Advanced Sensors and Controls

…A RIC Field Work Proposal at NETL

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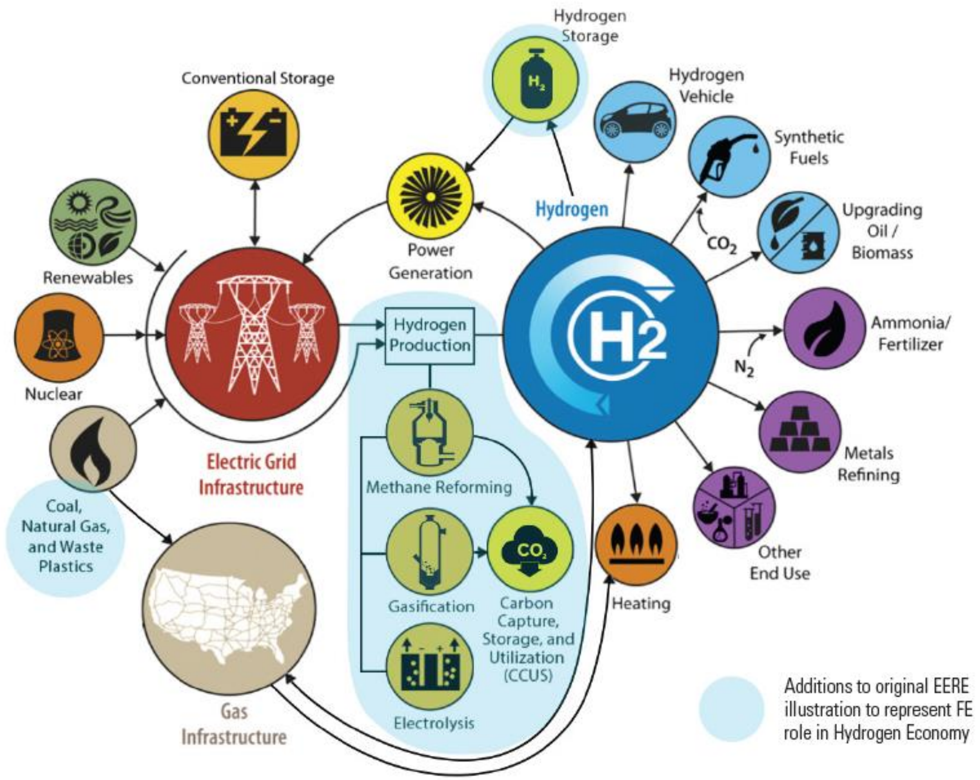
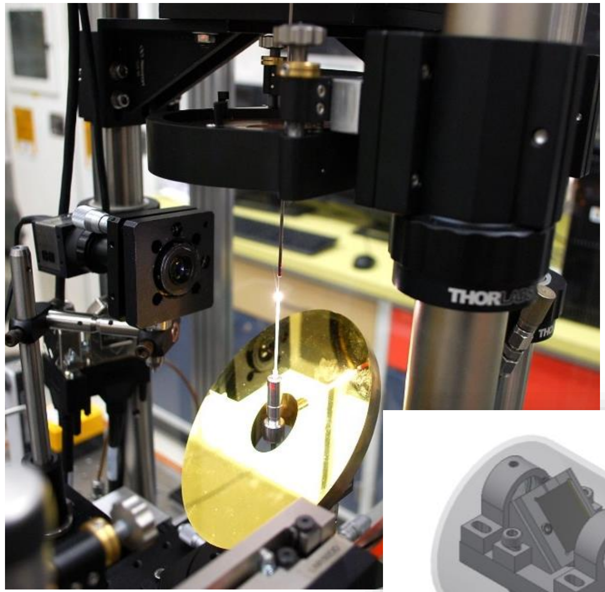
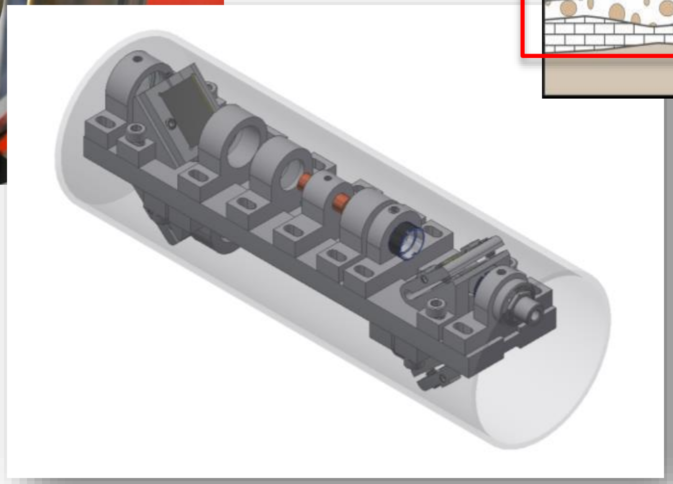
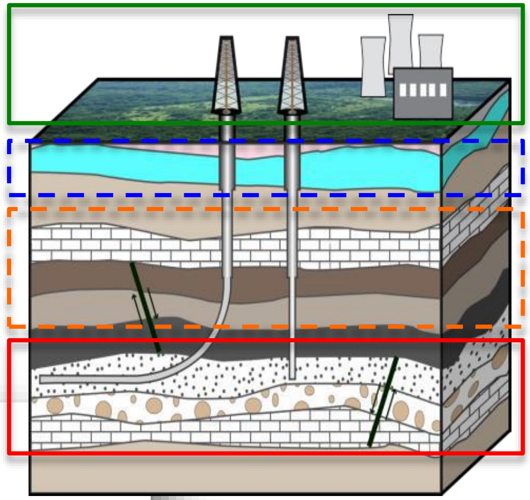








Advanced Sensors and Controls

High Level Goals of FWP

- Develop advanced sensors and controls to support development of technologies within FECM's portfolio
- Enable optimized monitoring and management using novel sensors and controls
  - Increase operational flexibility
  - Maintain or improve efficiency/availability
  - Sharply reducing carbon emissions

Net-zero carbon power

- NG turbines with Point-Source Capture
- Hydrogen as bulk clean **energy storage**
- **Hydrogen production from carbon-based fuels** with **carbon capture** **– support transition**
- Hydrogen utilization
  - Hydrogen/NG blend turbines
  - Hydrogen hybrid systems
- Carbon dioxide removal and direct air capture

Advanced Sensors and Controls

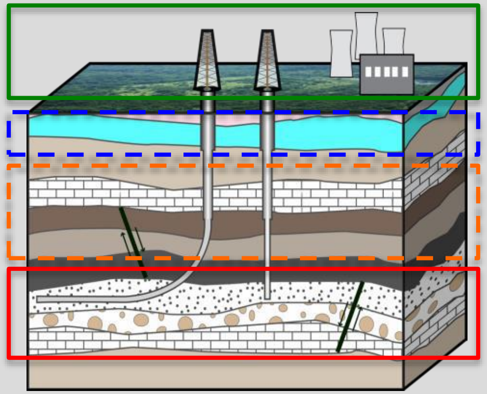
Fundamental challenges

- Provide **sufficiently resolved process data** to make operational optimization possible
  - Spatial and time resolution, extreme environments, sensor system cost
- Develop controls to **operate under static or dynamic operating conditions**, especially under load changes while optimizing for:
  - Efficiency
  - Operating cost
  - Safety margin

Examples:
- Boilers/gasifiers (slag, reducing gases, ash, acidic species)
- Solid oxide fuel cells (oxidizing and reducing flows) and reversible SOFCs (load cycling)
- Chemical looping (high temperatures and erosion)

Technology Areas for Sensors and Controls

Hydrogen and Carbon Management

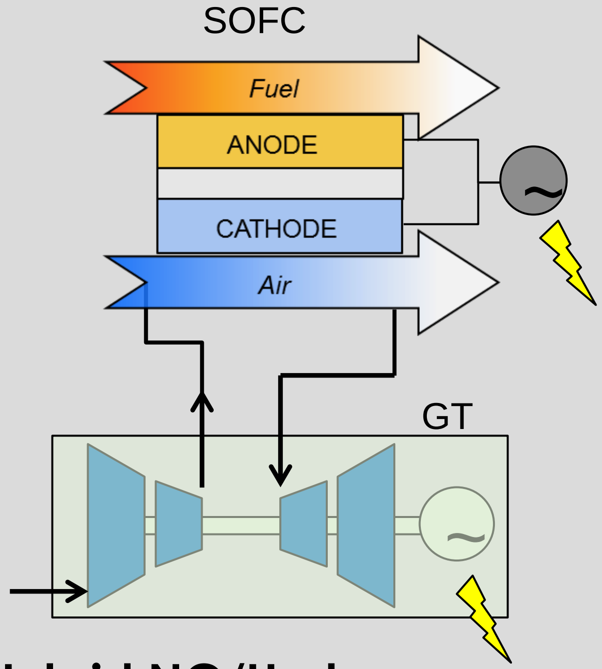


Carbon Storage and Subterranean chemistry

- Assure CO_2 storage stability
- At the Wellhead
- Downhole
- High pressure water or brine

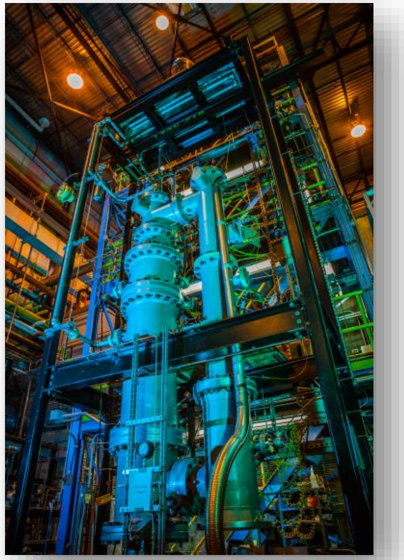
Hydrogen Production and Utilization

- Modular gasification
  - waste plastics / MSW
  - Sustainable biomass
  - Coal waste deposits
- Microwave fuel reforming
- Chemical Looping
- Hydrogen/Blend GT
- SOEC
- Ammonia systems



Hybrid NG/Hydrogen Systems

- 800°C in SOFC
- 1,500°C in GT
- Transient controls
- + CO_2 storage



Novel Systems

- Direct Air Capture
- Supercritical CO_2 cycles

Other relevant applications?

Advanced Sensors and Controls FWP

NATIONAL ENERGY TECHNOLOGY LABORATORY

Portfolio Overview

Sensors & Instruments

- High temperature optical fiber sensors
  - Crystalline fiber
  - Sensing materials
  - Interrogation
- Real-time gas composition analysis of hydrogen blends
- LIBS for subterranean sensing of fluid migration

Controls

- Cyber-physical systems as a zero-carbon integrated energy system development acceleration tool
- Online System Identification for power plants

Novel Concepts

- AI for screening and design of functional materials
- Quantum sensors for FECM applications
- VLC – Alternative to RF
- Direct Power Extraction (a.k.a. Magnetohydrodynamic power production)

Advanced Sensors Program Fiber Optic Sensor Projects

Speaker: *Michael Buric, Staff Scientist*
NETL, RIC-MEM

With: Guensik Lim, Jeff Wuenschell, and Gary Lander
(LEIDOS contractor scientists)

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Research Breakdown: Overall Objectives

- Task 24 – Single Crystal Fiber growth and sensing with Raman DTS
  - Perform distributed temperature sensing in extremely harsh environments including combustion, gasification, SOFCs, turbines, and others
  - Replace single-point with distributed measurements to enable full system visibility
- Task 22 – Functional Coatings for Hydrogen gas sensors in harsh-environments
  - Produce novel gas-sensitive coatings for optical fibers
  - Introduce gas sensors in high-value locations (inside SOFCs, high-temp combustor exhaust, etc.)
  - Use this sensor data for improved efficiency and control of hydrogen systems

Task 24: Why use single crystal fibers in energy applications?

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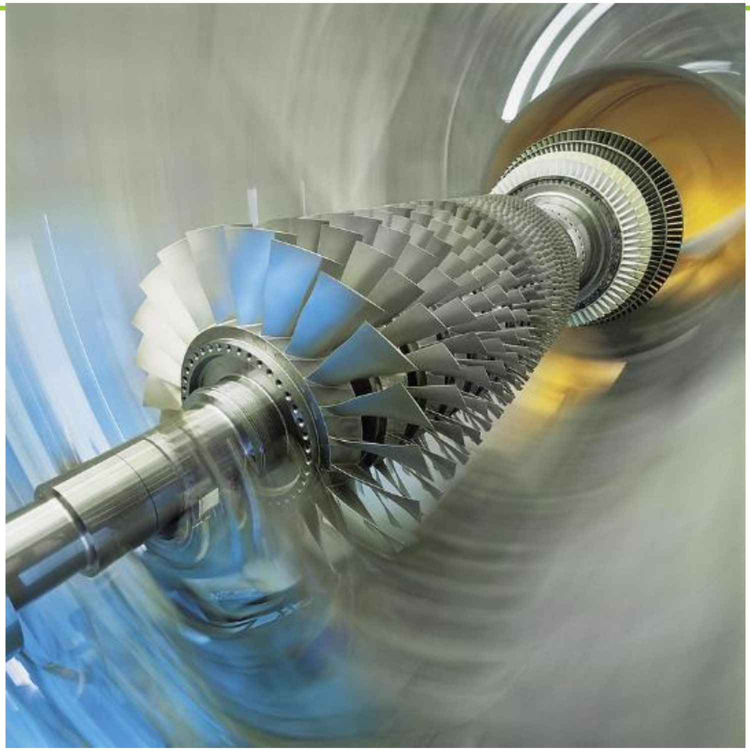


	Coal / Waste Plastic Biomass Gasifiers	Combustion Turbines (H2 or NG)	Solid Oxide Fuel Cells / Electrolyzers	Hybrid Systems	Nuclear	Solar Thermal
Temperatures	Up to 1600°C	Up to 1300°C	Up to 900°C	Up to 1000°C	Up to 1000°C	Up to 700°C
Pressures	Up to 1000 psi	Pressure ratios 30:1	Atmospheric	System dependent	High pressure steam	High pressure steam
Atmosphere	Highly reducing, erosive, corrosive	Oxidizing	Oxidizing and reducing	Oxidizing and reducing	Gamma and neutron radiation	Daily heating/cooling
Examples of Important Species	H_2, O_2, CO, CO_2, H_2O, H_2S, CH_4	O_2, gaseous fuels (natural gas to high hydrogen), CO, CO_2, NO_X, SO_X	Hydrogen from gaseous fuels and oxygen from air	H_2, NG components, contaminants	Head-space gases, water, molten salt	Water,brine, molten salts

❖ **Why optical fiber?**

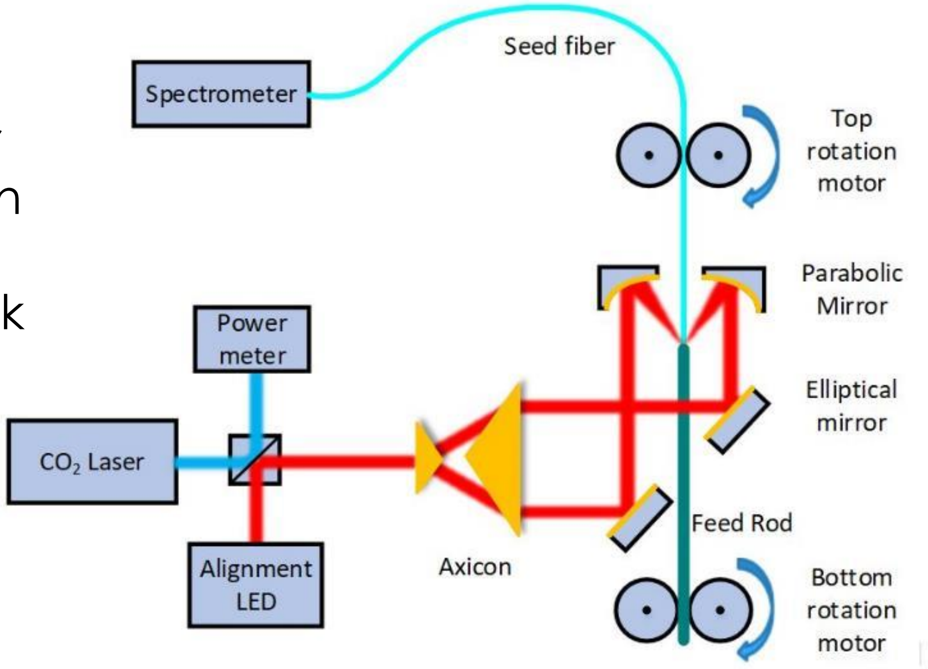
1. No electrical interference
2. Medium temperature (~800c)
3. Single feedthrough
4. Inexpensive
5. Easily functionalized
6. Distributed!

