Advanced Sensors & Controls FWP

Overview of NETL-RIC Research & Development

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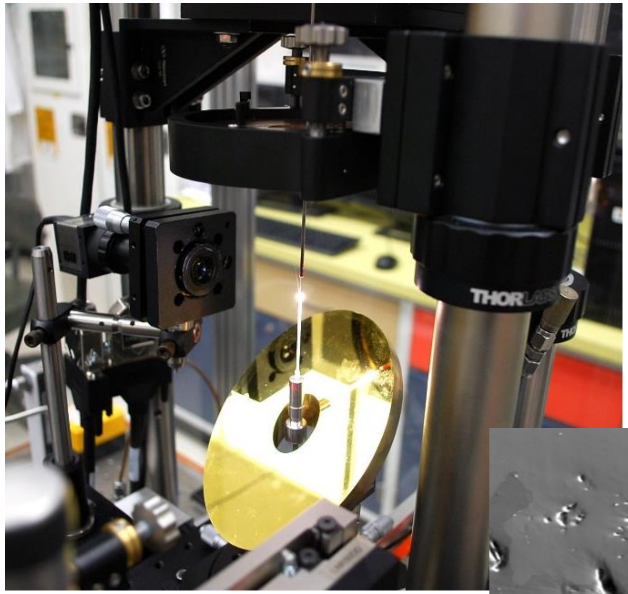
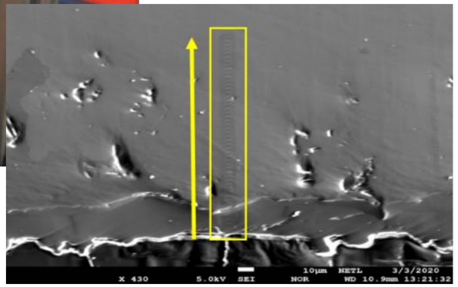
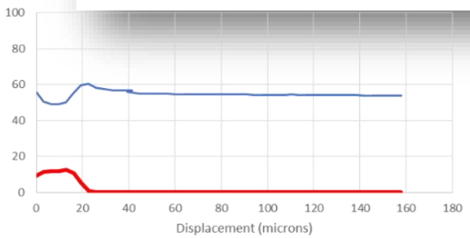
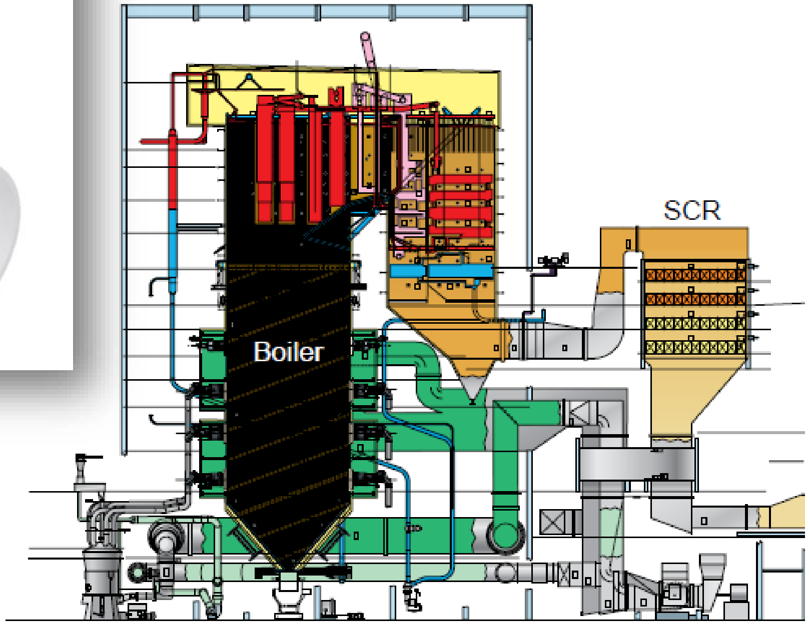
Presenter: Benjamin Chorpening, Ph.D.
Technical Portfolio Lead









UCR and HBCU-OMI FOA-2193 Joint Project Kickoff Meeting

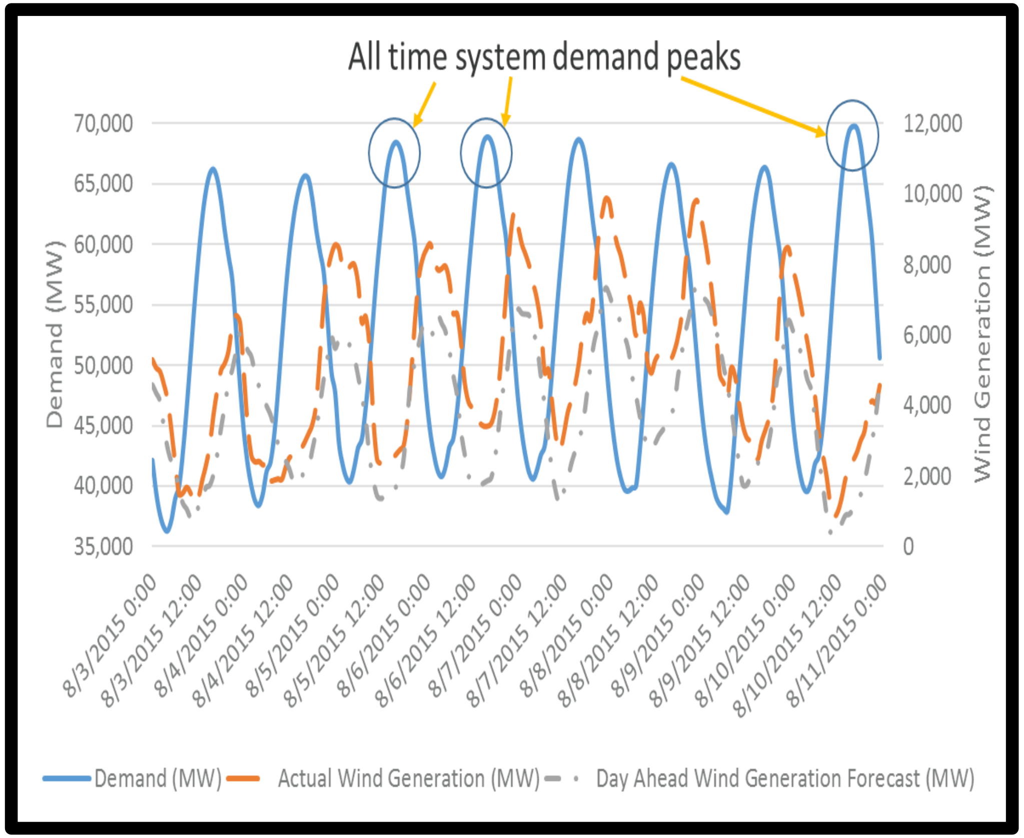
October 21, 2020

Changing Landscape for Fossil Energy Power

Adapting to Changing Role

Fossil energy power generation is needed now and in the future, but its role is shifting from baseload operation to fulfilling dispatchable power needs in regions of the United States.

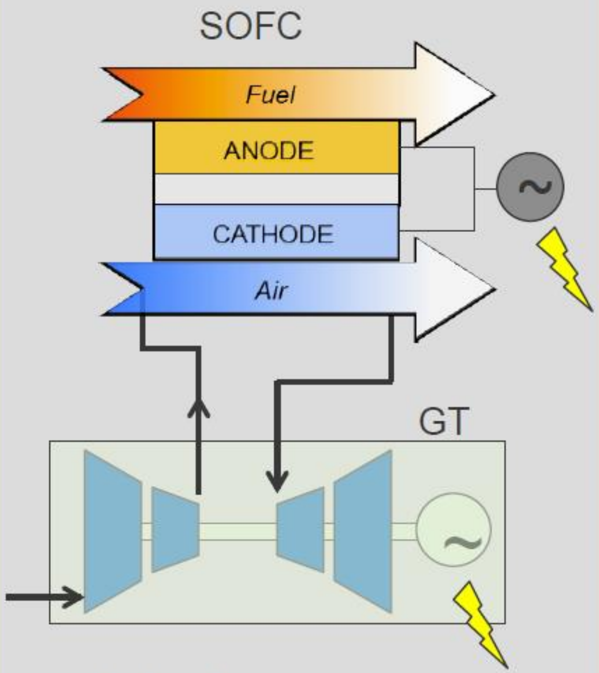
Novel sensors and controls will help to **increase efficiency**, **minimize emissions**, and **reduce operating costs** of existing power generation technologies under this increased load following role; and help enable next generation power systems with high efficiency and greater operational flexibility.



Data from Texas (ERCOT)

Renewable power production often does not match demand

Sensors & Controls Development for Harsh Environments



Hybrid systems
- 800°C in fuel cell
- 1500°C in GT

Meas. Challenges
- T and H_2 dist in SOFC
- Transient control

Gasification
- Radically engineered modular systems for gasification
- 1100 - 1500°C

Meas. Challenges
- Multipoint temp
- Species
- NDE of adv. manuf. components
- Multiphase flow

Coal-fired Boilers
- Steam 1110°F (600°C), 4000 psig
- Fire side 2500°F (1370°C) +
- Ash / slag / SOx

Meas. Challenges
- Tube temperatures / flow (cycling)
- Corrosion/erosion/exfoliation
- Steam chemistry
- Coal particle size
- Temperature / species dist. Inside boiler

