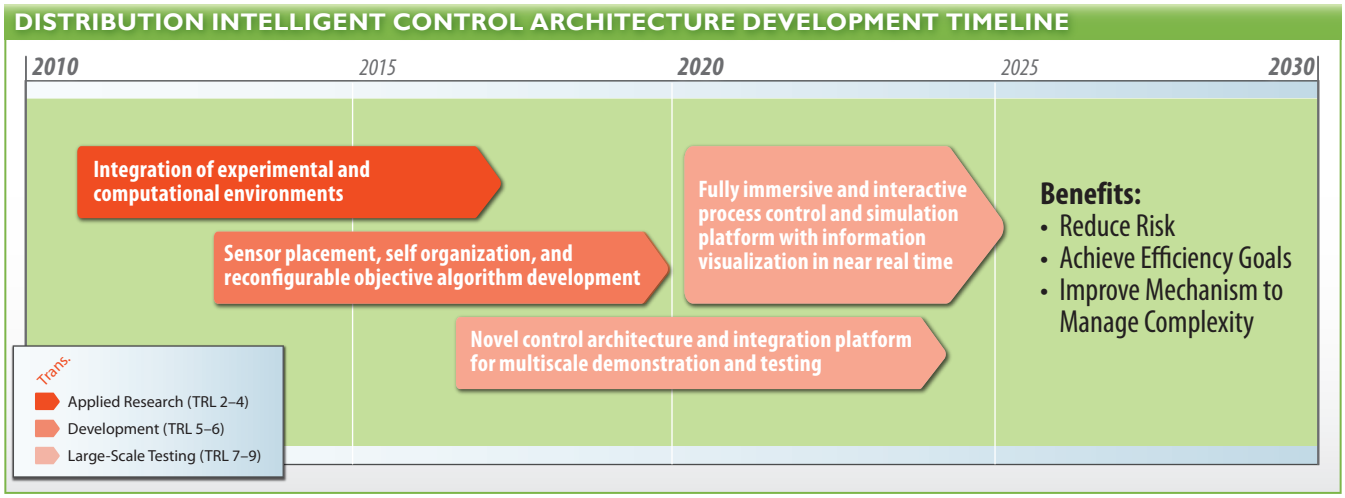


Project	Development Effort
Distributed Optical Sensing for High -Temperature Environments	Develop optical sensing devices capable of multiple sensors on a single fiber for temperature, pressure, and strain including signal processing, device fabrication, and sensor performance.
Self-Powered Wireless Sensor Systems	Develop of state-of-the-art self-powered sensor devices for highly distributed energy applications using energy harvesting technology, low-power sensors, and standard wireless communication devices.
Embedded Sensing Technology for Complex Geometries	Develop materials, synthesis techniques- and device fabrication to enable embedded and wireless sensing approaches for turbine applications.
Coaxial Cable Sensors for Highly Distributed Sensing Applications	Research toward the application of coaxial cable (variety of materials) to permit sensing of physical parameters for robust and highly distributed sensing capability in energy applications.



Benefits:
- Reduce Risk
- Achieve Efficiency Goals
- Improve Mechanism to Manage Complexity

Figure 3-7. Sensors, Controls, and Novel Concepts—Transformational Low-Cost Sensors Network Technologies Development Timeline



Project	Development Effort
Merged Environment for Sensor and Control Analysis and Development	Develop and utilize a merged experimental and computational environment to simulate new sensor and control algorithms based on stigmergic approaches.
Distributed Information Coordination for Objective-Based Control	Analyze sensor and data coordination to generate actionable information for system control and enable system to respond to multiple or changing objectives.
Information Theoretic Framework for Self-Organizing Agent-Based Architectures	Develop architecture and computational environment to enable agents to optimally collect, transmit, aggregate, and utilize data to produce actionable information.
Computational Techniques and Algorithms to Support Sensor Placement for Advanced Energy Systems	Apply emerging computational techniques to develop sensor placement algorithms for advanced energy systems that support a sensor network design and advanced control strategy that includes multiple control and condition monitoring objectives.

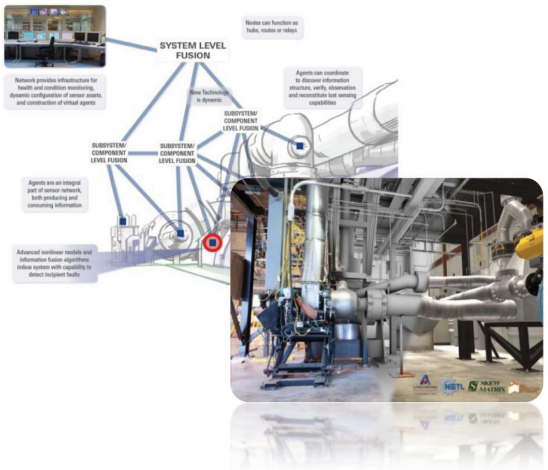


Figure 3-8. Sensors, Controls, and Novel Concepts—Transformational Distributed Intelligent Control Architecture Technologies Development Timeline

3.1.5 RESEARCH FOCUS AREA BENEFITS

The overarching benefits of implementing the Sensors, Controls, and Novel Concepts technologies relate to improvements in efficiency, availability, maintainability, and the overall operability of advanced energy systems. Under certain scenarios for both 2nd-Generation and Transformational technologies, the implementation of sensor and control technology is quantifiable. In future scenarios, primarily Transformational power systems with carbon capture, where novel and breakthrough sensor and control concepts are being pursued, the qualitative benefit and needs for the technology have been established. The benefits of 1st-Generation retrofits and upgrades of sensor and control technology are offered in the following sections.

Because sensor and control technology is an enabling technology, its value is derived and assessed from implementing the technology into a practical and real-world systems. While significant technical contributions have been realized through this program, these types of research advancements and associated breakthroughs are not used for establishing value or benefit of the program or Technology Area. However, patents, publications, and associated technology breakthroughs in this area serve as contributions to the energy and science communities.

Combining this analysis with the current state of the coal-fired fleet, the following conclusions were made regarding sensor and control investments:

- Advanced sensors and controls have the potential to be economically installed on 150–300 GW of the existing coal power-generation fleet.
- Availability is the key driver in determining the economics of refurbishment projects. Reducing forced outages by 10 percent alone would make it economical for most of the coal fleet to refurbish at capital costs under $1 million.
- Coal-fired power-plant CO_2 emissions could be reduced by around 1 percent or 20 million tonnes per year from advanced sensors and controls refurbishment. The cost per tonne of CO_2 avoided would be low, between $2 and $10 per tonne of CO_2.
- Funding NETL advanced sensors and controls research provides a return on investment of 5:1 or 15:1 depending on New Source Review requirements.
- With respect to benefits from implementing improved process control (via model-based algorithms) and placing sensors for better management of assets (via sensor placement algorithms), the following were estimated for projects conducted under the Sensors, Controls, and Novel Concepts key technology. The estimates are based on the assumption that the algorithms are fully implemented on a full-scale plant.
- An integrated model predictive control algorithm with integrated sensing can achieve the following if implemented on an IGCC system:
  - Improved steady-state and transient tracking during ramp-up and turndown of gasifier
  - Improved ramping of gasifier by 20–25 percent faster than that of current approaches
  - Significant savings in O_2 required, with 7–10 percent savings at partial load of the gasifier
  - A 1–2 percent improvement in unit capacity via enhanced operation of coal-fed IGCC systems
- An integrated algorithm for sensor placement and sensor hardware for asset management of a coal gasifier is estimated to contribute to overall gasifier performance in the following ways:
  - A 1–2 percent improvement in gasifier availability as realized over 3 years of refractory life in an entrained flow gasifier
  - A $5 million increase in revenue via improved availability
  - A 1 percent improvement in efficiency through better management of refractory degradation and other fouling issues

3.1.6 BARRIERS/RISK AND MITIGATION STRATEGIES

The overarching challenge to be addressed by the Sensors, Controls, and Novel Concepts key technology is economically generating clean power using fossil fuels in a deregulated power industry. Power systems that meet this challenge operate under extremely harsh conditions (high temperature, high pressure, corrosive, erosive, etc.). These systems cannot be operated optimally without suitable instrumentation and sensors capable of surviving and operating in harsh environments. In addition, advanced power systems operation is highly complex and cannot be sufficiently managed by current process control practices. The new classes of harsh-environment, high-priority sensors are based on a prioritized list of sensor needs as defined by industry and the Crosscutting Research program. Challenges with sensing in harsh environments are addressed by this key technology through the development of high-temperature sensor materials, new sensor designs, and sensor packaging. The risks and mitigation strategies for Sensors, Controls, and Novel Concepts are discussed in Table 3-2.

Table 3-2. **Sensors, Controls, and Novel Concepts Barriers/Risk and Mitigation Strategies**

Issue	Barrier/Risk	Mitigation Strategy
Achieve cost-effective clean energy with fossil fuels in a deregulated power industry	• Extremely harsh conditions (high temperature, high pressure, corrosive, erosive, etc.) • Complex advanced power systems operation management	• Develop high-temperature sensors capable of surviving and operating in harsh environments • Develop high-temperature sensor materials, new sensor designs, and sensor packaging • Develop process control of complex systems through both modeling and experimental techniques
Achieve capital cost reduction performance target	Material price increases	Employ minimal amounts of raw materials
Achieve efficiency gain performance target	Existing/new plants may not adopt advanced sensors and controls technologies	Perform studies and publish results to ensure designers have a basis to adopt new sensor and controls technologies
Achieve all performance targets by 2030	Delay in program execution; inadequate progress on cost and performance goals	Conduct near-, mid-, and long-term R&D projects as well as laboratory, proof-of-concept, and pilot-scale projects to foster the commercialization of the technologies

3.2 COMPUTATIONAL MODELING

3.2.1 BACKGROUND

Understanding the performance of complex multiphase flow reactors used in fossil-energy technology and having the means to impact their design early in the developmental process is important for two reasons. First, about 75 percent of the manufacturing cost of any product is committed at the conceptual design stage, even when the incurred cost might be very small (http://www.professionalpractice.asme.org/Design/Analytical/Impact_Design_Cost.cfm). Once the conceptual design stage has been completed, the opportunities for cost savings have already diminished. Computational models can be used to simulate the device and understand its performance before the design is finalized, which is important for reducing cost. Second, during new technology development—for example, the development of sorbent adsorber/desorber reactors for CO_2 capture—empirical scaleup information is not available because reactors at the large scales that are required have not been built. Furthermore, it is well known that traditional scaleup methods do not work well for multiphase flow reactors, such as the ones used for gasification or carbon capture. Therefore, science-based models with quantified uncertainty are important tools for reducing the cost and time required for their development.

Central to NETL's multiphase flow reactor modeling efforts is the laboratory's computational fluid dynamics (CFD) code—Multiphase Flow with Interphase eXchanges (MFIX)—developed specifically for modeling reacting multiphase systems. This open-source software has over two decades of development history and more than 2,700 registered users worldwide. This software has become the standard test for comparing, implementing, and evaluating multiphase flow constitutive models and has been applied to an extremely diverse range of applications involving multiphase flows. The successes achieved in modeling such complex problems have led to new and improved models that are now available to the modeling community, which feature greatly improved simulations of key attributes within multiphase flow systems such as drag, polydispersity, attrition, and agglomeration models, and other significant advances.

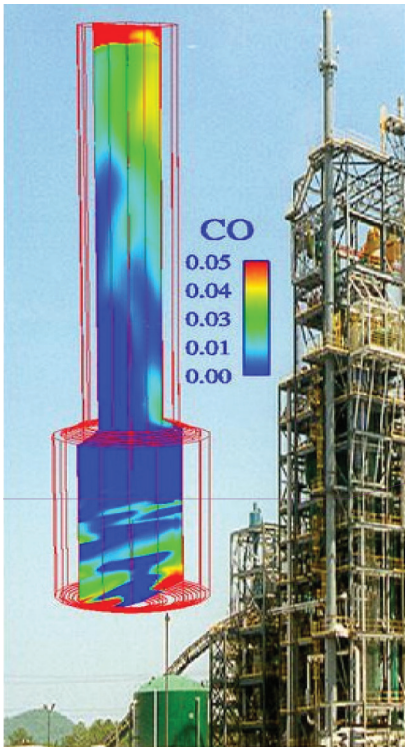


Figure 3-9. High Carbon Monoxide Mass Fractions Through a Center Plane Along the Reactor Length

The current research at NETL also seeks to ensure access to a comprehensive database of reaction kinetics models describing devolatilization, secondary tar cracking, soot formation, char gasification, and gas phase reactions for a wide variety of coals. Such reaction kinetics data exist in a number of commercial software packages (e.g., PC Coal Lab™ and Chemical Percolation Model), but these data/models are not generally easily implemented in CFD codes such as NETL's open-source code MFIX or commercial software such as Fluent or Barracuda. NETL's unique capabilities in multiphase flow science coupled with its extensive knowledge of carbonaceous fuel reactions enabled the development of a platform to incorporate carbonaceous reaction kinetics into multiphase flow models. This work has resulted in the development of the Carbonaceous Chemistry for Computational Modeling (C3M), a platform to perform virtual kinetics experiments that elucidate the effect of operating conditions (e.g., heating rate, temperature, pressure, fuel type) on output variables such as conversion rates and yield. C3M also provides a tool that can directly import kinetics information from NETL and other sources into a variety of computational software such as CFD models, ROMs, spreadsheet models, experimental planning software, and uncertainty quantification software.

C3M, MFIX, and commercial CFD software have been successfully used to model systems such as transport gasifiers. The results of the transport gasifier model offered a never-before-seen look at the hydrodynamics and chemistry inside a gasifier. For example, simulation results showed that oxygen reached the upper region of the mixing zone in the reactor, whereas it was expected that all the oxygen would be consumed in the lower region where the air contacts the hot recycled char. This prediction was later validated when sampling probes were installed in the mixing zone and the oxygen concentration in its upper region was measured. In another instance, the calculations showed a high concentration of carbon monoxide and solids near the disengager section of the reactor (Figure 3-9), which was also validated with subsequent measurements. The validated model was then successfully used to simulate a scaled up design of the gasifier.

Table 3-3. **Computational Modeling Technology Development Summary**

Key Technology	1st-Generation Technologies	2nd-Generation Technologies	Transformational Technologies
Computational Modeling	• Demonstration of available computational models within the suite of MFIX solvers with uncertainty quantification using the Transport Reactor Integrated Gasification (TRIG™) reactor at the National Carbon Capture Center (NCCC) • Continuum and discrete subgrid-scale modeling • Development of cohesive force models • Expansion of C3M database to include other kinetic processes (chemical looping, CO_2 sorbents, mercury capture, desulfurization) and add uncertainty quantification capabilities	• Validated hierarchy of high-fidelity reacting multiphase models • Integration of uncertainty quantification into the hierarchy of reacting multiphase models and ROMs within MFIX and C3M • Development of CFD-based ROMs • Multiscale modeling to incorporate particle morphology changes into a device scale models • Development of advanced hardware specific tools and algorithms to leverage advances in processor architecture for massively parallel multiphase simulations	• Development and application of a hierarchy of chemical looping models with uncertainty quantification • Development and application of a hierarchy of pressurized oxy-combustion models with uncertainty quantification

3.2.2 TECHNICAL DISCUSSION

One of the primary drivers in gaining acceptance and widespread use of computational models for advanced energy systems is the need for fast-running high-fidelity models where uncertainties in the predictions can be quantified. A developmental goal suggested during a workshop on multiphase flow science held at NETL in 2006 was that a high-fidelity simulation of a 25-MW transport reactor must finish overnight. The current time-to-solution is an order of magnitude greater than that target. At this point, there is no widely accepted, formal definition of the term "high fidelity"—other than to imply that the models will be based on CFD. There is a need to link the specified time-to-solution to a specified model fidelity. NETL is taking a leading role in meeting the goal identified in 2006 through the development and demonstration of reacting multiphase models with uncertainty quantification. Figure 3-10 graphically presents the development path for these efforts—i.e., a continuous effort to improve computational efficiency of the suite of models within MFIX into an industrially acceptable platform.

Performance estimates—for example the conversion, heating value, syngas composition, temperature, and pressure distribution in a gasifier—obtained from a computer model should provide the design engineer with a clear understanding of the range and likelihood of behavior resulting from variability in the operating parameters or design alternatives. Such variation in performance may result from uncertainties in the input parameters such as, coal feed rate, circulation rates, oxygen or steam feed rates. It is critically important to develop a practical framework to quantify the various types of uncertainties. The capability to assess these uncertainties and provide quantitative error-bars that might arise from their propagation in the computer models of any physical system provides valuable insight to help gasification designers, decision makers, and unit operators. There is a growing recognition of the fact that CFD model validation cannot be complete without explicit accounting of various uncertainties. A number of means have been developed to characterize uncertainty. Uncertainty quantification tool kits such as PSUADE from Lawrence Livermore National Laboratory or DAKOTA from Sandia National Laboratories can be coupled with NETL's in-house suite of multiphase software—such as MFIX-discrete element model (DEM), MFIX continuum, hybrid MFIX, or MFIX-particle in cell (PIC)—to other multiphase reduced order models (ROMs) and develop a hierarchy of computational models with quantified uncertainty.

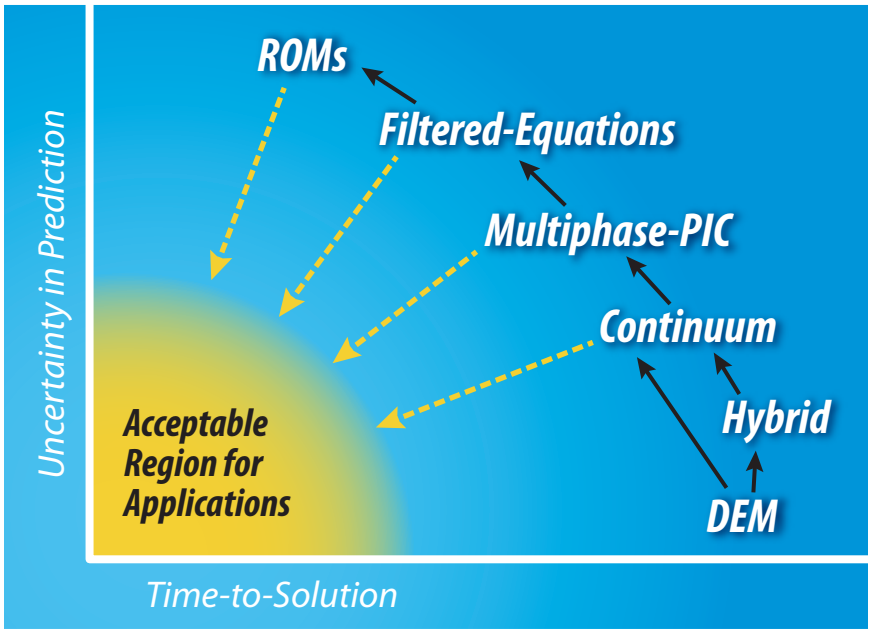


Figure 3-10. Development Path of Computational Models

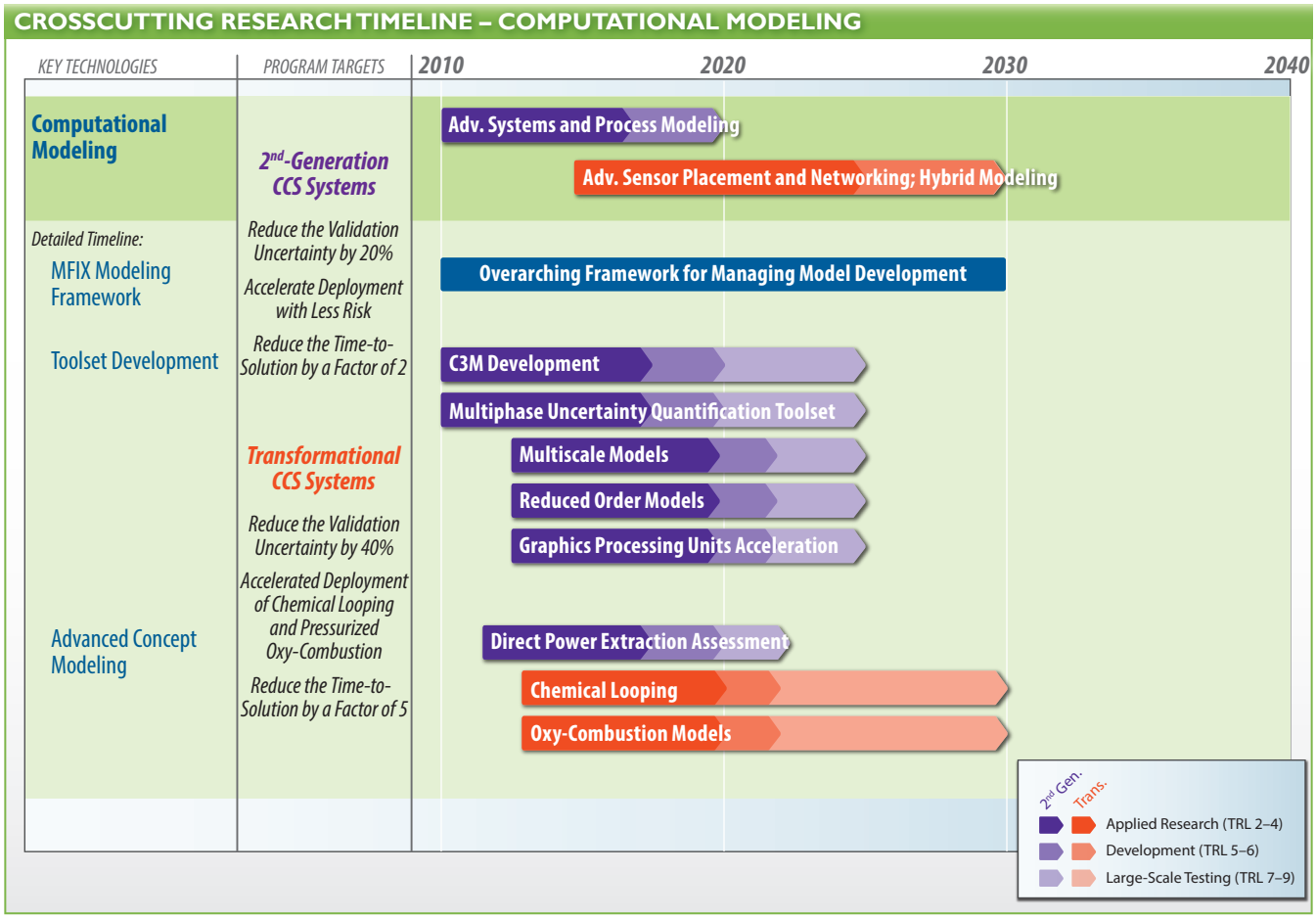


Figure 3-11. Computational Modeling—2nd-Generation and Transformational Technologies Development Timeline

2ND GENERATION TECHNOLOGIES

Reacting Multiphase Models with C3M and Uncertainty Quantification Hierarchy of Models—The primary impact of this research is that it will alter the role computational models play in gasifier design. To meet the needs of industry in the development and commercialization of advanced gasification systems, demonstrating a framework that enables quantification of uncertainty associated with numerical gasifier analysis and design will provide industry with the ability to pick from a range of models that can meet industrial constraints for turn-around-time and computational resources with assurances that the models can be run within each model's reliable, predictive capability, and with knowledge of the uncertainty associated with the results. NETL is deploying a suite of open-source multiphase solvers along with the PSUADE uncertainty quantification package from Lawrence Livermore National Laboratory to achieve the goals for this research focus area. At the start, the PSUADE package will be coupled with the MAX continuum model (one of the multiphase solvers) to develop a TRIG cofeed model. The model will be exercised and the uncertainty associated with key parameters—such as reaction rates and gas/solid flow rates—will be established. The next step will be to incorporate heat and mass transfer capabilities into the Eulerian-Lagrangian solvers to develop a reacting multiphase ROM. A TRIG cofeed model will then be constructed in MFIX-PIC, ROM, and hybrid MFIX models (with uncertainty associated with various parameters) and the models will be run and results will be compared.

Multiphase Uncertainty Quantification Toolset—To ensure the predictive ability of the computational tools used to model multiphase flow, fidelity to actual behavior in full-scale systems is essential. In addition, determining the degree of fidelity that can be attained when using fast-running ROMS can greatly enhance the value of these compu-

tational tools. Advances in computer hardware allow acceleration of the run time for models such as those included in the MFIX family of models. Developing an understanding of the accuracy possible at each level of complexity can lead to creation of a hierarchical set of modeling tools that allow for flexible computational strategies when starting to design novel components—including multiphase reactors—such as gasifiers, chemical looping combustors, and oxy-fired systems.

Development of Increased Fidelity ROMs—This portion of the research will use reacting multiphase CFD models to develop a high-fidelity basis for creation of the ROMs. Current weaknesses in existing proper orthogonal decomposition-based models will be addressed and/or new theories will be developed to develop fast-running ROMs that are based on high-fidelity reacting multiphase CFD models.

Graphics Processing Units (GPUs) and Other Acceleration Techniques—This research focuses on accelerating the family of models that serve as the core capability within this effort. Advances in computer hardware, using general purpose GPUs for the acceleration of MFIX-DEM and MFIX-PIC models, may lead to methodologies for performing similar acceleration on other NETL applications, such as the MFIX continuum model. High-end computing architectures are going through a transition from few cores on a chip to hundreds of cores or coprocessors. However, the efficient use of many-core architectures is dependent on the communication patterns and memory footprint of the algorithms used in MFIX. At present, MFIX is parallelized using MPI for multiprocessor calculations and with OpenMP for in-processor calculations over multiple cores. Efficient OpenMP implementation will provide a good starting point for efficient utilization of coprocessing architectures.

Multiscale Modeling—A conceptual framework for integrating models at different scales is shown in Figure 3-12. The models at different scales are bridged by using ROMs that capture the predictive behavior of the lower scale model while allowing the integrated formulation to be computationally tractable. The ROM included at each scale is a reduced representation of the model at the scale below, ranging from a set of parameters (e.g., elementary rate constants) to models derived using sophisticated model reduction techniques such as proper orthogonal decomposition. The goal of multiscale ROMs is that they allow feasible realizations of complex domain models and capture accurate complex model behavior over a wide range of the decision space.

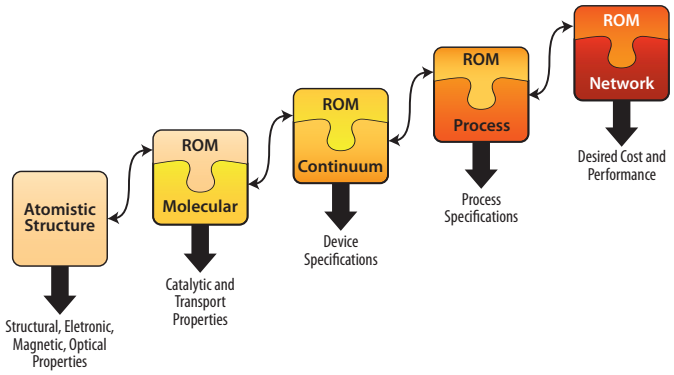


Figure 3-12. Hierarchy of Models that Exchange Information with the Help of ROMs

This approach allows evaluation of new hardware concepts and virtual exploration of systems such as gasifiers, chemical looping reactors, pressurized oxy-combustion units, and CO_2 capture vessels using a hierarchical, integrated framework of models coupled to uncertainty quantification methodologies.

Direct Power Extraction Assessment—The immediate goal of the computational modeling research is to expand the MFIX framework to include uncertainty quantification for all the various models under the MFIX framework. In parallel to this, reducing the time-to-solution will also be pursued through GPU acceleration and improved numerical algorithms. Activities will also include incorporation of microscale structure and properties of particles into the multiphase CFD models to increase the fidelity of these models. Using the C3M framework kinetic models will be

made available and coupled to MFIX and commercially available multiphase CFD models. This hierarchical structure will be demonstrated using the TRIG gasifier. Once testing is complete, new technologies (chemical looping and pressurized oxy-combustion) can be explored.

TRANSFORMATIONAL TECHNOLOGIES

Chemical Looping—Chemical looping combustion (CLC) is one of several Transformational technologies being developed by NETL for power and process heat generation (for a more detailed description of this technology see *CCRP Technology Roadmap*, Advanced Energy Systems). Bringing this technology to the marketplace in the least amount of time while reducing costs and risks, will require development of greatly improved computational tools such as reacting multiphase CFD models that can be extensively used to provide highly reliable predictions. Even though these tools exist today on a somewhat rudimentary level, significant improvements are needed. There are several specific areas needing improvement: interphase heat and mass transfer, the treatment of polydisperse solids phases where solids of different sizes and densities are reacted such that each of these may change, and ready availability of high-quality kinetics data for the simulations coupled with means to include the kinetics into the CFD simulations. For this, NETL's C3M provides a good starting point, but needs to be expanded to include quality data for these advanced reaction processes from continued work at NETL and elsewhere.

Pressurized Oxy-Combustion—Pressurized oxy-combustion concepts have been proposed in both combustor-boiler configurations as well circulating fluidized bed (CFB) boiler configurations. The technical challenges that will be addressed target the numerical simulation of the combustor-boiler configuration in both nonpressurized and pressurized forms. Key submodels for radiation, oxidation, and pyrolysis will be developed. Computational models will be developed for turbulence and the interaction with other phenomena (e.g., turbulence chemistry and turbulence radiation). Further, much more data are needed to cover the operating range for an oxy-fuel combustion system, because in contrast to air-fired systems the diluent composition and flow rate are variable. This also implies that more simulations are required to appropriately assess the design and operating space. Progress has been made on a number of fronts to address the previously stated issues. For example, some progress has been made in the standard design radiation models and ongoing research in the effect of gas composition on coal chemistry (oxidation, gasification, and pyrolysis). NETL's ongoing activities on coal chemistry for gasification (C3M) would be applicable for submodels of some of these systems.