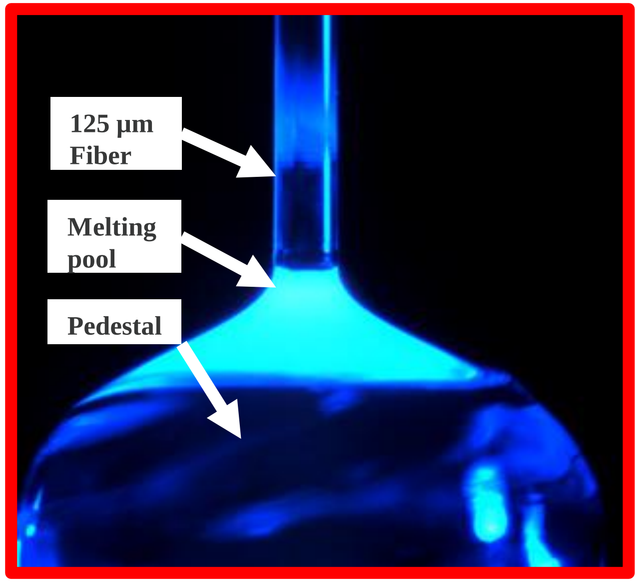
❖ **Single crystal fiber**

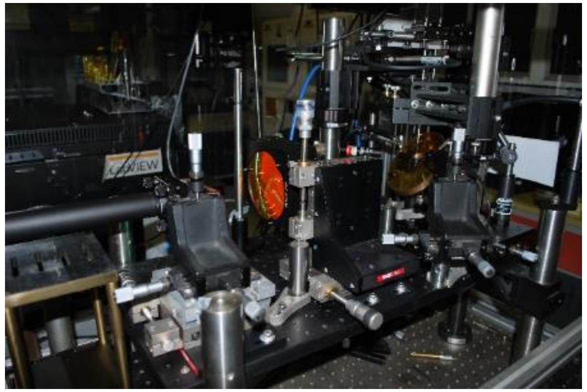
1. High melting point
2. Corrosion resistant
3. Compact size (100 microns)
4. Wide transmission window
5. Benefits of silica +low-OH absorption

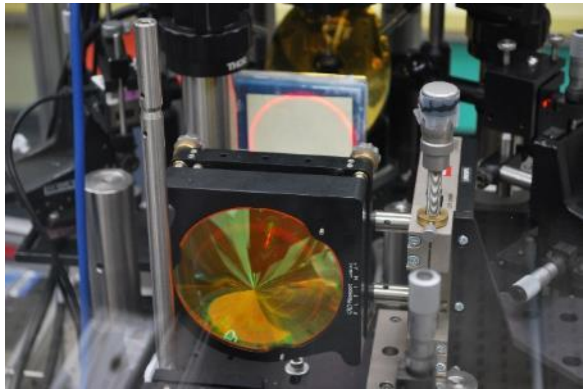
Tech info: Making single-crystal fiber with LHPG

- CO_2 laser source for heating
- "Doughnut" beam shaper surrounds molten zone with light
- Motors advance feedstock (pedestal) and fiber
- Slow process (mm/min)
- Grows pure crystals (no cladding)









Work approach: SC fiber cladding

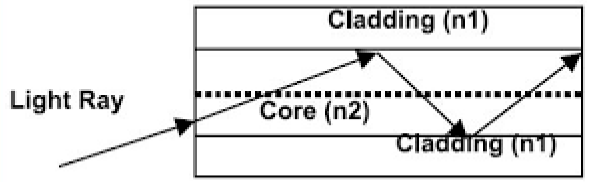
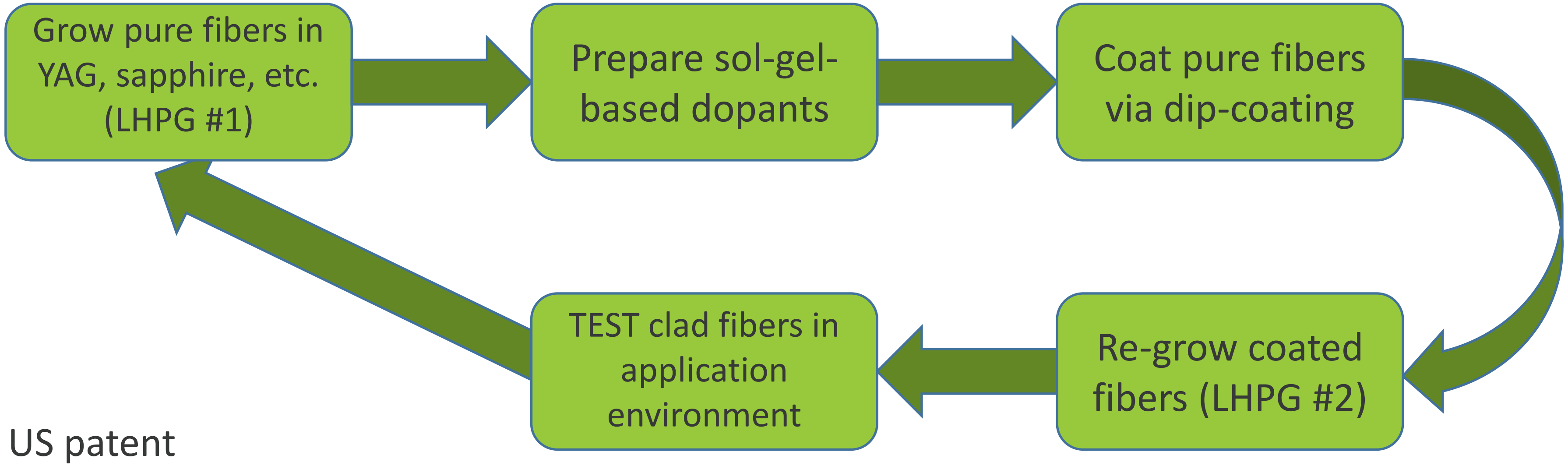


Figure 1: Light launched into the fiber core

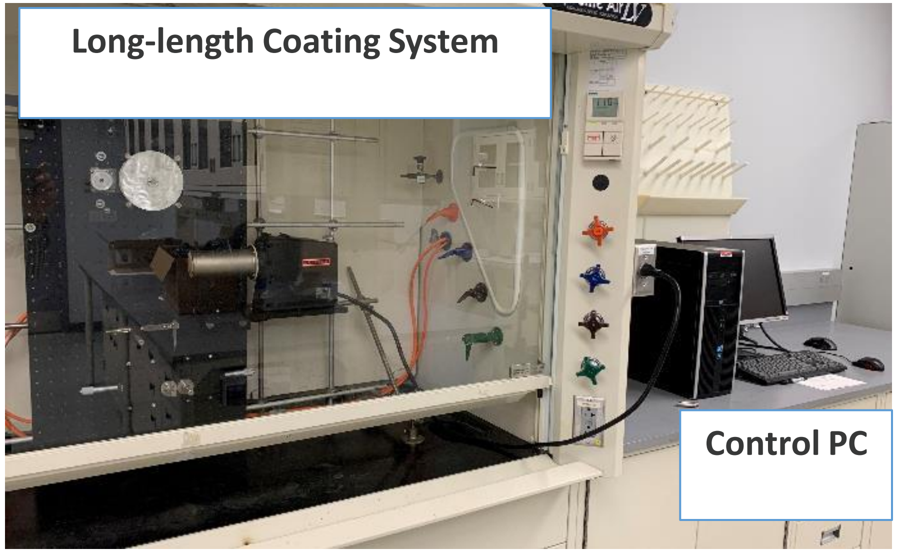
- Grow cladded fibers with 2-stage LHPG system
  - Sapphire or YAG
  - Sol-gel (or other) dopant additions
- Evaluate materials compatibility in energy systems
- Improve fiber performance

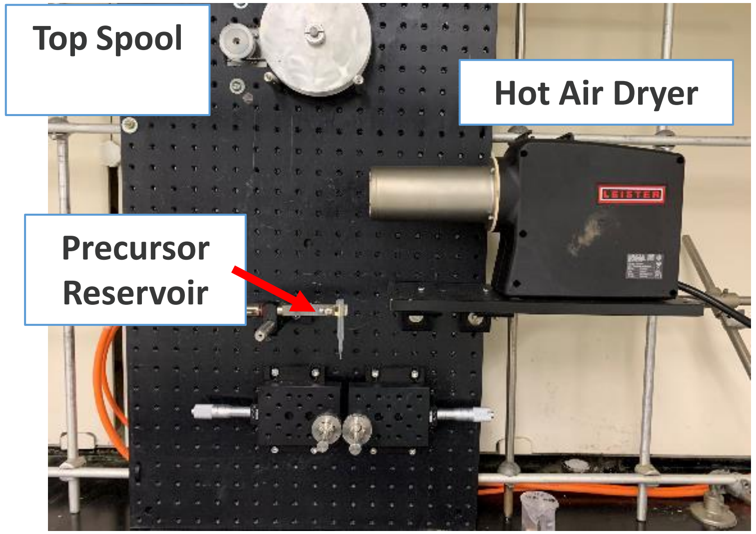


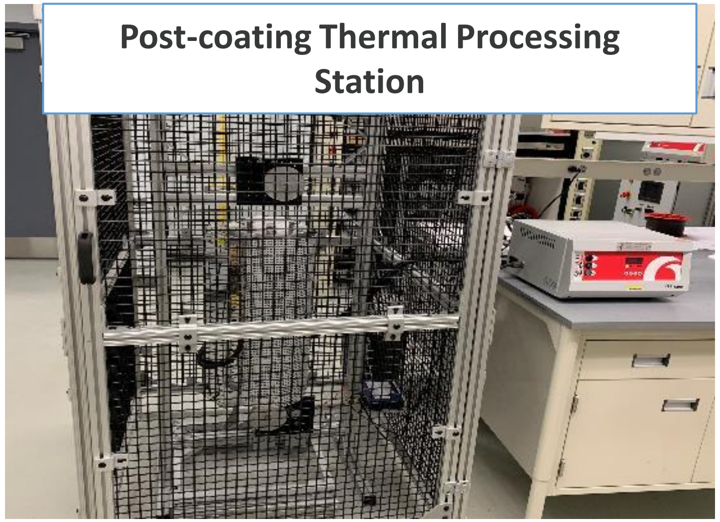
*provisional US patent

Work approach: Reel-to-Reel sol-gel processing system for cladding dopant additions

- Coater designed to coat long lengths of single crystal fiber (~several meters) in sol gel solution and "soft bake" with hot air dryer.
- Post-coating thermal processing – vertical furnace with 1200°C max temperature.
- Processed fiber used for re-growth and dopant distribution

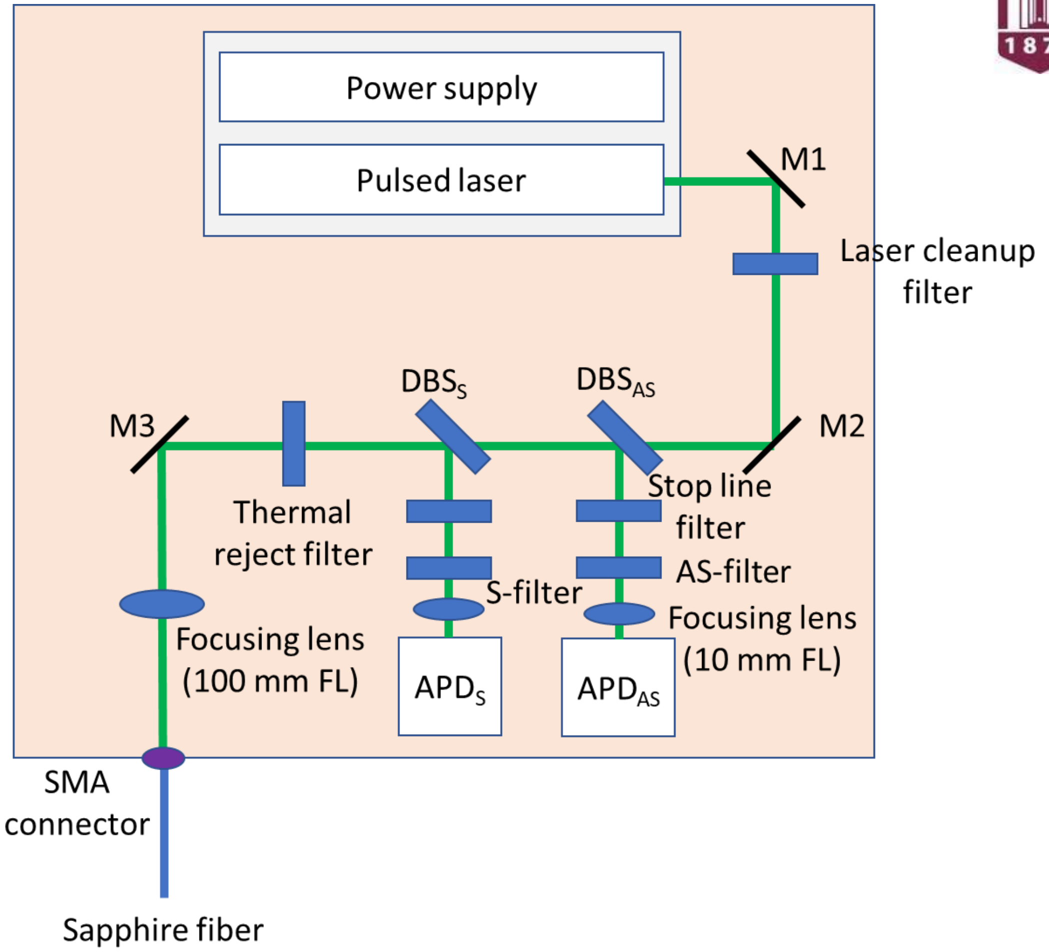






Tech info: How an SC-fiber becomes a T-sensor

- Introducing the NETL Raman DTS (distributed temperature sensor)
- Pulsed ~350ps 532nm green laser
- Excites Raman scattering as pulse propagates
- Collects Raman with fast avalanche photodiodes
- Optics designed for sapphire or YAG fiber
- First interrogator for SC-fiber
- First interrogator produced by NETL Interrogator Development Program



NETL Fiber Optic Interrogator Development Program

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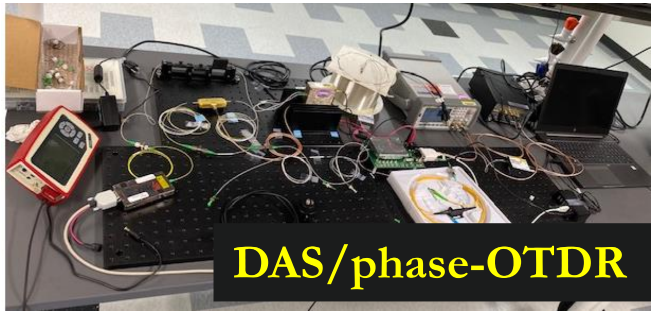
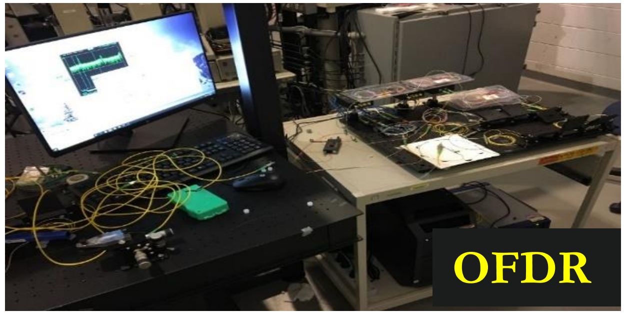
Cost: <$40k