Subterranean chemistry monitoring
- High pressure brine

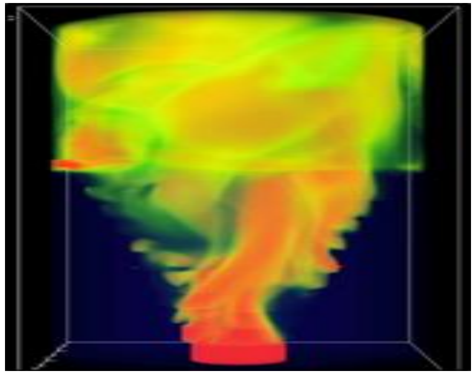
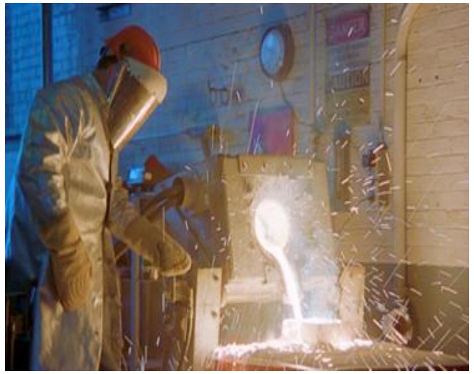
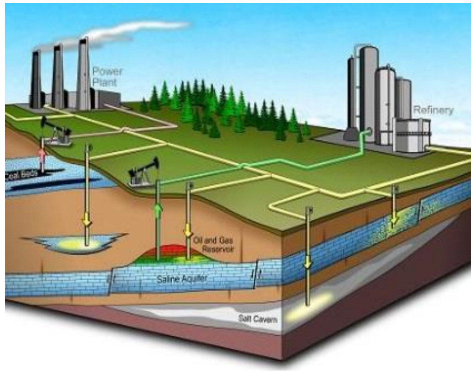
Meas. Challenges
- Salts in water
- Wellhead measurement
- Downhole measurement

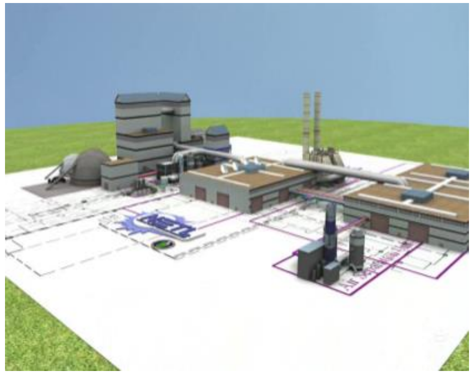
Chemical Looping
- > 1000°C
- Pressurized
- Erosive

Meas. Challenges
- Solids circulation
- Oxidation state
- Multipoint temp

Research and Innovation Center Core Capabilities

NATIONAL ENERGY TECHNOLOGY LABORATORY

APPLIED MATERIALS SCIENCE & ENGINEERING

Developing and deploying affordable, high-performance materials designed for severe service applications.

CHEMICAL ENGINEERING

Pioneering efficient energy conversion systems that can enable sustainable fossil energy utilization.

DECISION SCIENCE & ANALYSIS

Utilizing multi-scale computational approaches to provide in-depth objective analyses in support of the DOE mission.

SUBSURFACE SCIENCE

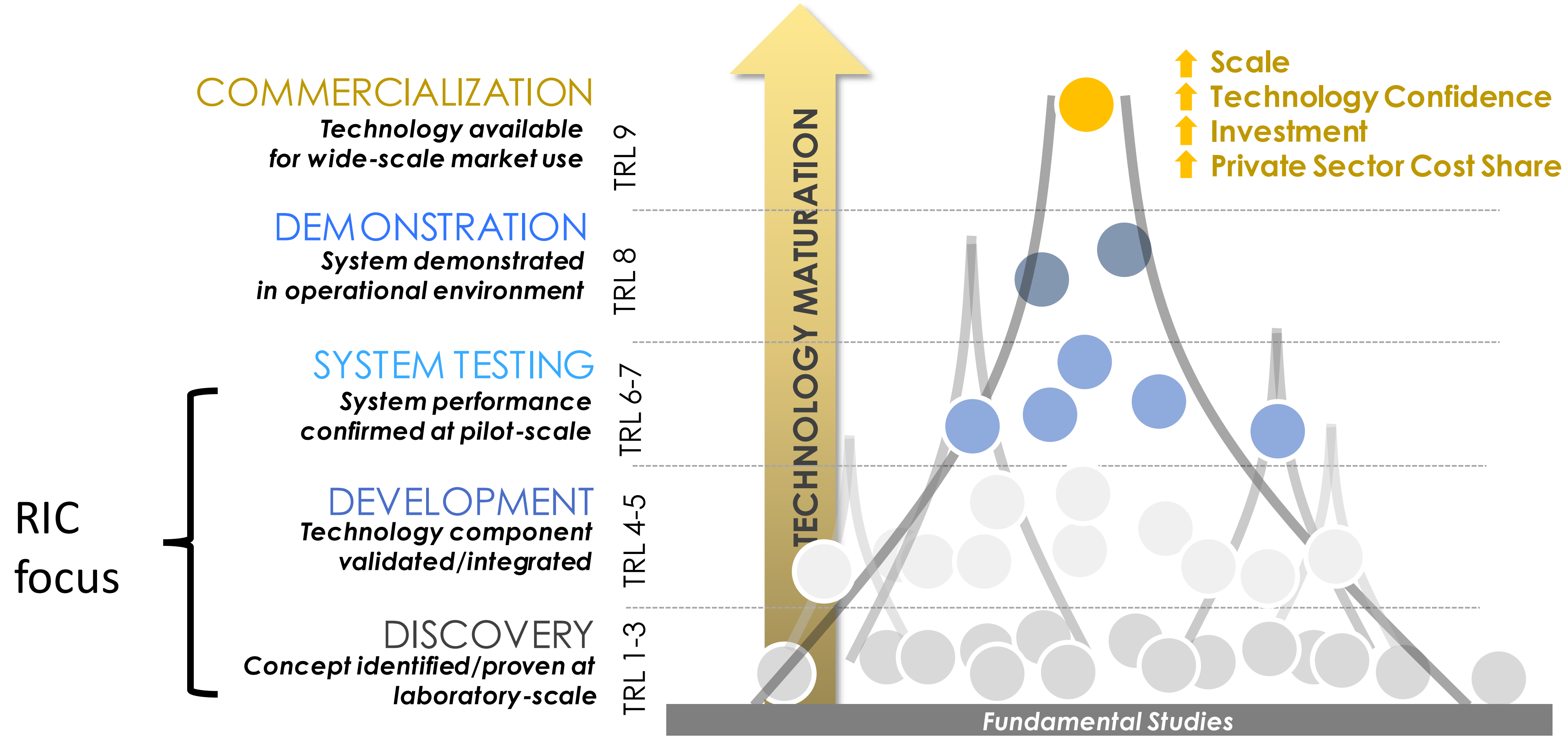
Enabling the sustainable production and use of fossil fuels through engineering of the subsurface.

SYSTEMS ENGINEERING & INTEGRATION

Accelerating technology innovation, development and deployment to enable new clean energy technologies to gain market acceptance.

Technology Development Pathway

An Active Portfolio from Concept to Market Readiness



Overview of Adv Sensors & Controls FWP

NATIONAL ENERGY TECHNOLOGY LABORATORY

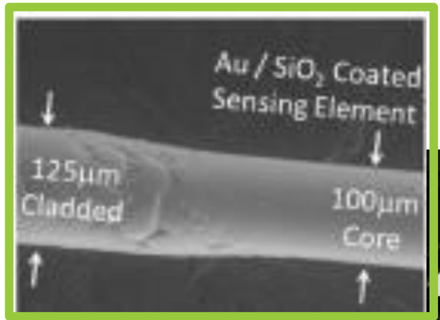
- Sensors and Instrumentation
  - High temperature optical fiber sensors
  - Functional materials for high temperature gas sensing
  - Raman Gas Analyzer
  - LIBS for Subterranean Chemical Sensing
  - In-Situ Temperature Measurements via Reactive Particles, & Lasers
- Controls
  - Advanced Controls for Power Systems
- Techno-Economic Analysis
  - TEA of Sensor and Control Technologies
- Cybersecurity and Novel Concepts
  - VLC – Alternative to WiFi
  - AI-based approach for screen and design of funct. materials for harsh env. (new)
  - Quantum sensors for fossil energy (new)

Optical Fiber Sensing for Harsh Fossil Energy Applications

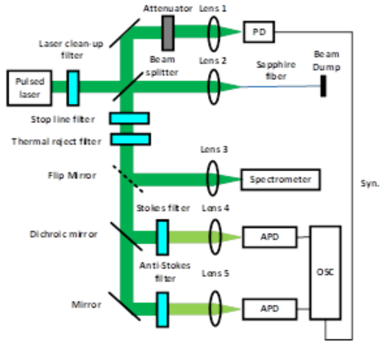
Michael Buric, Jeff Wuenschell, Subha Bera, Guensik Lim, Juddha Thapa

NATIONAL ENERGY TECHNOLOGY LABORATORY

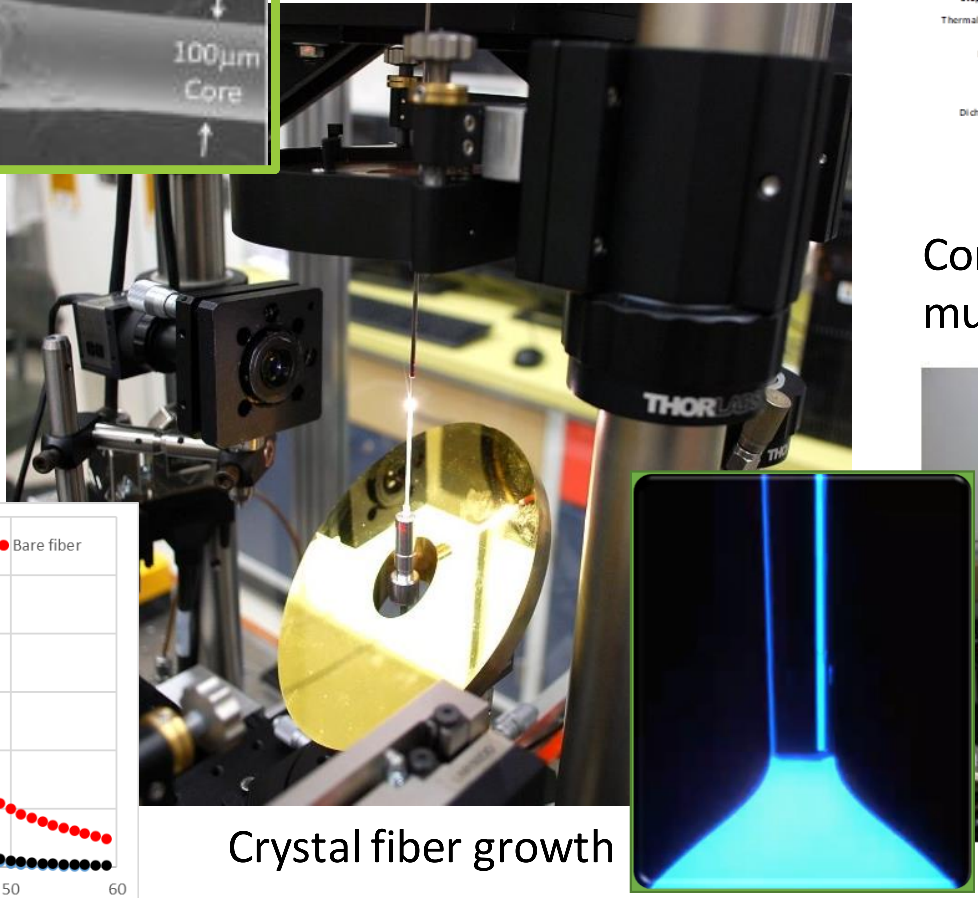
Developing materials and sensing approaches to develop a fiber-based sensing concepts that can provide spatially resolved chemical species and temperature measurements from an optical fiber at above 800°C