Circulating configurations add the additional complexity associated with the dynamics of dense-gas solid flows, due to the significantly higher volume occupied by solids (sand) in the system. On the other hand, the lower operating temperature associated with the CFB technology would indicate that radiative heat transfer is a less significant mode of heat transfer than that in the combustor boiler configuration. A number of different configurations exist for commercial concepts, in fact, many CFB configurations have the heat exchanger directly integrated with the reacting zone of the reactor. For Pratt & Whitney Rocketdyne's Zero Emission Power and Steam System (ZEPS™) process in particular, integration of the in-bed heat exchange in the reaction zone is a critical element to maximize the device efficiency. The necessity to tractably and accurately model in-bed heat exchangers is one of several challenges that modeling an oxy-CFB system shares with the modeling of other technologies built around multiphase reactors (e.g., sorbent-based CO_2 capture, chemical looping, gasification). NETL research in this area will be leveraged; as well as ongoing efforts within the CCSI project to develop such an approach for in-bed heat exchanger for post-combustion sorbent-based CO_2 capture.

3.2.3 R&D APPROACH—PERFORMANCE TARGETS AND MEASURES

The product of the computational modeling efforts will be a hierarchy of validated models within NETL's in-house code, MFIX. The models will be part of the open-source MFIX package made available to the public interested in using reacting multiphase computational models. These models will be coupled to NETL's C3M package, which will grant users of any of the models within MFIX immediate access to one of the largest sources of kinetics information in the world. All of the models within MFIX and C3M will allow users to (1) incorporate uncertainty

quantification into any reacting computational model's predictions to evaluate how uncertainties inherent to most model input parameters propagate through the model and (2) quantify the impact these uncertainties have on model predictions. Ongoing experimental programs at both the Morgantown, WV, and Pittsburgh, PA, sites will provide kinetics and hydrodynamics data for verification and validation of the models.

One of the success criteria of the computational modeling efforts is to apply this technology to industrially relevant problems to ensure transfer of this technology to industry. To achieve this goal, efforts will initially focus on development of a hierarchy of cofeed TRIG models based on the reactor in operation at the NCCC. The models being developed are general in nature, but the TRIG unit was selected for demonstration due the availability of experimental data, excellent working relationship with engineers at NCCC, and the current timelines of the commercialization of this technology. Another success criterion is the ability of the hierarchy of models to achieve the performance target of "overnight run" proposed in the 2006 workshop report.

To achieve success in the transition of the computational modeling efforts from 1st-Generation development and demonstration through 2nd-Generation to development of Transformational technologies, an integrated approach will be used to combine theory, in-house computational modeling expertise, experiment, and industrial input.

This section provides details on the performance measures and milestones for the allied projects that have project management plans in place.

2012–2020 MILESTONES

- Incorporate uncertainty quantification linked to the MFIX framework for transient multiphase CFD model
- Develop, verify, and validate new MFIX solvers to allow particle-in-cell computations and discrete element simulations
- Develop technology development roadmap for reduced order modeling
- Demonstrate the GPU acceleration of the Lagrangian models in MFIX and determine the suitability of the use of GPU acceleration for the continuum MFIX model
- Apply the uncertainty quantification toolset developed, kinetics in C3M, and the hierarchy of models in MFIX to the NCCC TRIG reactor. Validate and quantify uncertainty for each model against the TRIG experimental data
- Incorporate various multiscale models into MFIX to integrate microscale information into the CFD models
- Demonstrate the capability of the ROM and provide estimates of the predictive capabilities of the ROM

2020–2030 MILESTONES

- Incorporate intrusive sampling techniques into MFIX to perform uncertainty quantification
- Develop improved heat and mass transfer models and use multiscale modeling techniques to incorporate microstructure of a particular oxygen carrier into the CFD model
- Conduct ROM simulations of a TRIG with uncertainty quantification
- Use available in-house experimental data to develop appropriate kinetics submodels
- Create a hierarchy of models for chemical looping
- Develop improved modeling techniques for oxy-combustion to incorporate the coupling between turbulence and chemistry or radiation effects
- Incorporate kinetics submodels and available experimental data for oxy-combustion into the C3M framework
- Develop a hierarchy of verified and validated pressurized oxy-combustion models with uncertainty quantification

Deliverables associated with the aforementioned performance measures and milestones are provided in Table 3-4.

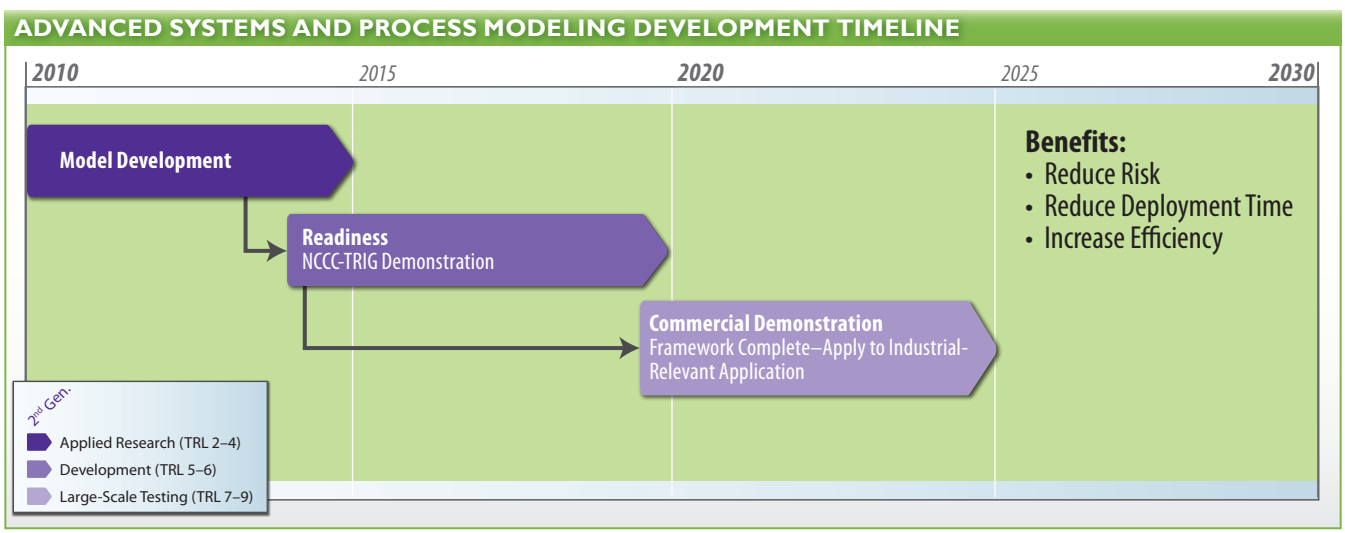
Table 3-4. **Computational Modeling Deliverables**

Deliverable	Date	Description of Software Components
Framework of High-Fidelity CFD Models	2015	Using MFIX as the underlying model, Eulerian-Lagrangian model will be added to the MFIX suite of solvers. This model tracks, in a Lagrangian framework, a computational model that statistically represents many actual particles in the system. This new model will allow faster turn-around times than those of the traditional MFIX continuum model by leveraging advances in GPU acceleration.
Incorporation of Multiscale Approach into MFIX	2017	The ability to couple microscale physics into device-scale submodels for improved heat and mass transfer calculations, drag, and particle-particle and particle-wall interactions will be incorporated into the MFIX framework.
Incorporation of Uncertainty Quantification	2018	Within the framework of MFIX solvers uncertainty quantification will be added to allow modelers to investigate how uncertainty in input parameters impact the model's predictions and quantify that amount of uncertainty.
Development of a Hybrid Solver	2020	A hybrid solver will be implemented into the MFIX framework to allow increased fidelity. The hybrid solver will allow modeling of discrete particle to be coupled to the continuum solver in MFIX. This model will allow, for example, detailed chemistry to be done on a particle level and be tracked to a point where the discrete particle could be incorporated into the continuum solid phase.
Reduced Order Models	2022	ROM development will allow a user to take high-fidelity CFD model results and regress these results into a ROM, which will allow for extremely fast turn-around times.

3.2.4 PROGRAM PLAN TIMELINE

The Computational Modeling capabilities for accelerating the deployment of 2nd-Generation and Transformational technologies will be developed as shown in Figure 3-13 and Figure 3-14, respectively. This modeling will represent a first-of-its-kind in terms of allowing users to select a model that meets the user requirements on computational time restrictions, fidelity, and level of acceptable uncertainty in a model's prediction.

2ND GENERATION TECHNOLOGIES



Model Development
Framework in MFIX of Continuum and Discrete Models
Incorporation of Uncertainty Quantification
Roadmap for High-Fidelity-Based ROM
Incorporation of Microscale Structure

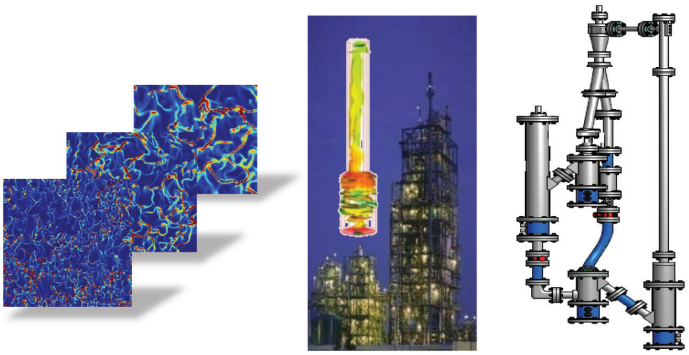
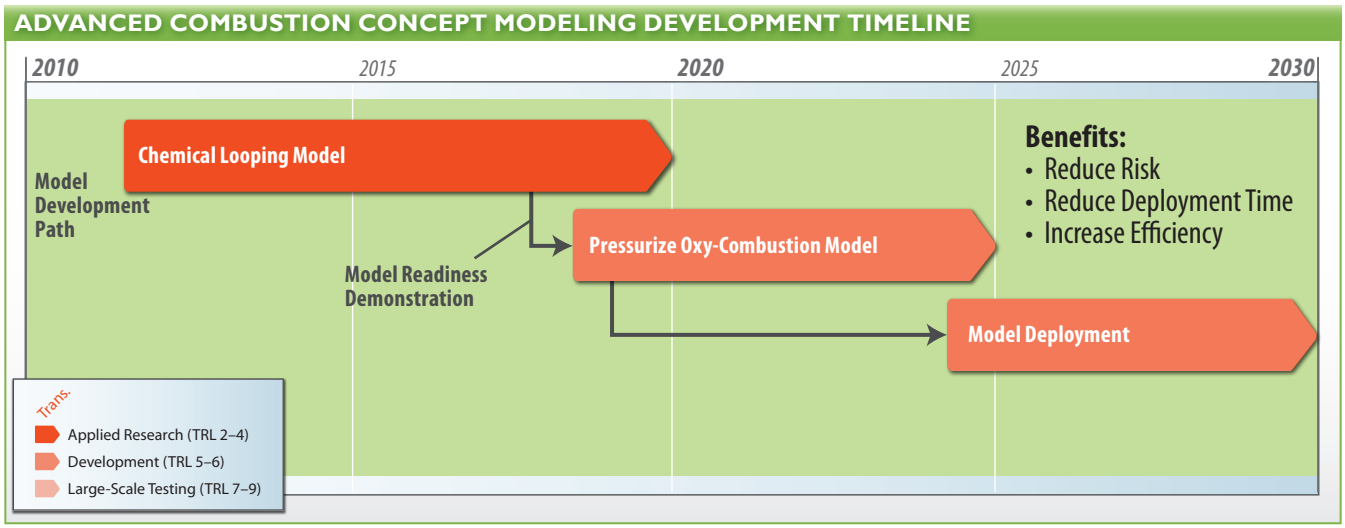


Figure 3-13. Computational Modeling—2nd-Generation Technologies Development Timeline

The 2nd-Generation Computational Modeling research will expand the MFIX framework to include uncertainty quantification for all the various models under the MFIX framework. These models will contain state-of-the-art kinetic submodels using C3M and incorporate microscale properties of the solid phase through multiscale techniques into the CFD model of choice. Users will not only have models that will leverage the latest developments in GPU acceleration, but will also have access to a high-fidelity-based ROMs.

TRANSFORMATIONAL TECHNOLOGIES



Chemical Looping Model Development	Pressurized Oxy-Combustion Model Development
Interphase Heat and Mass Transfer Submodels	Radiation Models
Effects of Polydispersity and Variable Solids Density	Oxidation and Pyrolysis Models
Kinetic Submodels	Models to Account for Turbulence, Chemistry, and Radiation Interactions
Incorporation of Oxygen Carrier Microscale Structure	Incorporation of Microscale Structure

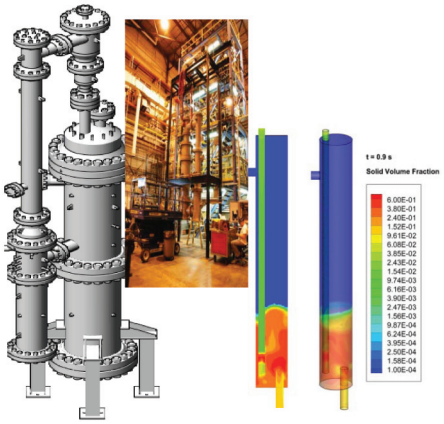


Figure 3-14. Computational Modeling—Transformational Technologies Development Timeline

The Transformational Computational Modeling activities will leverage the model developed, verified, and validated under the 2nd-Generation phase to advance development of chemical looping systems and pressurized oxy-combustion technology. New designs can be quickly considered using ROMs, while optimization and performance of a particular design can be probed using the models in the MFIX framework. Uncertainty in model predictions will be quantified and multiscale modeling will be used to incorporate oxygen carrier properties, improved heat and mass transfer, and radiation.

3.2.5 RESEARCH FOCUS AREA BENEFITS

The expected benefits and status of each of the research focus area pathways for Computational Modeling technologies are described subsequently and summarized as component features and benefits in Table 3-5.

Table 3-5. **Computational Modeling Component Features and Benefits**

Category of the Software Component	Description of the Software Component	Applications of the Software Component	Current State-of-the-Art and Limitations	Benefits the Software Component is to Deliver
MFIX Framework to Include a Hierarchy of Models	• Within MFIX there will be continuum, Lagrangian, and hybrid solvers.	• Ability to address computational requirements of a user through a choice of models within MFIX	• Currently, no single framework incorporates continuum, DEM, PIC, and hybrid solvers	• Address the need for faster running models • Provide a variety of modeling approaches to a single problem
Uncertainty Quantification Coupled to the MFIX Framework	• The uncertainty quantification will allow a user to run any solver within the MFIX suite of solvers and incorporate uncertainty in the model's predictions based on uncertainties in the model's input.	• Determine which input parameters have leading order effects • Quantify the uncertainty in a model's prediction	• Currently, there is no software that couples a hierarchy of multiphase CFD models with uncertainty quantification tools	• Allows a modeler to understand the tradeoff between turn-around times and uncertainty • Allows uncertainty to be quantified for a model's prediction
ROM Development	• A ROM will allow a user to regress MFIX or other high-fidelity CFD results, or even experimental results, into a fast-running ROM.	• Allow extremely fast turn-around times to probe new designs, or make initial progress into optimizing a particular device	• Currently, there is no existing fully-functional ROM based on transient multiphase CFD results	• Allow extremely fast turn-around times • Probe new designs • Optimization a particular device
Multiscale Modeling	• Allow the microscale structure of a reacting particle to be incorporated into a device-scale model.	• Multiscale models will be developed and coupled to existing CFD models within the MFIX framework	• Currently, there are very few multiscale models coupled to a CFD model for gasification, chemical looping, and capture	• Improved heat and mass transfer calculations • Improved drag models

3.2.6 BARRIERS/RISK AND MITIGATION STRATEGIES

The overarching challenge to be addressed by the Computational Modeling activity is the reduction of technology time and cost. This in turn requires increasing the confidence in the modeling predictions about the behavior of devices and systems at large scales based on a smaller number of intermediate-scale tests.

The risks and mitigation strategies for Computational Modeling are discussed in Table 3-6.

Table 3-6. **Computational Modeling Barriers/Risk and Mitigation Strategies**

Issue	Barrier/Risk	Mitigation Strategy
Development of a hierarchy of models	• Incorporation of microscale structure into the models • First-of-its-kind ROM • Validation • Significant computational costs associated with high-fidelity models and uncertainty quantification	• Perform well controlled small-scale experiments • Bring together leaders in the area of ROMs to develop a strategic development pathway • Leverage existing equipment and university labor in various field work proposals to produce required data • Continue with current efforts to keep pace with new computational hardware
Development of C3M	• Various proprietary and open-source computational models will require seamless coupling with C3M • Need to expand the kinetic database • Addition of new kinetic processes	• Maintain level of expertise in the computational science division to allow researchers to work with C3M team to incorporate information into all models • Continue to work with West Virginia University and Penn State University to incorporate cofeed and pressure kinetics into C3M • Use C3M as a repository for all relevant kinetic process research within NETL's Office of Research and Development—e.g., sorbent-based CO_2 and mercury capture and chemical looping
Demonstration of technology to industry	• Most industrial stakeholders have limited computational expertise and/or resources • Changing the mindset of industry on the acceptance of realistic computational times • Demonstrating the predictability of the models	• Seek industry feedback throughout development process and visit stakeholders to demonstrate recent development and success and how the computation models can be used • Include industrial participants in the activity and demonstrate to them the benefit of the models
Production of validation data	Need for both reacting and nonreacting experimental data for validation	Leverage both in-house and university experimental capabilities to obtain the required data

3.3 CARBON CAPTURE SIMULATION INITIATIVE

CCSI will develop and deploy state-of-the-art computational modeling and simulation tools to accelerate the commercialization of carbon capture technologies from discovery to development, demonstration, and ultimately widespread deployment to hundreds of power plants.

3.3.1 BACKGROUND

Current carbon capture technology, amine scrubbing, would increase the cost of electricity by as much as 80 percent in new PC power plants while reducing the power plant's net efficiency by about 30 percent. The cost of the CO_2 captured with 1st-Generation carbon capture technologies will be \$61/tonne. It is desired that this cost be reduced to \$40/tonne with 2nd-Generation technology made ready for demonstration in the 2020–2025 timeframe and to \$10/tonne with Transformational technology made ready for demonstration in the 2025–2030 timeframe. To achieve these cost targets many new technologies are under development. For every promising new technology, meeting the timeframe targets is a challenge because taking these promising new technologies from the lab to commercial deployment traditionally requires anywhere from 20 to 30 years.

An industrially proven approach for reducing the cost and time for technology development is the use of advanced modeling and simulation. A goal of CCSI is to use advanced modeling and simulation to reduce the cost and time required for taking carbon capture concepts from the lab to commercial deployment. The typical 20–30 years of

development time is the amount of time necessary to perform testing of technologies at progressively larger scales for commercial deployment. Advanced modeling can help save time and money early in the development phase by identifying promising capture concepts that are unlikely to be successful. Furthermore, modeling and simulation can be used to reduce the time required to accomplish the design, learning, and operation phases at each scale. Quantifying the confidence in model predictions and the technical risk of scaleup will shorten the time to achieve commercial deployment. Skipping tests at just one intermediate scale could reduce the development time by five or more years. It is known that the capital costs of energy technologies are initially high and reduce over a period of time during deployment. Enhanced learning enabled by virtual plant simulations—for example, from the virtual testing of a combination of technology options—has the potential to stabilize the costs more quickly. In summary, CCSI will accelerate the development and deployment of new carbon capture technologies in several important ways:

- Quick identification of promising concepts through rapid computational screening of devices and processes.
- Reduction in the time to design and troubleshoot new devices and processes through use of science-based optimal designs.
- Accurate quantification of the technical risk in taking technology from laboratory scale to commercial scale.
- Stabilization of deployment costs by using virtual power plant simulations in lieu of selected physical operational tests.

A summary of the high-level components developed under CCSI technology is provided in Table 3-7.

Table 3-7. **CCSI Technology Development Summary**

Key Technology	1st-Generation Technologies	2nd-Generation Technologies	Transformational Technologies
Carbon Capture Simulation Initiative	Does not address 1st-Generation capture technology	• Models for solving technical challenges in 2nd-Generation solid sorbent, solvent and oxy-combustion technologies • Toolset software infrastructure required for simulating 2nd-Generation technologies	• Models for solving technical challenges in Transformational sorbent, solvent, and oxy-combustion technologies • Toolset software infrastructure required for simulating Transformational technologies

3.3.2 TECHNICAL DISCUSSION

Models are currently used for conducting techno-economic analyses and describing carbon capture processes at the scale of particles, devices, and process. Particle-scale models are used as submodels for device- and process-scale models. These models are validated with separate datasets and the information exchange between the models is usually manual. Simulations are typically used for identifying the most promising concepts to pursue by screening materials, devices, and processes. Simulations are also employed for developing optimal designs that identify the tradeoffs among performance, cost, and reliability. Process dynamic simulations are used for analyzing the controllability and operability of plants.

Building upon those capabilities, CCSI will bring about innovations in four areas. First, the models will be made consistent and complete by integrating them so that the models are based on the same data and enable a knowledge transfer to develop other scales. Second, CCSI will develop a hierarchy of datasets for verifying and validating the integrated models to ensure high fidelity of the models at all scales. Third, CCSI will develop an end-to-end uncertainty quantification engine that will quantify uncertainties in the integrated models and develop the capability for optimizing process configurations with the integrated model. Finally, CCSI will develop risk acceptance metrics with the help of industry and develop the capability for assessing the scaleup risk through the computational results. With these innovations, CCSI will address the key industrial challenges of (1) developing a baseline for the uncertainty in simulation results, (2) quantifying and reducing the level of uncertainty, and (3) quantitatively assessing the

scaleup risk. The integrated CCSI Toolset will enable prototyping of designs with greater confidence and provide a uniform platform to evaluate options. More importantly, the CCSI Toolset will support decision making to move technologies to larger scales more quickly and with better designs, thereby accelerating development of carbon capture technologies.

The CCSI Toolset consists of models for specific carbon capture technologies and a simulation framework consisting of simulation tools and methodologies applicable to all technologies (see Figure 3-15). The development of these two parts of CCSI Toolset is described subsequently.

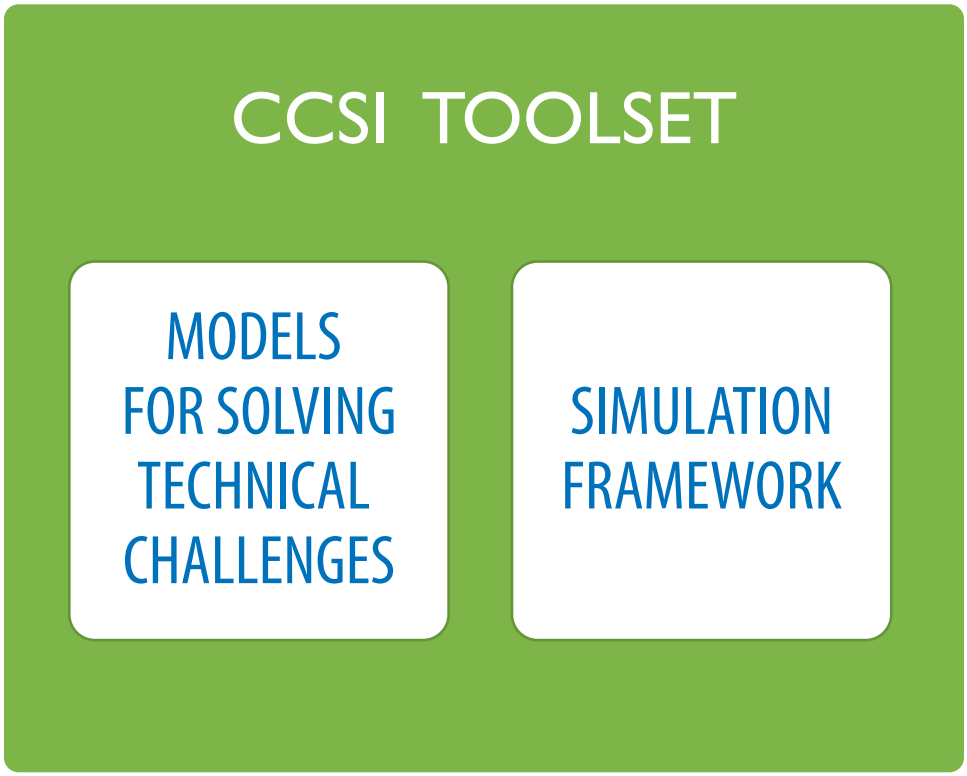


Figure 3-15. CCSI Toolset Consisting of Models for Specific Technologies and General Purpose Software Framework

The technologies to be developed supporting the CCSI program plan for models of CCS systems and software framework are shown with a timeline by research focus area in Figure 3-16.

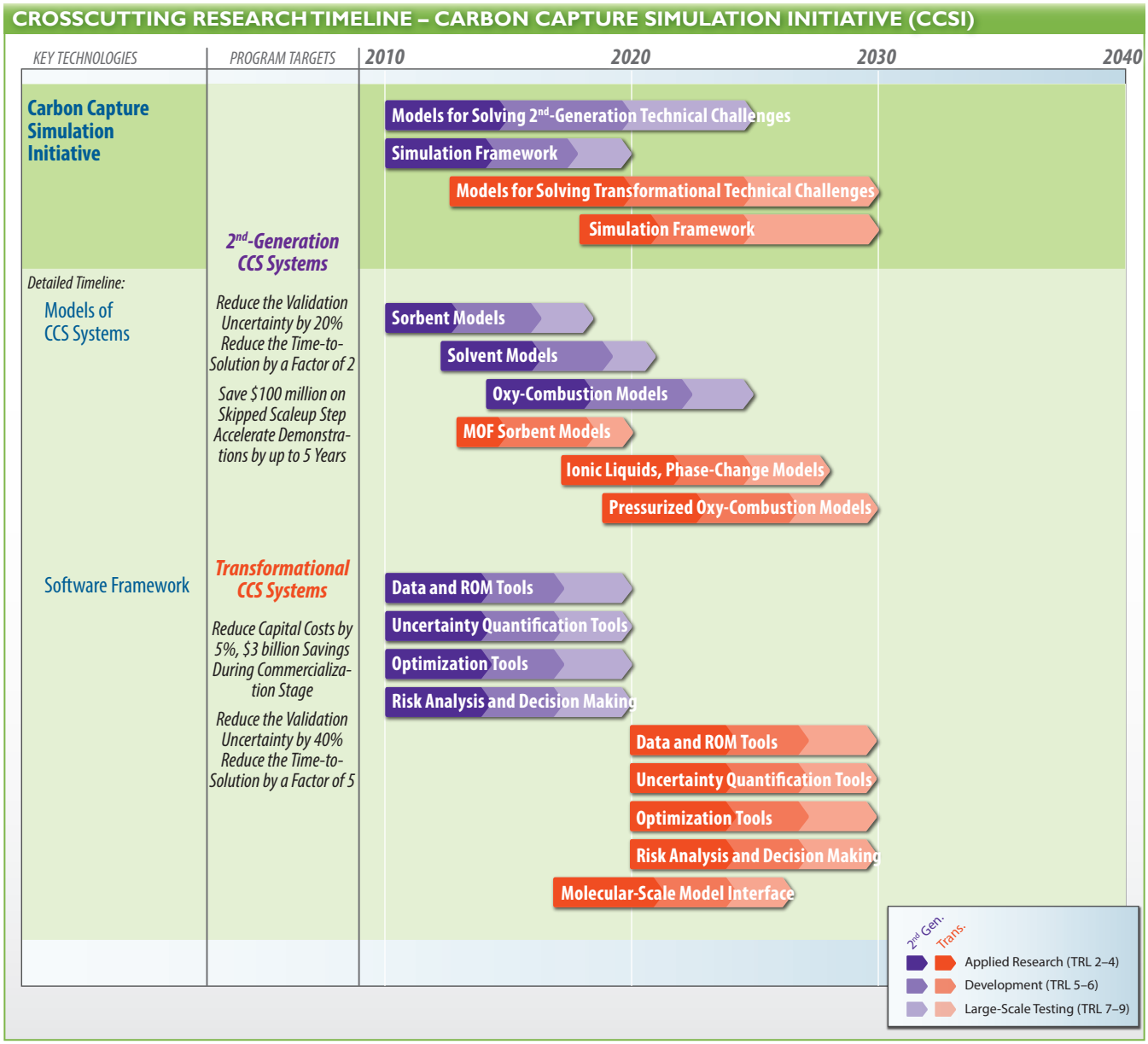


Figure 3-16. CCSI—2nd-Generation and Transformational Technologies Development Timeline

2ND GENERATION TECHNOLOGIES

MODELS FOR SOLVING 2ND-GENERATION TECHNICAL CHALLENGES

Solid sorbent-based post-combustion capture technology is the initial focus of model development. Sorbents offer an advantage because they can reduce the regeneration energy associated with CO_2 capture and reduce parasitic load. While there are a number of sorbent development efforts underway, significant work remains to be done to define and optimize the reactors and processes needed for successful sorbent capture systems. Most of the work on sorbents has been restricted to developing the sorbent itself with only very recent studies considering the design of the reactor system and integration with the power plant. Thus, solid-sorbent systems are at the start of the traditional process development cycle. The initial focus on solid sorbents will accelerate the analysis of options for this emerging technology. The target is to use the CCSI Toolset to help identify promising solid-sorbent processes and accelerate scaleup to 25 MWe and commercial demonstration scales.

While detailed component simulations for solid sorbents will be much different from those used for liquid solvents, the computational interfaces developed for either technology will share many common features (e.g., ability to handle multiphase devices). Advanced solvent-based post-combustion capture will be the second focus of model development.