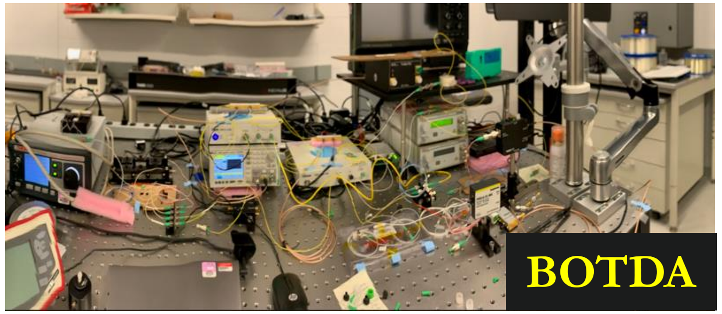
Sensing range = >50 km;
Spatial resolution = 1-2 m;
Acoustic frequency range: ≤20 kHz; (depends on the fiber length)**;**
Frequency resolution: <2 Hz;
Laser safety: Class 3B

Cost: <$35k

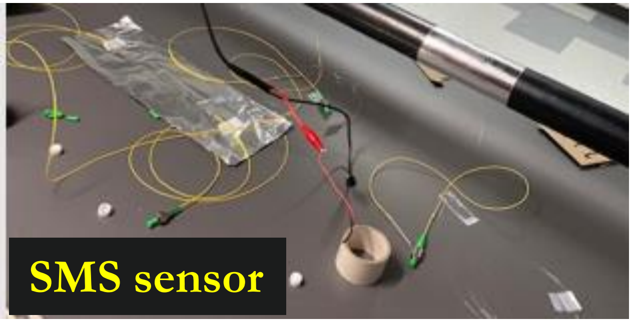


Sensing range = ≤1 km;
Spatial resolution = <1 mm;
Temperature resolution: 0.1°C;
Strain resolution: 2 με;
Laser safety: Class 1

Cost: <$70k



Sensing range = ≤150 km;
Spatial resolution = <5 m;
Temperature resolution: ±1 to 2°C;
Strain resolution: 10 to 20 με;
Laser safety: Class 3B



Cost: <$3k

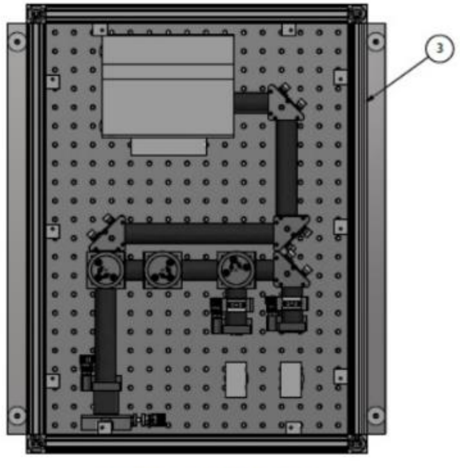
Acoustic frequency range: 5 Hz to 1 MHz;
Frequency resolution: <1 to 2 Hz;
Laser safety: Class 1

Cost: <$8k

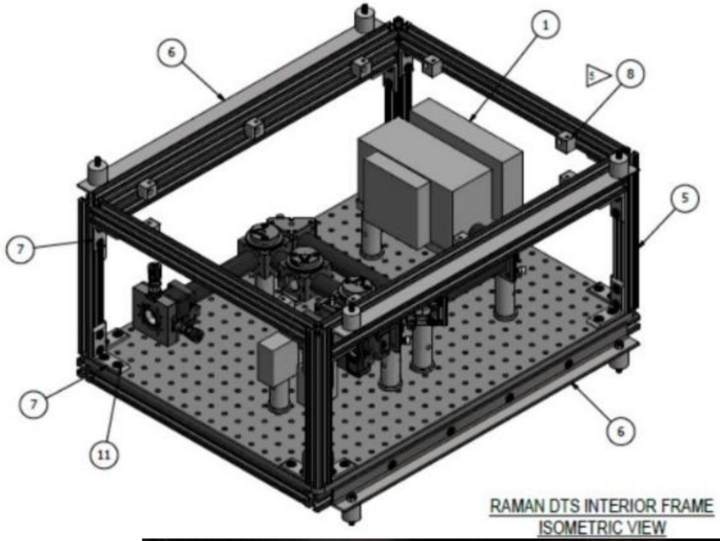
Acoustic frequency range: 1 Hz to 500 kHz;
Frequency resolution: <1 to 2 Hz;
Laser safety: Class 3B

Accomplishments: DTS field prototype

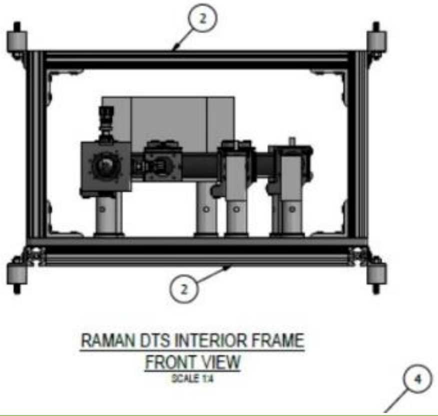
- FY22 Total re-work of optical design including laser path, optical filters, and detectors
- Increased collection efficiency by 10X enabling much longer sensor fibers
- Filed testing has occurred at INL, MIT research reactor, and at our pilot scale PPC



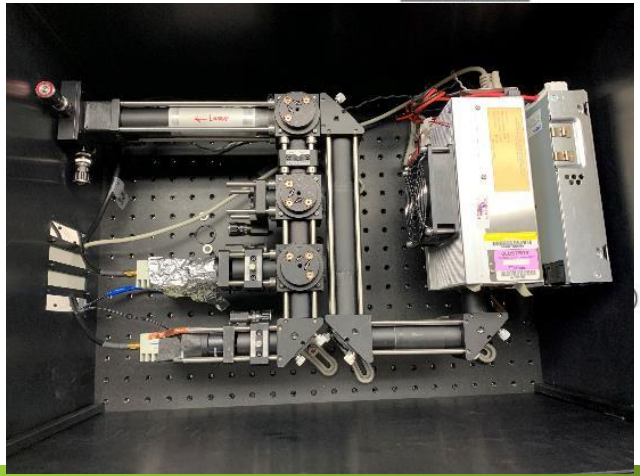
RAMAN DTS INTERIOR FRAME
TOP VIEW
SCALE 1:4



RAMAN DTS INTERIOR FRAME
ISOMETRIC VIEW

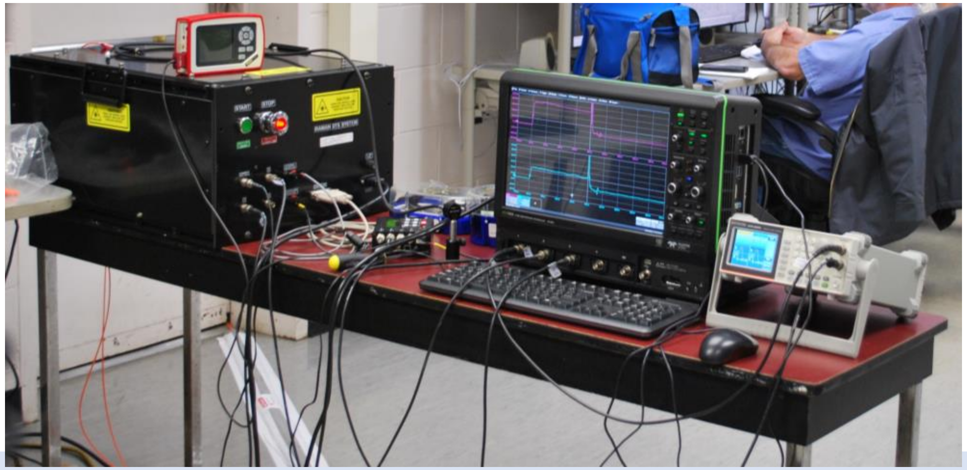


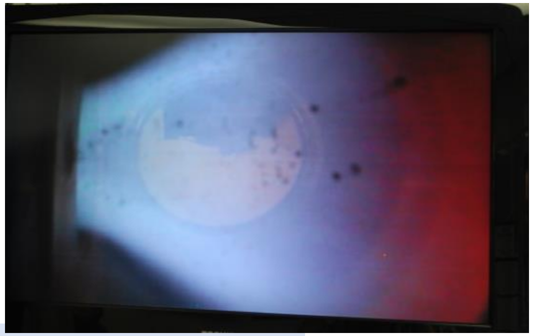
RAMAN DTS INTERIOR FRAME
FRONT VIEW
SCALE 1:4

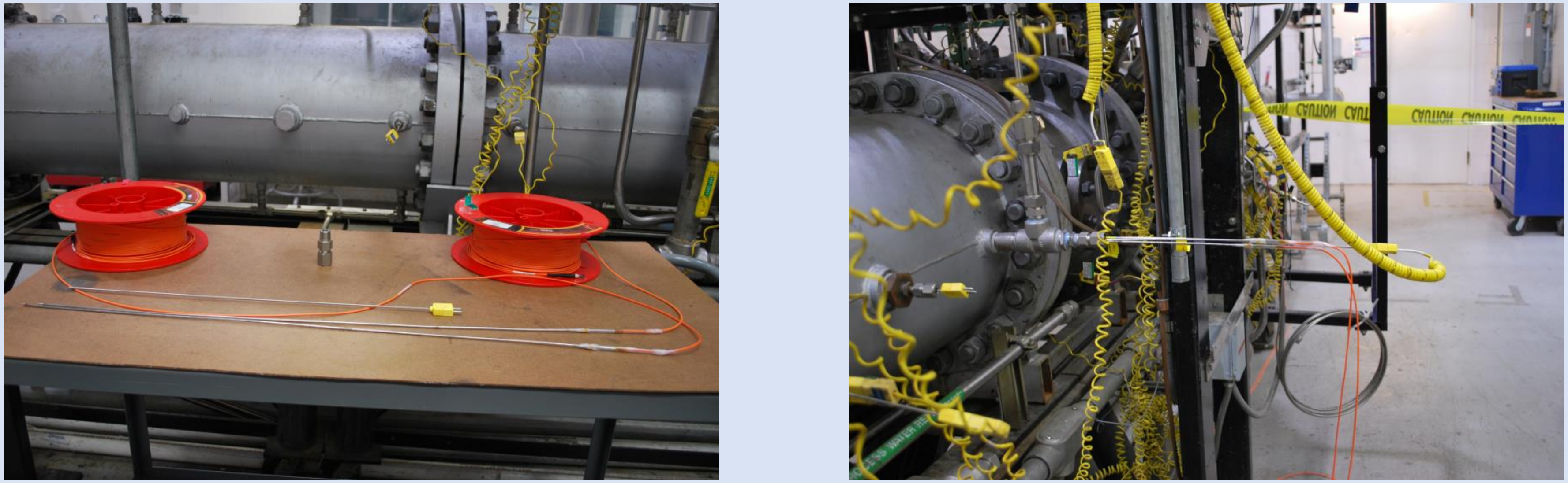


Accomplishments: DTS in fossil – Pressurized Pulse Combustor

- Fully distributed sensing – 5 cm resolution
- Temperature measurements above 1100°C
- Multiple probes deployed (sapphire and YAG)
- Transients observed easily
- ROI filed on single-crystal optical fiber cladding for high-temperature operations (22N-14)



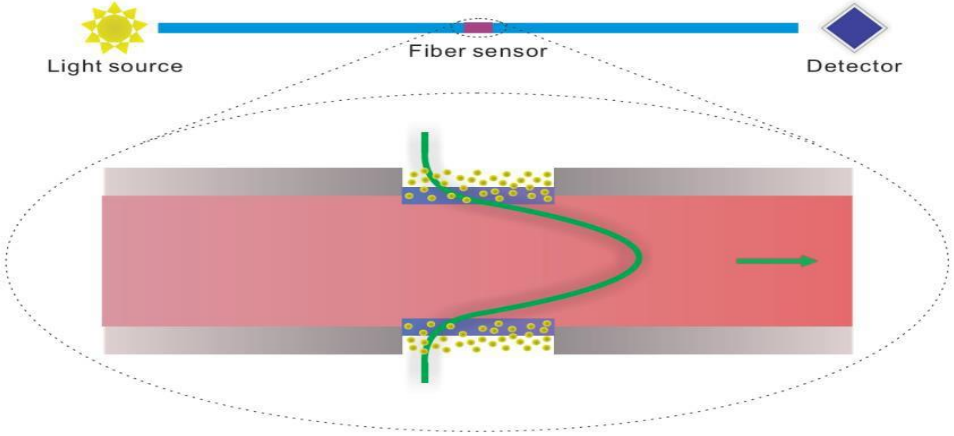


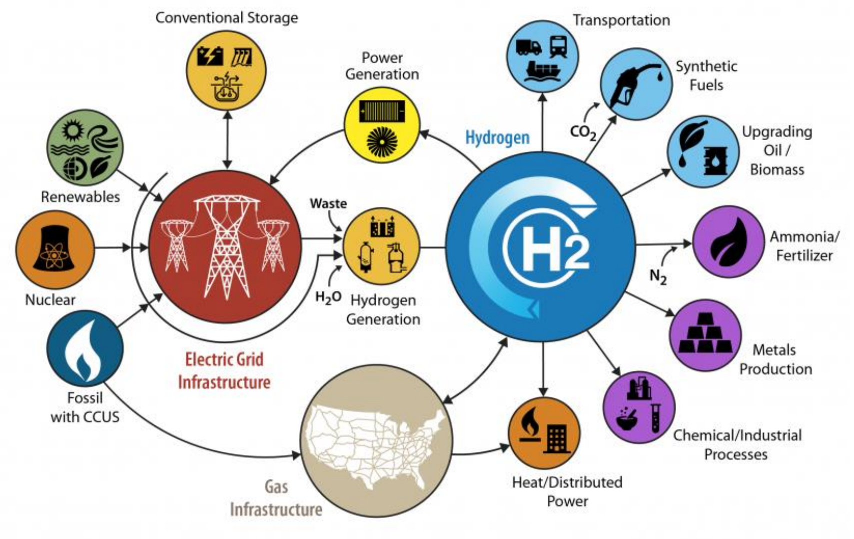


Two fiber-optic probes (sapphire and YAG) & thermocouple (left) and its installation on PPC test rig (right)

Tech info: Task 22 - optical fiber coatings for gas sensors

- **Task shifted from high-temperature O_2 sensing to H_2 sensing to support the new hydrogen economy**
- **Leverages new oxide materials, some from the SOFC world**
- **Begin with single-channel sensors; move to distributed**
- **Work approach:**
  - Deposition: sol-gel, sputtering, etc.
  - Select for responsivity, stability, and low cross-sensitivity
  - Explore cross-sensitivity mitigating over-layers for CH_4, CO, CO_2, H_2O
  - Initial tests on silica, later on SC fiber (target temperatures > 500 °C)