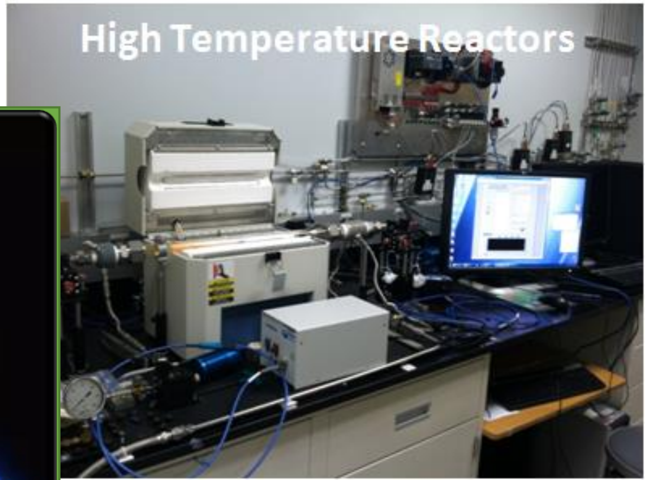
Functional nanomaterials



Commercial and novel multipoint interrogation

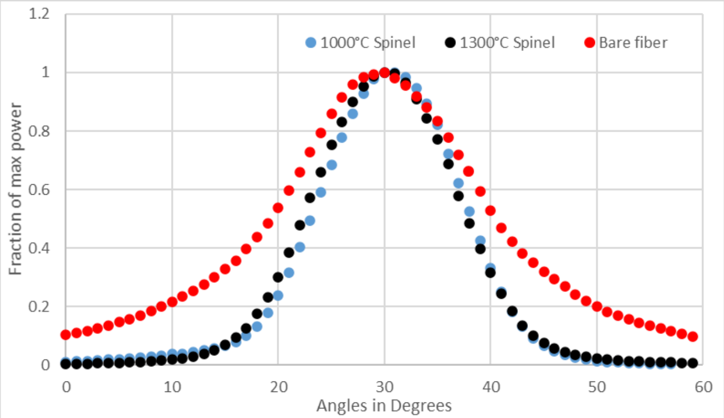


Crystal fiber growth



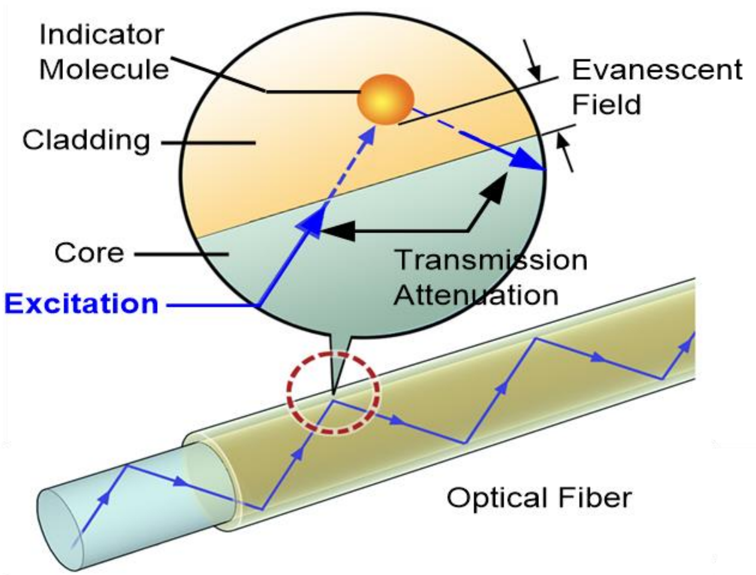
Fossil energy relevant gases

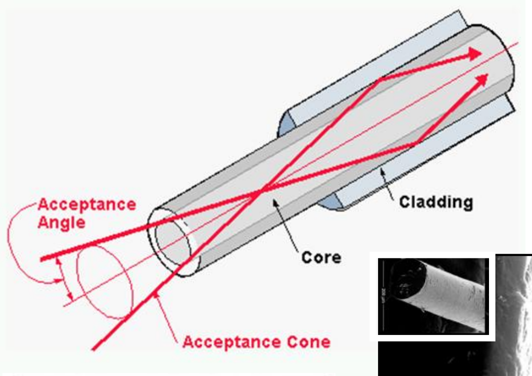
Crystal fiber cladding

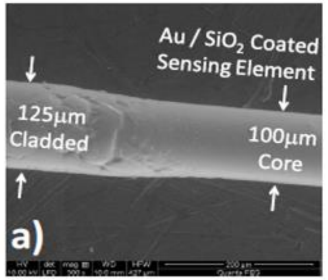


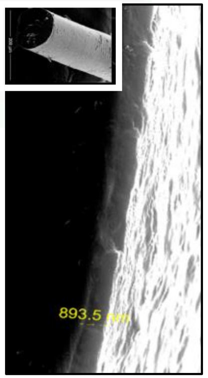
Functional Material Application to Sensors

DISTRIBUTED FIBER OPTIC SENSORS





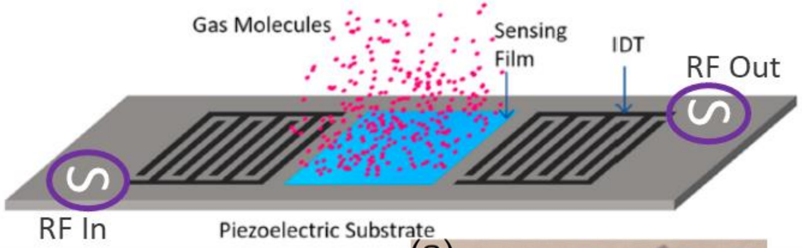


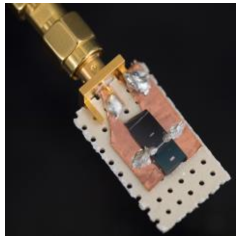


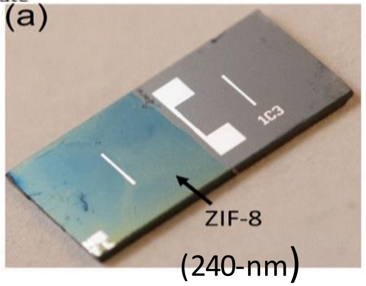
Single-Crystal Fiber Growth, Cladding, Sensing Materials & Distributed Interrogation

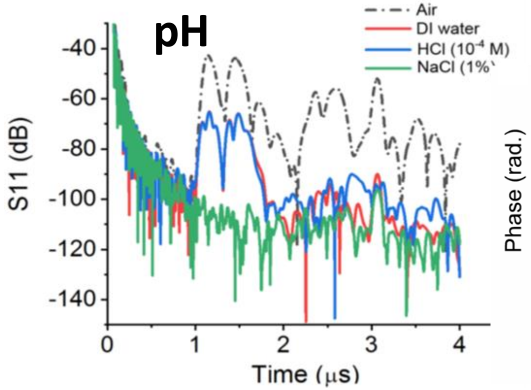
Temperature, Strain, Gas Chemistry, Early Corrosion/pH Detection