It is quite likely that solvent scrubbing will be deployed by industry as a CCS technology. Advanced solvents are currently in the middle of the traditional process development cycle, moving from pilot scale to commercial demonstration, so CCSI development can build logically on the prior developments for solid sorbents. Experimental validation data for advanced solvents are expected from pilot tests. Data from pilot testing of these existing solvents will be used to validate CCSI models and provide confidence that they can be used to model advanced solvents. Figure 3-17 shows the results of a CO_2 adsorber model overlaid on the physical device that supplied validation data. The CFD model, validated with data from small-scale capture devices, will be used to design larger scale devices.

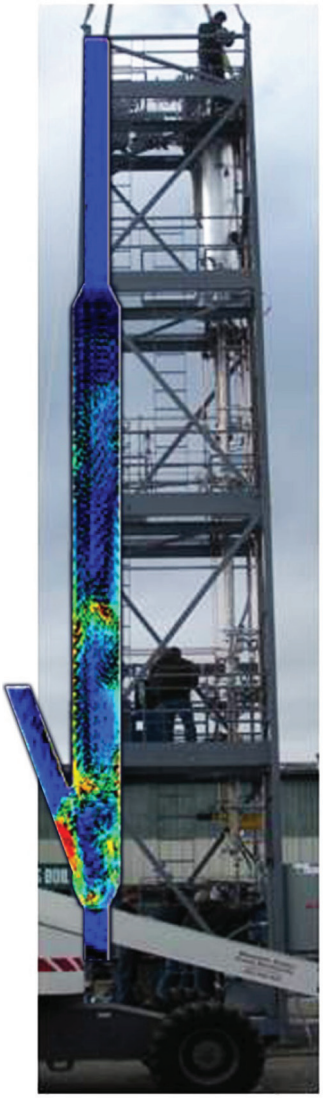


Figure 3-17. Example of Validated CFD Model

Oxy-combustion will be the third focus of model development because of the expected timelines for oxy-combustion pilot and demonstration projects. Validation data from these current projects will be used to gain confidence in the CCSI models. These will then be used to extrapolate demonstration project designs to 2nd-Generation configurations, analyze operation on different coal types, or retrofit analyses for existing plants. In contrast to sorbent- and solvent-based capture, the oxy-combustion case will add progressively more complex analysis capabilities to the CCSI Toolset. It will require adding details of the plant configuration (e.g., boiler interior, fuel handling, air preheating) that are not needed to assess an "add-on" technology, such as addressed in sorbent and solvent cases.

SIMULATION FRAMEWORK

The CCSI Toolset will be developed to ensure that all the models within its framework use consistent data formats (i.e., the same thermophysical properties are used in models at various scales). A model validation/uncertainty quantification hierarchy will be built to validate models at different scales (e.g., sorbent pellet, absorber column, capture process, capture process integrated with power plant) that constitute the virtual power plant with carbon capture.

The CCSI Toolset will ensure the consistency of models across all scales. Thus, knowledge gained from models at any scale will be available for making decisions with models at higher scales. One of the approaches of CCSI is to develop ROMs that allow models at different scales to readily exchange information in a computationally efficient manner, enabling the development of complete (knowledge preserving) and consistent models. The ability to create a ROM from higher fidelity models makes multiscale modeling, uncertainty quantification analysis, and advanced optimization possible. The ROM tools create new models that accurately capture the behavior of more detailed models over a specified range of input parameters. CCSI has two primary types of ROM tools. The first is designed primarily for computationally intense, detailed particle-scale or device-scale models that accurately simulate the detailed physics and chemistry. The ROMs from this approach can be embedded within higher scale models and used for uncertainty quantification. The second type of tool is targeted toward creating ROMs that can be used within advanced optimization codes.

Model predictions contain uncertainties that result from several sources including (1) uncertainties in basic input data (e.g., material properties or chemical reaction rates), (2) uncertainties in the output of one model that is used as the input to another model, (3) uncertainties that arise when a model validated at a certain scale is used for simulations at a larger scale, and (4) uncertainties due to "unknown unknowns" such as unanticipated chemistries, flow patterns, or materials problems that are encountered for the first time when a process is scaled up. The CCSI quantification framework can assess the effect of uncertainty in underlying parameters and models on the predicted performance of equipment and processes in a carbon capture system. Researchers will use the uncertainty quantification tool to conduct the required analyses for quantifying uncertainties in particle-, device-, and process-scale models. Existing uncertainty quantification analyses for carbon capture models lack (1) the capability to estimate model-form uncertainty and (2) the capability to transfer uncertainties across scales from particle-, device-, and process-scale models. Also, existing uncertainty quantification tools lack a user interface for the CCSI methodology. The CCSI uncertainty quantification tool will provide an estimate of the uncertainty in the predictions of capture models at various scales. This will also increase the confidence in the models used for making design decisions and potentially identify areas that need further smaller scale experimental investigation.

Optimization tools are essential for decision making as they (1) provide superior, consistent designs among practitioners with various levels of expertise, (2) provide new insights to novel designs, and (3) have been demonstrated to reduce the design cycle by one or two orders of magnitude. The technical and economic performance characteristics of a new technology are strongly dependent on the configuration, interconnecting operating conditions, and integration of equipment into a process. Thus, in order to rigorously screen and evaluate new technologies, it is important to ensure that an optimal process is used for the evaluation. The optimization tools being developed by CCSI will enable the identification of optimal equipment configurations for potential capture processes allowing more effective screening of materials and concepts, and identifying the types of devices and processes that should be the focus of more detailed modeling and analysis. The CCSI Toolset will provide a rigorous optimization and compress the development cycle by more quickly enabling process integration, which has taken decades in other industries. Figure 3-18 shows an example of how the CCSI Toolset can help optimize a capture process configuration by determining process flow and the correct number of adsorbers, desorbers, and heat exchangers.

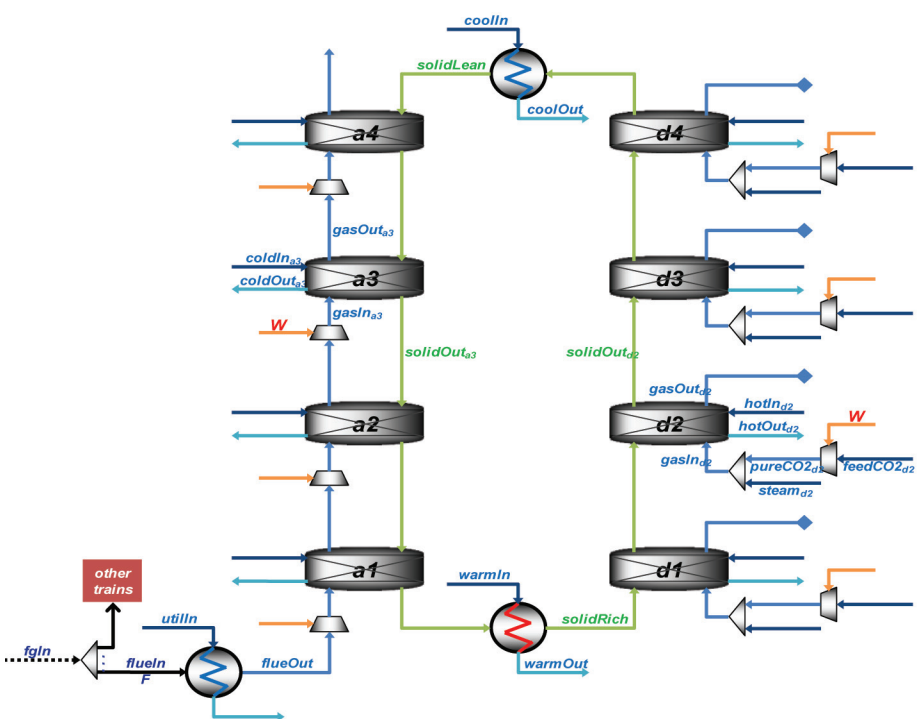


Figure 3-18. Example of Determining Optimal Capture Process Configuration via the CCSI Toolset

The CCSI risk analysis and decision making framework incorporates multiple risk contributors including technology readiness, uncertainty in models and simulations, economic uncertainty, and technical scaleup risk. This tool will be used to translate the results of science-based models described previously into the language used by decision makers, such as technical and financial risk metrics.

TRANSFORMATIONAL TECHNOLOGIES

MODELS FOR SOLVING TRANSFORMATIONAL TECHNICAL CHALLENGES

New sorbent materials are currently under development that could potentially lead to Transformational capture technologies. One such material is metal organic framework (MOF). A number of solvent technologies such as ionic liquids/switchable ionic liquids, enzyme-catalyzed absorption, and phase-change solvents are also under development. Process intensification or reducing the size of the solvent reactors is another objective of the program. The CCSI Toolset and models will be adapted to model these Transformational technologies and others such as pressurized oxy-combustion and pressurized gasification.

SIMULATION FRAMEWORK

Accurate molecular-scale simulations of materials such as MOFs are currently under development. It is expected that molecular-scale simulations and lab-scale experiments will identify a suite of candidate materials suitable for Transformational technologies. The capability for incorporating such molecular-scale models and manipulating the models will be incorporated into the toolset to aid in designing better Transformational materials and better devices and processes.

New validation/uncertainty quantification hierarchies and methods will be applied to develop and validate models used to describe the behavior of MOF materials, ionic liquids/switchable ionic liquids, enzyme-catalyzed absorption, phase-change solvents, and others. These methods will also be applied to all devices necessary for developing Transformational technologies (e.g., separation devices used with phase-change solvents).

The optimization methodologies will be developed to handle the modeling of Transformational technologies. The risk analysis and decision making component of the CCSI Toolset will be updated to use the results of science-based models of Transformational technologies.

3.3.3 R&D APPROACH—PERFORMANCE TARGETS AND MEASURES

The product of CCSI will be a comprehensive simulation toolset and infrastructure composed of data and validation/uncertainty quantification hierarchies, models, software, application programming interfaces, and best practices. The CCSI Toolset will incorporate commercial and open-source software currently in use by industry and will also develop new software tools, as necessary, to fill technology gaps identified during execution of the project. It will provide industry with an integrated suite of scientifically validated models for uncertainty quantification, optimization, risk analysis, and decision making.

CCSI will integrate models at various scales is to prevent knowledge loss and ensure model consistency across multiple scales.

CCSI targets are to:

- Enable the use of integrated models for the screening and rapid prototyping of designs.
- Develop a common integrated software platform that will allow designers and decision makers to readily exchange information and enable the development of complete and consistent models from the device scale to the full-plant scale.

- Make quantified uncertainty information, from science-based models, available to decision makers, who must make large capital investments.
- Build a computational infrastructure that industry can use to build a knowledge base of pre-competitive information.

Deliverables associated with the performance measures and milestones are given in Table 3-8.

Table 3-8. **CCSI Deliverables**

Deliverable	Date	Description of Software Components
CCSI Toolset Pre-Release	09/30/2012	• Kinetic model for amine-based solid sorbents (simple and multiscale kinetic/diffusion); high-fidelity full-scale model of solid sorbent adsorber/regenerator (RC1) • High-fidelity 1-MWe-scale model of solid sorbent adsorber/regenerator (RC1) • One-dimensional (1-D) process models of solid sorbent adsorber/regenerator (RC2) • Superstructure-based optimization framework (RC2) • Heterogeneous simulation-based process optimization framework (RC1) • Uncertainty quantification framework (RC2) • Risk analysis and decision making framework (RC1) • ROM development tools (RC1)
CCSI Toolset Release—1	01/31/2014	• ROM of the multiscale sorbent model; high-fidelity full-scale model of solid sorbent adsorber/regenerator (RC2) • Validated high-fidelity 1-MWe-scale model of solid sorbent adsorber/regenerator; high-fidelity intermediate-scale (≈25 MWe) model of solid sorbent adsorber/regenerator (RC1) • 1-D process models of solid sorbent adsorber/regenerator (RC3) • Superstructure-based optimization framework (RC3) • Heterogeneous simulation-based process optimization framework (RC2) • Uncertainty quantification framework (RC3) • Risk analysis and decision making framework (RC2) • ROM development tools (RC2)
CCSI Toolset Release—2	01/31/2015	• High-fidelity full-scale model of solid sorbent adsorber and regenerator (RC3) • Validated high-fidelity intermediate-scale (≈25 MWe) model of solid sorbent adsorber/regenerator; high-fidelity intermediate-scale (≈100 MWe) model of solid sorbent adsorber/regenerator (RC1) • Superstructure-based optimization framework (RC4) • Heterogeneous simulation-based process optimization framework (RC3) • Uncertainty quantification framework (RC4) • Risk analysis and decision making framework (RC3) • ROM development tools (RC3)
CCSI Toolset Release—3	01/31/2016	• Validated high-fidelity full-scale model of solid sorbent adsorber/regenerator (RC4) • Validated high-fidelity intermediate-scale (≈100 MWe) model of solid sorbent adsorber/regenerator; superstructure-based optimization framework (RC5) • Heterogeneous simulation-based process optimization framework (RC4) • Risk analysis and decision making framework (RC4)

3.3.4 PROGRAM PLAN TIMELINE

The CCSI Toolset models and software framework for accelerating the deployment of 2nd-Generation and Transformational technologies will be developed as shown in Figure 3-19 and Figure 3-20, respectively.

The CCSI Toolset development for 2nd-Generation technologies starts with the development of models for sorbent-based post-combustion capture. It is anticipated that 1-MWe-scale pilot plants will be operational by 2015, and 1-MWe device-scale models can be validated during the 2012–2015 timeframe. In parallel, models of 25-MWe, 100-MWe, and full-scale plants will also be developed to identify and solve issues related to larger scale models. After the sorbent models are developed, models of advanced solvents will be developed during the 2013–2020 timeframe. Also during this timeframe the data expected from 10-MWe-scale plants will be used for validating models. During

the 2020–2025 timeframe, models for oxy-combustion systems will be developed and validated. The validated models will be available to industry to help with the scaleup of 2nd-Generation processes to commercial scale by 2025.

During the 2012–2020 timeframe the 2nd-Generation simulation framework of the CCSI Toolset will be developed using an agile development methodology, an iterative and incremental method for ensuring rapid and flexible response to the evolving requirements of modeling carbon capture technologies. The framework will allow users from industry to conduct analyses with the capture models developed by them or provided by CCSI. The analyses include, for example, quantifying the uncertainty in model predictions, determining optimal capture process configurations, or quantifying technical risk. The classes of capabilities developed within the simulation framework are tools for ROM development, uncertainty quantification, superstructure-based optimization, heterogeneous simulation-based process optimization, and risk analysis and decision making. During this timeframe, Versions 1–6 of the CCSI Toolset will be released.

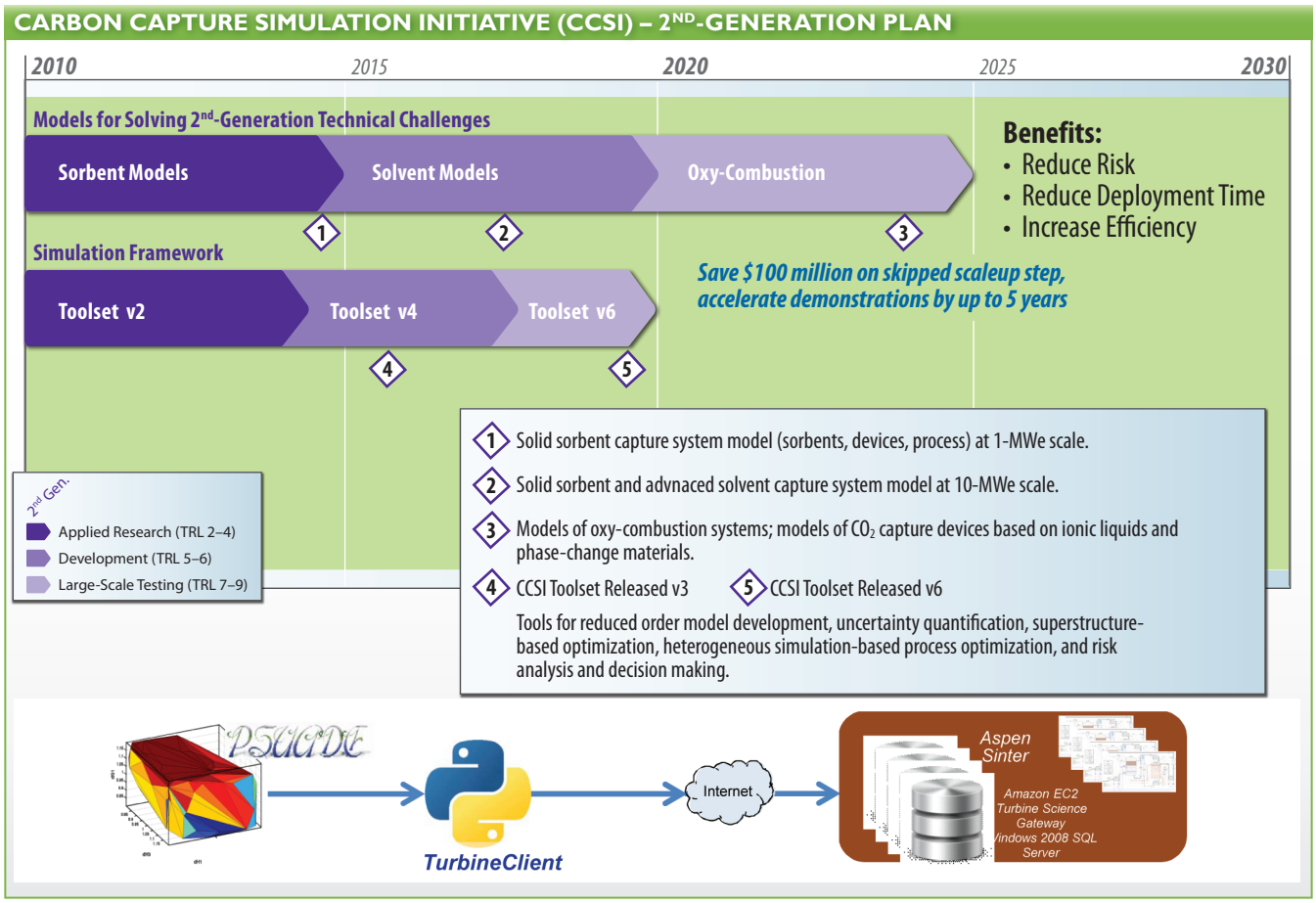


Figure 3-19. CCSI—2nd-Generation Technologies Development Timeline

The development of models for Transformational technologies will start before 2020 and proceed until 2030. The focus of model development will be on Transformational sorbent materials, solvents and oxy-combustion processes. During 2012–2020, processes based on sorbents such as MOF materials will be modeled. During 2020–2025 processes based on ionic liquids/switchable ionic liquids, enzyme-catalyzed absorption, and phase-change solvents will be modeled. During 2025–2030 pressurized oxy-combustion systems will be modeled to address issues with boiler design, solids handling, and heat transfer. Models will be used to identify promising Transformational capture materials, to design and troubleshoot novel separation devices, and to determine optimal designs for process intensification.

During the 2017–2030, timeframe the Transformational simulation framework will be developed. The agile development methodology will continue to be used and, during this timeframe, Versions 7–12 of the CCSI Toolset will be released. The framework will be extended to incorporate molecular-scale models. The capability for manipulating the models for designing better materials and better devices and processes based on those materials will be developed. The data formats will be updated to accommodate the requirements of Transformational technologies. New validation/uncertainty quantification hierarchies and optimization methods applicable to Transformational technologies will be developed. The risk analysis and decision making components of CCSI Toolset will be updated.

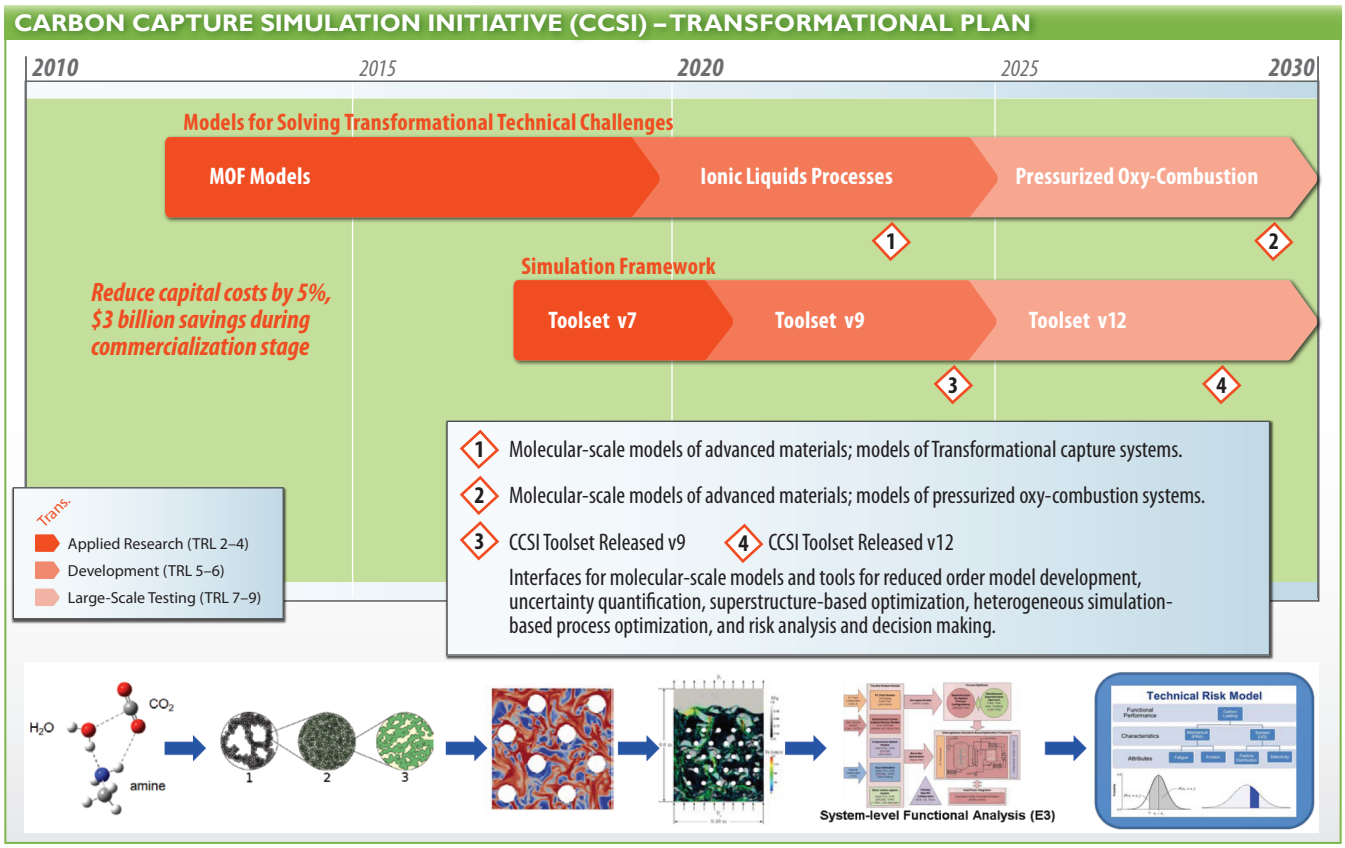


Figure 3-20. CCSI—Transformational Technologies Development Timeline

3.3.5 RESEARCH FOCUS AREA BENEFITS

CCSI Toolset component features and benefits and are discussed in the following paragraphs and summarized in Table 3-9.

CCSI will develop key component features for the CCSI Toolset:

- Validated submodels for candidate sorbents that can be used within both high-fidelity simulations and process simulations.
- Validated, high-fidelity models of solid sorbent carbon capture equipment at various scales, including 1-MW pilot scale, intermediate scales, and full scale.
- Models, computational tools, user interfaces, and accompanying methodology for optimal process synthesis and process design.
- An uncertainty quantification framework to assess the effect of uncertainty in underlying parameters and models on the predicted performance of equipment and processes in a carbon capture system.

- A risk analysis and decision making framework, which incorporates multiple risk contributors including technology readiness, uncertainty in models and simulations, economic uncertainty, and technical scaleup risk.
- ROM development tools to automatically develop ROMs in a form suitable for incorporation into larger scale models and simulations.

Benefits expected from the CCSI Toolset include the following:

- Submodels will predict the rate of adsorption and desorption of CO_2 under various operating conditions and provide an estimate of uncertainty in the model predictions.
- Model equations and validation methodology will be used to develop models of next-generation sorbents for CO_2 capture.
- CCSI device-scale models will reduce R&D cost and time.
- Models will allow industry to rapidly build simulations of potential processes to assess likely performance, as a means to not only screen new concepts, but also to identify promising system configurations.
- The uncertainty quantification tool will provide an estimate of the uncertainty in the predictions of capture models at various scales and increase the confidence in the models used for making design decisions and potentially identify areas that need further experimental investigation.
- CCSI risk analysis and decision making framework will translate the results of CCSI science-based models into the language used by decision makers, such as technical and financial risk metrics.
- Provide the capability to create ROMs to reduce R&D cost and time to build accurate multiscale models of capture processes.

Table 3-9. **CCSI Component Features and Benefits**

Category of the Software Component	Description of the Software Component	Applications of the Software Component	Current State-of-the-Art and Limitations	Benefits the Software Component is to Deliver
Particle-Scale Models	Validated sorbent submodels for candidate sorbents that can be used within both high-fidelity simulations and process simulations.	• Predict the rate of adsorption and desorption of CO_2 by sorbents	• Deficient number of industrially relevant sorbent models	• Fill a gap in the capture modeling capability • Provide the framework for models of new sorbents
Device-Scale Models	Validated, high-fidelity models of solid sorbent carbon capture equipment at various scales, including 1-MW pilot scale, intermediate scales, and full scale.	• Predict the performance of CO_2 capture devices • Help designers optimize and troubleshoot capture devices	Deficiencies in existing models: • Systematic approach to model validation • Methods for quantifying uncertainties • Ability to model features smaller than the computational grid	• Reduce R&D cost and time by providing confirmation of device designs • Ensure applicability of modeling and validation approaches to other devices
Process-Scale Models	Models, computational tools, user interfaces, and accompanying methodology for optimal process synthesis and process design.	• Predict with quantified uncertainty the efficiency of CO_2 capture process • Provide cost estimates at Class 5/4 levels with hooks for industry cost curves • Determine optimal capture process configurations	Deficiencies in existing software: • Confidence interval for simulation results • Ability to synthesize an optimal process configuration • Lack of submodels for capture devices	• Reduce R&D cost and time by identifying the most promising carbon capture process concepts and providing optimal carbon capture process designs
Uncertainty Quantification	Uncertainty quantification framework to assess the effect of uncertainty in underlying parameters and models on the predicted performance of equipment and processes in a carbon capture system.	• Conduct the required analyses for quantifying uncertainties in particle-, device-, and process-scale models	Deficiencies in existing uncertainty quantification analysis: • Model form uncertainty estimation • Lack of capability to transfer uncertainties across scales from particle to device to process scale models • Lack of user interface for the CCSI uncertainty quantification methodology	• Estimate the uncertainty in predictions, increase confidence in design decisions, and identify areas that need further investigation
Risk Analysis and Decision Making	Framework incorporates multiple risk contributors, including technology readiness, uncertainty in models and simulations, economic uncertainty, and technical scaleup risk.	• Translate the results of science-based models into the language used by decision makers, particularly focusing on technical and financial risk metrics	• Lack of capability to properly communicate results	• Provide quantitative information of financial and technical risks of scaleup, and help capture technologies reach larger scales earlier
Reduced Order Models	ROM development tools to automatically develop ROMs from high-fidelity models in a form suitable for incorporation into larger scale models and simulations.	• Make multiscale modeling and uncertainty quantification analysis possible	• Lack of tools for the model reduction tasks required in CCSI	• Reduce R&D cost and time by providing the capability to build accurate multiscale models of capture process

3.3.6 BARRIERS/RISK AND MITIGATION STRATEGIES

The overarching challenge to be addressed by the CCSI key technology is the reduction of the time period to scaleup the technology and cost. This in turn requires increasing the confidence in the modeling predictions about the behavior of devices and systems at large scales based on fewer intermediate-scale tests.

The risks and mitigation strategies for CCSI are discussed in Table 3-10.

Table 3-10. **CCSI Barriers/Risk and Mitigation Strategies**

Issue	Barrier/Risk	Mitigation Strategy
Complexity of the software toolset	Software integration and operability between proprietary and nonproprietary programs is complex, particularly with respect to the integration at different scales	• Assign dedicated teams for facilitating software integration and interoperability • Assign dedicated teams for frequent and open communication between developers involved in toolset development • Assign dedicated teams for formulation and execution of detailed software test plans
Diverse skill set required	The broad scope of CCSI requires that people with diverse skill sets and expertise are needed, who may not readily available on the open market	• Assemble a team with the requisite capabilities from national labs, industry, and academia • Train students to develop the required skill sets
Long computational time	High-fidelity multiscale models can be computationally expensive, leading to unacceptable simulation turnaround times	• Develop effective reduced order modeling strategies that offer a tradeoff between accuracy, range of applicability, and computational cost • Exploit parallel computing strategies to reduce the time-to-solution
Technology transfer to industry	Ineffective transfer of CCSI modeling and simulation tools to industry	• Seek industry feedback throughout development process • Include industrial participants in the development and application teams • Define technology transfer process • Identify and meet industry training needs
Change in the technologies pursued by industry	The capture technologies pursued by industry may change during the execution of the project because of a new discovery or changes in the prevailing market conditions	• Make semiannual go/no-go decisions on challenge problems with the help of industry • Develop reusable models and software components for each of the applications, whenever possible • Leverage the breadth provided by the applications to shift the focus of research as needed
Lack of validation data	It is difficult to obtain pilot-scale data for validating CCSI models and risk analysis methodology	• Form industrial partnership early in the project • Use nondisclosure/intellectual property protection plans accepted by industry • Define applications considering potential sources of industrial data

3.4 NATIONAL RISK ASSESSMENT PARTNERSHIP

NETL is conducting research to advance the science and engineering knowledge base for technologies that will accelerate the business case for CO_2 capture and storage, including prediction and quantification of risks that may relate to potential liabilities. As part of this effort, NETL (through its Office of Research and Development) is leading a multilaboratory effort that leverages broad technical capabilities across the DOE complex—NRAP. NRAP involves five DOE national laboratories: NETL, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, and Pacific Northwest National Laboratory. This team is

working together to develop a science-based method for quantifying the likelihood of risks (and associated potential liabilities) for CO_2 storage sites.