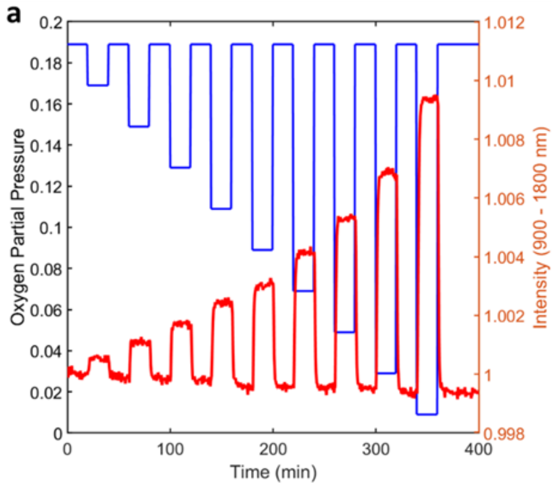


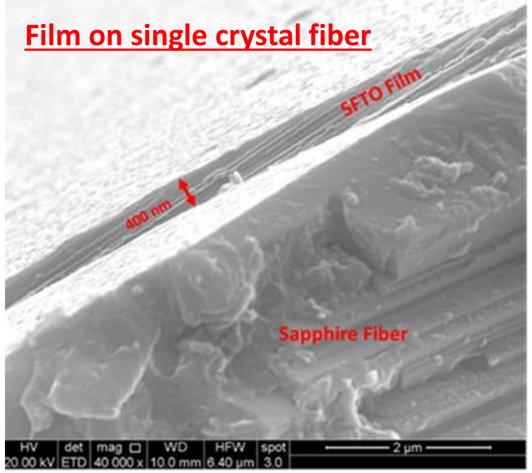
H_2@Scale

Accomplishments: Task 22 - optical fiber coatings for gas sensors

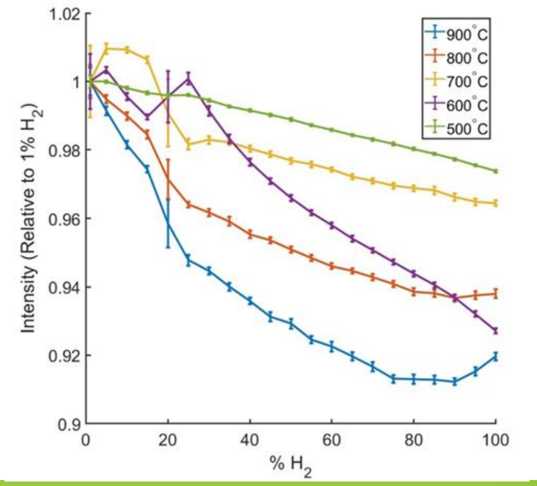
- **Completed testing of $La_{0.30}Sr_{0.70}TiO_3$ sensing layer on single crystal sapphire fiber:**
  - Alternate structures investigated to improve response – (Au nanorod embedded fibers).
  - Thin (~5 nm) silica overcoat investigated for improved stability and reduced cross-sensitivity.
- **Research Products:**
  - Presented at SPIE Photonics West 2023 and published in proceedings (Wuenschell, et al. "Optical gas sensing at extreme temperatures using perovskite oxides on single crystal fiber." *Oxide-based Materials and Devices XIV*. Vol. 12422. SPIE, 2023.)
  - ROI on single crystal fiber oxygen sensor presented to IRB, follow-up work currently in progress (23N-07).
  - Journal article submitted to *Sensors and Actuators B* and currently under review.

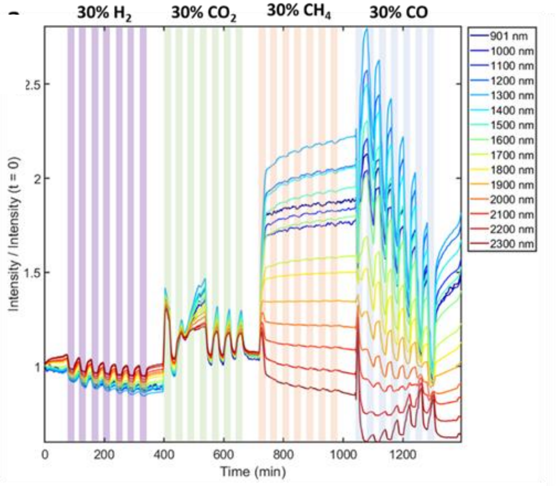
Oxygen Sensing w/ STFO film at 800 °C





Hydrogen Sensing w/ LSTO film at 500-900 °C





Major Conclusions

- 2 new inventions this year!
- World's only dual LHPG system for cladding application
- Unique DTS system for single-crystal optical fibers
- New functional coatings for hydrogen sensing
- Distributed Fiber-optic sensing enabling amazing new capabilities

Measure where it counts!

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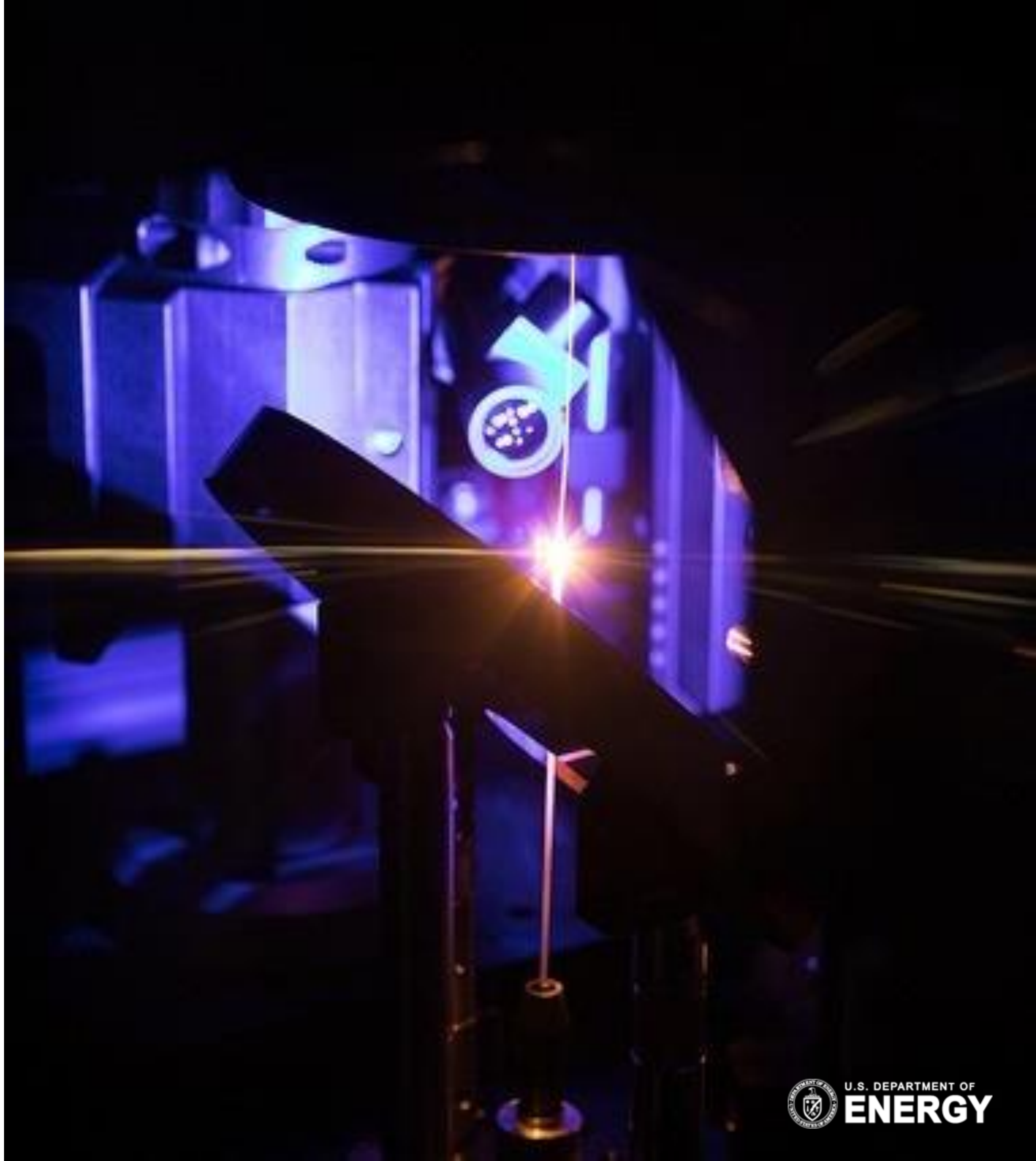


Application of Optical Fiber Distributed Temperature Measurement

J. Thapa, P. Muley, D. Shekhawat, B. Chorpening

Microwave reactor technology supports decarbonization

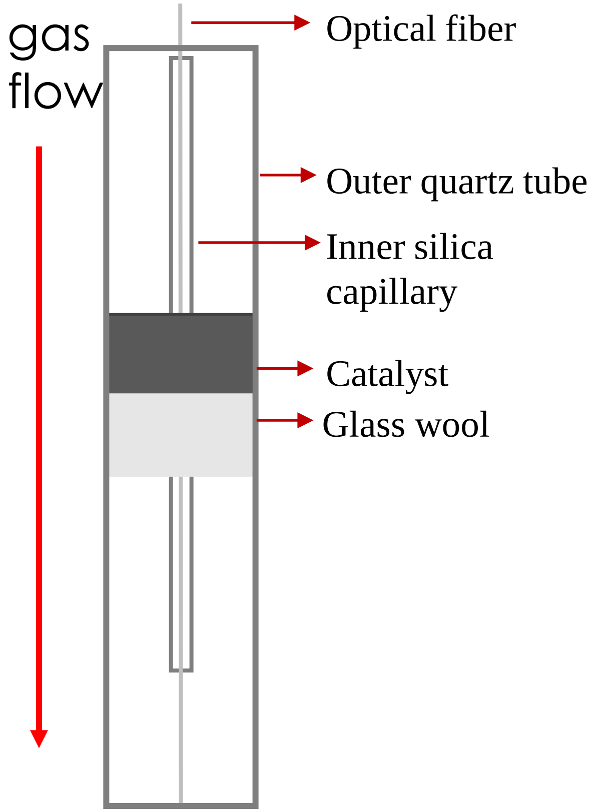
- Process intensification
- Methane mitigation
- Plastics conversion to H2
- Hydrogen or ammonia production

Difficult to perform measurements in the reactor

- High microwave energy
- Catalyst bed

Optical fiber sensing

ReACT Lab



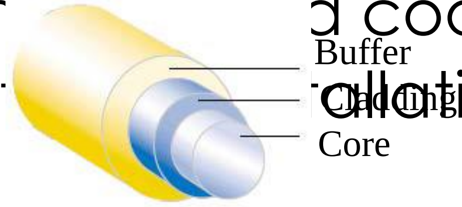
Apply COTS Interrogator

Assess performance

- Electrically heated plate system

Outside normal bounds for the optical fiber

- Singlemode fiber
- Beyond 300 C, plastic buffer melts and chars
- Car 'd coated
- Cus allation



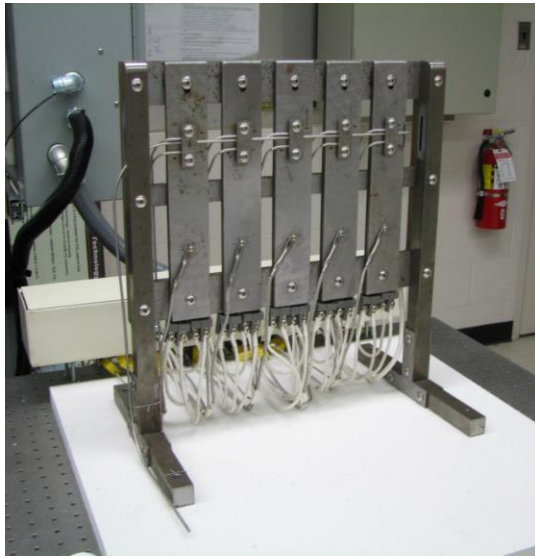
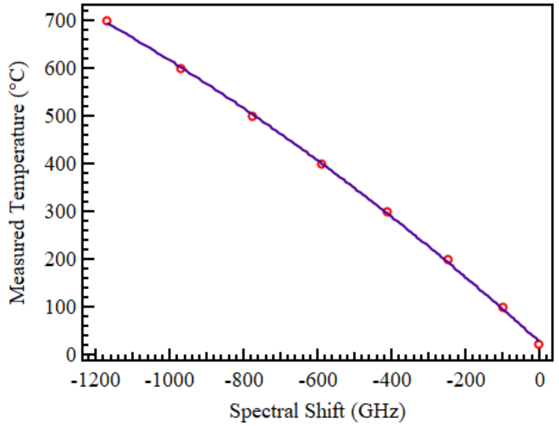
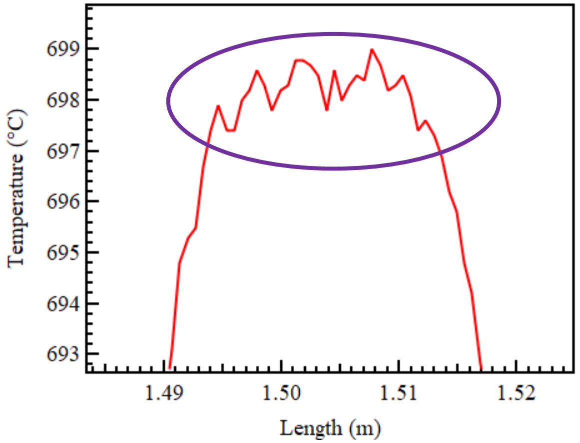


Plate heater test apparatus



Calibration curve



Fiber test in Plate Heater (plates heated to 701˚C per TC readings)

Application of Optical Fiber Distributed Temperature Measurement

Pretest

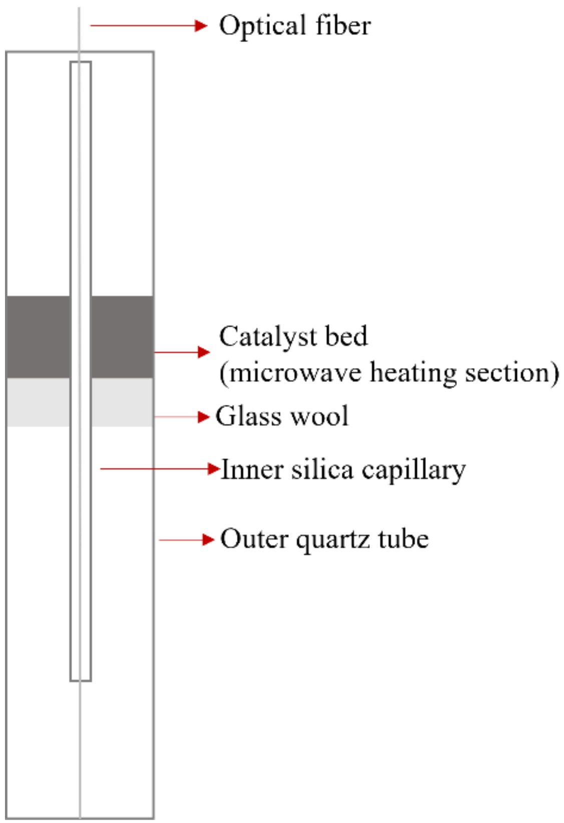
- Calibrated polyimide-removed silica optical fiber in the plate heater apparatus up to 700˚C at 0.65 mm gage pitch and 1 Hz
- Error less than 10˚C from 21→700˚C