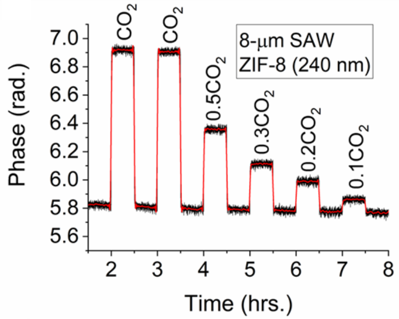
SURFACE ACOUSTIC WAVE SENSOR





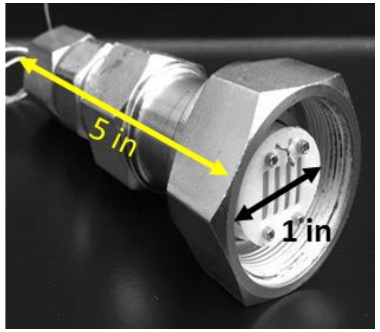






Temperature, Strain, Gas Chemistry, pH

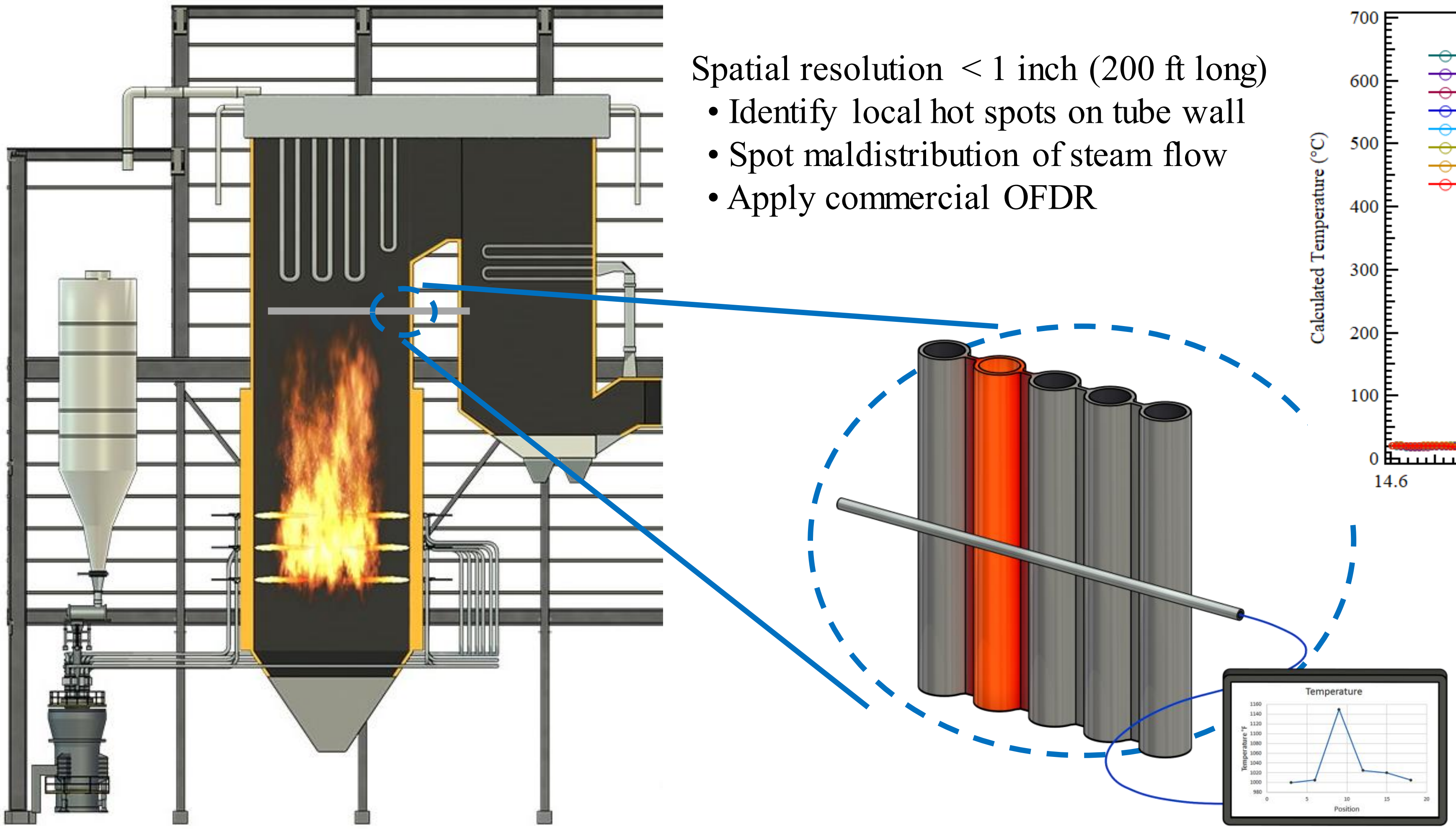
ELECTROCHEMICAL SENSORS



Capable of multiple-parameter measurement Failure prediction capabilities enabled by measuring corrosion precursors. Field Tested.

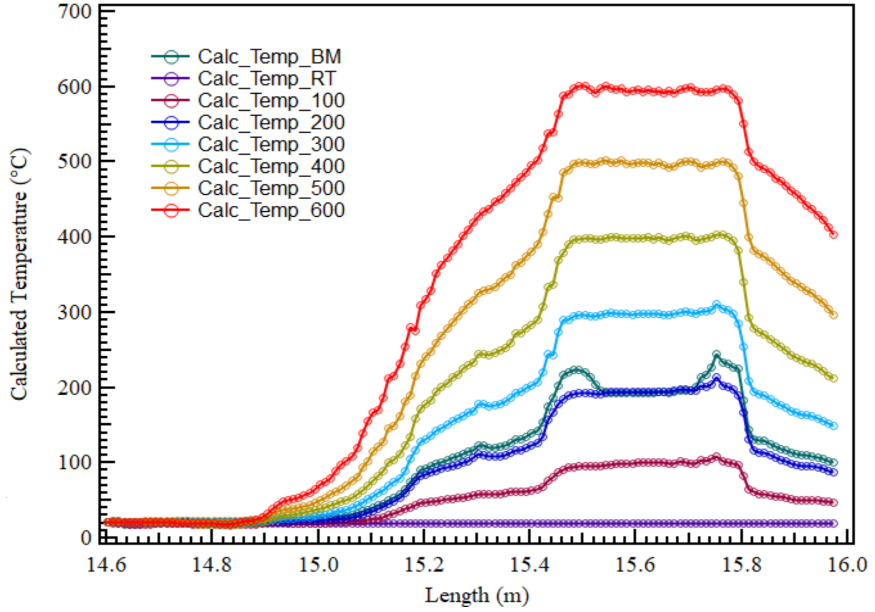
Gas, Chemical, Humidity, Corrosion Rate Monitoring

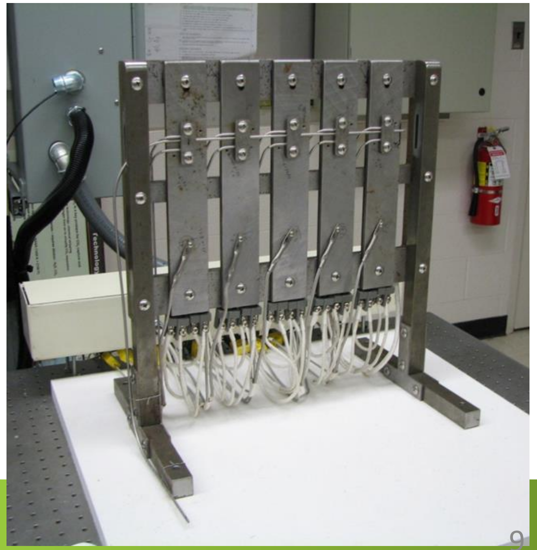
Multipoint Boiler Tube Temperature Monitoring



Spatial resolution < 1 inch (200 ft long)

- Identify local hot spots on tube wall
- Spot maldistribution of steam flow
- Apply commercial OFDR



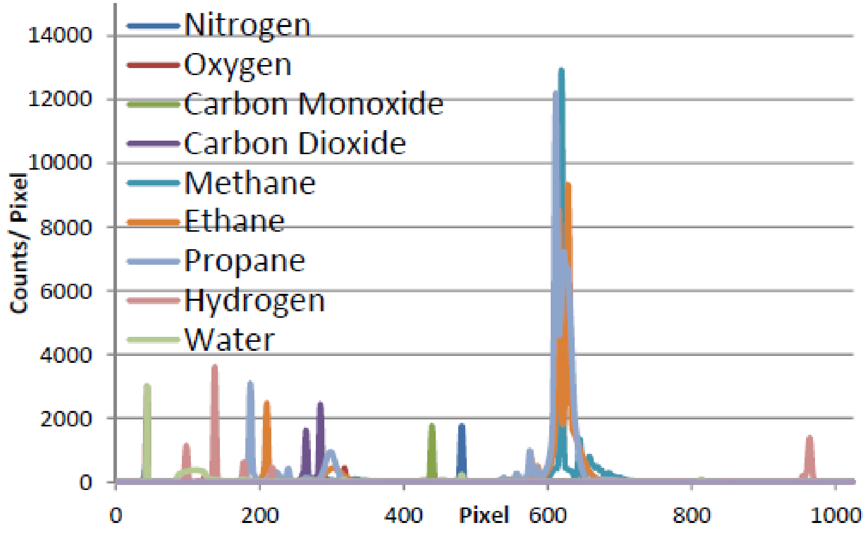


Gold-coated silica fiber useable: <1200°F (650°C), air

Fast Raman Gas Analyzer

- Applications to **power generation** and **chemical process control**
- Field prototype constructed for testing, up to 1000 psi
- Fast - 1 second measurement time
- Measures difficult gases: $\mathbf{H_2}$, N_2, O_2 (they have no IR transitions)
- Easily distinguishes CO from N_2 (difficult for mass spectrometer)
- Species concentrations measured to 0.1%
- Optical waveguide technology boosts Raman signal more than 1000X

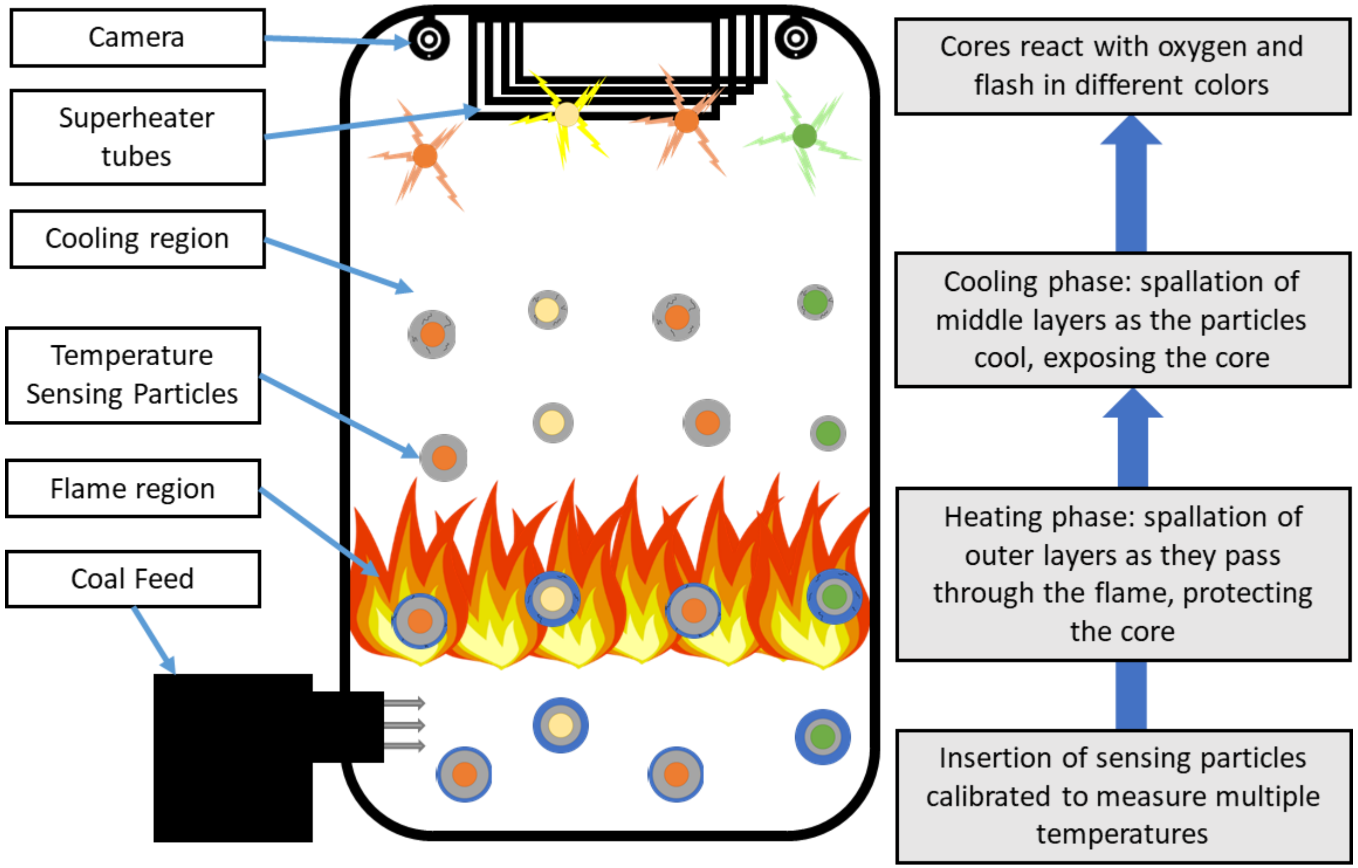
No commercial technology has this combination of speed, accuracy, and multi-gas capability.