The expected near-term (2010–2015) benefits of NRAP include:

- Removal of a key barrier to the business case for long-term CO_2 storage by developing the technical basis for quantifying long-term liability, through development of a robust methodology and platform (computational tools) for quantifying risks (and associated uncertainties) over time for long-term CO_2 storage at a site.
- Confidence in setting storage-security metrics by developing a science-based ability to identify safe operational envelopes that minimize potential risks across a range of storage environments.

The tools and/or underpinning science base can also inform regulators or their agents with respect to storage-site performance. Additionally, costs of long-term liability can be more easily estimated and with less uncertainty, thereby allowing greater confidence in a central component of the business case for CCS projects.

3.4.1 BACKGROUND

Successful large-scale carbon storage will require companies willing to invest in the injection of CO_2 into the subsurface. Operators and investors have extensive experience in valuing risks and liabilities for similar projects that have a well defined endpoint, such as enhanced oil recovery. However, there are currently two major barriers to the full-scale implementation of carbon storage in the United States and several other parts of the world: (1) critical uncertainties in the criteria and timeline for post-injection site care and monitoring and (2) the uncertainty in the responsibility and valuation for long-term liabilities associated with carbon storage. A science base that allows for better quantification of risks for carbon storage and a set of tested quantitative risk assessment tools will both be able to help establish performance-based criteria for post-injection site care and reduce uncertainty in long-term liability valuation. Thus, NRAP products will help remove two of the most critical barriers to carbon storage.

Risk assessment for CO_2 storage is an area of active investigation. Most efforts thus far have relied on a qualitative assessment of risks based on features, events, and processes (FEPs) analysis, which involves creating a catalog of "Features" of an engineered geologic system that impact its behavior, discrete events that can impact behavior, and other processes that can influence its behavior. The FEPs approach has been the primary method for risk assessment used in most of the initial CO_2 storage efforts, including many of the Regional Carbon Sequestration Partnerships.

Quantitative risk assessment can benefit from FEPs analysis, but requires going beyond the catalog to a methodology for predicting the behavior and performance of the engineered geologic system represented by the storage site. FEPs analysis and the associated representation methodologies can be incorporated as part of a three-step approach to integrating simulation and risk assessment for an engineered geologic system: (1) development of site-specific conceptual models for critical scenarios (sometimes referred to as scenario analysis), which typically relies on a prioritized set of FEPs for the site, followed by identification of FEPs interactions; (2) development of mathematical descriptions for the critical scenarios, which can be based on empirical assessments of analogs or deterministic simulations of the geologic system's response based on fundamental physical and chemical phenomena; and (3) assessment of potential consequences resulting from the critical scenarios, which can include health/safety/environment risks as well as various non-health/safety/environment risks. The first two steps are sometimes referred to as a site performance assessment; some also group the third step as part of performance assessment.

The three-step approach is typically used in quantitative environmental risk assessments. Computational models range from the process level (such as related to the flow and reactivity of fluids in the reservoir) to the system level (such as coupling the reservoir to the other natural and engineered systems at the site). In process models, fundamental phenomena can be described from first principles at a range of scales. Due to the challenges in addressing the entire site at a process level, however, several approaches are often employed to simplify the calculations, ranging

from simplified analytical expressions to describe various complex processes to hybrid computational models that couple system-level models to more detailed simulators for components of the system.

Uncertainty quantification is a critical element of environmental risk assessments. Uncertainty in engineered natural systems is usually traceable to specific parameters of the natural system and results from both the difficulty in quantifying a parameter and the variability exhibited by multiple parameters, making the uncertainty quantification in such systems a significantly different exercise than that of a completely engineered system. Accurate quantification of the parameters that characterize the engineered geologic system is fundamental to the quality of the simulation and prediction. Parameter quantification can rely on direct observations from an analogue system, laboratory measurements, theoretically derived values, and/or expert opinion. Efforts are underway internationally to develop various components of these risk assessment tools for CO_2. Many of these efforts are actively engaged in the International Energy Agency Greenhouse Gas R&D Programme's Risk Assessment Network, an international forum for scientific experts to identify technical needs related to CO_2 risk assessment. NRAP teams participate in the International Energy Agency Greenhouse Gas R&D Programme's Risk Assessment Network.

Progress toward the NRAP goals has been very good over the past year. The 1st-Generation integrated assessment model (IAM) and risk profiles for all of the leakage profiles were completed on schedule, and the IAM for ground motion has also been completed. Two meetings were held with the NRAP stakeholder group that represents operators, regulators, insurers, governmental and nongovernmental organizations, and Regional Carbon Sequestration Partnerships. Their guidance has been incorporated into the research and operations plans to ensure that NRAP products will be useful to the various stakeholders.

The NRAP approach is summarized in Figure 3-21.

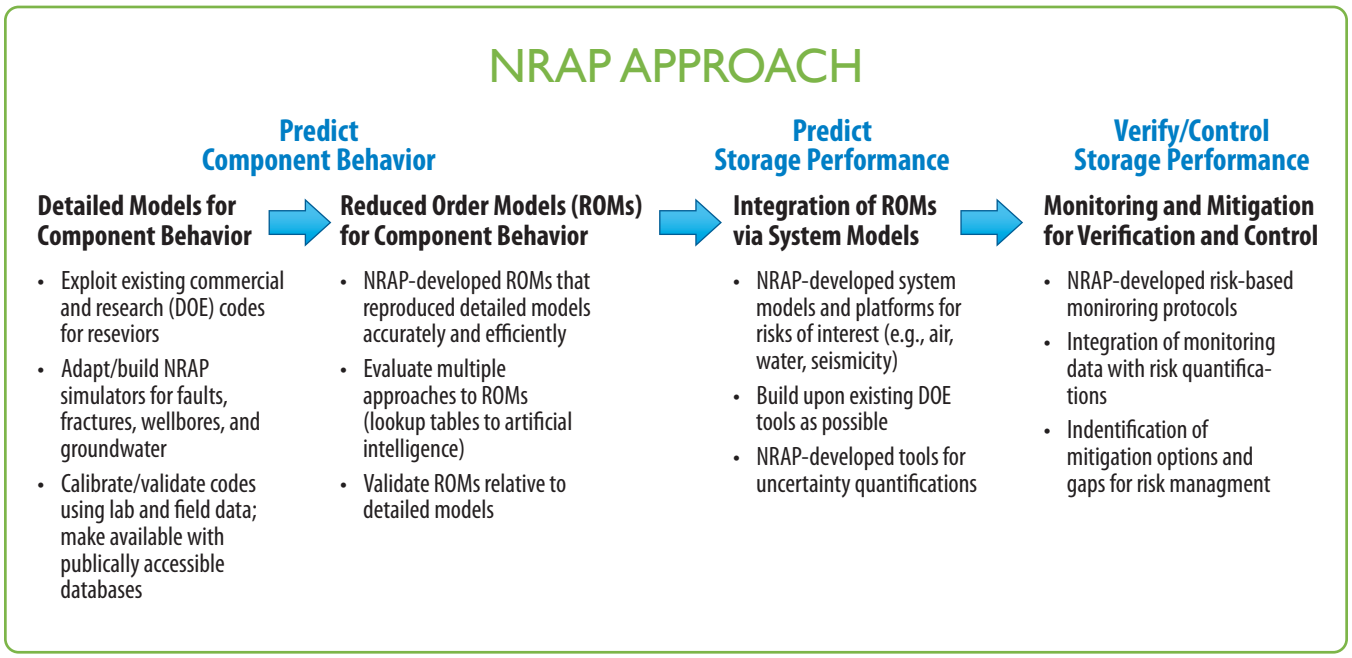


Figure 3-21. NRAP Technical Approach

A summary of the high-level components developed under NRAP is provided in Table 3-11.

Table 3-11. **NRAP Technology Development Summary**

Key Technology	1st-Generation Technologies	2nd-Generation Technologies	Transformational Technologies
Science-Based Risk Management for Engineered Natural Systems	• FEPs identification • Site-specific qualitative and semi-quantitative screening tools • Reservoir component model development (science-base, validation/calibration) • Wellbore transmissivity model • Groundwater component model development • IAM for leakage	• Basin component model development (long-term behavior, ROM) • Wellbore component model (geomechanics, chemistry, valid/calibration, ROM) • Natural seal component model • Basin-scale groundwater component model • Field-scale IAMs with integrated monitoring and mitigation and uncertainty quantification • Basin-scale IAM for leakage • IAMs for ground motion • Basin-scale uncertainty quantification methodology	• Validated, calibrated multiscale physics-based models for subsurface components • ROMs for subsurface components with ability to integrate high-resolution real-time data • IAMs with uncertainty quantification for multiscale real-time data for risk management

3.4.2 TECHNICAL DISCUSSION

The primary objective of NRAP is to develop a defensible, science-based methodology and platform for quantifying risk profiles at most types of CO_2 storage sites to guide decision making and risk management. NRAP will also develop monitoring and mitigation protocols to reduce uncertainty in the predicted long-term behavior of a site.

To assist in effective site characterization, selection, operation, and management, NRAP is considering potential risks associated with key operational concerns, as well as those associated with long-term liabilities. Operational issues include the management of reservoir pressure and stress to avoid conditions that might induce seismic activity. Issues associated with long-term liabilities include groundwater protection and storage permanence to avoid CO_2 leakage.

The technologies under development are shown in the timeline by research focus area in Figure 3-22.

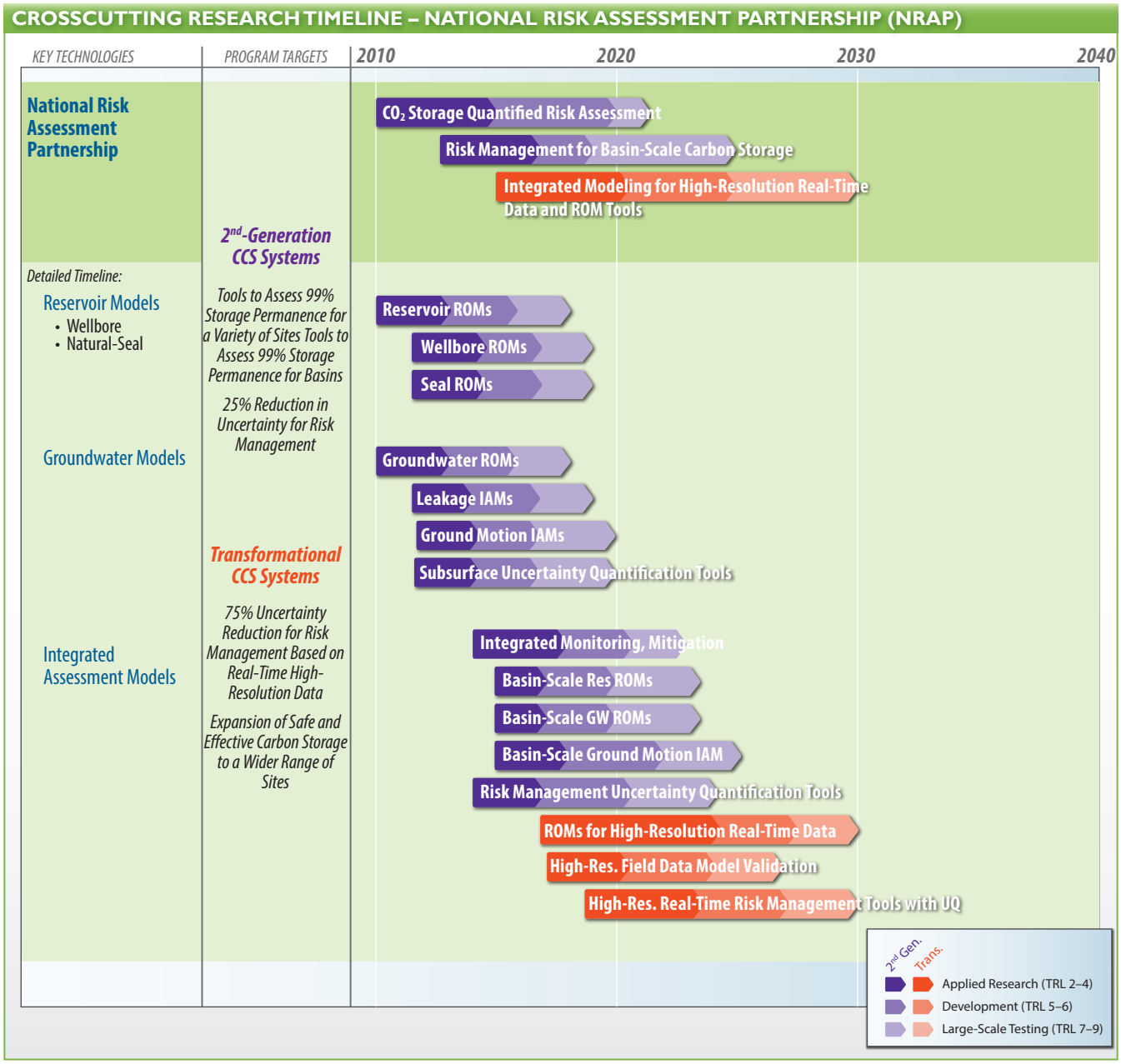


Figure 3-22. NRAP—2nd-Generation and Transformational Technologies Development Timeline

2ND GENERATION TECHNOLOGIES

One of the key strategies NRAP uses is the development of ROMs for each of the subsurface components. In the near term, the sets of ROMs for system components are being developed in accordance with Table 3-12.

Table 3-12. **NRAP Component Models**

NRAP Component Models	January 2012, complete	January 2013	January 2014
Reservoir	• Flow only • Two reservoir classes • Multiple reservoir simulators • Stochastic permeability • Both commercial and research simulators	• Flow and geomechanics • Three reservoir classes (oil and gas, bounded, depleted) • Additional reservoir simulators • Quantified trapping mechanisms	• Four reservoir classes • Coupled effects between reservoir flow and flow along release pathways
Release and Transport	• Wellbores (flow + phase change) • Faults (flow + phase change) • 1-D flow into thief zones	• Wellbores (flow + chemistry) changing k (permeability) due to chemistry, flow through caprock fractures/faults (flow + geomechanics) • Porous flow through homogeneous overburden • Field-based initial state of wells, wellbore failure, fault-zone complexity	• Wellbores/fractures (flow, chemistry, geomechanics) • Field-based initial state of wells (completion and abandonment history) • Wellbore failure • Fracture distribution complexity • Two-dimensional (2-D) flow into thief zones • Coupled flow in wells, faults, and porous overburden
Induced Seismicity	• Hazard	• Hazard and damage risk	• Hazard, damage, and nuisance risk
Groundwater	• Total dissolved solids (TDS), pH • Equilibrium geochemistry • Two end-member aquifers • CO_2 and brine flux	• TDS, pH, metals in brine • Multiple leakage sources • Fault orientation, trace metal chemistry in aquifer, impermeable, and semipermeable caprocks	• TDS, pH, metals, organics • Kinetic geochemistry • Multiple leakage sources • Fault orientation, coconstituent effects, pathway dependent effects on gigawatt quality (pending resource evaluation)
Atmosphere	• Total flux only		• Atmospheric dispersion

The NRAP program will develop several products to better understand the behavioral and performance characteristics involving CO_2 storage. The final products will consist of a suite of ROMs that can be integrated with the structure required by the IAMs. The final products will also include for each ROM a report (1) outlining the methodology used to produce the ROMs, (2) detailing the limitations on conditions of applicability for the ROMs, and (3) documenting that the ROMs can reproduce predictions from simulators to within +/-10 percent.

Further descriptions of each technology emphasis are as follows:

Reservoir Behavior—Full physics research- and commercial-grade reservoir simulators have been under development for decades in the DOE complex and in industry, so NRAP is not focused on developing new reservoir models for carbon storage. Instead, NRAP is focused on developing an improved capability for predicting long-term behavior within existing reservoir simulators and on the development of ROMs that accurately describe the predicted evolution of pressure and saturations at the reservoir-seal interface over time. The 1st-Generation ROMs account both for multiphase flow (brine and CO_2) and for uncertainty in key parameters (such as permeability, compressibility, etc.).

Wellbore Behavior—Wells provide the most likely potential leakage pathway for reservoir fluids to the near surface. NRAP is focused on two areas related to wellbore behavior: (1) the statistics of wellbore failure and its impact on well transmissivity and (2) the long-term behavior of leaky wells in the presence of CO_2 with and without additional constituents. Models will be developed to simulate the near- and long-term behavior of wellbore transmissivity and how it relates to geomechanical, thermal, and geochemical interactions. These ROMs will accurately

describe the predicted multiphase flow of CO_2 and brine through the wells as a function of pressure and saturations at the reservoir-seal interface over time. They will be based on predictions from a variety of detailed process models and will represent those predictions accurately. ROMs will account for (1) flow in open wellbores, intact wellbores, and degraded wellbores; (2) multiphase flow (brine and CO_2), including CO_2 phase changes associated with pressure and temperature; and (3) uncertainty in key parameters (such as transmissivity).

Natural Seal Behavior—Natural seals constitute the most uncertain aspect of CO_2 leakage processes. NRAP considers the potential for leakage through faults, natural fractured systems, and high-permeability zones within a caprock. NRAP is developing and calibrating coupled flow and fractured models that are capable of addressing the issues of how fracture transmissivities are affected by changing stresses and geochemistry due to the injection of CO_2. ROMs that accurately describe the predicted multiphase flow of CO_2 and brine through seals as a function of pressure and saturations at the reservoir-seal interface over time are being developed. They will be based on predictions from a variety of detailed process models and will represent those predictions accurately. ROMs will account for (1) porous flow and flow through a fault/fracture; (2) multiphase flow (brine and CO_2), including CO_2 phase changes associated with pressure and temperature; and (3) uncertainty in key parameters (such as permeability, etc.).

Groundwater Impacts—If CO_2 and/or brine migrates to underground sources of drinking water, it has the potential to affect drinking water quality. As in reservoirs, there are existing groundwater models that have been used for decades to simulate groundwater flow, so NRAP is not developing new groundwater models. Instead, NRAP is focused on identifying the most appropriate processes to use in groundwater models for CO_2 storage risk and for determining the appropriate parameters to use in such models, such as reaction rates, etc. NRAP is using existing models to predict impacts to pH, TDS, metals, and organics in a groundwater aquifer as a function of CO_2 and/or brine flow into the aquifer over time. ROMs are being developed based on predictions from a variety of detailed groundwater models and will represent those predictions accurately. ROMs will account for (1) multiphase flow (brine and CO_2), (2) equilibrium geochemical interactions with key mineralogical and aqueous constituents of the aquifer, and (3) uncertainty in key parameters (such as permeability, etc.).

Ground Motion—Induced seismicity is a potential risk that has received much discussion lately. NRAP is using existing models, where possible, to incorporate a time-dependent pressure field to simulate tectonic and fluid-induced earthquake catalogs. These ROMs utilize approximate analytical calculations that enable rapid simulation of large sequences of earthquakes. NRAP is combining ROMs developed for pressures and saturations with models being developed for fluid flow in faults. The corresponding pressure field will be combined with the catalogs discussed previously. This information, together with site-specific, physics-based deterministic ground motions calculated using existing codes, form the input to time-dependent hazard calculations. Ground motion IAMs will complete the hazard part of the risk estimation for bedrock ground motion frequencies for multiple faults.

IAMs for Leakage—Component ROMs developed by NRAP are being incorporated into a series of IAMs that can be used to calculate profiles for various risk metrics (return of CO_2 to atmosphere, changes to groundwater chemistry—pH and TDS). The IAMs will be used to calculate probabilities of failing or meeting selected performance criteria/thresholds for specific risk metrics. Calculations of probabilities will require multiple simulations with IAMs utilizing approaches such as Monte Carlo simulations coupled with efficient parameter sampling algorithms for uncertainty quantification. The probabilities will be converted into time-dependent risk profiles.

The IAMs will be applied to real-world scenarios with respect to parameters to quantify uncertainty characterizations. The assessment of uncertainties in the underlying ROMs will build an understanding of the propagated errors through the system to assess the overall impact on risk quantification as well as to identify relative importance of various parameters to the models. This information will be used to identify critical science gaps in order to refine research priorities for future risk calculations.

The final product for this task will consist of a report assessing (1) the probabilistic magnitude of various impacts across a range of anticipated geological environments, (2) the key drivers for both the magnitude of risk and the underpinning uncertainty, and (3) general trends/observations on the variation of trapping mechanisms and storage integrity with respect to storage site characteristics.

TRANSFORMATIONAL TECHNOLOGIES

Transformational technologies in the area of science-based risk management for engineered natural systems will center around the expected gains in our ability to collect high-resolution real-time data. As smart fields are becoming more common in the oil and gas industry, similar technology will be available for carbon storage at a significantly lower cost. Additionally, as advances occur in the development of nanotechnology, novel sensors will be able to monitor much higher resolution data in the field. One of the most significant challenges will be the development of computational tools that will allow us to analyze such data and incorporate it into predictive simulation tools for carbon storage and other engineered natural systems.

Research in the 2020–2030 timeframe will focus on the development and validation of real-time processing tools that will allow for the integration of real-time high-resolution data. New simulation technology will benefit from field data that can be collected at the pore scale and used to generated predictive models of field-scale behavior. These models can then be integrated to develop risk assessments with much greater certainty than could previous generation technology.

3.4.3 R&D APPROACH—PERFORMANCE TARGETS AND MEASURES

A detailed schedule for NRAP products can be found in NRAP's project management plan. A high-level list of NRAP products by 2015 includes (1) simulation toolsets (including component ROMs and IAMs) and protocols, (2) broadly applicable quantitative predictive models, (3) a web-accessible database of critical parameters for prediction of CO_2 storage and potential risks, and (4) comprehensive technical assessments of key storage security relationships and issues. Peer-reviewed products will be made available through the Energy Data eXchange, as series of models, reports, and conference proceedings.

Key targets for NRAP are to:

- Develop a suite of tools and a science base that is capable of addressing post-injection site care issues and assessing the goal of 99 percent storage permanence at a range of storage sites by 2015.
- Develop capability to evaluate 99 percent storage permanence goals at the basin scale by 2020.
- Provide a 25 percent reduction in uncertainty associated with risk between current IAMs and 2nd-Generation IAMs that incorporate monitoring and mitigation strategies in 2020.
- Demonstrate the ability to analyze high-resolution real-time datasets within predictive models by 2030.

A summary of the high-level deliverables are addressed in Table 3-13.

Table 3-13. **NRAP Deliverables**

Deliverable	Date	Description of Deliverable
Integrated Assessment Models for Migration and Ground Motion	2013	• 2nd-Generation ROMs will be incorporated into IAMs for risk profiles calculation. • Metrics—(1) return of CO_2 to atmosphere, (2) changes to groundwater pH, (3) changes to groundwater TDS, and (4) changes to metal concentrations in groundwater. • ROMs with improved portability—(1) 1st-Generation ROMs updated, (2) new ROMs added to address oilfield storage, (3) time-dependent mechanical impacts on wellbores, (4) thief zones, (5) leakage through fractured seals, (6) leakage through intact caprock, and (7) metals in groundwater. • The final product will consist of a set of IAMs that integrate results from component ROMs to predict stochastically, spatially, and temporally the impacts of interest.
System Model for Potential Impacts due to Ground Motion	2013	• This system model will use the RSQSim, SimRisk®, and EMPSYN codes to predict both hazard and risk from damage due to ground motions. • Calculations will be expanded to include earthquakes that occur on geostatistically generated three-dimensional (3-D) stochastic distributions of fractures in addition to larger faults. The earthquake catalog and ground motion simulations will be calibrated against an injection site dataset from a well characterized injection site. • The final product will consist of a system-level model that predicts time-dependent hazards and risks from damage resulting from ground motion induced by CO_2 injection and associated pressure changes.
Integrated Assessment Models	2014	• Completed ROMs will be incorporated into for risk profiles calculation. • Metrics—(1) return of CO_2 to atmosphere, (2) changes to groundwater pH, (3) changes to groundwater TDS, (4) changes to metal concentrations in groundwater, (5) changes to organics concentrations in groundwater, and (6) ground motion. • 2nd-Generation ROMs will be updated and new ROMs will be added to address (1) fully integrated multilayer leakage, (2) chemical and mechanical time-dependent wellbore effects, (3) mechanical time-dependent effects on faults and fracture leakage, (4) organics in groundwater, and (5) amplification and other effects due to the shallow geology at surface sites. • The final product for this task will consist of a set of system models that integrates results from the component ROMs to predict stochastically, spatially, and temporally the impacts of interest.

3.4.4 PROGRAM PLAN TIMELINE

The NRAP toolset models to address risk management of technologies will be developed as shown in Figure 3-23 and Figure 3-24.

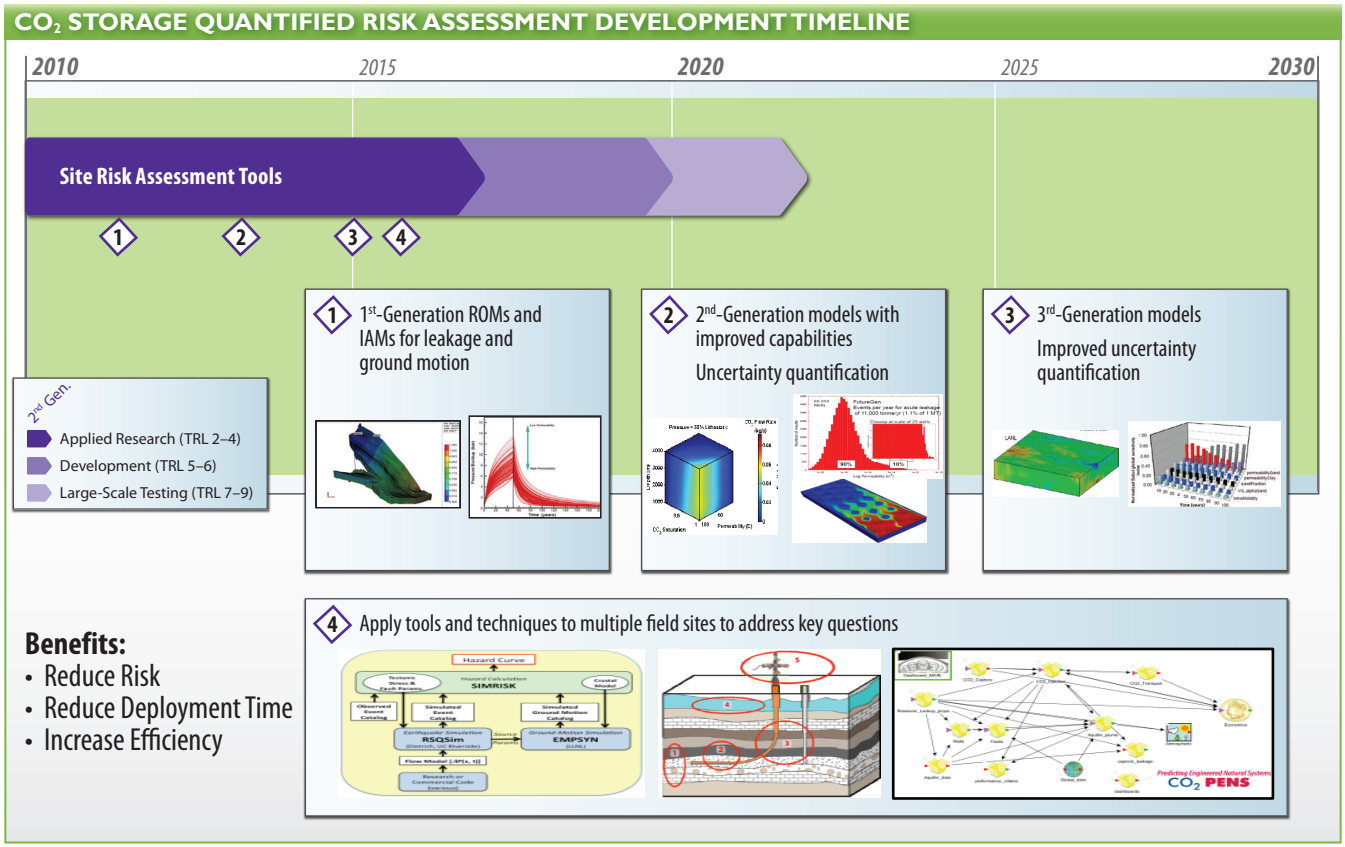


Figure 3-23. NRAP—2nd-Generation Site Risk Assessment Tools Technologies Development Timeline

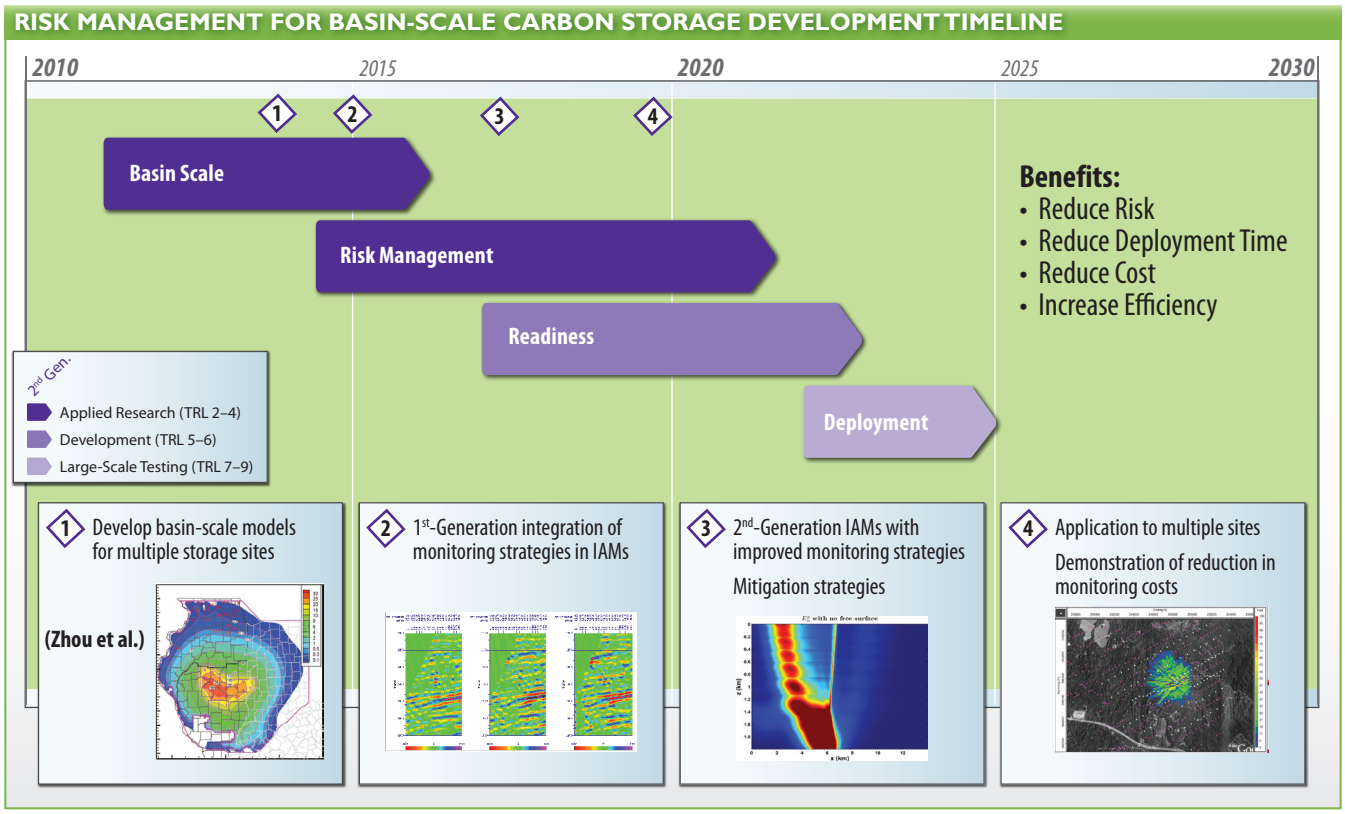


Figure 3-24. NRAP—2nd-Generation Basin-Scale and Risk Management Technologies Development Timeline

3.4.5 RESEARCH FOCUS AREA BENEFITS

The NRAP project will be executed in three phases, each of which improves the science-based platform.