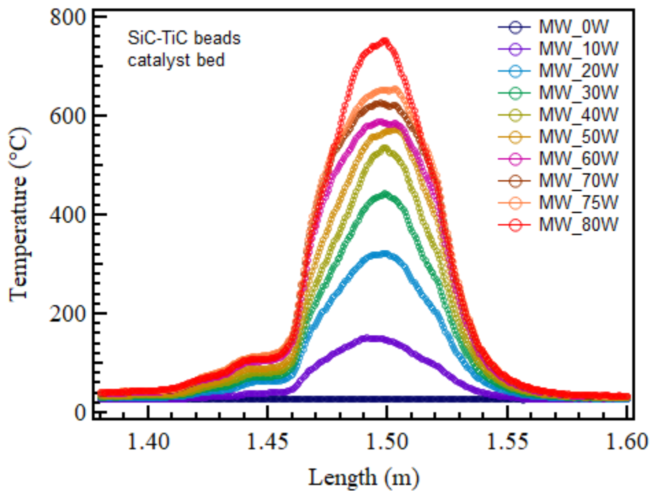
Optical fiber testing in microwave reactor conducted with 4 different catalysts

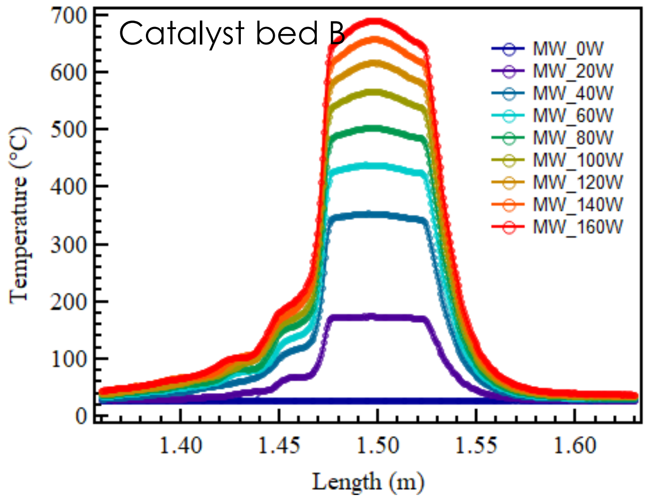
- Temperature profiles found to differ with catalyst
- Within bed temperature higher than the bed surface temperature (optical pyrometer)
  - Varies, ΔT up to 200°C observed
  - Results to be published

Future work

- Comparison with model of reactor bed
- Reacting flow testing
- Bed radial profile testing
- Higher resolution performance testing



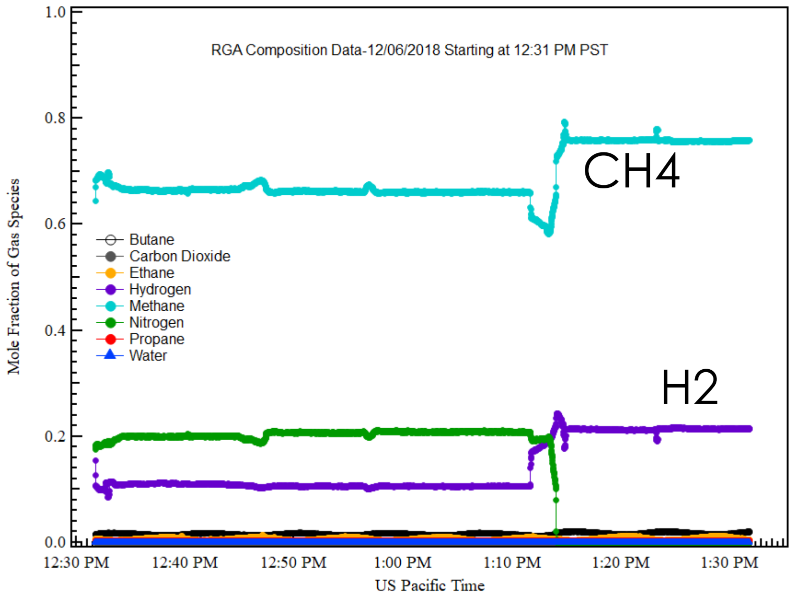


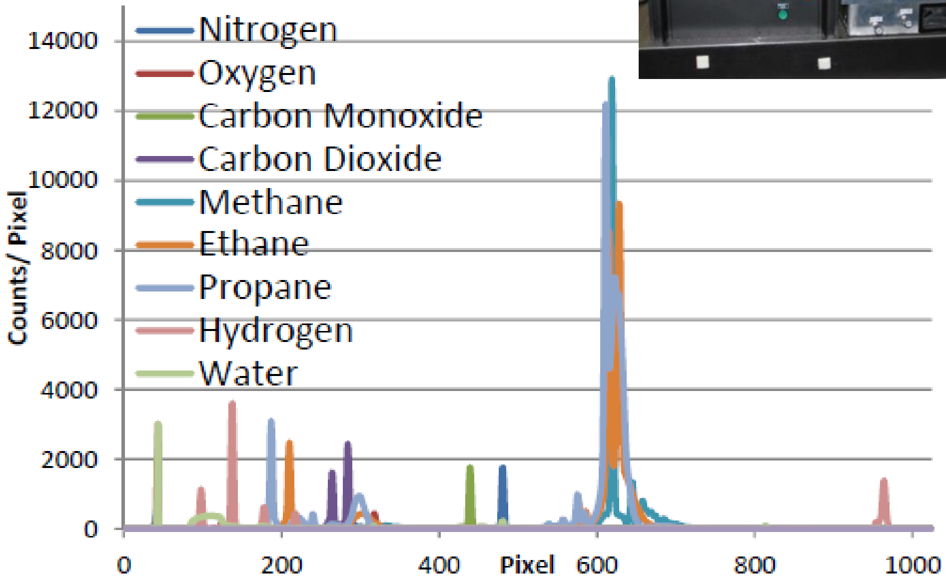


NETL Fast Raman Gas Analyzer

- Support transition to H_2 through H_2/NG blend turbines & systems
- Prototype tested in pilot scale laboratory applications (TRL 5-6)
- Fast - 1 second measurement time
- Species concentrations measured to 0.1%
- Optical waveguide technology boosts Raman signal more than 1000X
- EY23: Program and lab testing of smaller rack mount version

- 1000 psi
- Design for NEC Class 1 Div 2



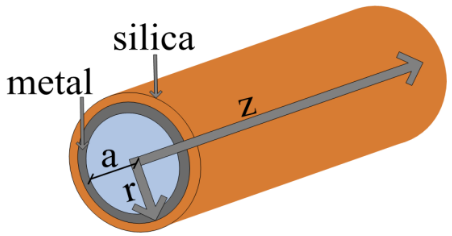


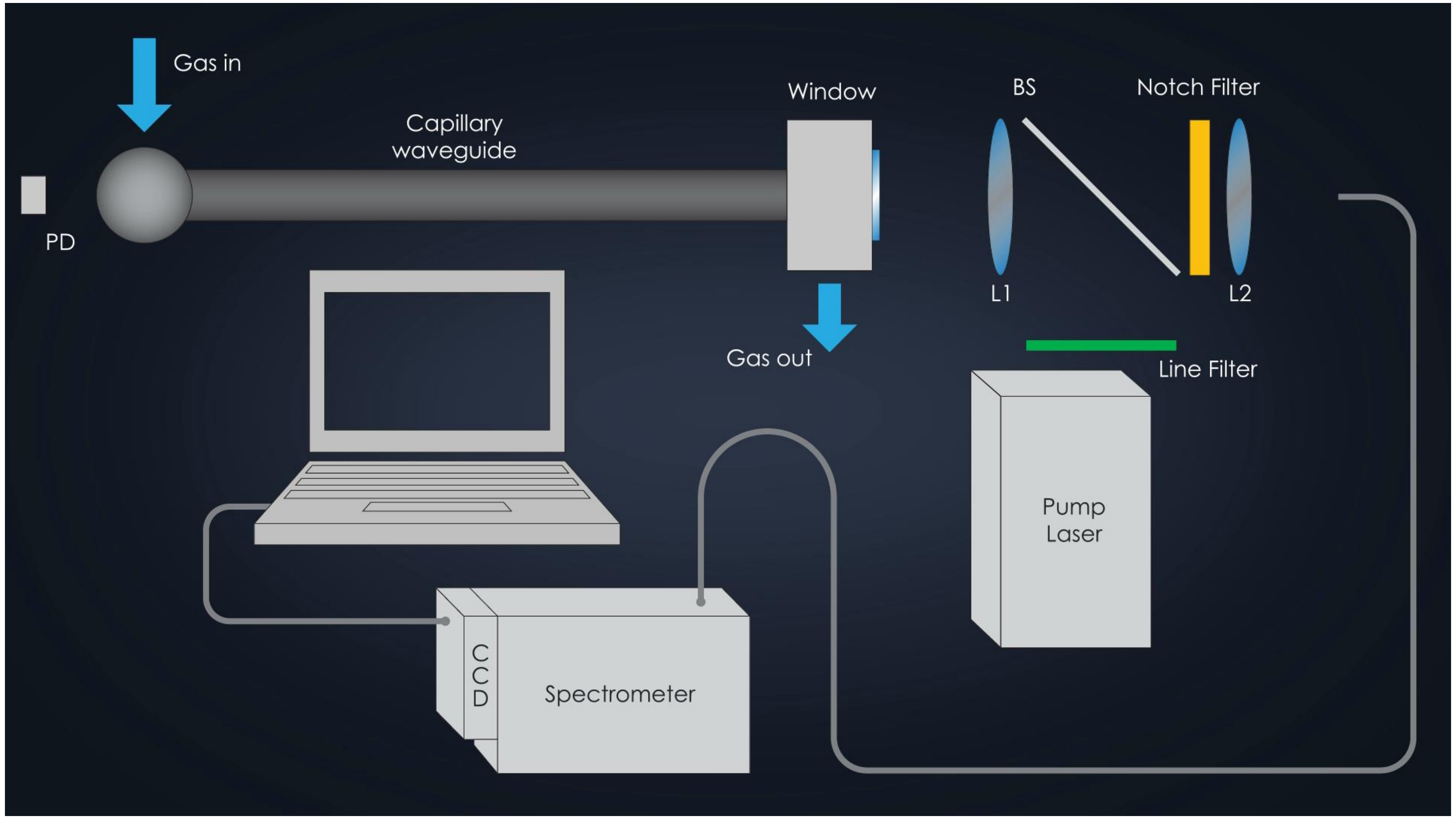
Waveguide Enhanced Raman System

- **SPEED**: One-second response time
- **ACCURACY**: Sub-percent for all molecular species with little cross sensitivity
- **SIMPLICITY/STABILITY**: Obtains all species at once with no tunable lasers, no pump power control

Novel configuration with capillary waveguide enables speed and accuracy.

US Patent 8,674,306, NETL and University of Pittsburgh

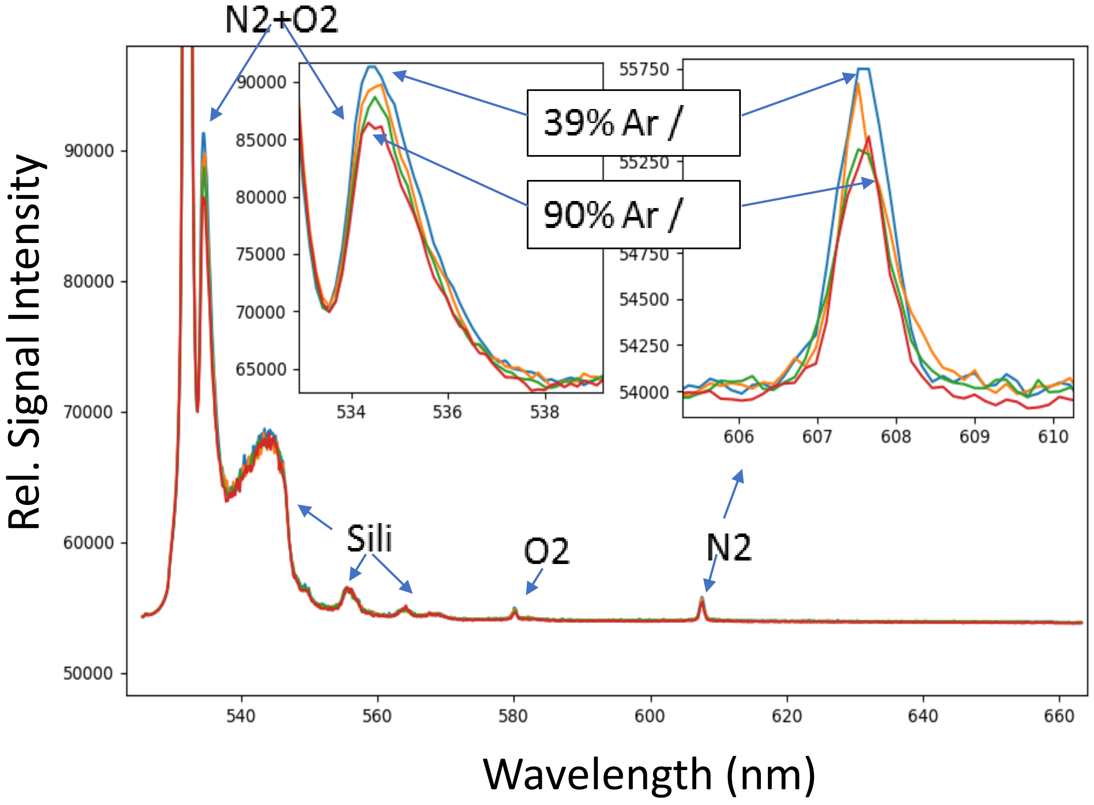




Ultrafast Laser Measurements for Harsh Environments

Task 48 Objectives

- Design pulsed Raman system for spatially resolved measurements in gasifiers or other large industrial systems
- Assemble higher resolution prototype using existing laser, detector, and optics
- Test and apply to field measurements
- Explore Scheimpflug LIDAR as an alternative approach with lower equipment costs



Laser-based measurement of species/temperature along a line of sight with spatial resolution and single point access

Ultrafast Laser Measurements for Harsh Environments

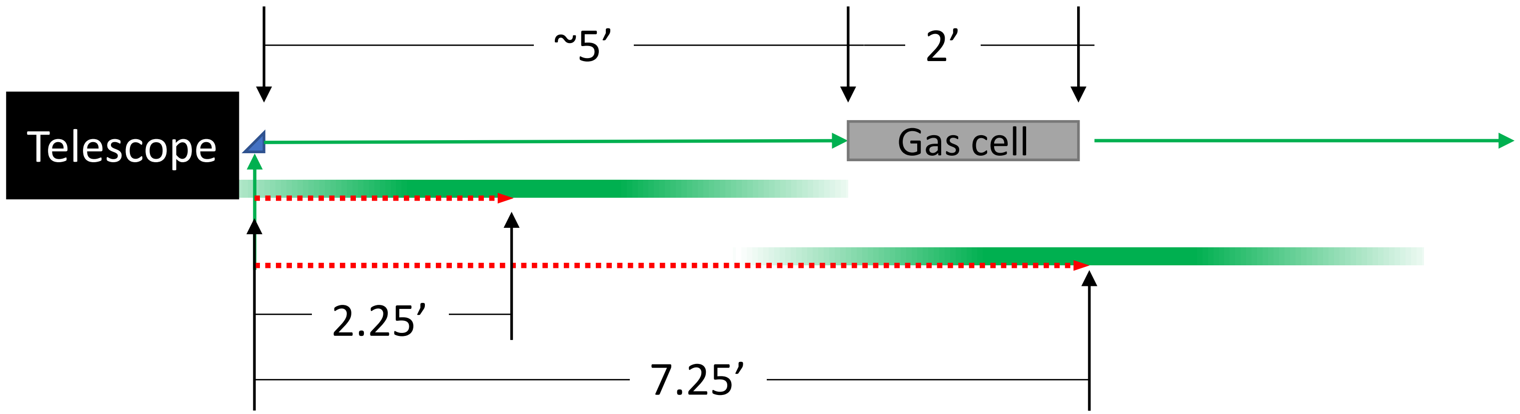
NATIONAL ENERGY TECHNOLOGY

Task 48 Initial exploration

Time Domain Raman Scattering Spectroscopy
- Line of sight molecular measurement

Resolution based on laser pulse width (6ft)
- Shorter laser pulse improves resolution