US Patent 8,674,306, NETL and U. of Pittsburgh

In-situ Temperature Measurements via Reactive Particles

- Developing multilalyer particles for injection into boiler with coal
- Temperature to be mapped from reaction pattern



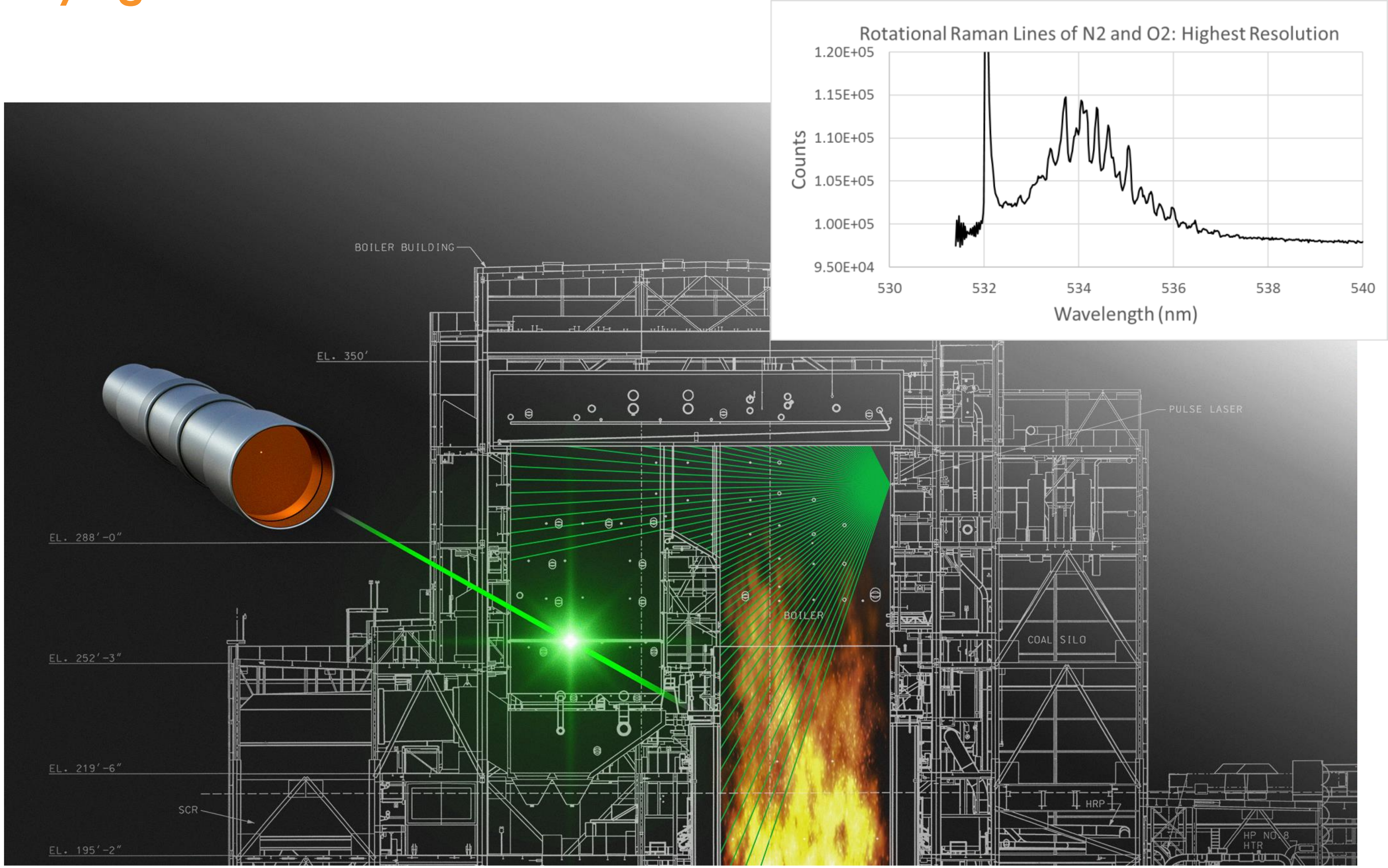
$BaCl_2/KClO_4/Sn^0$/Ethyl Cellulose

Ba(NO3)2/$KClO_4/Mg^0$/Ethyl Cellulose/PVC

Ultrafast Laser Measurements for Power Generation Environments

Improve boiler operation at varying loads

Laser-based measurement of species or temperature inside a coal-fired boiler or HRSG along a line of sight with spatial resolution better than 1 meter and a single point of access



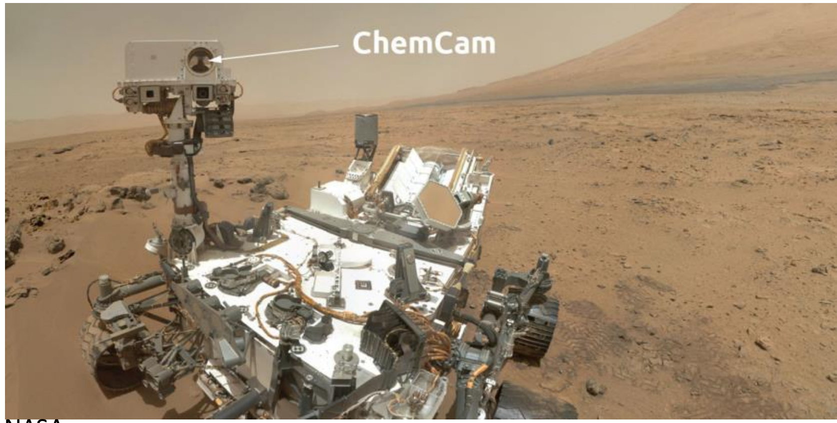
LIBS Sensor Development

What is LIBS?

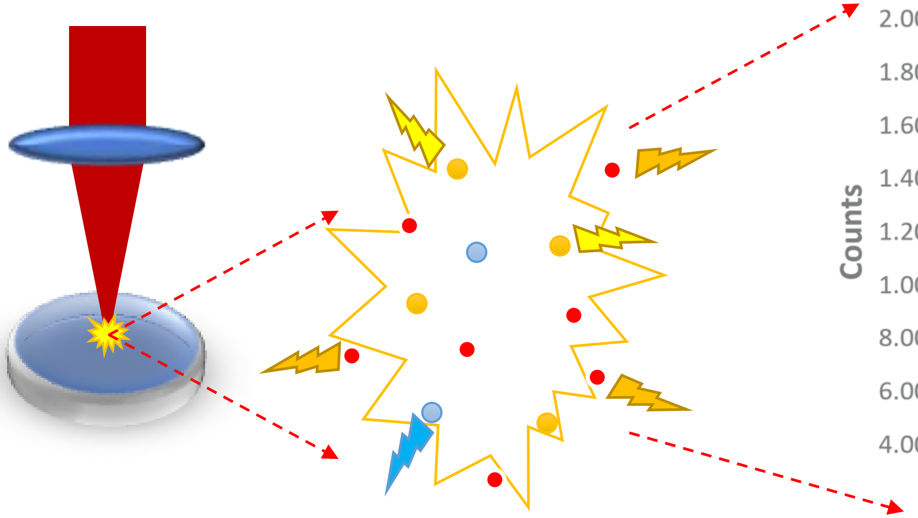
Dan Hartzler, Chet Bhatt, Jinesh Jain, Dustin McIntyre

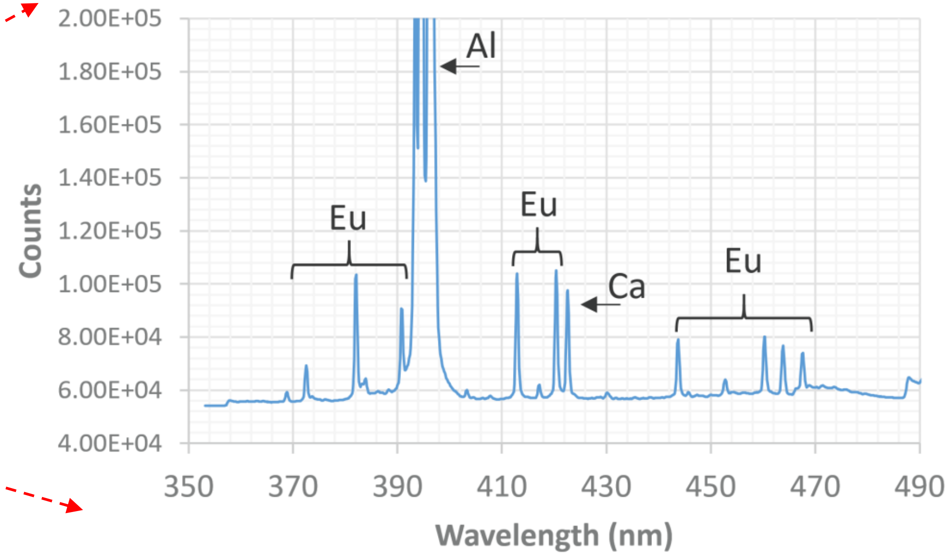
NATIONAL ENERGY TECHNOLOGY LABORATORY

- **Laser Induced Breakdown Spectroscopy (LIBS)**
  - Elemental analysis
  - Rapid
  - Minimal sample preparation
  - Hostile environments
    - Ex: ChemCam (Mars)