- Phase I is underway for the FY10–FY14 timeframe and focuses on quantification of risk profiles, trapping mechanisms, and associated uncertainties.
- Phase II is ongoing and runs to FY14. Phase II focuses on the identification and development of risk management approaches that include strategic monitoring to verify system performance and lower uncertainty.
- Phase III addresses a potential need for additional data from field tests. An integral component of the NRAP approach is to utilize laboratory and field data to calibrate and validate models. NRAP's strategy in Phase I is to exploit existing data and ongoing field efforts to the extent possible, augmenting these data through the use of targeted laboratory-data and field-data efforts. Consequently, a Phase III field effort may be proposed for FY14 and FY15.

The NRAP research effort is divided into five technical components:

- Development of a methodology and computational platform for quantifying risk profiles (the increase and decrease of risk over time) based on IAMs and uncertainly quantification.
- Targeted scientific investigations at the laboratory and field scale to calibrate component behavior and reduce uncertainties in predicted risk profiles.
- Integration of risk-based monitoring and mitigation strategies to reduce uncertainty and overall risk.
- Potential additional field-scale tests of specific processes to validate predicted behaviors of natural systems.
- Incorporation of phenomena specific to potential risks associated with storage of CO_2 captured from industrial facilities (other than coal-fired power plants).

The tasks associated with the first four components address general issues associated with CO_2 storage. The fifth addresses potential issues in capturing carbon from large stationary sources other than power plants. Though initial research efforts focused on managing CO_2 emissions from coal-fired power plants, CO_2 can be captured at other industrial sources, which present unique challenges.

Expected results and benefits of NRAP's efforts include:

- Removal of a key barrier to the business case for CO_2 storage by providing the technical basis for quantifying long-term liability through development of a robust methodology and platform (computational tools) for quantifying risks (and associated uncertainties).
- More effective and efficient management of long-term storage sites by providing a protocol for integrating risk-based strategic monitoring and mitigation to reduce uncertainties and risk at a site.
- Confidence in setting storage-security metrics by providing a science-based ability to identify safe operational envelopes that minimize potential risks across a range of storage environments.

The tools and improved scientific base developed by the collaborative will help operators design and apply monitoring and mitigation strategies. They will help regulators and their agents quantify risks and perform cost-benefit analyses for specific CCS projects. Finally, financiers and regulators will be able to invest in and approve CCS projects with greater confidence because costs of long-term liability can be estimated more easily and with less uncertainty.

The expected benefits and status of each of the research focus area pathways for NRAP technologies are described subsequently and summarized as component features and benefits in Table 3-14 and Table 3-15.

Table 3-14. **NRAP Component ROM Features and Benefits**

Component ROM	Applications of ROM Software	1st-Generation Features	2nd-Generation Features	3rd-Generation Features	Component ROM Benefits
Reservoir ROMs	• Predict area of review for operators/ regulators • Predict quantities of CO_2 trapped over time	• Multiphase flow • Two reservoir classes • Multiple commercial and research simulators • Stochastic permeability	• Three reservoir classes • Quantified trapping mechanisms	• Four reservoir classes • Coupled effects between reservoir flow and flow along release pathways	• Reduce time in permitting and monitoring processes (post-injection site care) • Improve quantification of trapping over the long term (liability)
Release and Transport ROMs (for wellbores and seals)	• Predict leakage rates of CO_2 and brine • Assess impact on other subsurface resources • Determine "buffering capacity" of subsurface (i.e., how much CO_2 can migrate out of storage formation before it reaches a sensitive receptor—e.g., groundwater)	• Wellbores (flow + phase change) • Faults (flow + phase change) • 1-D flow into thief zones	• Wellbores (flow + mechanics) changing k (permeability) • Flow through caprock fractures/faults (flow + geomechanics) • Porous flow through overburden • Initial state of wells • Wellbore failure and fault-zone complexity	• Wellbores/fractures (flow, chemistry, geomechanics) • Well history stats • Fracture distribution complexity • 2-D flow into thief zones • Coupled flow in wells, faults, and porous overburden	• Reduce time in permitting process (post-injection site care) • Address long-term behavior of seals (liability) • Assist in deep subsurface monitoring design
Groundwater ROMs	• Predict likelihood of an effect on groundwater resources • Assess potential volume and locations of affected areas • Address potential mitigation costs	• TDS, pH • Equilibrium geochemistry • 2 end-member aquifers • CO_2 and brine flux	• TDS, pH, metals inbrine • Multiple leakage sources • Fault orientation, trace metal chemistry in aquifer, impermeable, and semipermeable caprocks	• TDS, pH, metals, organics • Kinetic geochemistry • Coconstituent effects, pathway-dependent effects on groundwater quality	• Reduce time in permitting process (post-injection site care) • Aid in valuation of long-term liability • Assist in shallow subsurface monitoring design

Table 3-15. **NRAP Software Features and Benefits**

Type of Software Component	Applications of Software	1st-Generation ROM Features	2nd-Generation ROM Features	3rd-Generation ROM Features	Model Benefits
Atmospheric Models	• Predict zone of influence of a leaky well at the ground's surface	• Total flux only		• Atmospheric dispersion	• Aid in potential liability quantification
Induced Seismicity IAMs	• Determine chance of increase in seismic risk due to carbon storage	• Hazard risk only	• Hazard and damage risk	• Hazard, damage, and Nuisance risk	• Aid in site selection for seismic hazard • Aid in developing mitigation strategy
Migration IAMs	• Perform quantified risk assessment and develop risk profiles • Address needs for monitoring systems • Address needs for mitigation strategy	• Integrate multiple 1st-Generation ROMs • Sensitivity analysis	• Integrate multiple 2nd-Generation ROMs • Multivariate uncertainty quantification	• Integrate multiple 3rd-Generation ROMs • Improved multivariate uncertainty quantification	• Valuate long-term liability • Determine potential risks over the long term and uncertainty bounds • Aid in design of monitoring systems • Aid in planning mitigation strategy

3.4.6 BARRIERS/RISK AND MITIGATION STRATEGIES

Project risk events are defined as uncertain future events that, if realized, negatively or positively impact the success of the project. Identified project risks should be assessed on a regular basis to measure the probability of occurrence and consequence or impact to the project. Periodic assessments serve two main purposes: (1) keeping the project team aware of risk triggers leading to potential project risks and (2) providing a mechanism for classifying identified risks at key decision points along the critical path. Risk management is also necessary to assure that negative risks—ones that would impede or preclude the timely achievement of established goals and targets—are identified and reasonably mitigated; and positive risks are considered and possibly pursued. Risk probabilities commonly diminish as the project progresses.

Table 3-16 outlines risks and mitigations that have been identified for NRAP.

Table 3-16. **NRAP Barriers/Risk and Mitigation Strategies**

Issue	Barrier/Risk	Mitigation Strategy
Technical	Information available may be insufficient to make decisions to proceed.	This risk is managed by the use of a technical group of experts from each national laboratory to identify the important research topics in individual subtasks.
Technical	An appropriate research strategy to develop a science-based quantitative methodology for determining risk profiles at storage sites is not identified resulting in project failure.	This risk is managed by the use of a technical group of experts from each national laboratory to identify the important research topics in individual subtasks. These priorities will be reevaluated on an annual basis by the technical working groups and vetted with the executive committee and stakeholders group.
Technical	Inaccurate quantification and/or incomplete/incorrect identification of processes at the field scale could result in incorrect quantification of risk profile and/or uncertainties in risk profile.	NRAP's strategy is to utilize multiple field datasets to evaluate field-scale behavior. Short-term processes will be evaluated by observations primarily from anthropogenic analogs whereas long-term processes will be evaluated by observations from natural analog sites. NRAP is pursuing multiple opportunities in parallel to maximize the potential to build the field-database sufficiently.
Management	Inefficiency and/or missed cross-organizational milestones or deliverables due to lack of coordination among researchers, research organizations, or national labs arising from poor integration and coordination.	The working groups and Technical Leadership Team (TLT) are designed to encourage and ensure communication among researchers in each technical area of NRAP work. Annual technical workshops and working group teleconferences will be held to exchange information, progress, upcoming work, and technical ideas. The executive committee was formed to ensure high-level communication among the national laboratories for NRAP. The TLT ensures working level communication among the national laboratories (through the technical coordinators). The TLT will use cross-organizational project planning and monitoring to track and coordinate tasks across components of the project
Management	Staffing challenges due to conflicting national laboratory staffing needs or unexpected loss of staff.	This can be addressed by careful discussion of timelines and staff availability during regular TLT meetings.

3.5 HIGH-PERFORMANCE MATERIALS AND MODELING

The goal for this research is to develop new materials that will enable the next generation of fossil fuel power-generation technologies to operate at higher pressures and temperatures to achieve increased efficiency and lower operating costs. These new materials will need to sustain their superior properties for lifetimes up to 30 years in extreme environments. This research covers the entire realm of materials design and manufacturing. The High-Performance Materials and Modeling key technology leverages the funding available in the University Coal Research

and Historically Black Colleges and Universities programs to maximize the extensive amount of materials research required. This is to ensure that the materials technology necessary to meet the technical performance and market-based goals are achieved for the Advanced Energy Systems technologies.

New alloys are being designed to increase their capability to withstand higher temperatures, corrosion, and erosion at higher pressures that will be experienced by components in advanced power plants. Designing new alloys to perform under these conditions requires an understanding of the interrelationships among composition, microstructure, and properties. Successful designs will result in new coating materials to protect major components such as the steam turbine and primary furnace (boiler).

Focused research to evaluate and develop advanced materials technologies is currently being conducted. These materials will allow the use of advanced steam cycles in coal-based power plants to operate at steam conditions of up to 760 °C (1,400 °F) and 5,000 psi.

A goal of the High-Performance Materials and Modeling key technology includes shortening material development timelines to facilitate FE goals. Experimental and computational investigations cut across many scientific and technological disciplines to address materials requirements for all fossil-energy systems. To bridge the gap between basic and applied research, "breakthrough" concepts are pursued to develop materials with unique thermal, chemical, and mechanical capabilities. High-Performance Materials and Modeling has two basic parts. The first is the computational materials portion (design) and the second is actual material development (manufacture, testing, and qualification). The computational materials effort focuses on a predictive computational framework that accelerates the development of materials and utilizes multiscale computational materials modeling methods with focused validation experiments. Utilization of these techniques is expected to accomplish many results that include: rapid alloy design, manufacture, simulation of an alloy's environmental and mechanical performance, and component life.

The High-Performance Materials and Modeling key technology recognizes that materials research can be cost-effectively conducted at a basic level and then transferred to the appropriate Technology Area for specific performance evaluation and deployment. Moreover, because materials are in many cases the primary enabler of a technology's performance, the benefits of materials can be measured by the benefits of the technology achieving its performance goal.

3.5.1 BACKGROUND

Under the High-Performance Materials and Modeling key technology, 1st-Generation technologies center on the identification and development of materials capable of increasing coal-based electricity generation from the current industry average of 34–46 percent. Current and future research is developing materials that will enable coal-fired power plants not only to operate at higher temperatures, but also to be economically viable.

Efficiency improvements are directly proportional to operation temperatures. Current materials limit the use of advanced steam cycles in coal-based power plants to operate at steam conditions of up to 760 °C (1,400 °F) and 5,000 psi. Higher temperatures are necessary to achieve higher efficiency as shown in Figure 3-25. Plants operating above 22 MPa at 538–565 °C are supercritical, above 565 °C are ultra-supercritical (USC), and above 700 °C are A-USC.

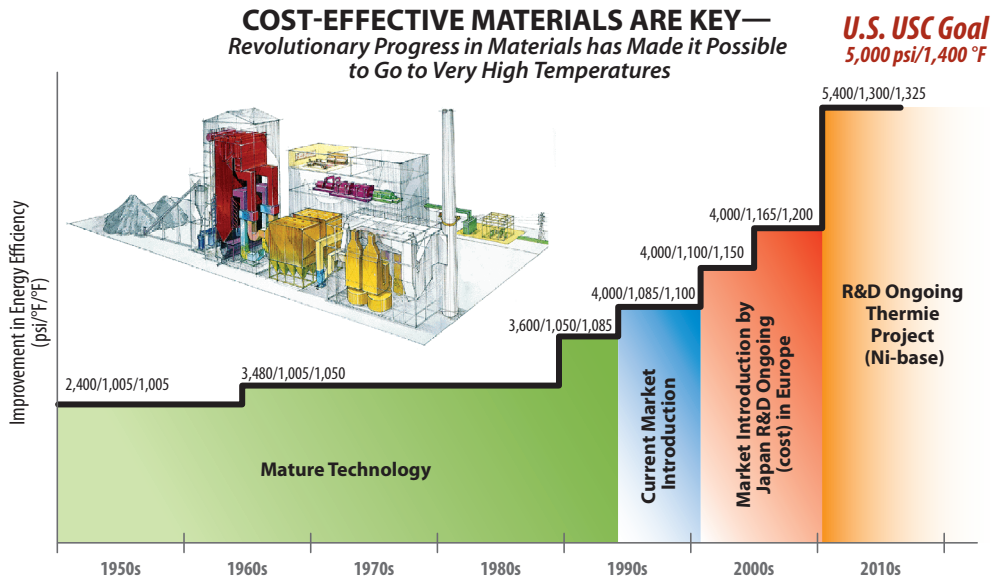


Figure 3-25. Efficiency Improvements Directly Proportional to Operation Temperatures

Currently, creep-strength-enhanced ferritic steels are used up to approximately 600 °C and are increasingly being specified and used for superheater tubing and main steam piping in coal-fired steam boilers, as well as in heat-recovery steam generators used in combined cycle gas turbine units. The High-Performance Materials and Modeling key technology is conducting research to enable the use of creep-strength-enhanced ferritic steels up to 650 °C (or higher).

The increased efficiency of A-USC steam cycles has the potential to reduce CO_2 emissions from coal combustion by up to 30 percent. A-USC plants designed with CO_2 systems will use this increased efficiency to offset the power loss resulting from operating the CO_2 capture systems.

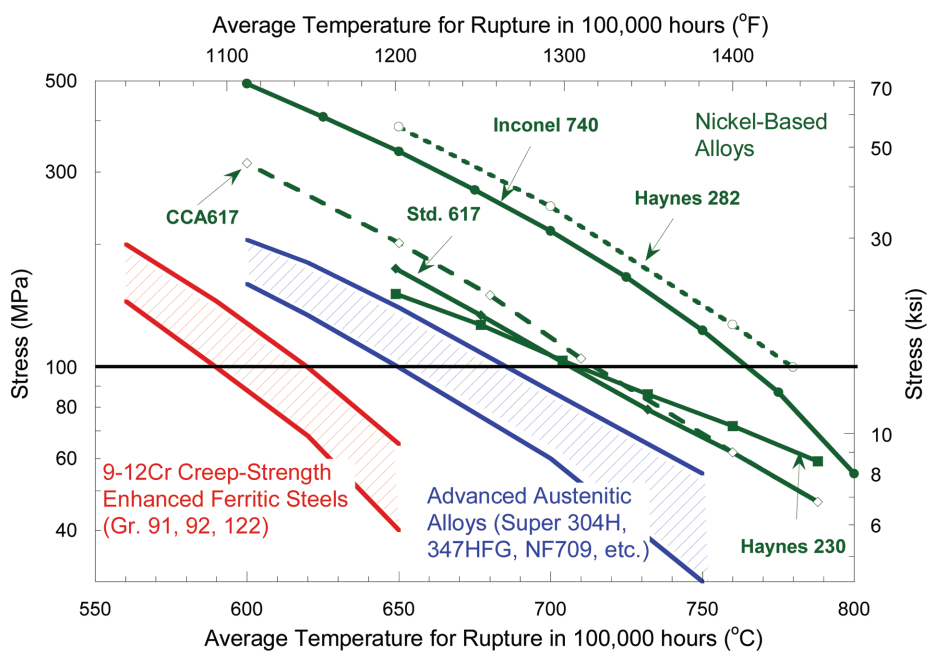


Figure 3-26. Design Requirements for Boiler Materials

Design requirements for boiler materials include a minimum strength of 100 MPa at operational temperatures to withstand high internal water/steam pressure. As shown in Figure 3-26, nickel (Ni)-based alloys are required to withstand 100 MPa at temperatures above 700 °C.

The High-Performance Materials and Modeling key technology sponsors work of uniquely formed A-USC boiler and steam turbine consortia that include all of the major U.S. boiler and steam turbine manufacturers along with national laboratories and industry associations. Over the last decade the A-USC boiler and steam turbine consortia have conducted extensive laboratory testing, shop fabrication studies, field corrosion tests, and design studies. These efforts supported the materials data generation needs of the consortium and lead to a number of successes including the identification of materials that will meet the strength performance requirements at high temperatures.

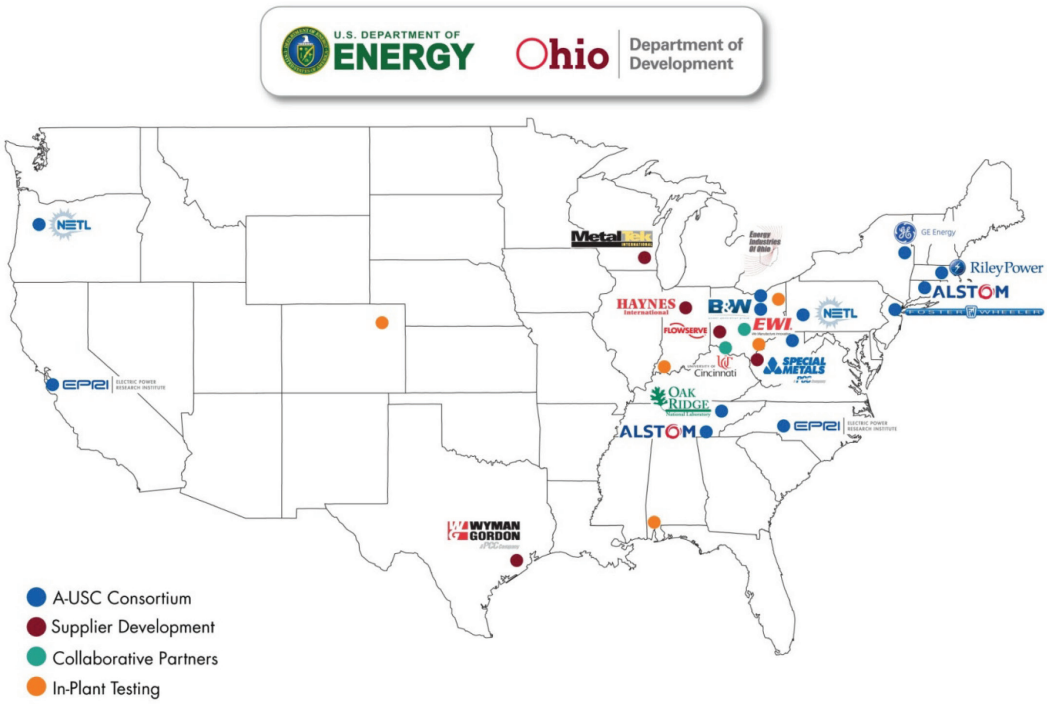


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Figure 3-27. A-USC Consortium Activities Conducted Across the Country

The uniquely formed A-USC Consortium has activities being conducted across the country at facilities of all the major U.S. turbine and boiler manufacturers as shown in Figure 3-27. A brief summary of selected activities and accomplishments are described below.

- Completed the testing that led to the American Society of Mechanical Engineers (ASME) Boiler and Pressure Code Standards Committee's approval of the use of precipitation-hardenable Inconel® 740 wrought sheet, plate, rod, seamless pipe and tube, fittings and forgings in welded construction for service up to 800 °C under Section I rules. The nickel-based alloy has proven to be the best candidate material of construction for components such as steam headers and piping of a boiler operating at A-USC steam conditions (760 °C; 5,000 psi).
- Conducted creep-rupture tests to confirm nickel-based superalloy HR 282 as a candidate alloy for A-USC steam turbines supporting the commercial scaleup for additional testing.
- Installed a steam loop containing a variety of candidate alloys in a host utility plant to evaluate the corrosion performance of various materials at A-USC conditions as shown in Figure 3-28.

- Performed pilot-scale oxy-combustion tests burning bituminous coal under staged and unstaged conditions in the burner flow reactor at Brigham Young University. These tests were designed to produce the boiler conditions with a warm recycle of the flue gas.
- Members of the A-USC Consortium, including the Ohio Coal Development Office, the Electric Power Research Institute, Alstom, General Electric, Foster Wheeler, and The Babcock & Wilcox Company, organized a workshop for U.S. utilities, suppliers, and manufacturers to discuss the accomplishments of the consortium and the next steps for moving A-USC technology forward. As a result of that meeting an Advanced Generation Advisory Panel was established with the purpose of guiding the A-USC Consortium in finalizing its material development activities by identifying the concerns and requirements of the power industry associated with the deployment of the A-USC technology.

Figure 3-28. Steam Loop Installed at Host Utility Site, Targeted 2 Years of Exposure at 1,400 °F

Materials research for oxy-fired A-USC plants is simultaneously being conducted to meet the goals of the Advanced Combustion Systems 2nd-Generation program. A workshop to review materials development and boiler fireside corrosion research being performed for oxy-fired boilers under the program was held with participating researchers from NETL Office of Research and Development, Argonne National Laboratory, and Oak Ridge National Laboratory. During the workshop, researchers from each organization presented information describing the scope of the effort they are conducting, including alloys being developed and tested, mechanical testing plans and testing parameters, corrosion test conditions (temperatures, pressures, gas and ash environment, coal types being tested or simulated in lab tests, duration, sampling and post-exposure analysis protocols) and expected output of the work—experimental data, predictive models, new products. Industry representatives from Alstom, The Babcock & Wilcox Company, Electric Power Research Institute, Foster Wheeler, and General Electric participated in the discussions and provided feedback to the researchers.

The overall objective of the High-Performance Materials and Modeling key technology for Transformational technologies is to develop and demonstrate a predictive materials modeling and computational framework. This modeling and computational framework will accelerate the design, development, and optimization of efficient, cost-effective structural and functional materials for Transformational power-generation cycles. To accomplish this objective, a variety of projects are tackling different aspects of materials modeling. The varied work areas range from first-principle atomistic modeling through the mesoscale modeling to predict thermodynamic and kinetic properties of complex materials.

Current work involves the modeling of alloys based on refractory metal elements to withstand the high temperatures and aggressive environments predicted for components such as oxy-fuel turbines, hydrogen turbines, and syngas turbines; and ab initio modeling of thermomechanical properties of molybdenum (Mo)-based alloys for fossil energy conversion.

A summary of the high-level components developed under the High-Performance Materials and Modeling key technology is provided in Table 3-17.

Table 3-17. **High-Performance Materials and Modeling Technology Development Summary**

Key Technology	1st-Generation Technologies	2nd-Generation Technologies	Transformational Technologies
High-Performance Materials and Modeling	• A-USC materials and materials technology including Inconel 740 ASME Boiler Code approval; coatings handbook; fabricability handbook • Oxy-combustion materials modeling	• Computational materials modeling • Structural and functional performance materials - Thermal-fatigue-resistant alloys for PC plants - Low-cost alloys and coatings for A-USC plants - Next-generation alloys and thermal barrier coatings (TBCs) for high-temperature gas turbines • Computational models for high-temperature alloy design and performance modeling	• Predictive materials modeling and computational framework • New structural materials for Transformational power-generation cycles • Stable, high-capacity CLC oxygen carriers • Integrated modeling system

3.5.2 TECHNICAL DISCUSSION

The High-Performance Materials and Modeling key technology is building on the aforementioned successes to ensure that materials will be ready to meet deployment targets of the 2nd-Generation and Transformational coal power plants. Figure 3-29 shows the High-Performance Materials and Modeling 2nd-Generation and Transformational technologies development R&D program plan timeline.

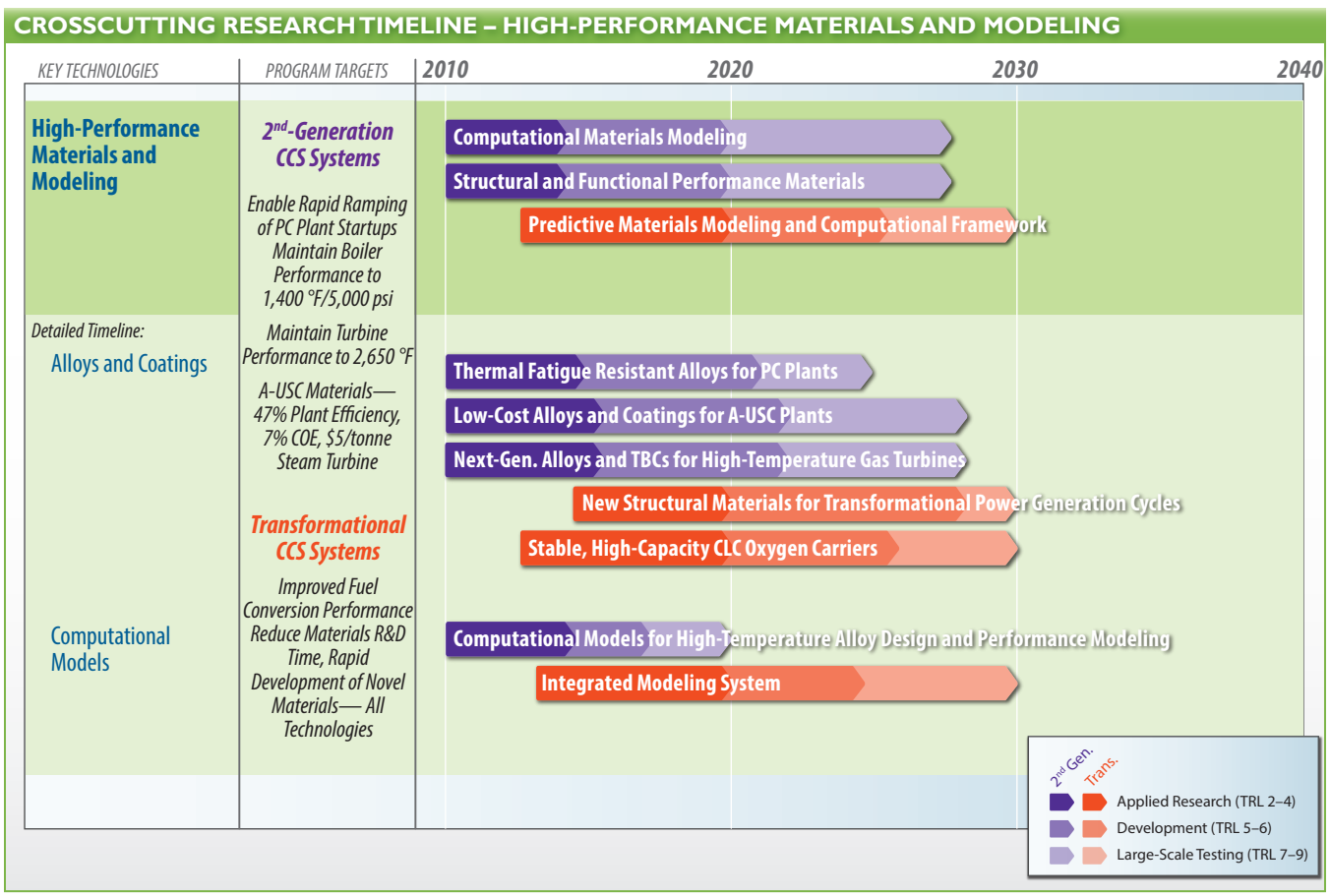


Figure 3-29. High-Performance Materials and Modeling—2nd-Generation and Transformational Technologies Development Timeline

2ND GENERATION TECHNOLOGIES

Materials research develops predictive structural and functional modeling capabilities to provide for timely design of new alloys. Materials research uses computational modeling and simulation tools to guide the design of new materials capable of operation under the extreme temperature, pressure, and corrosive conditions found in coal-fueled power plants. Experimental and computational methodologies are being pursued to decrease the time and cost required to develop new materials compared to traditional trial-based methodologies. This work includes the exploration of developing chemistries that will form either protective chromia-oxide scales or alumina-oxide scales depending upon the application environment and performance requirement needs. The overall objective of the High-Performance Materials and Modeling key technology is to develop and demonstrate a predictive computational framework that will accelerate the design, development, and optimization of efficient, cost-effective functional materials. This includes developing an integrated computational framework, ranging from first-principle atomistic modeling through the mesoscale modeling capable of predicting thermodynamic and kinetic properties of complex materials.