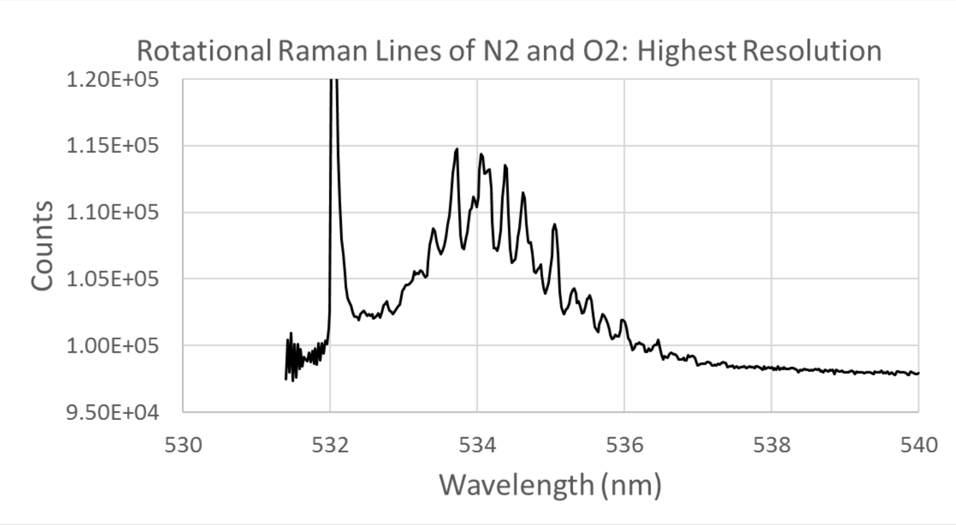
Detector timing is critical to capturing data
- Temperature
- Molecular Species

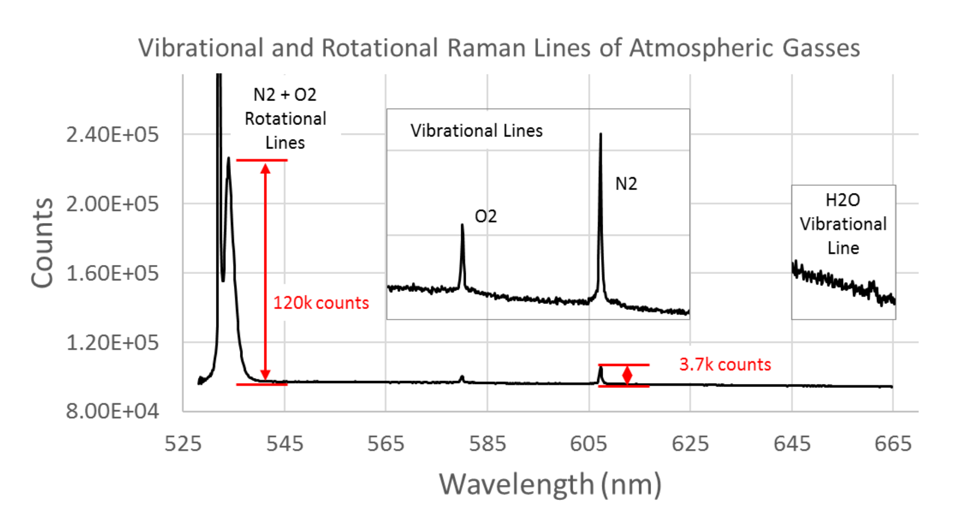


Ultrafast Laser Measurements for Harsh Environments

Task 48 Update

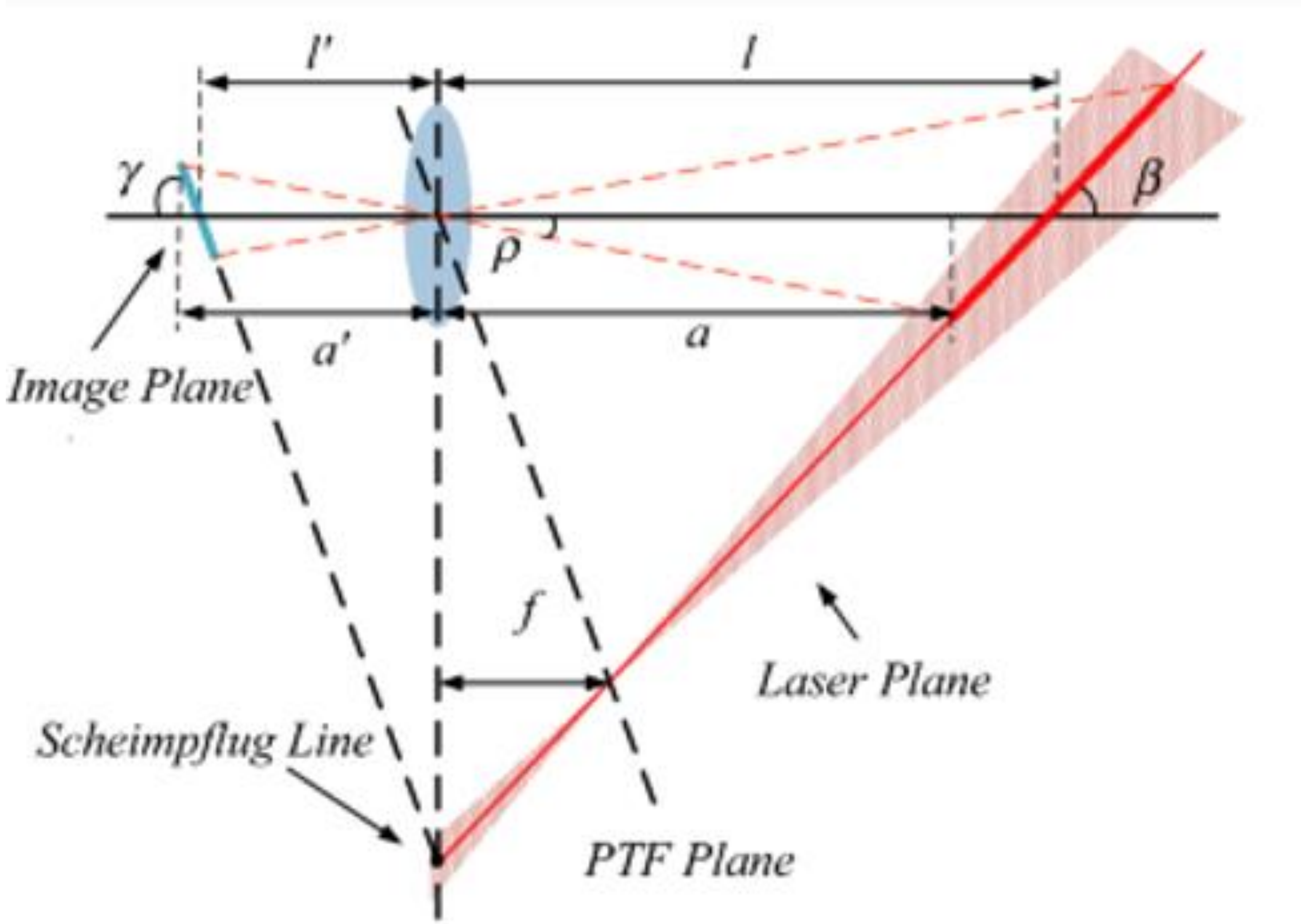
- Proof of concept Raman LIDAR system built
  - Pure vibrational and rotational Raman lines of N_2 and O_2 (rotational lines are ~30x more intense) at room temperature
- Preparations for high temperature testing completed
  - Tube furnace configured to test flue gas components (e.g., N_2, O_2, H_2O, CO_2)
- Custom optical arrangement for improving resolution has been designed and components ordered
- Scheimpflug optical arrangement currently under test to improve spatial resolution.
- Precise gas mixing apparatus has been engineered and constructed completed, testing to follow.

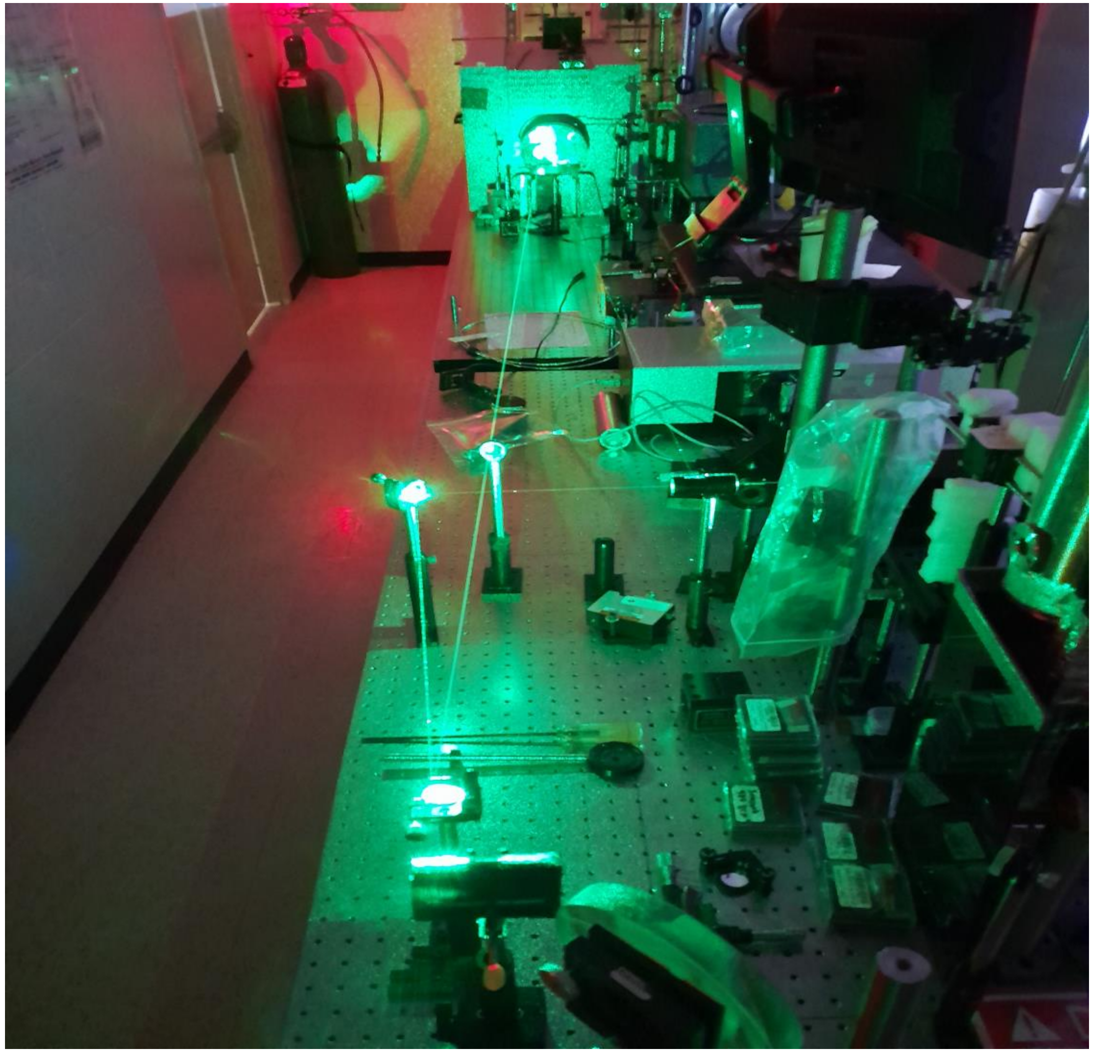




Ultrafast Laser Measurements for Harsh Environments

Task 48 Scheimpflug Optical measurements





Ultrafast Laser Measurements for Harsh Environments

Task 48 Scheimpflug measurements

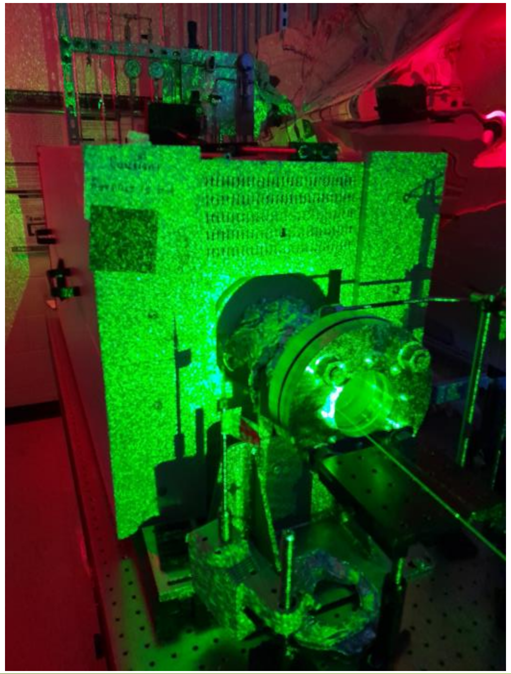
Initial Scheimpflug measurements show ability to measure temperature and species well

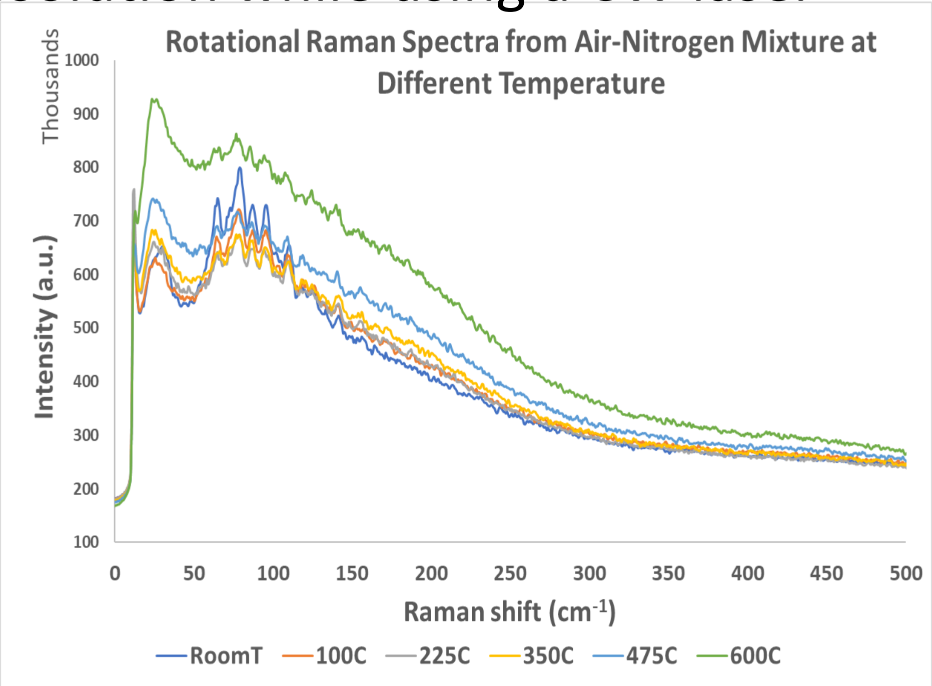
Significantly reduce laser probe requirements