NASA






Springer

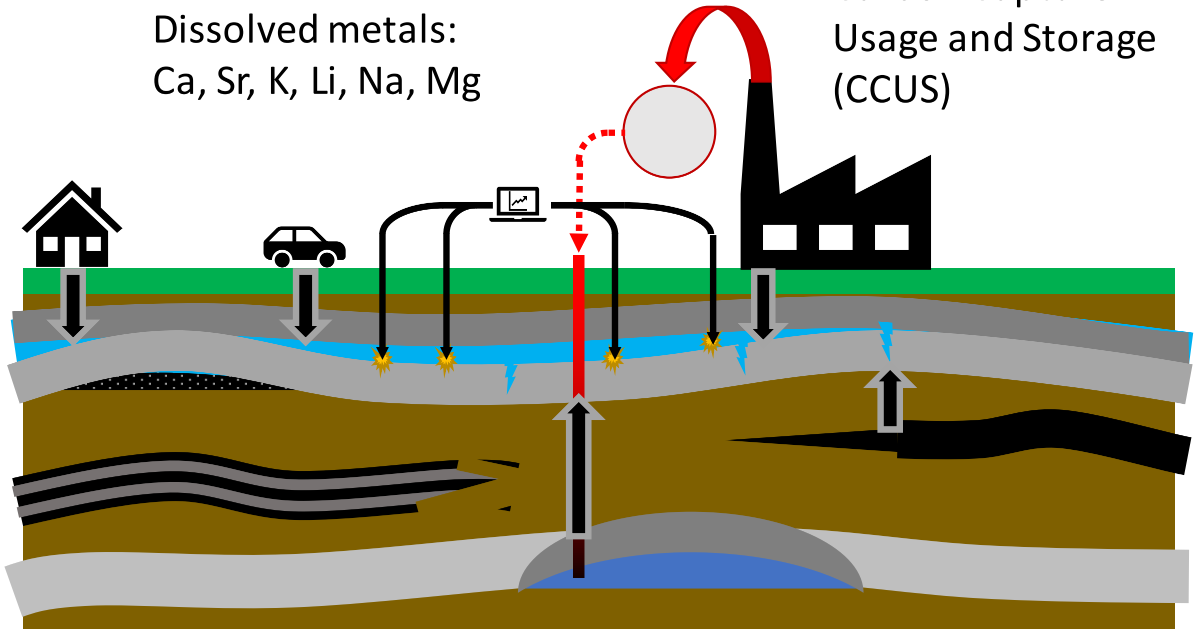
LIBS Sensor Development

Fossil Energy Applications

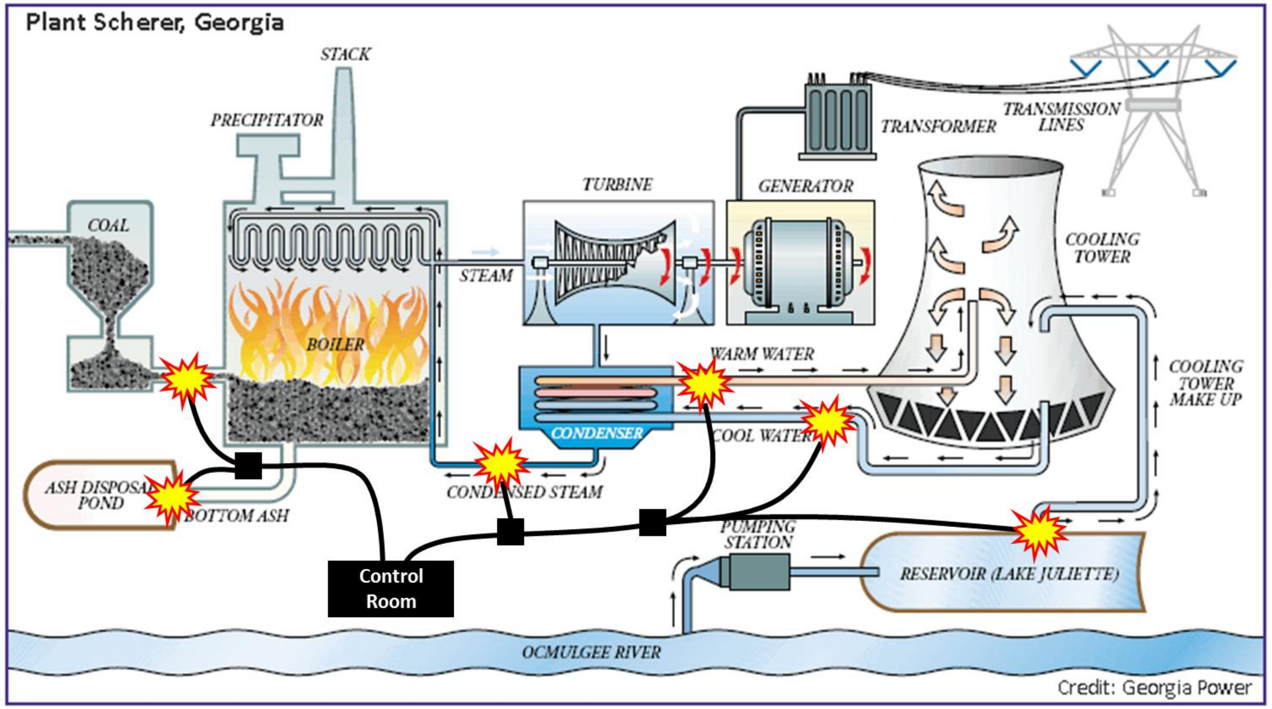
CCUS Downhole Monitoring

Dissolved metals:
Ca, Sr, K, Li, Na, Mg

Carbon Capture Usage and Storage (CCUS)