The High-Performance Materials and Modeling key technology will demonstrate a discovery, design, and manufacturing methodology that is generally applicable to materials needed for advanced fossil-energy systems. The goal is to develop a validated computational framework that facilitates the design and development of materials by elucidating chemical and mechanical properties at conditions and time scales consistent with application. The computational tools developed through this research will assist in accelerating the design, development, and deployment of materials for fossil-energy applications. Research is focused on developing computational frameworks to (1) predict alloy oxidation behavior in a variety of relevant environments; (2) predict microstructure stability—and therefore materials properties and performance—under relevant time scales for alloys under consideration for application in advanced fossil-energy systems, including A-USC power plants; and (3) aid in the electroslag remelting processing of alloys under consideration for advanced fossil-energy systems, including A-USC power plants, by establishing the thermodynamics of electroslag remelting and developing a thermodynamic database for oxide and fluoride slag components used in electroslag remelting melting of Ni-alloys. The outcome of this research will benefit the public by developing and validating advanced virtual engineering computer-aided design tools (for designing, assessing the performance, and processing of materials) that will contribute to reducing the cost and accelerating the deployment of advanced materials for fossil-energy applications.

Materials research is focused on developing new high-performance materials for structural and functional A-USC power-plant applications and advanced turbines. Such materials also are needed to develop new systems and capabilities for coal combustion and gasification, gas separation, hydrogen storage, and improve performance and reduce costs of existing power-generation systems. New alloys will fulfill the need to use advanced materials in boilers and steam turbines for achievement of higher efficiencies, emissions reductions, lower cooling water requirements, and lower fuel costs. Research is needed to develop materials that can sustain high temperatures, elevated pressures, and corrosive environments (e.g., reducing and oxidizing conditions, molten salts, and gaseous alkali compounds). Research in this area develops materials of construction and includes processing and fabrication methods.

This will assist in accelerating the commercialization of advanced power-generation systems and carbon capture technologies from discovery to development, demonstration, and ultimately to widespread deployment.

TRANSFORMATIONAL TECHNOLOGIES

Transformational technologies will require novel materials solutions to meet requirements of yet undeveloped processes. The High-Performance Materials and Modeling key technology expects to meet these challenges through development of a comprehensive and fully verified predictive materials modeling and computational framework. Such a toolkit will enable rapid development of materials required to meet future specifications of transformational systems. For example, a computationally designed material could be quickly prototyped by future 3-D printing via stereolithography or direct metal laser sintering within a matter of hours of design completion. The prototype could then be tested and qualified for plant system applications. The following paragraphs include a brief description of Transformational technologies that are anticipated to require High-Performance Materials and Modeling support.

Pressurized oxy-combustion will feature combustion of fuel with a pressurized mixture of nearly pure oxygen and recycled flue gas rather than air. There would be no emissions of particulate, mercury, heavy metal, hydrogen fluoride, hydrogen chloride, nitrogen oxides, or sulfur oxides from an oxy-combustion plant. Only a small amount of nitric oxide, carbon monoxide, and CO_2 is emitted to the atmosphere. Flue gas is recycled back to the boiler to control flame temperature, dilute corrosive constituents, and provide mass for convective heat transfer. Radiant and convective heat transfer in the boiler is balanced by the gas mass flow. Heat transfer to the water and steam contained in pressure boundary metal tubes is accomplished by radiation and convection. The hotter the flame, the higher the heat fluxes in the boiler tubing furnace. Water is used to cool the furnace tubes and steam cools superheater tubing, which is generally located in the convection pass where heat fluxes are lower. However, steam is about one-fifth as effective as water at cooling the tubes. Pressurized oxy-combustion superheater tubing will have ultra-supercritical steam temperatures of 1,300 °F or higher and require Transformational materials with high creep resistance.

Coal-fueled CLC is a flameless combustion technology where there is no direct contact between air and fuel. This process utilizes oxygen from metal oxide oxygen carriers for fuel combustion and yields CO_2 and water (H_2O) vapor as combustion products. Benefits of this combustion process include minimizing production of nitrogen oxides and production of a CO_2 stream ready for storage that does not require additional CO_2 separation units. Transformational materials are necessary to support development of advanced oxygen carriers with optimum attrition-resistance and thermal-stability properties for diversified coal types.

Energy storage materials are being developed and demonstrated at laboratory scale using an integrated electrochemical architecture with performance characteristics suitable for grid-scale power electronics. The emphasis is on the continued development of a potentially Transformational magnesium (Mg)-based battery system for large energy storage applications. Research is focused on improving the electrochemical materials systems through interrogating pertinent structure-property relationships and improving processing methods. Benefits of large-scale electrical energy storage for grid-scale applications include providing a more stable, efficient, and reliable grid for the delivery of electrical power and the capacity to "peak shave or load shift." This will result in more stable and efficient delivery of electrical power while reducing overall CO_2 emissions.

3.5.3 R&D APPROACH—PERFORMANCE TARGETS AND MEASURES

This section provides high-level milestones describing the effort for each of the 2nd-Generation and Transformational categories identified within the overall timeline (Figure 3-29). A portfolio of projects is managed within each category to address stakeholder needs, to accelerate development timelines for approaches that are viable, and down-select those that are deemed not viable for commercialization.

The 2nd-Generation technologies are expected to result in materials capable of withstanding rapid ramping of PC plants to provide timely support of electric grid demands placed on generating plants by system operators. This generation of materials will also support increased plant efficiency and availability through materials capable of operating up to 1,400 °F/5,000 psi for A-USC steam turbine and boiler performance. Additionally, 2nd-Generation materials will enable increased combustion turbine performance to 2,650 °F.

Transformational materials are needed to support future power systems such as pressurized oxy-combustion, chemical looping, and energy storage. New materials developed with advanced Transformational computational modeling design technologies are expected to possess superior properties for enhanced durability and lifetime while operating under extreme conditions. The development of new Transformational materials and an integrated modeling system for material design will ensure and enable a reliable and stable electrical supply from coal-powered generating plants to meet any rapid changes in future grid requirements.

THERMAL FATIGUE RESISTANT ALLOYS FOR PC PLANT

- FY 2012: Identify R&D need
- FY 2013: FOA to solicit projects
- FY 2015: Identify potential alloys
- FY 2020: Testing and computational modeling of material properties
- FY 2025: Component testing and technology transfer to Advanced Combustion Systems

LOW-COST ALLOYS AND COATINGS FOR A-USC PLANTS (AIR- AND OXY-FIRED)

- FY 2013: Design studies based on selected materials
- FY 2015: Complete steam turbine casting development
- FY 2028: Technology transfer to Advanced Combustion Systems

NEXT-GENERATION ALLOYS AND TBCS FOR HIGH-TEMPERATURE GAS TURBINES

- FY 2012: Computational design/experimental testing
- FY 2020: Component testing

NEW STRUCTURAL MATERIALS FOR TRANSFORMATIONAL POWER-GENERATION CYCLES

- FY 2013: Identify research need
- FY 2014: FOA to solicit projects
- FY 2016: Identify potential alloys
- FY 2020: Testing and down-selection of alloys
- FY 2025: Long-term testing
- FY 2028: Material assessment and refinement
- FY 2035: Technology transfer to Advanced Energy Systems Technology Areas

STABLE, HIGH-CAPACITY CLC OXYGEN CARRIERS

- FY 2013: FOA to solicit projects.
- FY 2015: Identify potential alloys
- FY 2020: Lab-scale testing and computational modeling of material properties
- FY 2025: Technology transfer to Advanced Combustion Systems

COMPUTATIONAL MODELS FOR HIGH-TEMPERATURE ALLOY DESIGN AND PERFORMANCE MODELING

- FY 2020: Able to model mechanical performance for several alloy systems

PREDICTIVE COMPUTATIONAL FRAMEWORK FOR RAPID DEVELOPMENT OF NEW MATERIALS

- FY 2014: Identify alloy systems to be modeled
- FY 2016: Identify framework
- FY 2020: Integrated modules
- FY 2035: Component testing

Deliverables associated with the aforementioned performance measures and milestones are provided in Table 3-18.

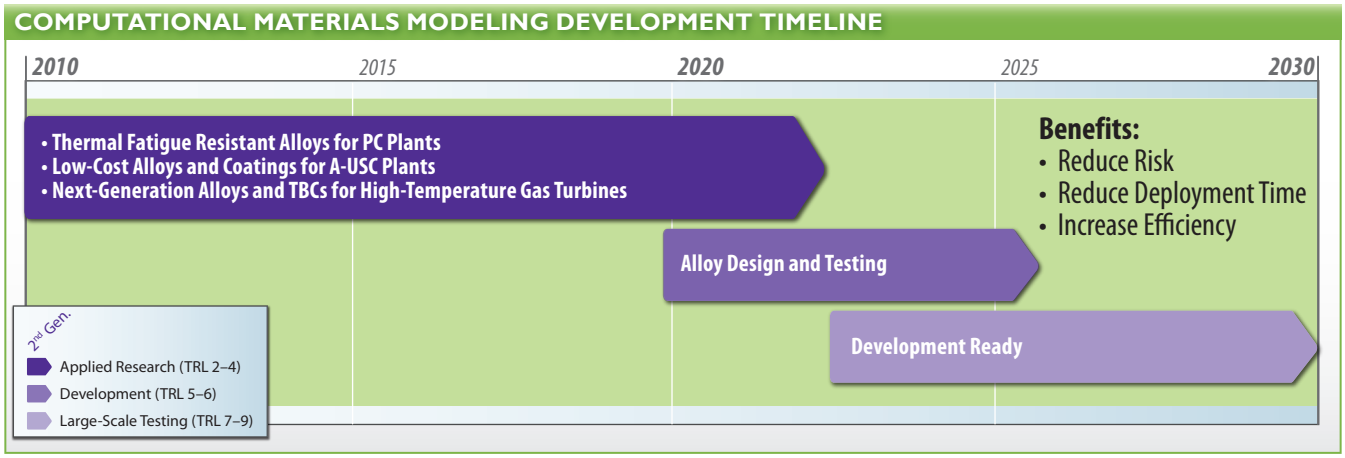
Table 3-18. **High-Performance Materials and Modeling Deliverables**

Deliverable	Date	Description of Deliverable
Complete Corrosion Evaluation of Turbine Materials in CO_2 Plus Steam Environments	2013	• Continue corrosion evaluation of advanced nickel-based alloys in monolithic and dissimilar metal weldments in the presence of alkali sulfate/alkali chloride and ash in simulated fireside combustion environments
Computational Modeling	2013	• Predict corrosion wastage of boiler tubing in reducing and oxidizing environments
Atomic-Level Oxide Dispersion Strengthened (ODS) Interface Models	2015	• Improved software codes for large-scale-molecular dynamics simulations to enable design of new ODS steel alloy compositions that have improved high-temperature mechanical and corrosion-resistance properties for advanced fossil-energy applications
High-Entropy Alloys Material Characterization Models	2015	• Computational thermodynamic models that characterize material phase mechanical properties for new AlCrCuFeMnNi high-entropy alloys along with an enhanced thermodynamic database
Quantitative Creep Models	2015	• Computational models for design of a wide range of advanced precipitation-strengthened alloys
MAX* Simulations	2016	• Large-scale simulations of the mechanical properties of layered transition metal ternary compounds • Electronic structure characterized for specified crystalline phases in the MAX system
A-USC Materials for Components: Steam Turbine, Boiler, Turbine Blades	2023	• Improved nozzles and powder formation techniques for applications to materials used in A-USC boilers • Lower cost steels capable of operation at 760 °C • Thermal coatings with high corrosion/erosion resistance • High-temperature Ni-based alloy castings for turbine subcomponents • Creep-strength-enhanced ferritic steels • ODS alloys designed for A-USC pressures and temperatures
High-Capacity Oxygen Carrier Materials	2023	• Oxygen carrier materials for coal-fueled CLC
Predictive Computational Material Models	2024	• Validated computational models capable of predicting performance of materials in various types of Transformational power plants, including pressurized oxy-combustion, pressurized gasification, and CO_2 cycle plants
Advanced High-Temperature, High-Pressure Alloys	2025	• High-nickel-based superalloys with ability to operate at high temperatures and high pressures • Additional properties include ability to resist corrosion/erosion in an oxygen-rich environment containing abrasive particles

NOTE:
* MAX: Layered Ternary Transition Metal Carbides and Nitrides.
Formula: $M_{n+1}AX_n$, where M is Early Transition Metal; A is A-group element; X is Carbide or Nitride; n = 2–5, n = 1 also possible.
Most phases are 211 or 312 compounds; 413 and 514 are very rare.

3.5.4 PROGRAM PLAN TIMELINE

High-Performance Materials and Modeling research for 2nd-Generation technologies will be developed for new materials and materials modeling as shown in Figure 3-30 and Figure 3-31. Materials modeling is being developed and alloys shown in Figure 3-30 are discussed subsequently.



Materials Model Development
Atomic-Level Oxide Dispersion Strengthened Steel Alloy Interface Models
High-Entropy Alloys
TBCs
Nickel-Based Alloys

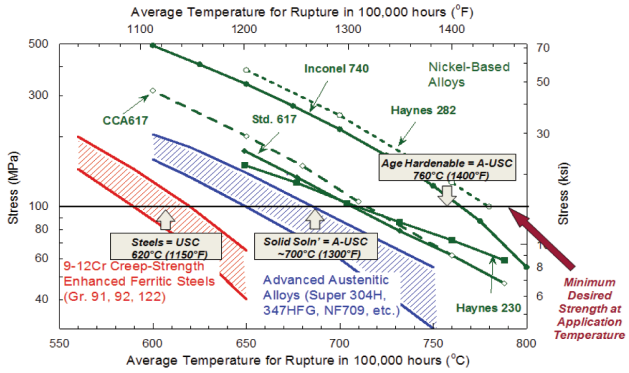


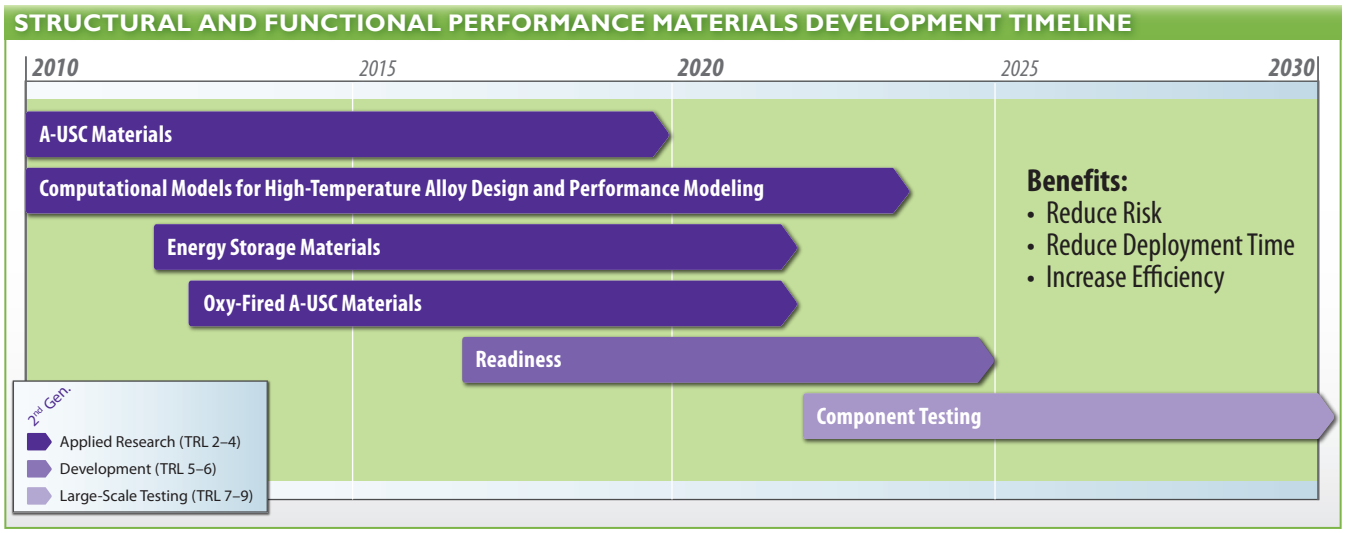
Figure 3-30. High-Performance Materials and Modeling—2nd-Generation Technologies Development Timeline (Part 1)

Thermal-Fatigue-Resistant Alloys for PC Plants—Computational materials modeling will be used to develop 2nd-Generation materials with enhanced properties required to support optimized operation of PC plants. The business environment requires the ever increasing need to rapidly ramp up power plants to quickly support electrical grid demands. Existing power plants were designed with materials that limit the ramp rates due to their thermal fatigue properties. Advanced 2nd-Generation computational materials modeling will result in thermal-fatigue-resistant alloys able to transfer heat at a faster rate and/or capable of withstanding higher stresses through enhanced material microstructures with new compositions.

Low-Cost Alloys and Coatings for A-USC Plants—A-USC power plants will operate at high temperature and pressure under harsh conditions. High-nickel alloys are applicable to A-USC harsh conditions, but low-cost alloys and corrosion/erosion-resistant coatings need to be developed to keep the costs as low as possible to optimize the economics. In addition to developing appropriate low-cost alloys, joining of the materials is important. The friction stir welding process is being investigated as a new method to economically weld the latest ferritic ODS alloys.

Next-Generation Alloys and TBCs for High-Temperature Gas Turbines—Advanced single-crystal alloys and TBCs are necessary to support high-temperature applications such as turbine blades and combustors in A-USC turbines. Experimental and computational investigation is being performed on high-entropy alloys for elevated-temperature use in boilers and steam and gas turbines at temperatures above 760 °C and stress of 35 MPa. Current materials work includes efforts to develop a tool for rapid assessment of potential material formulations to find candidate materials for construction of high-temperature gas turbine components and reduce new material development time by performing comparisons using formation enthalpy data. TBCs are added to the blade surface to provide additional heat resistance. The TBCs must also be able to withstand thermal cycling and provide resistance to erosive particles such as loose scale from the internal surfaces of boiler tubing and main steam piping.

Novel materials are being developed and applications shown in Figure 3-31 are discussed subsequently.



Materials Development
Materials Property Characterization Models
Turbine Castings
Ferritic and Austenitic Stainless Steels
Nickel-Based Alloys
TBCs (Turbine Blades, A-USC Tubing)

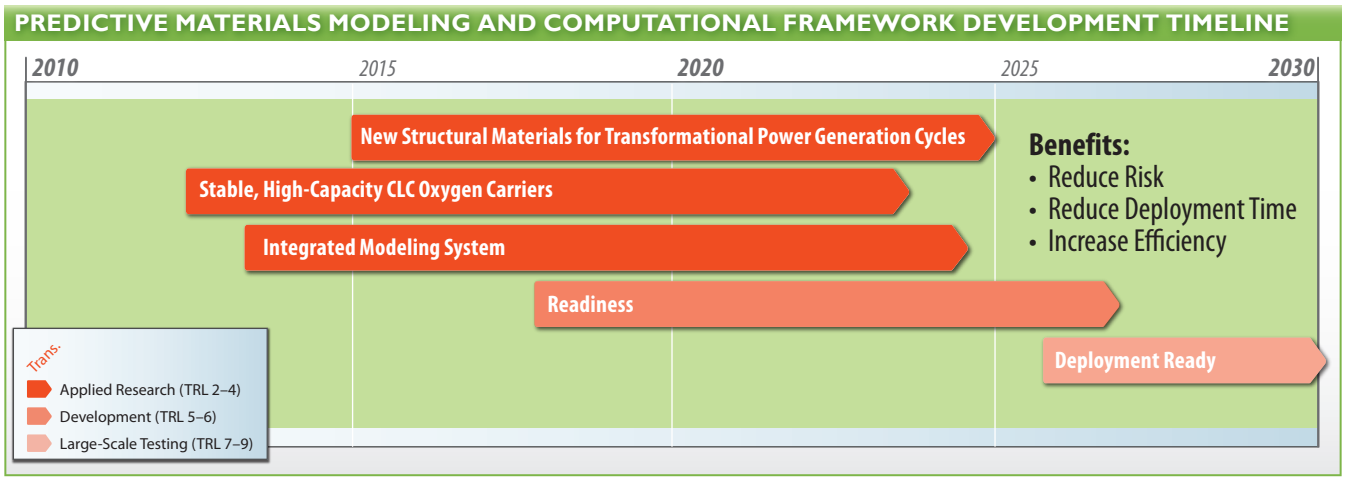
Figure 3-31. High-Performance Materials and Modeling—2nd-Generation Technologies Development Timeline (Part 2)

A-USC Materials—New A-USC materials and coatings are necessary to support efficient operations at higher temperatures and pressures with all types of coal. Promising materials, such as Ni-based alloys, are being evaluated to develop data necessary for the design of a steam turbine operable at A-USC conditions through research on the mechanical properties, oxidation resistance, weldability, and suitability of alloys and coatings. In addition to Ni-based alloys, new ferritic steels with high iron and chromium (Cr) concentrations are being developed along with novel strengthening mechanisms/microstructures.

Computational Models for High-Temperature Alloy Design and Performance Modeling—Computational models are being developed to study the physical properties of various alloys. For the niobium (Nb)-Si alloy system a computational tool is in development to assess thermodynamics properties relative to ordered and disordered lattice structures. The model will be interfaced to Thermo-Calc® with the goal of evaluating the Nb-Si alloy, which is a top candidate for next-generation hot section material for turbines. This process will speed up the development of Nb-Si-based refractory alloys for energy applications. Synergistic computational and microstructural design is being performed for next-generation high-temperature austenitic stainless steels. This will involve careful design of the microalloy composition and heat treatments to control microstructure. Other computational modeling efforts are focused on layered transition metal ternary compounds, Ni-Cr alloys, ferritic superalloys, and novel Cr-based alloys.

Energy Storage Materials—Discovery of new materials and components can lead to new technologies meeting the performance and cost requirements for grid-scale energy storage applications. Optimization of materials is required for anodes, cathodes, and electrolytes to support a viable energy storage system. Current efforts are focused on anode, cathode, and electrolyte development, and primarily involve magnesium-based alloys, silicates, and salts.

Oxy-Fired A-USC Materials—Oxy-fired A-USC boiler/furnace tubing will be exposed to higher concentrations of oxygen while operating at higher temperatures. These materials will need to be able to form protective oxide scales that are able to adhere to the exterior surface of the tubing. The tubing in A-USC boilers will experience thermal cycling through a greater range of temperatures as compared to supercritical plants operating at lower maximum temperatures. Oxy-fired systems are under study to determine the temperature-dependent corrosion mechanisms of candidate high-temperature alloys and coatings in oxy-firing systems.



Materials Modeling and Computational Framework Development
Comprehensive Material Design Framework
Nickel-Based Superalloy Models
Refractory Alloys
Age-Hardenable Alloys
Oxygen Carrier Materials

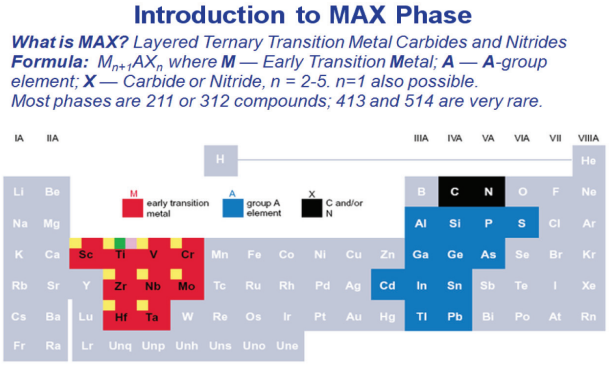


Figure 3-32. High-Performance Materials and Modeling—Transformational Technologies Development Timeline

The High-Performance Materials and Modeling research for Transformational technologies that will be developed for new materials and materials modeling is shown in Figure 3-32 and discussed subsequently.

New Structural Materials for Transformational Power-Generation Cycles—Multiscale computational design and synthesis of protective smart coatings for refractory metal alloys will enable the implementation of new structural materials in fossil fuel energy generation. The combination of a protective smart coating on a refractory metal alloy will provide a 200–400 °C increase in material operating temperature beyond the limitation of current Ni-based superalloys. The enabling technology underlying this advance is based on the computational design of a novel multifunctional integrated coating strategy that will provide both environmental and thermal protection in advanced combustion systems. Another structural material candidate involves $MoSi_2$-based composites. A novel and competitive processing route needs to be developed for manufacturing $MoSi_2$-based composites.

Stable, High-Capacity CLC Oxygen Carriers—Material processing techniques need to be developed to manufacture next-generation oxygen carrier materials for CLC. This will be performed for two new groups of oxygen carrier materials based on a crystal structure. The oxygen carrier material formulations will be investigated by using these new oxygen carriers in CLC systems.

Integrated Modeling System—Transformational materials will be designed with a comprehensive computational modeling framework for rapid design and development. This framework will be composed of computational models capable of providing candidate compositions of new alloys, predicting phase formation, microstructure stability, material performance, formability, and weldability.

Current modeling efforts include microstructural optimization of alloys. High-resolution methods for modeling the three dimensional mechanical response of metallic alloys when exposed to high temperatures are being developed by simulating plastic deformation and damage accumulation of polycrystalline materials at the grain scale. Another modeling effort involves a quantitative model for predicting grain boundary embrittlement in refractory alloys.

Investigations of strengthening mechanisms and model development are ongoing for the precipitation kinetics and deformation behavior of aluminum-alloyed, Laves phase-strengthened, austenitic steels. These steels have improved oxidation resistance and are potential candidate materials for fossil fuel energy systems operating at temperatures greater than 800 °C.

Additional science-based computational methods and modeling are being assessed for selecting chemical composition of nanostructure coatings to develop advanced coating application processes, assess the lifetimes of the coatings, and characterize the creep-fatigue-environment interactions in steam turbine rotor materials.

3.5.5 RESEARCH FOCUS AREA BENEFITS

The expected benefits of each of the research focus area technologies, are described subsequently and summarized as component features and benefits in Table 3-19.

Table 3-19. **High-Performance Materials and Modeling Component Features and Benefits**

Category of the Material Component/Software	Description of the Material/ Software Component	Applications of the Material/ Software Component	Current State-of-the-Art and Limitations	Benefits The Material/ Software Component is to Deliver
Thermal-Fatigue-Resistant Alloys for PC Plant	• ODS steels • High-entropy alloys	• Superheater headers • Turbine casings • Main steam piping	• Current PC fleet unable to respond in a timely manner to grid demands due to alloys utilized in thick-walled components	• Enable flexible operation of PC power plants
Low-Cost Alloys and Coatings for A-USC Plants	• High-chrome ferritic steels • Chromia-oxide/alumina-oxide forming coatings • TiC and TiB_2 nanoparticles	• Boiler tubing • Superheater headers • Main steam connection piping from the boiler to the steam turbine • Turbine casings	• Steam temperature 620 °C limiting plant efficiency	• Higher efficiency plants • Materials export
Next-Generation Alloys and TBCs for High-Temperature Gas Turbines	• Pyrochlore oxide-based double-layer coatings • TiC and TiB_2 nanoparticles • Mo-Ni-Al alloys	• Turbine blades and combustor components	• TBC condition is limited to visual inspection	• Nondestructive evaluation methods can be used to assess the quality of new coatings, identify defective components that could cause unscheduled outages, monitor degradation rates during engine service, and provide data for reaching rational decisions on replace/ repair/reuse of components
Computational Models for High-Temperature Alloy Design and Performance Modeling	• Atomic-level alloy interface models	• ODS steel alloy design	• Long materials design and testing time	• Shorten time to develop materials for high-temperature/high-pressure applications
Stable, High-Capacity CLC Oxygen Carriers	• Metal oxides	• CLC reactors	• Costly, unstable oxygen carriers	• High-efficiency power generation

Table 3-19. **High-Performance Materials and Modeling Component Features and Benefits**

Category of the Material Component/Software	Description of the Material/ Software Component	Applications of the Material/ Software Component	Current State-of-the-Art and Limitations	Benefits The Material/ Software Component is to Deliver
Predictive Computational Framework for Rapid Development of New Materials	• Multiphase CFD models	• Transformational power plants, including pressurized oxy-combustion, pressurized gasification, and CO_2 cycle plants	• Long materials design and testing time	• Shorten time to develop materials for high-temperature/high-pressure applications

2ND GENERATION TECHNOLOGIES

The benefits of 2nd-Generation technologies for High-Performance Materials and Modeling will include improvements in operational flexibility, efficiency, emissions, availability, reliability, and lower costs for advanced coal-fueled power plants. Improvements to materials are being made in two primary areas: (1) materials modeling and (2) improved materials for advanced power-plant applications.