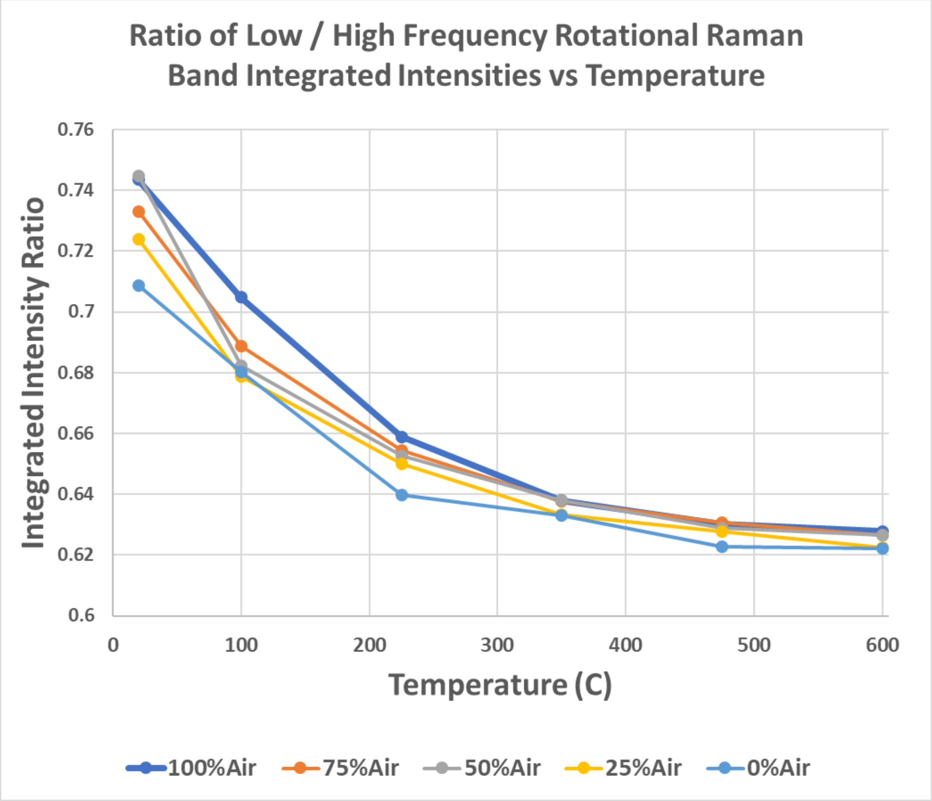
Increase measurement integration time

Eliminate need for precise timing

Significantly improve resolution while using a CW laser



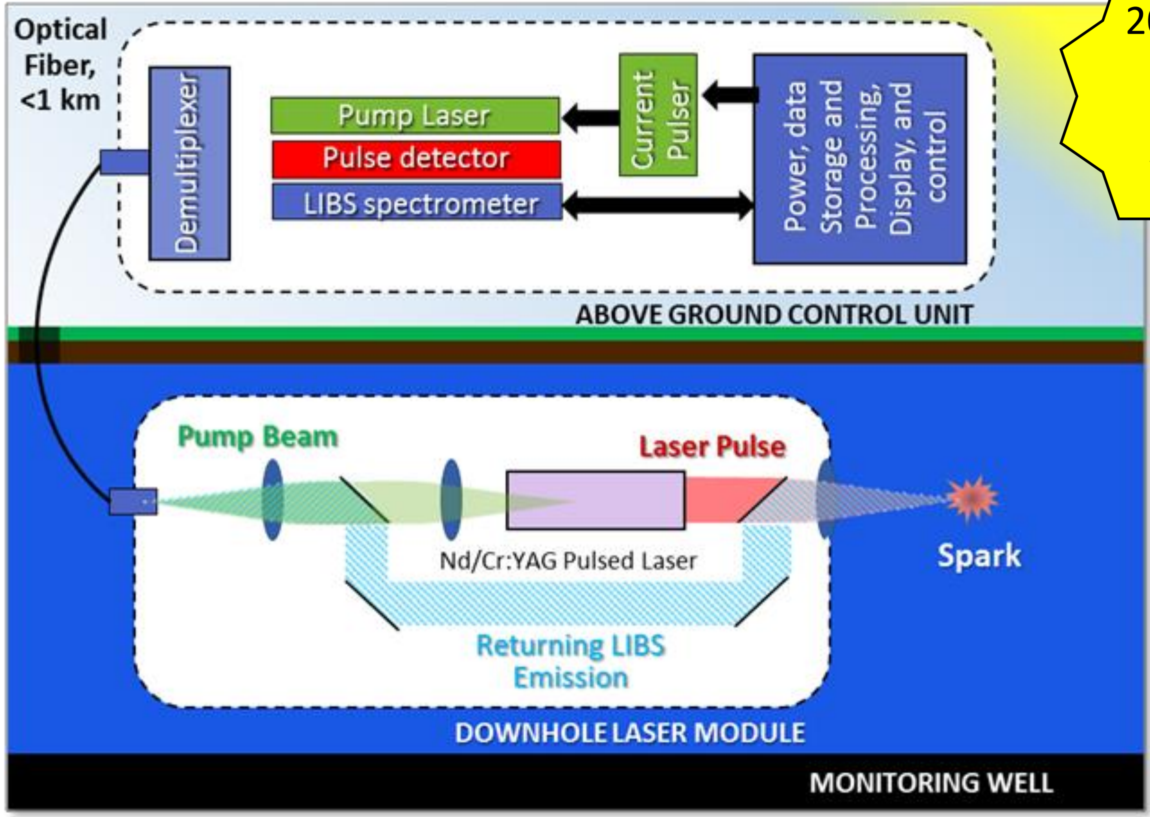




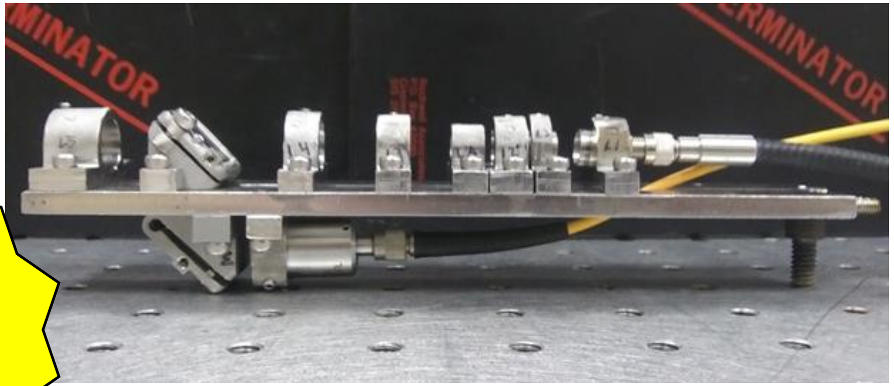
LIBS for Subterranean Sensing

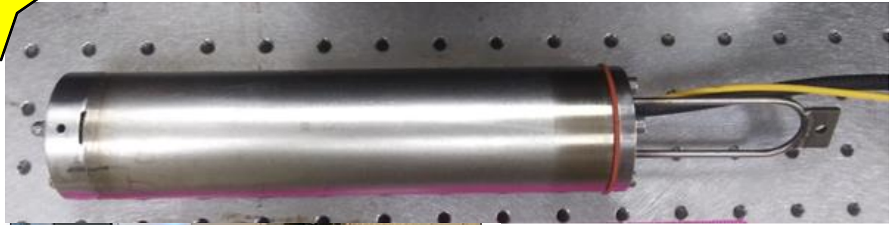
Task 71 Objectives

- Development, optimization and testing of a deployable miniaturized LIBS system for subterranean chemical sensing



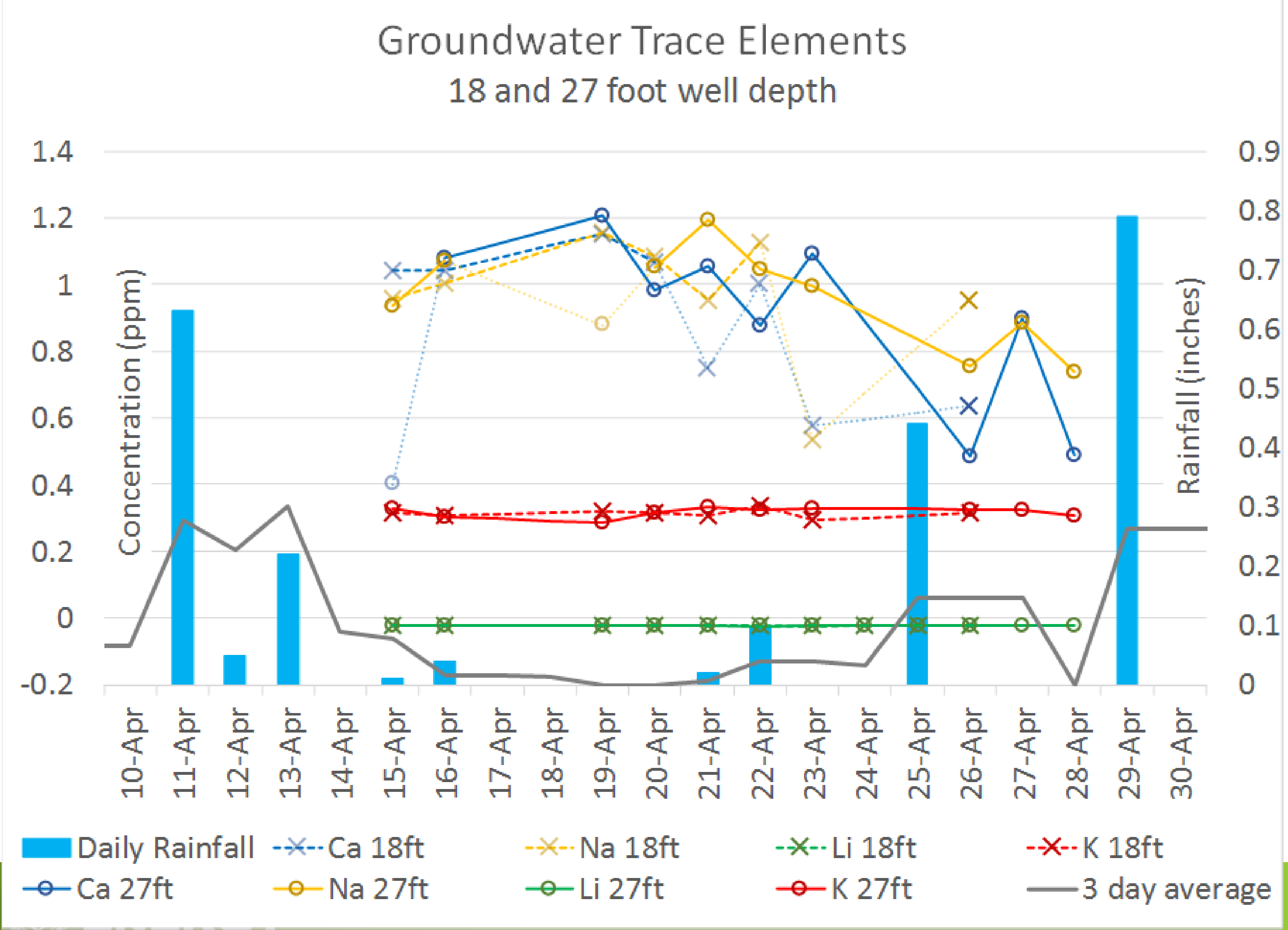
2019 R&D 100 Award Winner





LIBS for Subterranean Sensing

Task 71 downhole data



Element calibrations performed prior

Multiple depths interrogated

Each data point is a few hundred spectra

Rainfall dilution indicated for Na and Ca

K appears unaffected

Li too low to measure (LOD = 8ppb in lab)

LIBS for Subterranean Sensing

Task 71

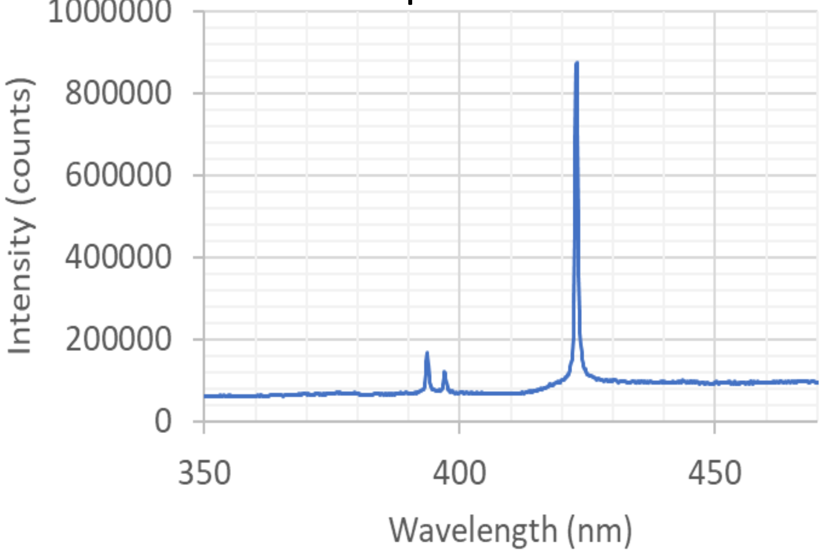
Bubble production during measurements forced a minor change in probe design

LIBS for Subterranean Sensing

Task 71 Update

- Replacement parts on order
- Planning of next deployment complete
- Publications in process
- Patent issued 11,451,004

Calcium spectra in water



US011451004B2

(12) **United States Patent**
McIntyre et al.

(10) **Patent No.: US 11,451,004 B2**
(45) **Date of Patent: Sep. 20, 2022**

(54) **DOWNHOLE LASER SYSTEM WITH AN IMPROVED LASER OUTPUT PRODUCTION AND DATA COLLECTION**

(71) Applicant: **United States Department of Energy**, Washington, DC (US)

(72) Inventors: **Dustin McIntyre**, Washington, PA (US); **Daniel Hartzler**, Westover, WV (US)

(73) Assignee: **U.S. Department of Energy**, Washington, DC (US)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 23 days.

(21) Appl. No.: **17/074,162**

(22) Filed: **Oct. 19, 2020**

(65) **Prior Publication Data**

US 2021/0119403 A1 Apr. 22, 2021

Related U.S. Application Data

(60) Provisional application No. 62/916,508, filed on Oct. 17, 2019.

(51) **Int. Cl.**
G01J 3/46 (2006.01)
H01S 3/106 (2006.01)
H01S 3/094 (2006.01)
H01S 3/11 (2006.01)
G01N 21/31 (2006.01)

(52) **U.S. Cl.**
CPC ***H01S 3/106*** (2013.01); ***G01N 21/31*** (2013.01); ***H01S 3/094038*** (2013.01); ***H01S 3/094053*** (2013.01); ***H01S 3/094096*** (2013.01); ***H01S 3/11*** (2013.01); *G01N 2201/0633* (2013.01); *G01N 2201/0634* (2013.01); *G01N 2201/0636* (2013.01); *G01N 2201/06113* (2013.01); *G01N 2201/08* (2013.01)

(58) **Field of Classification Search**
CPC H01S 3/106; H01S 3/094038; H01S 3/094053; H01S 3/094096; H01S 3/11; H01S 3/1024; H01S 3/113; G01N 21/31; G01N 2201/06113; G01N 2201/0633; G01N 2201/0634; G01N 2201/0636; G01N 2201/08; G01N 21/718; G01N 2021/1793; G01J 3/0208; G01J 3/021; G01J 3/0218; G01J 3/443
USPC 356/402
See application file for complete search history.

(56) **References Cited**

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10,145,737 B1 * 12/2018 McIntyre H01S 3/0941
2019/0386449 A1 * 12/2019 McIntyre H01S 3/094038

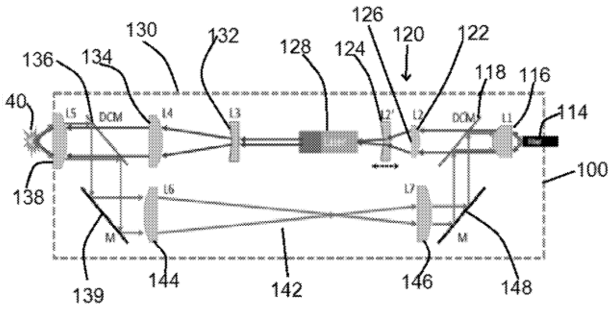
* cited by examiner

Primary Examiner — Md M Rahman
(74) *Attorney, Agent, or Firm* — Timothy L. Harney; Michael J. Dobbs; Brian J. Lally

(57) **ABSTRACT**

One or more embodiments relates to a method of growing ultrasmooth and high quantum efficiency CsTe photocathodes. The method includes exposing a substrate of Cs using an alkali source such as an effusion cell; and controlling co-evaporating growth and co-deposition forming a CsTe growth. The method further includes monitoring a stoichiometry of the CsTe growth.