Power Plant Process Waters

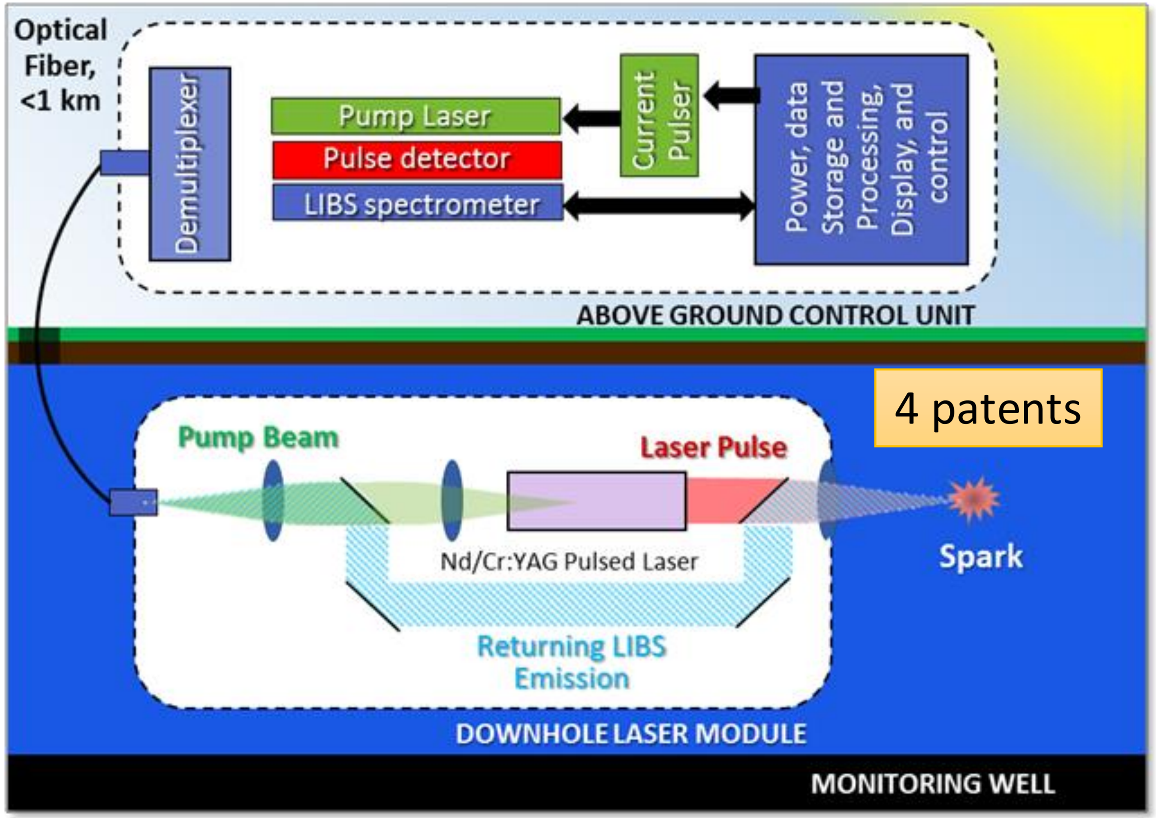


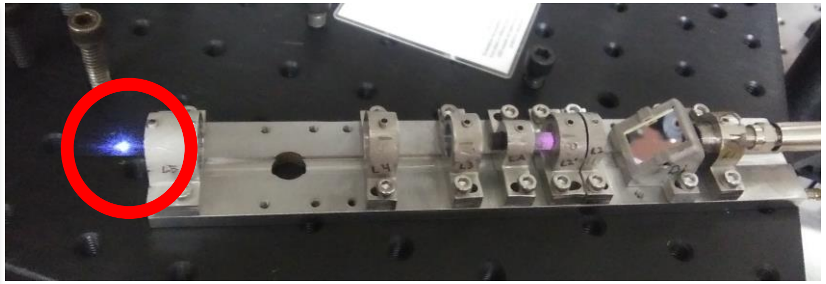
REE Prospecting and Refining

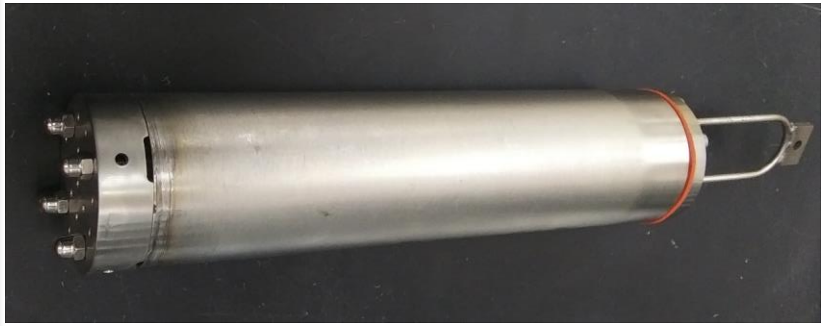
LIBS Sensor Development

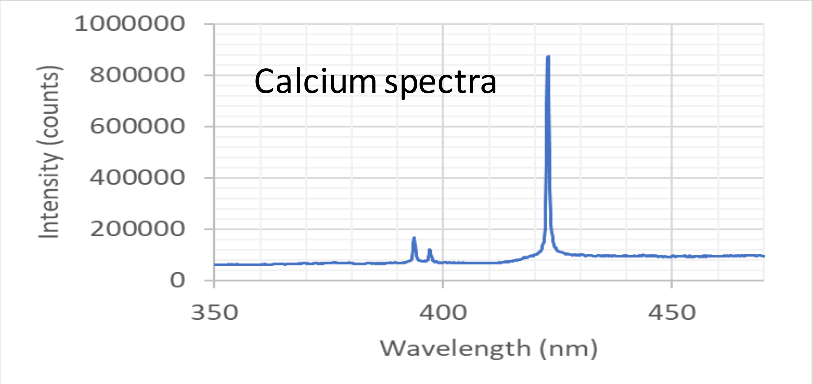
Submersible Prototype

- Construction: < 50 mm (2 in) diameter
- < 200 mm (8 in) long, watertight







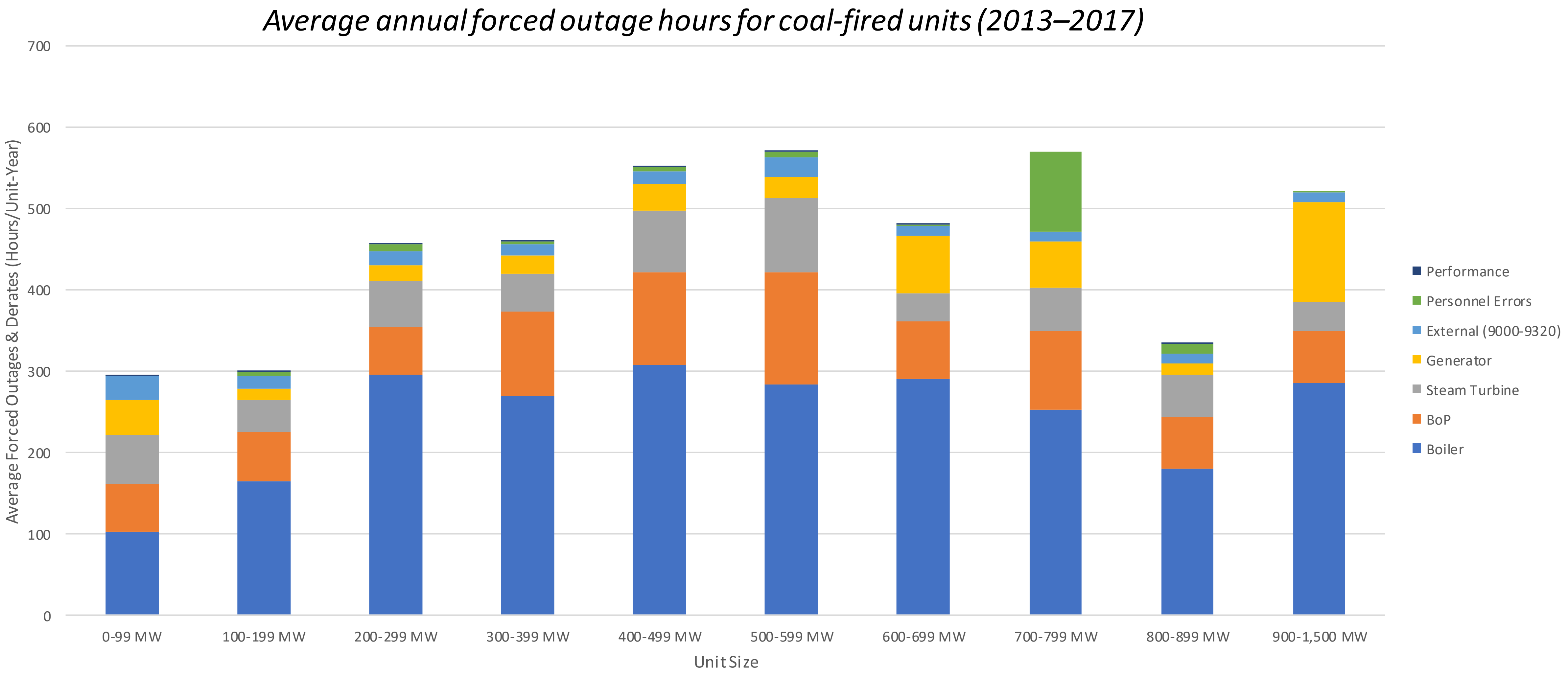


APPLIED SPECTRA

TRONIX3D

Hartzler, D.A., Jain, J.C., McIntyre, D.L., “Development of a subsurface LIBS sensor for in situ groundwater quality monitoring with applications in CO2 leak sensing in carbon sequestration,” Scientific Reports, (2019) 9:4430, DOI:10.1038/s41598-019-41025-3

TEA Analysis: Forced Outages for Coal-Fired Power Boilers



Source: NERC GADS PC GAR-MT,

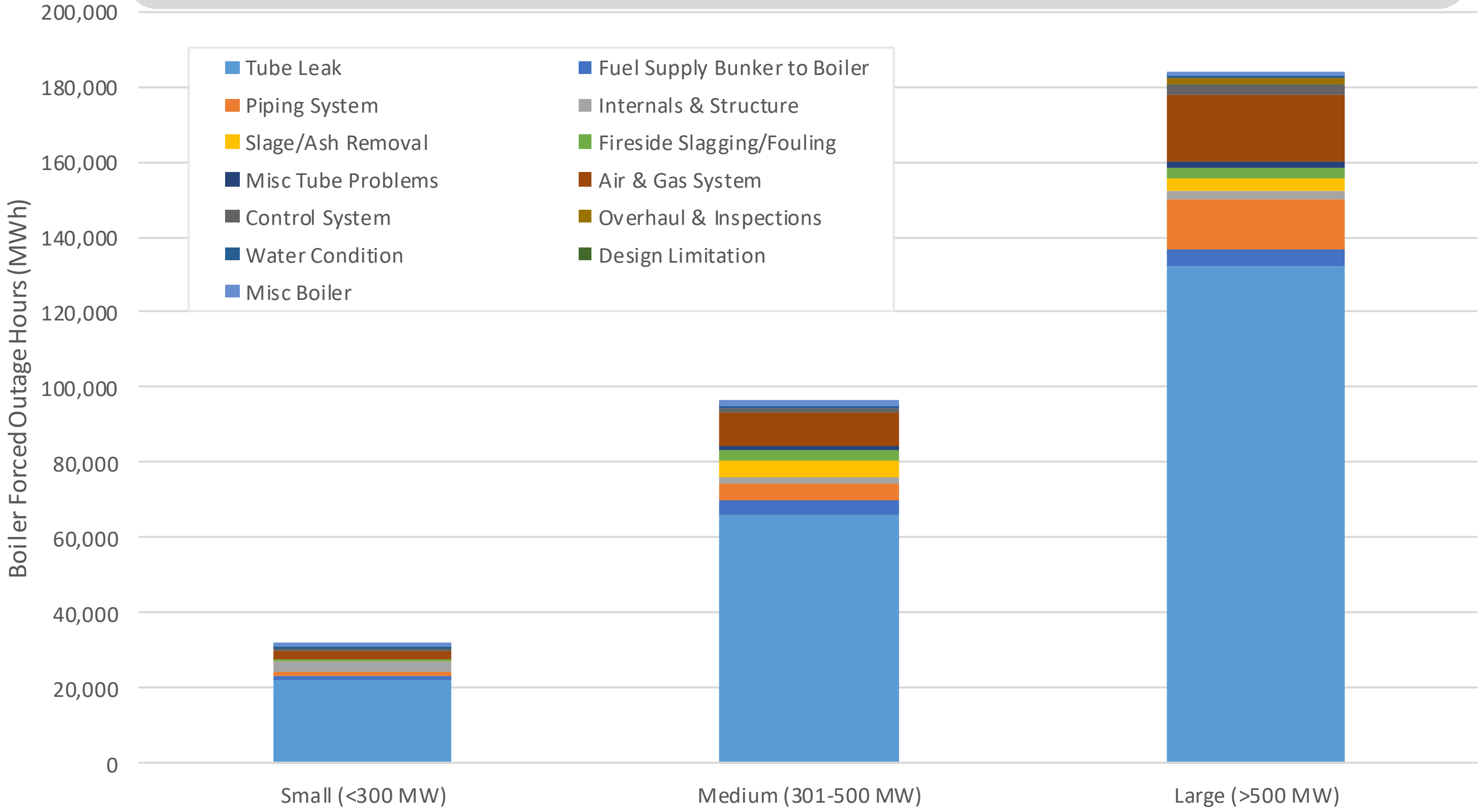
TEA Analysis: Boiler Instrumentation Gap Analysis