Computational modeling efforts will focus on high-temperature alloy design and performance modeling. Improved modeling will identify novel material compositions with increased fatigue and creep resistance at high temperatures. Material modeling benefits include shortening the materials design time period that is required to discover and qualify new alloys. The capability to quickly identify new material compositions and shorten the materials design period will result in savings by making new materials available earlier than would be possible without advanced computational tools.

Improved materials features include increased thermal fatigue resistance, lower cost alloys, low-cost erosion/corrosion-resistant coatings, TBCs, and higher temperature operation. Materials with increased fatigue- and creep-resistant properties will allow power-plant operators to have faster ramp-up rates for power plants from cold-start conditions and enable flexible operation of PC power plants to meet grid demands. Lower cost alloys and corrosion/erosion-resistant coatings will lower the cost of electricity by reducing capital costs for replacement materials in existing plants and new materials in A-USC power plants. New materials will enable operation of A-USC power plants up to 14,00 °F (760 °C) as compared to today's operation of the John W. Turk, Jr. USC power plant with a turbine inlet temperature of 1,110 °F (599 °C) at 3,515 psi. USC plants operate with efficiencies in the 39–40 percent range. A-USC plants will be able to operate at a higher temperature of up to 1,400 °F (760°C) at 5,000 psi with 47 percent plant efficiency. Less fuel will be required for A-USC power plants than USC coal-fired plants to produce the same amount of electricity with lower emissions. These factors will contribute to lowering the COE up to 7 percent. Materials with enhanced properties will also provide industry with new material products for export.

TRANSFORMATIONAL TECHNOLOGIES

Future High-Performance Materials and Modeling Transformational technology efforts will result in novel materials, and design and performance modeling tools to support new alloy materials for advanced power plants, including pressurized oxy-combustion, pressurized gasification, CLC, and CO_2 cycle plants. In addition, A-USC power-plant materials technologies will be further optimized as new materials performance data are acquired from plants operating under increased grid demand conditions. The predictive computational modeling framework will be refined and validated as new alloys gain operational time. Also, the constructability, weldability and long-term material performance will yield new data to further refine computational modeling efforts.

The benefits of the new materials and advanced modeling computational tools will include high-efficiency power generation; optimization of plant operations for diversified fuels; operation at higher temperatures and pressures for increased efficiency, lower emissions, and lower costs; and shortened times to develop materials for high-temperature/high-pressure applications.

3.5.6 BARRIERS/RISK AND MITIGATION STRATEGIES

The main issues for the High-Performance Materials and Modeling 2nd-Generation and Transformational technologies are listed in Table 3-20 along with the risks and mitigation strategies.

Table 3-20. **High-Performance Materials and Modeling Barriers/Risk and Mitigation Strategies**

Issue	Barrier/Risk	Mitigation Strategy
Economically generating clean power using fossil fuels in a deregulated power industry	Extremely harsh conditions (high temperature, high pressure, corrosive, erosive, etc.) Supply chain unavailable Complex component fabrication	Develop high-temperature materials capable of maintaining performance in harsh environments Evaluate supply chain, including raw material availability Include fabrication methodology development in program
Achieve capital cost reduction performance target	Material price volatility	Develop multiple alloys capable of meeting performance requirements
Achieve efficiency gain performance target	Existing/new plants do not adopt advanced materials technologies	Maintain relationships with manufacturers, industry groups and other stakeholders so that they have buy-in to new materials Perform studies and publish results to ensure designers have a basis to adopt new materials technologies
Achieve all performance targets by 2030	Delay in program execution; inadequate progress on cost and performance goals	Near-, mid-, and long-term R&D projects as well as laboratory, proof-of-concept, and pilot-scale projects to foster the commercialization of the technologies Multiple strategies (projects) with similar goals Computational techniques to reduce development time
Lack of funding	Program will not be able to realize its materials development goals	Look for collaboration opportunities with industry, industry associations, and other Government organizations, both domestic and international

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CHAPTER 4: IMPLEMENTATION AND COORDINATION PLAN

4.1 IMPLEMENTATION PLAN

The CCRP has adopted a comprehensive, multipronged R&D approach on a portfolio of technologies along multiple paths to enhance the probability of success of research efforts that are operating at the boundaries of current scientific understanding. The R&D covers a wide scale, integrating advances and lessons learned from fundamental research, technology development, and large-scale testing. The success of this effort will enable cost-effective implementation of technologies throughout the power-generation sector.

The funding request for DOE's Crosscutting Research in FY 2013 is $27,450,000, and higher levels are needed in subsequent fiscal years. At lower levels, key next-generation technology will not be pursued. This will result in DOE discontinuing research on advanced concepts and not pursuing others that would have significant national benefit.

4.2 COORDINATION WITH OTHER TECHNOLOGY AREAS

The Crosscutting Research Technology Areas provide a consistent focus on important technologies. The interrelationships between the Crosscutting Research Technology Areas help ensure that critically important key technologies receive adequate R&D. In turn, these important key technologies support various Technology Areas in other subprograms. For example, the Plant Optimization Technology Area develops technologies (i.e., high-temperature sensors, novel control architectures, and high-performance materials and modeling) that support the Advanced Turbines, Gasification Systems, Advanced Combustion Systems, and Solid Oxide Fuel Cells Technology Areas within the Advanced Energy Systems subprogram. The Sensors, Controls, and Novel Concepts key technology in the Plant Optimization Technology Area has 2nd-Generation and Transformational technologies to support current and future power-generation needs. These include manufacturing of high-temperature nanomaterials and microsensors that will be utilized for in situ and embedded component monitoring in gasifier and turbine applications that depend on and benefit from accurate, real-time temperature and gas composition data to optimize plant operations. These sensors will be self-powered and wireless to lower initial capital costs and lower maintenance for ease of plant operation and higher reliability. Crosscutting R&D for individual 2nd-Generation novel sensors, controls, and other architecture technologies will be completed to support A-USC and oxy-combustion boilers, and advanced IGCC plants with advanced turbines. Crosscutting R&D for high-performance modeling of 2nd-Generation materials will be done for improved refractory life and higher temperature pressure boundary materials to withstand higher temperatures while having improved corrosion/erosion-resistance properties. The Coal Utilization Sciences key technologies will support CCS activities through CCSI and NRAP efforts. Storage reservoir modeling and simulation capabilities will be further developed to ensure proper selection, use, monitoring, verification, and risk minimization. University Training and Research will support other Technology Areas through maintaining and upgrading the education, training, and research capabilities in the fields of science and technology related to fossil energy resources in order to ensure a workforce with applicable knowledge and skills. The University Training and Research Technology Area supplements important technologies that are not completely encompassed by the Plant Optimization and Coal Utilization Sciences Technology Areas within the Crosscutting Research subprogram. The University Training and Research R&D is directly applicable to Technology Areas in the Advanced Energy Systems subprogram.

The Sensors, Controls, and Novel Concepts technologies and research focus areas support the Advanced Energy Systems Gasification Systems Technology Area by providing harsh-environmental sensors and controls to assist in the operation of the high-temperature and high-pressure power-generation components being developed by their respective technologies. The Advanced Turbines Technology Area has 2nd-Generation technologies to have an H_2 turbine with 2,650 °F turbine inlet temperature and a Transformational technology to produce a fossil-fueled turbine with a 3,100 °F turbine inlet temperature. To achieve optimal operation and control of these high-temperature components, the Sensors, Controls, and Novel Concepts key technology has 2nd-Generation and Transformational technologies that address the need for high-temperature sensors and controls.

The Crosscutting Research Sensors, Controls, and Novel Concepts technologies and research focus areas will be utilized to support Advanced Post-Combustion, large-scale pilot tests for state-of-the-art solvents, sorbents, and membranes. The 2nd-Generation Sensors, Controls, and Novel Concepts technologies and research focus areas will be integrated in Clean Coal Power Initiative demonstrations, and performance data will be gathered and utilized to identify additional Transformational Sensors, Controls, and Novel Concepts technologies and research focus areas.

The Carbon Storage program will utilize Crosscutting Research's technologies for CCS infrastructure; MVA; carbon use and reuse; and geologic storage advanced tools. Crosscutting Research's simulation and modeling technologies (via CCSI and NRAP) will help ensure the proper design and implementation of CCS projects during the planning, injection, and long-term storage phases.

4.3 NEXT STEPS

Implementation of the planned technologies requires funding for continuing the R&D of existing successful projects, new R&D requests that will be solicited by issuing FOAs, and integration and demonstration of selected technologies.

Continued R&D of existing successful projects will allow relatively rapid commercial deployment of several promising technologies for substantially increasing existing and advanced power-plant efficiency and environmental performance. These technologies are typically ready for pilot-scale development and pre-commercialization, representing relatively low risk and high probability of return on investment and positive impact in increased deployment in existing plants in the short term.

New R&D requests will be necessary for many Crosscutting Research subprogram key technologies, particularly to spur commencement of development of Transformational, novel sensors and controls technologies, and novel modeling and simulation technologies. Accordingly, funding over the long term will be required in some areas; however, risk is attenuated by scaleup of budgetary funding from lower levels at early study and bench-scale phases of development to larger amounts of funding (and continued R&D as discussed previously) for projects demonstrating success in the early developmental phases.

Key technologies may or may not be known; in particular, novel technologies emerging from initial study may become essential elements of the Transformational sensors and controls and computational modeling technology portfolio. However, as the broad areas of novel technology development move forward, these key technologies will become identified. Ultimately, funding supporting early development stages must continue into integration and large-scale testing of the technologies as an essential aspect of pre-commercialization leading to commercial deployment.

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APPENDIX A: ACTIVE CROSSCUTTING RESEARCH PROJECTS

(AS OF OCTOBER 2012)

Table A-1. **Crosscutting Research Sensors, Controls, and Novel Concepts Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
AL-06-205-020	Ames Laboratory	High-Density Sensor Network Development	3	Develop understandings, algorithms, and control strategies to utilize sensor networks in power plants to help achieve efficiency gains of 2% by integrating work with the HYPER facility to demonstrate a proof-of-concept for high-density sensor networks.
AL-12-470-009	Ames Laboratory	Merged Environment for Simulation and Analysis (MESA)	n/a	Develop a MESA at NETL's hybrid fuel cell turbine laboratory. The MESA sensor lab developed as a component of this research will provide a development platform for investigating (1) advanced sensor control strategies; (2) testing and development of sensor hardware; (3) various modeling in the loop algorithms; and (4) other advanced computational algorithms for improved plant performance using sensors, real-time models, and complex systems tools.
FE0007270	Case Western Reserve University	An Information Theoretic Framework and Self-Organizing Agent-Based Sensor Network Architecture for Power-Plant Condition Monitoring	2	Develop an information theoretic framework for monitoring power-plant conditions to help reduce forced outages 5–10% by incorporating distributed software agents and companion computational algorithms to maximize collection, transmission, aggregation, and conversion of data.
FE0010116	GE Global Research	Multipoint Pressure and Temperature sensing Fiber-Optic Cable for Monitoring CO_2 Sequestration	n/a	Enable the development of "smart" wells by addressing the need for novel sensing techniques to continuously and remotely monitor CO_2 sequestration wells, thus contributing to the emission reduction of CO_2 from fossil fuel-based electric/industrial sources.
FE0010318	Intelligent Optical Systems, Inc.	Intrinsic Fiber-Optic Chemical Sensors for Subsurface Detection of CO_2	n/a	Develop fiber-optic chemical sensors to detect subsurface CO_2 for monitoring of CO_2 leakage from storage reservoirs.
FE0001127	Missouri University of Science and Technology	Microstructured Sapphire Fiber Sensors for Simultaneous Measurements of High Temperature and Dynamic Gas Pressure in Harsh Environments	3	Develop unique single-crystal sapphire fiber sensors to measure temperature and gas pressure and contribute to a ≥10% gasification system efficiency gain by using a novel cladding and excitation techniques to assure signal integrity and sensor robustness.
FE0009878	New Mexico Institute of Mining and Technology	Development of a CO_2 Chemical Sensor for Downhole CO_2 Monitoring in Carbon Sequestration	n/a	Develop a downhole CO_2 sensor that can in situ, continuously monitor CO_2 concentration change in deep saline. The sensor is a Severinghaus-type CO_2 sensor with small size, which can be embedded in monitoring well casing or integrated with pressure/temperature transducers, enabling the development of "smart" wells.
NT42439	New Mexico Institute of Mining and Technology	Development of Nanocrystalline-Doped Ceramic-Enabled Fiber Sensors for High-Temperature In Situ Monitoring of Fossil Fuel Gases	5	Develop sensors for monitoring of syngas in advanced power systems to contribute to ≥10% gasification system efficiency gain by designing, fabricating, and testing nanocrystalline ceramic films and silicalite layers on structured optical fibers.
FE0001249	Prime Research	Ultrahigh-Temperature Distributed Wireless Sensors	5	Develop an ultrahigh-temperature wireless sensor to help increase systems reliability ≥5%, by understanding radio frequencies, electromagnetic properties of materials, optimum electromagnetic design, and testing of packaged wireless sensors.
FE0007190	The Research Foundation of State University of New York	Heat-Activated Plasmonics-Based Harsh-Environment Chemical Sensors	n/a	Develop a suite of plasmonic-based gas sensors capable of operating in 500–900 °C mixed gas environments. The approach is based on optical interrogation of electron beam patterned gold nanoparticles embedded within metal oxide nanocomposites.
NT0007918	The Research Foundation of State University of New York	Plasmonics-Based Harsh-Environment-Compatible Chemical Sensors	n/a	Develop a plasmonics-based all-optical sensing technique that utilizes the optical properties of tailored nanomaterials as the sensing layer while further developing a detailed understanding of the sensing mechanism as a function of temperature and humidity.
12-014451	Sandia National Laboratories	Laser-Based Detection of Trace Level Contaminants	n/a	Development of an instrument for high-sensitivity, real-time detection of hydrogen chloride. This instrument will employ a novel cavity ring-down spectrometer that enables collection of a broad bandwidth, high-resolution absorption spectrum with a single laser pulse. The detection approach developed will enable selective detection of trace-level species in the flue gas with greater sensitivity than currently achievable.
FE0005666	Siemens Energy	Conditioned-Based Monitoring of Turbine Blades Demonstrated in H-Class Engine	3	Develop a sensor suite to enable real-time, high-accuracy, remote monitoring of rotating turbomachinery and help achieve ≥10% turbine system efficiency gain by combining fast area sensors with point sensors connected to wireless transmitters.

Table A-1. **Crosscutting Research Sensors, Controls, and Novel Concepts Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
NT0006833	Siemens Westinghouse Power Corporation	Condition-Based Monitoring of Turbine Combustion Components	5	Develop an integrated condition-monitoring system to contribute to system reliability increase ≥5% by developing direct measurement systems, software, and algorithms for a simulated test turbine.
FE0001180	Stanford University	Tunable Diode Laser Sensors to Monitor Temperature and Gas Composition in High-Temperature Coal Gasifiers	5	Improve measurement of temperature and gas composition to optimize gasifier output and gas turbine input and assist in a 2% plant efficiency gain, by designing, building, and testing a tunable diode laser sensor.
NT0005654	Tech4Imaging	Development and Implementation of 3-D, High-Speed Capacitance Tomography for Imaging Large-Scale, Cold-Flow Circulating Fluidized Bed	5	Enable more inexpensive exploration of options to contribute to a system efficiency ≥10% in producing power using cold-flow CFBs by developing a three-dimensional, high-speed capacitance tomography system for imaging large-scale CFBs.
FE0001241	University of Central Florida	Online In Situ Monitoring Combustion Turbines Using Wireless Passive Ceramic Sensors	3	Develop a set of sensors to solve issues related to real-time turbine monitoring and contribute to system reliability increase >5%, by using high-temperature wireless passive ceramic and microelectro-mechanical systems technologies.
FE0007004	University of Central Florida	Wireless Passive Ceramic Strain Sensors for Turbine Engine Applications	n/a	Develop an accurate and robust wireless passive high-temperature sensor for in situ measurement of strains inside turbine engines in coal-based power systems for advanced sensor technologies that will contribute to higher energy efficiency, increased reliability, and decreased pollution.
NT0008062	University of Cincinnati	Development of Novel Ceramic Nanofilm Integrated Optical Sensors for Rapid Detection of Coal-Derived Synthesis Gas	n/a	Develop new types of high-temperature (greater than 500 °C) devices to monitor coal-derived gases by physically and functionally integrating advanced nanoceramic materials with fiber-optic chemical sensors that possess the desired stability, sensitivity, and selectivity for in situ, rapid gas detection in coal-derived syngas streams.
FE0000870	University of Connecticut	Multifunctional Nanowire/Film Composites Based Bi-Modular Sensors for In Situ and Real-Time High-Temperature Gas Detection	3	Develop high-temperature in situ real-time gas sensors to facilitate the production of hydrogen from coal and help achieve system efficiency >10% by using a unique class of multifunctional metal oxide/perovskite core-shell composite nanostructures.
FE0007379	University of Maine System	High-Temperature Wireless Sensor for Harsh Environment Condition Monitoring	2	Develop a novel high-temperature embedded wireless component-monitoring sensor to assist in reducing forced outages 5–10% by using prototype temperature sensors embedded in critical components at operating power plants.
FE0009843	University of Missouri-Rolla	Robust Ceramic Coaxial Cable Downhole Sensors for Long-Term In Situ Monitoring of Geologic CO_2 Injection and Storage	n/a	Develop a distributed and robust ceramic coaxial cable sensor platform for in situ downhole monitoring of geologic CO_2 injection and storage with high spatial and temporal resolutions. The research will demonstrate the feasibility of the proposed coaxial cable Bragg gratings and coaxial cable Fabry-Perot interferometers sensors for in situ measurement of temperature, pressure, and strain in downhole environments. The research will also develop a novel looped coherent amplification signal processing methodology.
FC26-08NT43291	University of North Dakota	EERC-DOE Joint Program on Research and Development for Fossil Energy-Related Resources	2–6	Make fossil-energy systems nonpolluting and more efficient, capture and sequester GHGs, and integrate fossil and renewable energy sources to permit continued use of domestic fossil fuels as a mainstay of U.S. energy production by conducting basic, fundamental, and applied research.
FE0007225	University of Texas at El Paso	Gallium Oxide Nanostructures for High-Temperature Sensors	n/a	Engineered nanostructures of pure and tungsten-doped gallium oxide materials will be used to develop high-temperature O_2 sensors with enhanced selectivity, sensitivity, and long-term stability when compared with their conventional counterparts.
NT0008022	University of Texas at El Paso	Investigation of WO_3-Based H_2S Sensor Materials for Coal Gasification Systems	n/a	Develop high-quality new sensor materials to achieve improved response time and controlled microstructure for long-term stability, and to narrow particle-size distribution for improved sensor characteristics and performance.
FE0003780	University of Texas at San Antonio	Development of High-Temperature and High-Sensitivity Novel Chemical-Resistive Sensor	n/a	Conduct research to understand the mechanisms of mixed ionic electronic conductive $LaBaCO_2O_5$ highly epitaxial thin-films and to establish the relationship between the electrochemical properties and the surface/interface structure of the mixed conductive thin films for the purpose of fabricating high-temperature ultrasensitive chemical sensors in high-temperature environments.

Table A-1. **Crosscutting Research Sensors, Controls, and Novel Concepts Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
FE0006947	The University of Utah	In Situ Acoustic Measurements of Temperature Profiles in Extreme Environments	n/a	Develop and validate methods for noninvasive ultrasound measurements of temperature distribution inside refractories during coal gasification and for measuring refractory thickness in terms of their accuracy, response time, and robustness.
FE0007272	University of Washington	High-Temperature Thermoelectric Oxides Engineered at Multiple Length Scales for Energy Harvesting	n/a	Develop 'n' type thermoelectric oxides materials that can be used together with the already well established 'p' type thermoelectric oxides to make highly efficient thermoelectric devices for waste heat recovery in coal-fired power by conducting combinatorial materials exploration and developing processing approaches.
FC26-08NT43293	University of Wyoming Research Corporation	DOE-WRI Cooperative Research and Development Program for Fossil Energy-Related Resources	2–7	Develop, commercialize, and deploy technologies of value to assist industry with efficient, nonpolluting energy technologies and competitively meet requirements for clean fuels, chemical feedstocks, electricity, and water resources by conducting fundamental and applied research.
FE0003859	University of Pittsburgh	Metal-Oxide Sensing Materials Integrated with High-Temperature Optical-Sensor Platforms for Real-Time Fossil Fuel Gas Composition Analysis	n/a	Objectives of this proposal are to perform nanoengineering on functional metal oxide materials and to integrate them with high-temperature optical sensor platforms for real-time fossil fuel gas composition analysis.
FE0005703	Virginia Polytechnic Institute and State University	Distributed Fiber-Optic Sensor for Online Monitoring of Coal Gasifier Refractory Health	3	Develop a high-temperature distributed sensing platform for monitoring a gasifier's refractory wall to help reduce forced outages 5–10% by placing the photonic crystal fiber sensor at the back side of the innermost gasifier liner.
FE0007405	Virginia Polytechnic Institute and State University	Embedded Active Fiber-Optic Sensing Network for Structural Health Monitoring in Harsh Environments	2	Develop a sensing network for structural health monitoring to provide real-time information on critical power-plant components and help reduce forced outages 5–10% by using embedded active fiber-optic technology.
FT40685	Virginia Polytechnic Institute and State University	Single-Crystal Sapphire Optical Fiber Sensor Instrumentation	6	This project is to develop and demonstrate the full capability of an integrated sapphire optical temperature sensor through the development of sapphire-based sensor assemblies and performance evaluation of the sensor on a full-scale coal gasifier and a bench-scale aerothermal turbine combustion rig.
FT42441	Virginia Polytechnic Institute and State University	Novel Modified Optical Fibers for High-Temperature In Situ Miniaturized Gas Sensors in Advanced Fossil-Energy Systems	3	Develop modified optical fibers for high-temperature in situ gas sensors to increase measurement capability and contribute to lowering sensor costs more than 20% over the cost of discrete sensors by developing a process to produce holes in optical fibers.
NT0005591	Virginia Polytechnic Institute and State University	Multiplexed Optical Fiber Sensors for Coal-Fired Advanced Fossil-Energy Systems	3	Develop a sensor network for measurement of strain, temperature, and pressure in supercritical and UCS boiler systems to help reduce forced outages 5–10% by packaging multiplexed IFPI fiber-optic sensors and demonstrating performance in simulated conditions.
FE0003872	West Virginia University	High-Temperature Nanoderived Micro-H_2 and -H_2S Sensors	n/a	Develop microscale, chemical sensors and sensor arrays composed of nanoderived, metal-oxide composite materials to detect H_2 and H_2S within high-temperature environments (500–1,200 °C).
FE0005717	West Virginia University Research Corporation	Development of Self-Powered Wireless-Ready High-Temperature Electrochemical Sensors of In Situ Corrosion Monitoring for Boiler Tubes	3	Develop in situ corrosion-monitoring sensors to detect fireside corrosion on USC boiler tubes, generate a life prediction toolbox, and help reduce forced outages 5–10% by designing, constructing, and demonstrating initial performance of a prototype corrosion sensor.

Table A-2. **Crosscutting Research Computational Modeling Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
NT0005395	Alstom Power, Inc.	Process/Equipment Cosimulation of Oxy-Combustion and Chemical-Looping Combustion	3	Upgrade the Advanced Process Engineering Cosimulator computational toolkit to allow systematic evaluations of various oxy-combustion and chemical-looping concepts by coupling user-defined functions and modifying an existing process model of a commercial chemical-looping facility.
FC26-07NT43095	Alstom Power, Inc.	Development of Computational Approaches for Simulation and Advanced Controls for Hybrid Combustion-Gasification Chemical Looping	5	Develop computational approaches for simulation and advanced controls to enable and contribute to increasing systems reliability ≥5% for chemical-looping plants by developing and testing advanced control algorithms.
AL-00-470-001	Ames Laboratory	Technology Crosscut (Kinetic Theory of Multiphase Flow)	3	Further understanding of CFBs to provide underpinning for computer code construction and aid in developing energy systems with efficiency gains of 2% by performing analytical studies to enable theoretical estimates for transport coefficient analogues that parameterize computer simulations.
AL-00-470-002	Ames Laboratory	Coal Utilization Science (Development of Virtual Power Plants)	4	Develop virtual engineering tools to provide power-plant designers and trainers with a robust computational environment and help predict plant performance <10%, by incorporating multibody physics, hotlinks to physics-based engines, and human interaction for optimization.
AL-07-450-004	Ames Laboratory	Coal Utilization Science (Virtual Advanced Power Training Environments)	4	Develop a set of advanced virtual power-plant training environments to provide future operators with an improved understanding of the plant by integrating these tools into the training and research environment.
49629	Argonne National Laboratory	Fundamental Studies of Clay and Clay-Rich Mineral Reactions with H_2O-CO_2 Fluids: Applications to Geological Sequestration	3	Understand CO_2 injection interaction with swellable clay to enhance the predictive capability of geological sequestration models by integrating observations of key geochemical processes under simulated in situ sequestration conditions.
FE0007260	Florida International University	Development of a Two-Fluid Drag Law for Clustered Particles Using Direct Numerical Simulation and Validation Through Experiments	n/a	Apply advanced experimental and computational techniques to develop and validate new drag force correlations for the case of particle clustering based on direct numerical simulation of gas-solids flow structures in risers and vertical columns, and validate the proposed drag law using the MFIX multiphase flow simulation code.
FE0005712	GE Global Research	Model-Based Optimal Sensor Network Design for Condition Monitoring in an IGCC Plant	2	Identify an optimal sensor network design for IGCC plant condition monitoring and help reduce forced outages 5–10% by developing a model-based algorithm for sensor placement that considers refractory degradation and radiant syngas cooler fouling impacts on sensors.
NT43069	Georgia Tech Research Corporation	Prediction of Combustion Stability and Flashback in Turbines with High-Hydrogen Fuel	n/a	Develop the scientific understanding and validated design tool that can predict flashback and combustion instability in lean premixed combustors operating on syngas/high-hydrogen content fuels in order to mitigate damaging pressure oscillations (excited by the combustion process) for low-emissions gas turbines using a three-pronged R&D approach: experiments, computational kinetic calculations, and analytic modeling.
FE0003997	Illinois Institute of Technology	Computational Fluid Dynamics Simulations of a Regenerative Process for Carbon Dioxide Capture in Advanced Gasification-Based Power Systems	n/a	Develop a CFD model and to perform CFD simulations to describe the heterogeneous gas-solid absorption/regeneration and water-gas-shift reactions in the context of multiphase CFD for a regenerative magnesium oxide-based process for simultaneous removal of CO_2 and enhancement of H_2 production in coal gasification processes.
FE0006946	Iowa State University	Uncertainty Quantification Tools for Multiphase Gas-Solid Flow Simulations Using MFIX	n/a	Develop a nonintrusive uncertainty quantification approach based on PC methodology together with reconstruction of a multivariate probability density function, and apply it to the uncertainty quantification for multiphase gas-solids flow simulations.
FEAA046	Oak Ridge National Laboratory	Computational Fluid Dynamics for Multiphase Flow	n/a	Support of the development of a computer simulation model that can be used by U.S. energy industry to improve their competitiveness, increase energy efficiency and decrease emissions. The Oak Ridge National Laboratory contribution involves work with the MFIX fluidization code.