Focus on outages due to boiler problems – causes, sensing, tech gaps

Boiler outage cause codes from EV / GADS data

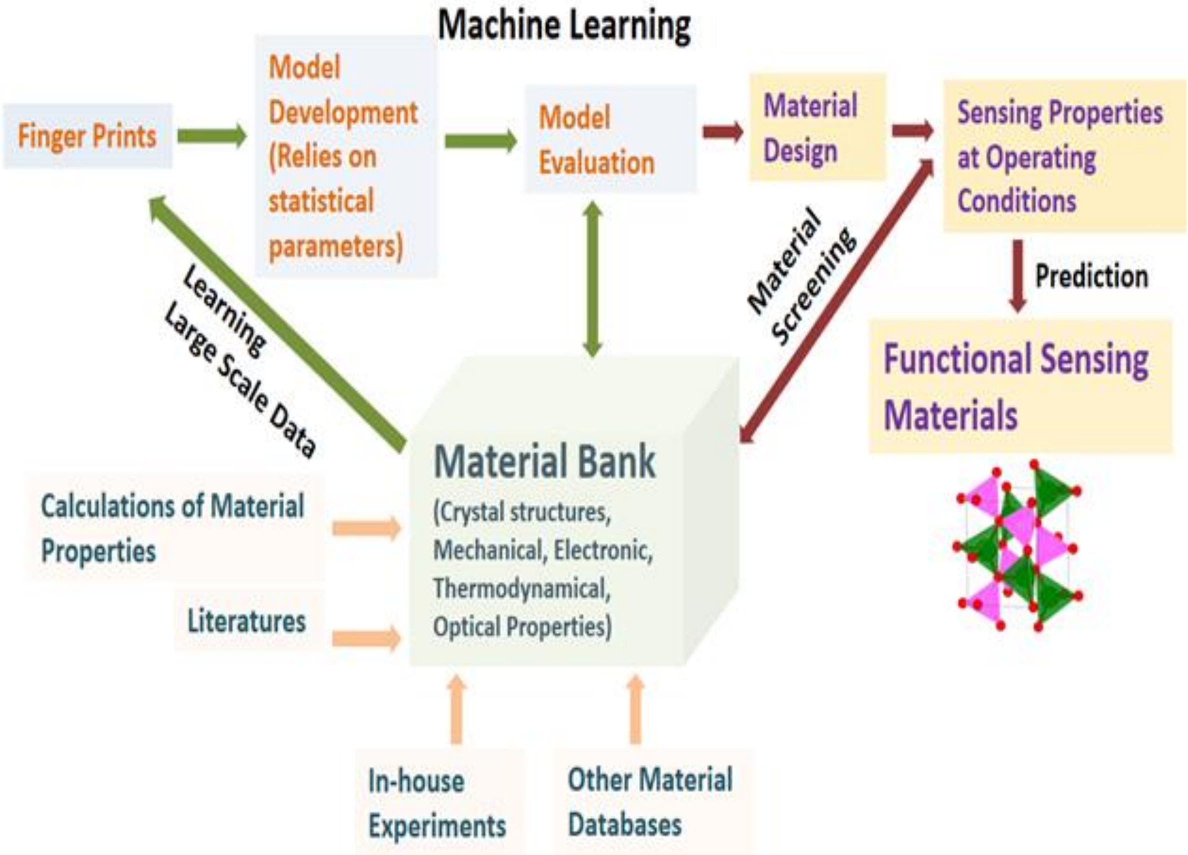
- Fuel supply bunker to boiler
- Piping system
- Internals and Structure
- Slag/Ash removal
- Tube leak
- Fireside slagging/ fouling
- Misc tube problems
- Air and Gas system
- Control system
- Overhaul and inspections
- Water condition
- Design limitation
- Misc boiler

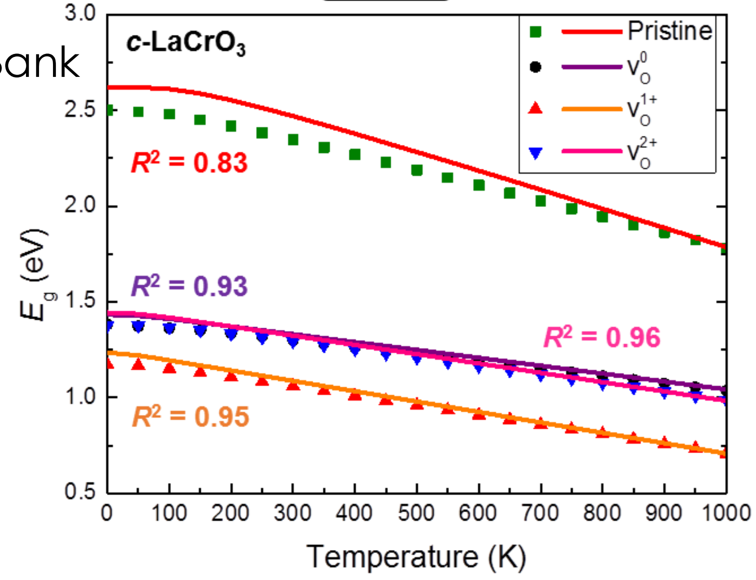
Tube leaks cause forced outages for coal boilers at more than 10x the rate of next highest failure



Machine Learning-Based Theoretical Approach for Screening and Design of Functional Materials for the Harsh Environment Applications

- Establishing gas sensor utilized materials database
  - Collected optical gas sensor materials from literature to build the Material Bank
  - Semiconducting metal oxides (> 50) and perovskite oxides (> 20)
- Focus on observable vs. temperature relationships





	E_o (eV)	S	$<\hbar\omega>$ (meV)
Pristine	2.62	5.9	33
v_O^0	1.43	2.4	10
v_O^{1+}	1.23	3.2	5
v_O^{2+}	1.44	2.8	10

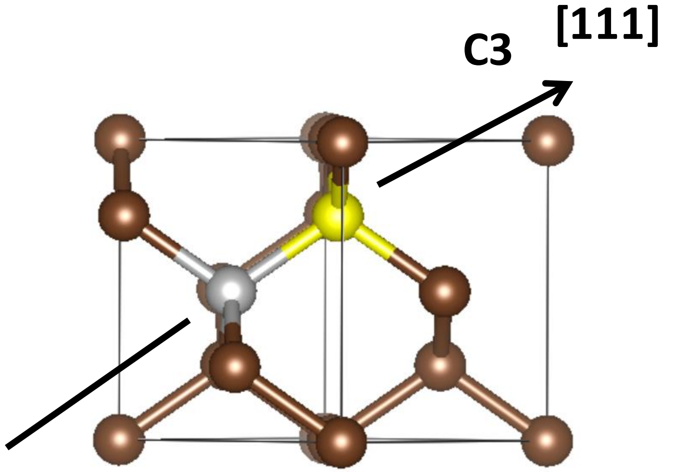
Data input from the Materials Project

		crystal system	space group	m.p. (C)	Ehull (eV/atom)	Eform (eV/atom)	density (g/cm3)		band gap (eV)	dielectr
Semiconductig MOx metal oxide										
1	TiO2	tetragonal	P4_2/mnm	1855	0.037	-3.475	4.13	direct	1.781	
		tetragonal	I4_1/amd	1843	0.006	-3.506	3.76	indirect	2.062	
2	SnO2	tetragonal	P4_2/mnm	1630	0	-2.123	6.61	direct	0.648	
3	SiO2	trigonal	P3_221	1720	0.01	-3.268	2.48	[-]	5.708	
4	TeO2	tetragonal	P4_12_12	733	0.011	-1.494	5.64	indirect	2.896	
5	CeO2	cubic	Fm3m	2727	0	-3.938	6.99	indirect	1.867	[-]
6	HfO2	monoclinic	P2_1/c	2790	0	-4.03	9.97	indirect	4.017	
7	ZrO2	monoclinic	P2_1/c	2690	0	-3.824	5.56	indirect	3.474	
8	GeO2	tetragonal	P4_2/mnm	1115	0.004	-2.085	5.94	direct	1.231	[-]
9	MnO2	tetragonal	P4_2/m	535	0.384	-1.437	3.22	[-]	1.015	[-]

Quantum Sensing for Fossil Energy Applications

Progress Highlights

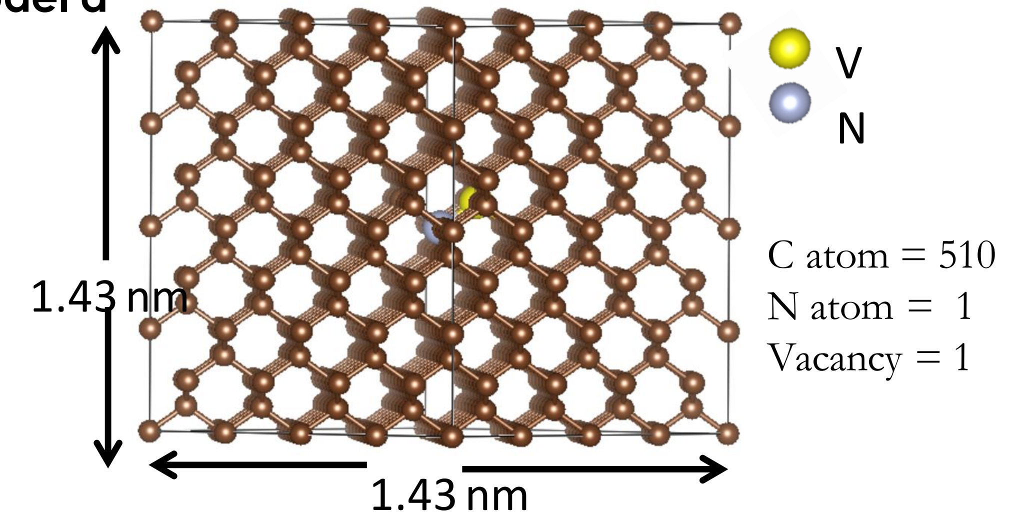
- Review manuscript submitted for publication
  - Quantum sensing: Focused to fossil energy applications
  - Quantum networking: For energy applications
  - Quantum simulations: Focused on quantum chemistry problems
  - Quantum computing: Combinatorial and material chemistry problems
- Modeling of diamond with nitrogen-vacancy (NV) center
  - Orientation of stable NV center is along [111] direction
  - A C-defect formation is found to be energy = 6.78 eV
  - **A 512-atom supercell model is found to be good enough to model a NV center for sensing applications**
  - Neutral NV center formation energy = 7.5 eV



Unit cell of diamond enclosing a NV center

Outlook

- NV center electronics structures
- Surface model for nano-diamond with NV center
- NV center responses to the external light and magnetic fields
- Adding experimental work



Supercell model (cubic structure) of diamond enclosing a NV center

Questions?

Collaborative Research and Testing
https://netl.doe.gov/business/partnerships
https://netl.doe.gov/news-room-news-stories

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