Table A-2. **Crosscutting Research Computational Modeling Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
NT0007428	The Ohio State University Research Foundation	Process/Equipment Cosimulation on Syngas Chemical-Looping Process	n/a	Conducts cosimulation that validates the technical and economical attractiveness of chemical looping systems using a combination of CFD software Fluent and process simulator Aspen Plus® on the platform of NETL's advanced process engineering cosimulator and provide (1) thermodynamic analysis on syngas chemical-looping systems, (2) reaction mechanisms between porous oxygen carries and gas reactants, (3) distributed gas-solid contacting pattern, and (4) heat and energy balance for different configurations of the whole syngas chemical-looping process.
FE0000857	Oregon State University	Distributed Sensor Coordination for Advanced Energy Systems	2	Improve coordinated behavior in large sensor networks to provide a solution to a scalable and reliable sensor coordination issue and help increase systems reliability by ≥5% by deriving, implementing, and testing agent-objective functions.
FE0006932	Princeton University	Implementation and Refinement of a Comprehensive Model for Dense Granular Flows	n/a	Implement and validate a new granular stress model in MFIX to improve the model to capture more complex flow behavior by using a steady shear rheological model, performing MFIX simulations of various test problems, examining the effect of refined boundary conditions on flow, and modifying MFIX implementation and conducting validation tests.
FE0001074	Reaction Design	Package Equivalent Reactor Networks as Reduced-Order Models for Use with CAPE-OPEN-Compliant Simulations	4	Develop simulation modeling software to provide an alternative to existing high-fidelity fluid-dynamics models and help achieve systems efficiency gains of ≥10% by integrating ROMs and computer-aided process engineering (CAPE)-OPEN architecture.
FE0007450	The Regents of The University of Colorado	Quantifying the Uncertainty of Kinetic-Theory Predictions of Clustering	n/a	Determine the relative importance of the driving forces for instabilities in high-velocity, gas-solid flows, and to establish the suitability first-principles theory, with no adjustable parameters, to accurately predict the type, onset, evolution, and steady-state characteristics of such instabilities.
FEW0709	Sandia National Laboratories	Advanced Coal Combustion and Gasification Science	3	Develop fundamental information on the kinetics of advanced combustion and gasification systems to assist with design and commercialization and help achieve efficiency gains of 2% by obtaining experimental measurements of gasification kinetics of coal char at high temperature and pressure.
FE0005749	Texas Tech University	Model-Based Sensor Placement for Component-Condition Monitoring and Fault Diagnosis in Fossil-Energy Systems	2	Improve sensor networks for monitoring gasification plant component health and diagnosing faults to help increase systems reliability by >5% by developing a two-tier (distributed and plant-level) sensor placement algorithm and enhancing models with incorporation of identified system level faults.
FE0007520	Tuskegee University	Study of Particle Rotation Effect in Gas-Solid Flows Using Direct Numerical Simulation with a Lattice Boltzmann Method	n/a	Use the direct numerical simulation method to investigate the drag force between solid particles and gas phases, generate a database, formulate, test, conduct studies, and compare the new model with other traditional drag models to predict gas-solid flow interactions at microscopic scales.
FE0003801	University of California, Merced	High-Fidelity Multiphase Radiation Module for Modern Coal Combustion Systems	n/a	Develop optimal radiation tools to allow efficient high-fidelity determination of radiative fluxes and sources in real time in two-phase coal combustion systems toward a level that is commensurate with their importance in such high-temperature reacting flows.
NT43098	University of Colorado	Development, Verification, and Validation of Multiphase Models for Polydisperse Flows	4	Upgrade MFIX to help predict plant performance <10% by deriving constitutive relations for a polydisperse solid phase, developing a drag law for polydisperse flows, and extending gas-phase turbulence models to account for polydisperse particles.
NT0007649	University of Michigan	A Study of Horizontal Gas Jets in a Bubbling Fluidized Bed of Nonspherical Particles	n/a	Perform a comprehensive study of horizontal gas jets injected into a 2-D bubbling fluidized bed of nonspherical particles. This project will expand NETL's computational capabilities with experimentally verified physical models for dilute turbulent fluid/nonspherical particle flow. The project will focus on obtaining time resolved measurements and modeling of a gas jet penetrating a bed of spherical particles.
FE0003742	University of Texas at El Paso	Investigation of Gas-Solid Fluidized Bed Dynamics with Nonspherical Particles	n/a	Develop a high-speed particle imaging technique and obtain full-field visualization of rotational motions of nonspherical particles in semi-dilute (volume fractions of 10 or 15 percent) flows for the development of multiphase flow code being developed to model gas-solid systems such as fluidized beds.

Table A-2. **Crosscutting Research Computational Modeling Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
NT0008064	University of Texas at San Antonio	Use of an Accurate Direct Numerical Simulation Particulate Flow Method to Supply and Validate Boundary Conditions for the MFIX Code	n/a	Improve the performance and accuracy of the MFIX code that is frequently used in multiphase flow simulations. The specific objectives of the project are to use first principles embedded in a validated direct numerical simulation particulate flow program that uses the immersed boundary method in order to establish, modify, and validate needed energy and momentum boundary conditions for the MFIX code.
NT0043326	Virginia Polytechnic Institute and State University	Experimental and Computational Investigations of Boundary Condition Effects on CFD Simulations of Thermoacoustic Instabilities	n/a	Determine the sensitivity of transient thermoacoustic CFD simulations to poorly defined, or misrepresentation of prescribed time domain impedance acoustic boundary condition and enhance simulation capabilities to predict performance of power-generation systems.

Table A-3. **Crosscutting Research CCSI Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
2012.04.02	Multiple Partners	Carbon Capture Simulation Initiative	3	Develop the CCSI Toolset to accelerate commercialization of carbon capture technologies with reduced risk by increasing confidence in designs and reducing risk associated with incorporating multiple innovative technologies.

Table A-4. **Crosscutting Research NRAP Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
2012.04.03	National Energy Technology Laboratory	National Risk Assessment Partnership	3–5	Develop a science-based methodology, associated science base, and computational tools for quantifying long-term risks and reducing uncertainties in liability associated with carbon storage sites, to support the business case for full-scale carbon utilization and storage projects at a wide range of potential locations.

Table A-5. **Crosscutting Research High-Performance Materials and Modeling Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
AL-07-360-019	Ames Laboratory	Computational and Experimental Development of Novel High-Temperature Alloys	3	Develop a tool for rapid assessment of potential material formulations to find candidate materials for construction of high-temperature gas turbine components and reduce new material development time by performing comparisons using formation enthalpy data.
AL-10-450-007	Ames Laboratory	Materials (Design of Multiscale Systems)	n/a	Develop computational algorithms, strategies, and informational framework needed to design materials in an integrated manner across length and time scales, creating the ability to design and tailor material properties for specific applications.
AL-99-501-032	Ames Laboratory	Improved Atomization Processing for Fossil-Energy Applications	3	Develop improved nozzles and powder formation techniques for applications to materials used in A-USC boilers to decrease costs of materials that will improve power-plant efficiencies through a detailed analysis of atomization process responses to alloy and parameter modifications.
FWP-49640-02	Argonne National Laboratory	Corrosion and Mechanical Properties of Materials in Combustion and Mixed-Gas Environments	3	Identify suitable materials with adequate mechanical properties to solve issues with high-temperature service and reduce ASME Code approval time by conducting experiments to establish the corrosion behavior of materials developed for the oxy-fuel environment.

Table A-5. **Crosscutting Research High-Performance Materials and Modeling Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
NT43097	The Babcock & Wilcox Company	Development of Computation Capabilities to Predict the Corrosion Wastage of Boiler Tubes in Advanced Combustion Systems	3	Develop computation capabilities to help develop better alloys and increase plant efficiency by developing accurate equations to predict the fireside corrosion of boiler tubing in the reducing and oxidizing zones as a function of a number of variables.
FE0008742	Brown University	Advanced Thermal Barrier Coatings for Next-Generation Gas Turbine Engines Fueled by Coal-Derived Syngas	n/a	Investigate the feasibility of developing two-layer air-plasma sprayed TBCs with low thermal conductivities that can operate at higher gas-inlet temperatures while maintaining integrity in high-impurity, high-moisture environments by conducting laboratory experiments.
FE0003840	Carnegie Mellon University	High-Resolution Modeling of Materials for High-Temperature Service	n/a	Develop high-resolution methods for modeling the 3-D mechanical response of metallic alloys when exposed to high temperatures by simulating plastic deformation and damage accumulation of polycrystalline materials at the grain scale.
FE0003892	Clemson University	Multiscale Modeling of GB Segregation and Embrittlement in Tungsten for Mechanistic Design of Alloys for Coal-Fired Plants	n/a	The project will develop a quantitative model for predicting grain boundary segregation in refractory alloys. Researchers will utilize this model to develop a multiscale modeling strategy to predict grain boundary embrittlement from grain boundary segregation.
FE0008857	Dartmouth College	Laves Phase-Strengthened Austenitic Steels for Coal-Fired Power Systems	n/a	Investigate the strengthening mechanisms and develop models of both the precipitation kinetics and deformation behavior of aluminum-alloyed, Laves phase-strengthened, austenitic steels, which have improved oxidation resistance and are potential candidate materials for fossil fuel energy systems operating at temperatures greater than 800 °C by assessing and documenting material behavior under a variety of conditions.
NT43096	Electric Power Research Institute	Computational Modeling and Assessment of Nanocoatings for Ultra-Supercritical Boilers	n/a	Utilize science-based computational methods for selecting chemical composition of coatings to develop advanced coating application processes for depositing nanostructured coatings by using computational approaches to assess the lifetime prediction of the coating.
NT41175	Energy Industries of Ohio	Boiler Materials for Ultra-Supercritical Coal Power Plants	5	Develop materials for use in USC and A-USC boilers that work well with all types of coal to increase combustion efficiency through field exposure testing (via a steam loop) at A-USC service conditions.
FE0000234	Energy Industries of Ohio	Steam Turbine Materials for Ultra-Supercritical Coal Power Plants	3	Evaluate promising materials to develop data necessary for the design of a steam turbine operable at A-USC conditions through research on the mechanical properties, oxidation resistance, weldability, and suitability of alloys and coatings.
FE0005859	GE Global Research	Modeling Creep-Fatigue-Environment Interactions in Steam Turbine Rotor Materials for Advanced Ultra-Supercritical Coal Power Plants	3	Develop multiscale computational algorithms and guidelines to help reduce the time required to develop new materials ≤5 years and assist in reducing the time required for ASME Code approval ≤3 years by conducting bench-scale experiments on a steam turbine rotor superalloy.
FE-1168(100159)	Idaho National Laboratory	Influence of Processing on Microstructure and Properties of Iron Aluminides and Coatings	n/a	Determine the influence of thermal spray processing parameters on the microstructure, stress state, and performance of advanced coatings for high-temperature corrosion/oxidation resistance by measuring coating adhesion, durability, and corrosion/oxidation resistance.
FE0008868	Indiana University	Novel Functional-Gradient Thermal Barrier Coatings in Coal-Fired Power-Plant Turbines	n/a	Develop a manufacturing process to produce novel low thermal conductivity and high thermal stability pyrochlore oxide-based double-layer coatings with improved high-temperature corrosion resistance. Compared with the current standard TBC, pyrochlore oxides have demonstrated lower thermal conductivity and better thermal stability, which are crucial to the high-temperature applications such as coal-fired power-plant turbines.
FE0004007	Missouri University of Science and Technology	Ab Initio Modeling of Thermomechanical Properties of Mo-Based Alloys for Fossil Energy Conversion	n/a	Develop extensive computational modeling techniques for Mo-based composite alloys that can be used in a high-temperature high-pressure environment for applications in fossil energy conversion technology.
NT0001473	North Carolina Agricultural and Technical State University	Fabrication of Pd/Pd Alloy Films by Surfactant-Induced Electroless Plating	n/a	Investigate the applicability of the pulsed laser deposition technique as an activation step followed by surfactant induced electroless deposition as a novel route to fabricate hydrogen-selective Pd/Pd-alloy composite membrane on microporous substrate for use in production and separation of hydrogen at elevated temperature and pressure.

Table A-5. **Crosscutting Research High-Performance Materials and Modeling Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
NT0008066	North Carolina Agricultural and Technical State University	Bimetallic Nanocatalysts in Mesoporous Silica for Hydrogen Production from Coal-Derived Fuels	n/a	Develop a novel approach for in situ synthesis of bimetallic nanostructured mesoporous silica materials and study their utility for production of hydrogen for coal-derived syngas.
FEAA069	Oak Ridge National Laboratory	Ultra-Supercritical Steam Cycle Turbine Materials	3	Contribute to the development of A-USC turbine materials to promote more efficient power production through development of high-temperature Ni-based alloy castings and evaluation of long-term performance including understanding modes of degradation.
FEAA105	Oak Ridge National Laboratory	Bespoke Materials Surfaces	3	Develop a family of material coatings for coal-fired waterwall tube fireside protection that allows for higher temperature, more efficient power production through thermochemical/mechanical modeling, development of coating deposition methods, and testing of coatings under operational conditions.
FEAA106	Oak Ridge National Laboratory	Understanding Corrosion in Oxy-Fired Systems	3	Determine the temperature-dependent corrosion mechanisms of candidate high-temperature alloys and coatings in oxy-firing systems to facilitate the development of cost-effective oxy-combustion systems through corrosion testing under realistic combustion gas and ash/slag conditions.
FEAA107	Oak Ridge National Laboratory	Improving the Performance of Creep-Strength-Enhanced Ferritic Steels	3	Develop methods to improve the performance of creep-strength-enhanced ferritic steels to promote more efficient A-USC power production through fundamental and applied studies of the effects of heat treatment, welding, and process control on microstructural evolution and material properties.
FEAA109	Oak Ridge National Laboratory	Qualification of New, Commercial ODS Alloys for Use in Advanced Fuel Processes	3	Determine the viability of oxide dispersion-strengthened steel in USC boilers to increase efficiency of oxy-combustion systems through corrosion and fatigue testing under A-USC pressure, temperature, and gas composition conditions.
FEAA031	Oak Ridge National Laboratory	Development of Electrochemical Sensors for Fossil-Energy Applications	n/a	Develop robust, low-cost microsensors for measurement of gas constituents and trace gases associated with fossil power plants. This project seeks to develop and exploit the natural redox behavior in mixed gas streams to develop electrochemical sensors to detect SO_2 at temperatures in the range of 500–800 °C, with the aim of allowing the sensors to be placed anywhere from the cold flue gas to close to the hot zone, allowing improved control of combustion processes.
FE0008960	Ohio State University	Effective Exploration of New 760 °C-Capability Steels for Coal Energy	n/a	Research new steels capable of operating at 760 °C in the aggressive environments of A-USC boilers and steam turbines to identify new compositions and new strengthening mechanisms/microstructures by using steel compositions with high iron and chromium concentrations.
FEAA061	Oak Ridge National Laboratory	Materials for Ultra-Supercritical Steam Power Plants	n/a	Develop materials technology required to design, construct and operate an USC steam boiler with much reduced heat rate and increased efficiency by researching precipitation-strengthened alloys and generating creep data, mechanical property data and metallurgical understanding needed for both ASME Code approval and general acceptance by the utility industry.
FWP-12461	Pacific Northwest National Laboratory	Joining of Advanced High-Temperature Materials	3	Prove that friction stir welding can be used to fuse materials and that the materials can withstand the environment within a USC boiler to enable cost-effective oxy-combustion systems through creep testing, microstructure characterization, and mechanical properties testing.
FWP-60098	Pacific Northwest National Laboratory	Low-Cost Fabrication of ODS Materials	n/a	Conduct testing of a new one step friction stir processing-based powder metallurgy process to produce ferritic ODS alloys for high-temperature applications in advanced power plants for increased efficiency and lower emissions.
FE0008864	Southern Illinois University	High-Velocity Oxy-Fuel Thermal Spray TiC/TiB_2 Coatings of A-USC Boiler/Turbine Components for Enhanced Corrosion Protection	n/a	Develop new coatings to improve corrosion resistance of boiler materials, fireside corrosion protection of tubes and turbine blade materials. The new coating will be prepared by high-velocity oxy-fuel spray coating of TiC and TiB_2 nanoparticles synthesized by a patented process.
FE0008382	Southern University and A&M College	Novel Nanosize Oxide Dispersion Strengthened Steels Development Through Computational and Experimental Study	n/a	Identify ab initio molecular dynamic atomic level modeling and computer simulation to find the most promising ODS steel alloy compositions by building interface models, performing high-performance computing simulations, and developing experiments on high-temperature oxidation.

Table A-5. **Crosscutting Research High-Performance Materials and Modeling Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
FE0003693	Southern University and A&M College System	Computer Simulation and Experimental Validation on the Oxidation and Sulfate-Corrosion Resistance of Novel Chromium-Based High-Temperature Alloys	n/a	Develop a computer model for determining the most promising Cr alloys with regard to oxidation and sulfate corrosion resistance for use in advanced coal gasification systems.
FE0007220	Southern University and A&M College System	An Integrated Study on the Novel Thermal Barrier Coating for Nb-Based High-Temperature Alloy	n/a	Integrate high-performance computer simulation and experimental validation in material sciences to study the elastic constants, interface bonding, high-temperature microstructures, melting points, diffusion coefficients, and oxidation resistance of the proposed bond coat and top coat of Nb-based alloys for exploration of new TBCs.
FE0000103	Tennessee State University	Computational Studies of Physical Properties of Boron Carbonate	n/a	Provide valuable insight in to the mechanisms and processes that could lead to better engineering of boron carbide. Boron carbide is a high-temperature material that could withstand the environments necessary for operation of improved-efficiency.
FE0003798	Tennessee State University	Computational Studies of Physical Properties of Nb-Si Alloy	n/a	Develop a computational tool for thermodynamics properties assessment for order and disordered lattice and interfacing the package to Thermo-Calc® with the goal of evaluating the Nb-Si alloy, which is a top candidate for next-generation hot section material for turbines, thereby breaking new ground for computer aided material design and speeding up the development of Nb-Si-based refractory alloy for energy applications.
FE0008719	Texas Engineering Experiment Station	Synergistic Computational and Microstructural Design of Next-Generation High-Temperature Austenitic Stainless Steels	n/a	Develop the next-generation advanced austenitic stainless steels that are capable of operating at the extreme conditions associated with advanced fossil energy power-generation plants, including temperatures above 850 °C by carefully designing microalloying composition and heat treatments to control microstructure.
NT43073	University of California, San Diego	Solid State Joining of High-Temperature Alloy Tubes for USC and Heat Exchanger Systems	n/a	Develop materials enabling joining technologies for use in forward looking heat-exchanger fabrication concepts capable of operating at temperatures in excess of 1,000 °C as well as conventional technology upgrades via USC Rankine-cycle boilers capable of operating at 760 °C (1,400 °F)/38.5 MPa (5,500 psi) steam, while still using coal as the principal fossil fuel.
FE0005865	University of Missouri, Kansas City	Large-Scale Simulations of the Mechanical Properties of Layered-Transition-Metal Ternary Compounds for Fossil Energy Power System Applications	3	Develop predictive modeling of a new class of materials to fulfill demanding applications in the next generation of fossil energy power systems and contribute in reducing development time <5 years by modeling and performing laboratory testing of layered transition-metal carbides or nitrides.
FE0008648	University of North Texas	Computational Microstructural Optimization Design Tool for High-Temperature Structural Materials	n/a	Develop a methodology for microstructural optimization of alloys and develop a new computationally designed Ni-Cr alloy for coal-fired power-plant applications. The broader outcome of these objectives will be the creation of an integrated approach for materials development by microstructural design.
FE0005868	University of Tennessee	Computational Design of Creep-Resistant Alloys and Experimental Validation in Ferritic Superalloys	3	Design and optimize a class of ferritic superalloys to improve the thermal efficiency and help reduce the time required to develop new materials by up to 5 years by developing computational tools for ternary alloys and phases.
FE0008855	University of Tennessee	Experimental and Computational Investigation of High-Entropy Alloys for Elevated-Temperature Applications	n/a	Perform fundamental studies on the high-entropy alloy system to use in boilers and steam and gas turbines at temperatures above 760 °C and stress of 35 MPa by developing an integrated approach to coupling thermodynamic calculations and focused experiments.
NT0008089	University of Tennessee	Computational and Experimental Design of FE-Based Superalloys for Elevated Temperature Applications	n/a	Utilize a science-based engineering approach to design iron-based superalloys capable of operating in the temperature range of 873–1,033 °K by using computational experiments to study phase stability, microstructure design and coarsening dynamics.
FE0008400	University of Texas at El Paso	A Computational-Experimental Study of the Plasma Processing of Carbides at High Temperatures	n/a	Investigate the effects of the plasma flow dynamics within the pores to form oxycarbide and amorphous phases, which ultimately would impede oxygen ingress through the scale. Determine the effect of the potential gradient established by the electromagnetic field on mass transfer to seal pores, as a result of the temperature spikes on pore surfaces. Investigate the surface kinetics within the pore wall of the packed bed, as a result of the plasma coupling with the surface reaction of the carbide.

Table A-5. **Crosscutting Research High-Performance Materials and Modeling Projects**

Agreement Number	Performer	Project Title	TRL	Relevancy Statement
FE0008470	University of Texas at El Paso	Mechanically Activated Combustion Synthesis of $MoSi_2$-Based Composites	n/a	Develop a novel and competitive processing route for manufacturing $MoSi_2$-based composites that are promising candidates for using as structural materials in advanced fossil-energy applications.
FE0008548	University of Texas at El Paso	Design Optimization of Liquid-Fueled High-Velocity Oxy-Fuel Thermal Spraying Technique for Durable Coatings for Fossil Power Systems	n/a	Develop a knowledge database of liquid-fueled high-velocity oxy-fuel thermal spraying technique processes and coatings developments so that durable coatings suitable for extreme environments of fossil-fueled power systems can be developed by studying the particle dynamics of liquid-fueled high-velocity oxy-fuel process for a range of operating and process parameters and the effects of operating and process parameters on coating characteristics.
NT0007636	University of Texas at Dallas	Novel Zeolitic Imidazolate-Framework Polymer Membranes for Hydrogen Separations in Coal Processing	n/a	Prepare novel mixed-matrix membranes based on polymer composites with nanoparticles of zeolitic imidazolate frameworks and related hybrid frameworks. Membranes containing these new materials will be used to evaluate separations important to coal gasification (e.g., H_2, carbon monoxide, O_2, CO_2). The goal is to exploit the high surface areas, adsorption capacities, and selectivities of the nanoporous zeolitic imidazolate frameworks additives to achieve unprecedented transport of gases critical to coal processing.
FE0008774	University of Toledo	Processing and Evaluation of Next-Generation Oxygen Carrier Materials for Chemical Looping Combustion	n/a	Devise a material processing technique for the development and evaluation of two new groups of oxygen carrier materials based on a crystal structure and will systematically investigate their carrier formulations by using these new oxygen carriers in CLC systems.
FE0007377	University of Wisconsin System	Active Multiscale Computational Design and Synthesis of Protective Smart Coatings for Refractory Metal Alloys	n/a	Enable the implementation of new structural materials based on refractory alloys in fossil fuel energy generation in order to provide a 200–400 °C increase in material operating temperature beyond the limitation of current Ni-based superalloys. The enabling technology underlying this advance is based on the computational design of a novel multifunctional integrated coating strategy that will provide both environmental and thermal protection in advanced combustion systems.

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APPENDIX B: DOE-FE TECHNOLOGY READINESS LEVELS

Table B-1. **Definitions of Technology Readiness Levels**

TRL	DOE-FE Definition	DOE-FE Description
1	Basic principles observed and reported	Lowest level of technology readiness. Scientific research begins to be translated into applied R&D. Examples might include paper studies of a technology's basic properties.
2	Technology concept and/or application formulated	Invention begins. Once basic principles are observed, practical applications can be invented. Applications are speculative, and there may be no proof or detailed analysis to support the assumptions. Examples are still limited to analytic studies.
3	Analytical and experimental critical function and/or characteristic proof of concept	Active R&D is initiated. This includes analytical studies and laboratory-scale studies to physically validate the analytical predictions of separate elements of the technology. Examples include components that are not yet integrated or representative. Components may be tested with simulants.
4	Component and/or system validation in laboratory environment	The basic technological components are integrated to establish that the pieces will work together. This is relatively "low fidelity" compared with the eventual system. Examples include integration of "ad hoc" hardware in a laboratory and testing with a range of simulants.
5	Laboratory scale, similar system validation in relevant environment	The basic technological components are integrated so that the system configuration is similar to (matches) the final application in almost all respects. Examples include testing a high-fidelity, laboratory-scale system in a simulated environment with a range of simulants.
6	Engineering/pilot scale, similar (prototypical) system demonstrated in a relevant environment	Engineering-scale models or prototypes are tested in a relevant environment. This represents a major step up from a TRL 5. Examples include testing an engineering scale prototype system with a range of simulants. TRL 6 begins true engineering development of the technology as an operational system.
7	System prototype demonstrated in a plant environment	This represents a major step up from TRL 6, requiring demonstration of an actual system prototype in a relevant environment. Examples include testing full-scale prototype in the field with a range of simulants. Final design is virtually complete.
8	Actual system completed and qualified through test and demonstration in a plant environment	The 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. Examples include developmental testing and evaluation of the system within a plant/CCS operation.
9	Actual system operated over the full range of expected conditions	The technology is in its final form and operated under the full range of operating conditions. Examples include using the actual system with the full range of plant/CCS operations.

APPENDIX C: ADMINISTRATION AND DOE PRIORITIES, MISSION, GOALS, AND TARGETS

ADMINISTRATION PRIORITIES

Presidential Goal—Catalyze the timely, material, and efficient transformation of the nation's energy system and secure U.S. leadership in clean energy technologies

PRESIDENTIAL ENERGY TARGETS

- Reduce energy-related greenhouse gas emissions by 17 percent by 2020 and 83 percent by 2050, from a 2005 baseline.
- By 2035, 80 percent of America's electricity will come from clean energy sources.

DOE STRATEGIC PLAN—HIERARCHY OF RELEVANT MISSION, GOALS AND TARGETS

SECRETARIAL PRIORITIES

- ***Clean, Secure Energy:*** Develop and deploy clean, safe, low-carbon energy supplies.
- ***Climate Change:*** Provide science and technology inputs needed for global climate change negotiations; develop and deploy technology solutions domestically and global.

MISSION

The mission of the Department of Energy is to ensure America's security and prosperity by addressing its energy, environmental, and nuclear challenges through transformative science and technology solutions.

GOALS

- Catalyze the timely, material, and efficient transformation of the nation's energy system and secure U.S. leadership in clean energy technologies.
- Maintain a vibrant U.S. effort in science and engineering as a cornerstone of our economic prosperity, with clear leadership in strategic areas.

TARGETS

- Sustain a world leading technical work force
- Deploy the technologies we have
  - Demonstrate and deploy clean energy technologies
  - Enable prudent development of our natural resources
- Discover the new solutions the nation needs
  - Accelerate energy innovation through pre-competitive research and development
  - Facilitate technology transfer to industry
  - Establish technology test beds and demonstrations
  - Leverage partnerships to expand our impact
- Deliver new technologies to advance our mission
  - Lead computational sciences and high-performance computing

- Use Energy Frontier Research Centers where key scientific barriers to energy breakthroughs have been identified and we believe we can clear these roadblocks faster by linking together small groups of researchers across departments, schools and institutions
- Use ARPA-E, a new funding organization within the Department, to hunt for new technologies rather than the creation of new scientific knowledge or the incremental improvement of existing technologies

FOSSIL ENERGY RESEARCH AND DEVELOPMENT

MISSION

The mission of the Fossil Energy Research and Development program creates public benefits by increasing U.S. energy independence and enhancing economic and environmental security. The program carries out three primary activities: (1) managing and performing energy-related research that reduces market barriers to the environmentally sound use of fossil fuels; (2) partnering with industry and others to advance fossil energy technologies toward commercialization; and (3) supporting the development of information and policy options that benefit the public.

CLEAN COAL RESEARCH PROGRAM

MISSION

The CCRP will ensure the availability of near-zero atmospheric emissions, abundant, affordable, domestic energy to fuel economic prosperity, increase energy independence, and enhance environmental quality.

STRATEGIC GOAL

Catalyze the timely, material, and efficient transformation of the nation's energy systems and secure U.S. leadership in clean energy technologies.

STRATEGIC OBJECTIVES

- Deploy the technologies we have
- Discover the new solutions the nation needs
- Deliver new technologies to advance our mission

STRATEGY

- Accelerate energy innovation through pre-competitive research and development
- Demonstrate and deploy clean energy technologies
- Facilitate technology transfer to industry
- Establish technology test beds and demonstrations
- Leverage partnerships to expand our impact

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ABBREVIATIONS

1-D	one-dimensional
2-D	two-dimensional
3-D	three-dimensional
Al	aluminum
ASME	American Society of Mechanical Engineers
A-USC	advanced ultra-supercritical
Btu	British thermal unit
°C	degrees Celsius
C3M	Carbonaceous Chemistry for Computational Modeling
CAPE	computer-aided process engineering
CCRP	Clean Coal Research Program
CCS	carbon capture and storage
CCSI	Carbon Capture Simulation Initiative
CFB	circulating fluidized bed
CFD	computational fluid dynamics
CLC	chemical looping combustion
CO_2	carbon dioxide
COE	cost of electricity
Cr	chromium
Cu	copper
DEM	discrete element model
DOE	Department of Energy
EOR	enhanced oil recovery
°F	degrees Fahrenheit
FE	Office of Fossil Energy
Fe	iron
FeO	iron oxide
FEPs	features, events, and processes
FOA	funding opportunity announcement
FY	fiscal year
GHG	greenhouse gas
GPU	graphics processing unit
GW	gigawatt
GWe	gigawatt electric
H_2	hydrogen
H_2O	water
H_2S	hydrogen sulfide
HBCU	Historical Black Colleges and Universities
HHV	higher heating value
IAM	integrated assessment model
IGCC	integrated gasification combined cycle
°K	degrees Kelvin
kWh	kilowatt-hour
MESA	merged environment for simulation and analysis
MFIX	Multiphase Flow with Interphase eXchanges
Mg	magnesium
Mn	manganese
Mo	molybdenum
MOF	metal organic framework
MPa	megapascal
MW	megawatt
MWe	megawatt electric
MWth	megawatt thermal
Na	sodium
NASA	National Aeronautics and Space Administration
Nb	niobium
NCCC	National Carbon Capture Center
NETL	National Energy Technology Laboratory
Ni	nickel
NRAP	National Risk Assessment Partnership
O&M	operating and maintenance
O_2	oxygen
ODS	oxide dispersion strengthened
OMI	Other Minority Institutions
PC	pulverized coal
Pd	palladium
PIC	particle in cell
ppm	parts per million
psi	pounds per square inch
psia	pounds per square inch absolute
R&D	research and development
RD&D	research, development, and demonstration
ROM	reduced-order model
S	sulfur
Si	silicon
syngas	synthesis gas
T&S	transport and storage
TBC	thermal barrier coating
TDS	total dissolved solids
Ti	titanium
TiB_2	titanium diboride
TiC	titanium carbide
TLT	Technical Leadership Team
TRIG™	Transport Reactor Integrated Gasification
TRL	Technology Readiness Level
UCR	University Coal Research
USC	ultra-supercritical
ZEPS™	Zero Emission Power and Steam System

FOR MORE INFORMATION

National Energy Technology Laboratory
http://www.netl.doe.gov/technologies/coalpower

U.S. Department of Energy, Office of Fossil Energy
http://www.fossil.energy.gov/programs/powersystems

If you have any questions, comments, or would like more information about the DOE/NETL Crosscutting Research effort, please contact the following persons:

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