6 Claims, 5 Drawing Sheets



- Metrolaser TTO Phase I
- Further simplify and productize
- Improve laser probe output
- Provide lower cost sensing options
- Metrolaser TTO Phase II
- License technology
- Finalize design of system
- Offer system for sale
- Collect in-situ data at multiple sites
- Continue collaboration to document technical success

Advanced Control Sensors – David Tucker, Farida Harun, Nana Zhou

Task 52.0: Cyber-Physical Systems as an Integrated Energy System (IES) Development Tool

NATIONAL ENERGY TECHNOLOGY LABORATORY

Milestones

Development of cycle concepts that include thermal energy storage and CO_2 capture

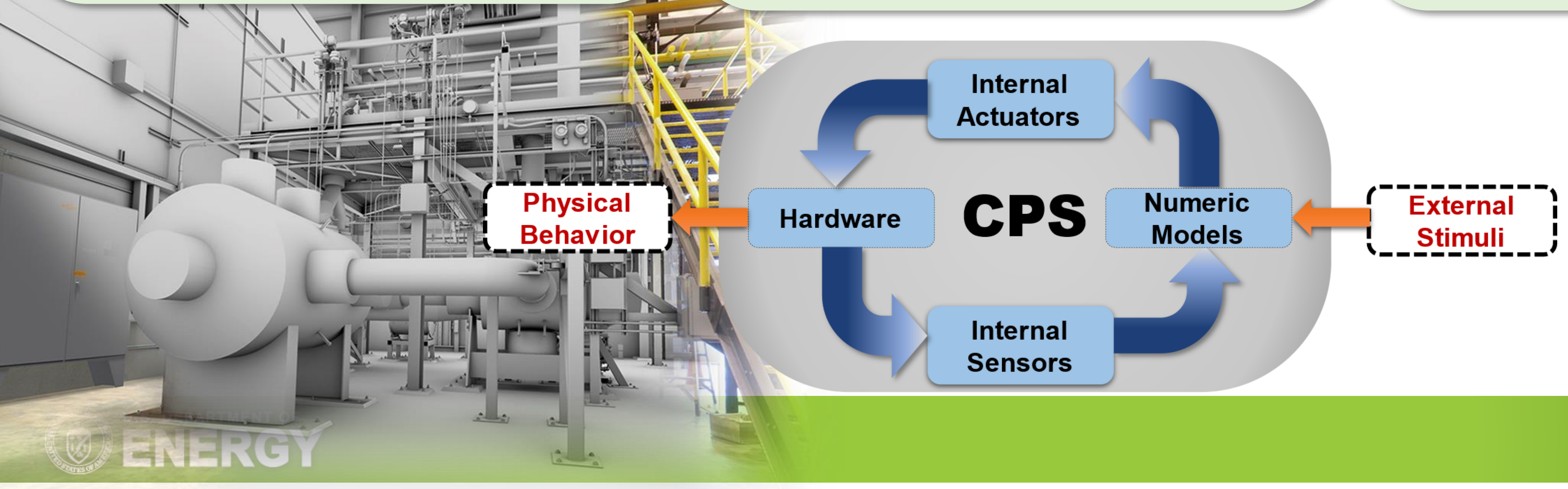
Identified cycle configurations that would have **high efficiency** and include thermal energy storage and CO_2 capture

Development of conceptual design of an IES with thermal energy storage and CO_2 capture

Developed a complete conceptual design with **anticipated costs and benefits**

Preliminary control evaluation of the concept cycle

Assessed **possible issues and opportunities** that could be further identified using **cyber-physical** approach.

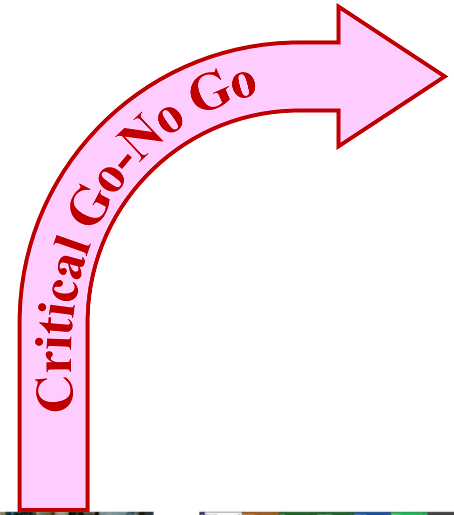


Cyber Physical Systems are used to replace physical components that:

1. *are irreplaceable*
2. *are expensive*
3. *are unable to meet performance targets*
4. *don't exist…yet*

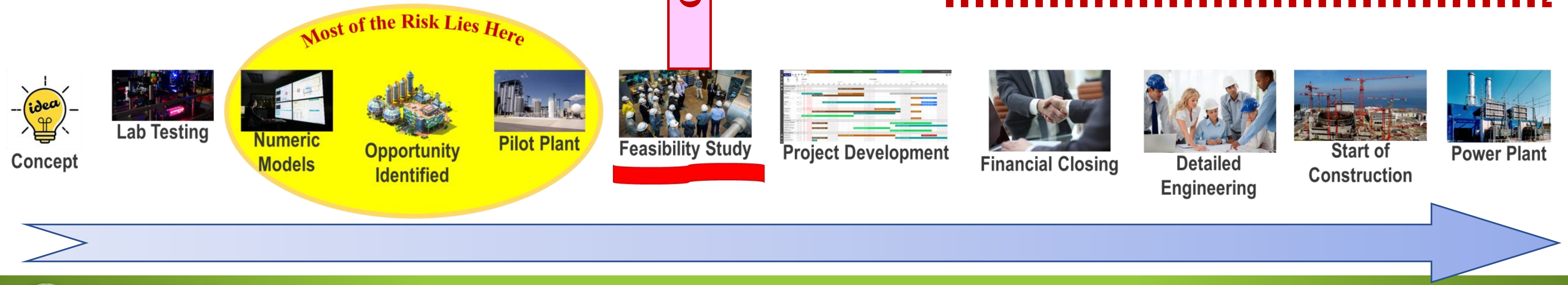
Technology Development Today

- The current technology paradigm requires two decades (P&CM)
- The highest risk is always associated with pilot development
- Critical Go-No Go relies on a pilot scale technical assessment

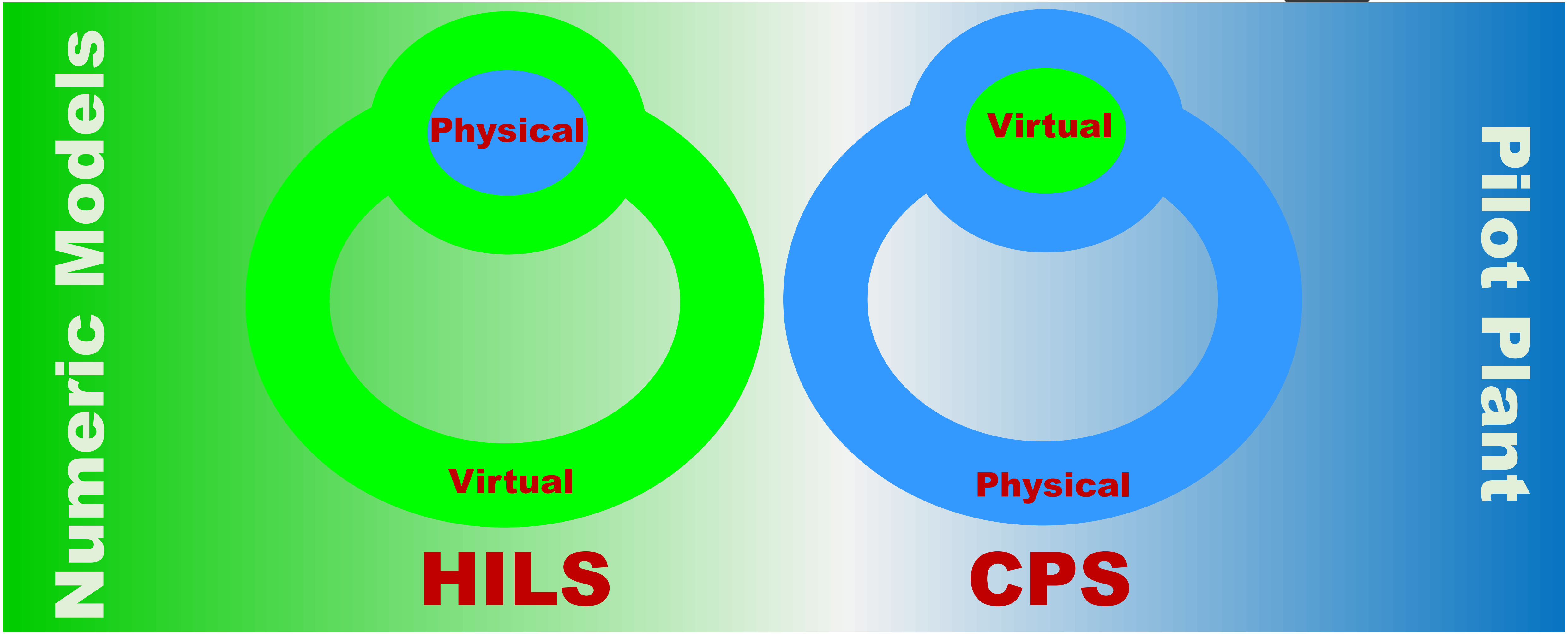


1. Conduct Initial Assessments
   a. Engineering
   b. Environmental
   c. Economic
   d. Legal
2. Technical Assessment
3. Conceptual Costs and Schedule
4. Summarize Results
5. Management Direction

1. Fuel Type/Availability
2. Technical Risk
3. Controls Development
4. Uprate Capability
5. Time to Construct
6. Emissions
7. Reliability, Availability, Maintainability
8. Footprint
9. Delivery Schedule
10. Delivery Logistics
11. Cycling Capability
12. Fuel Flexibility
13. Equipment Costs

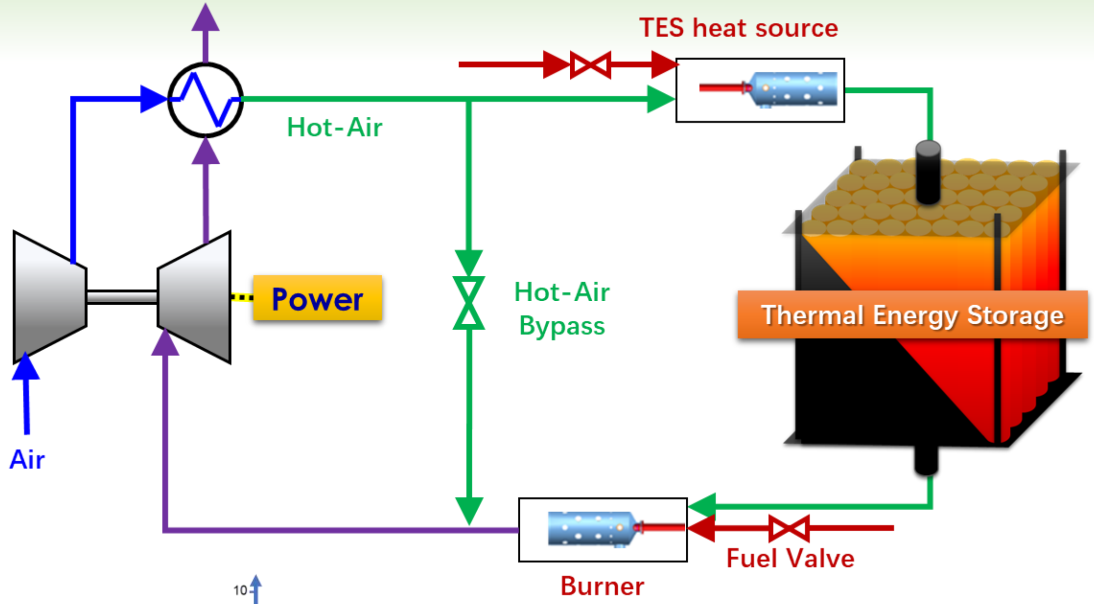


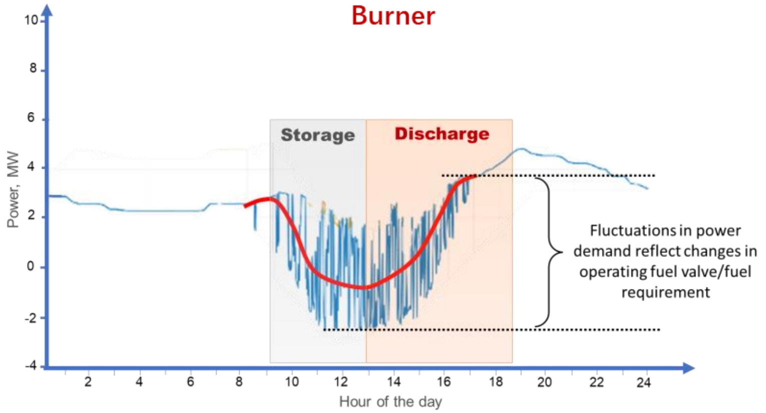
Hardware in the Loop vs Cyber Physical



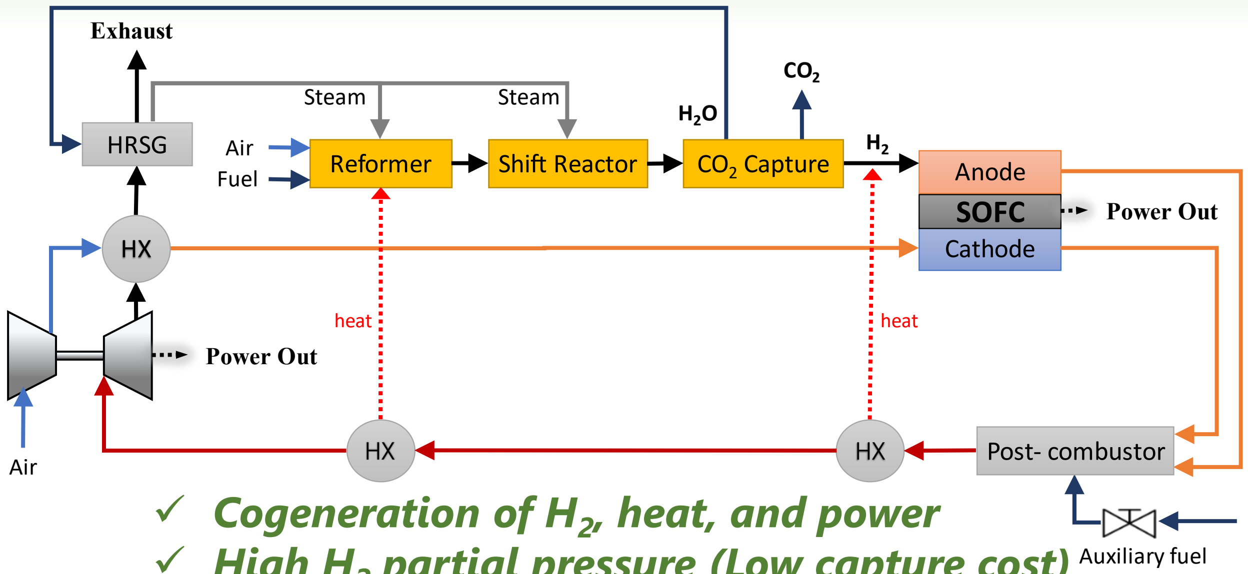
IES Cycles: Thermal Energy Storage and CO_2 Capture

Concept 1: Thermal Energy Storage





Concept 2: CO_2 Capture Cycle

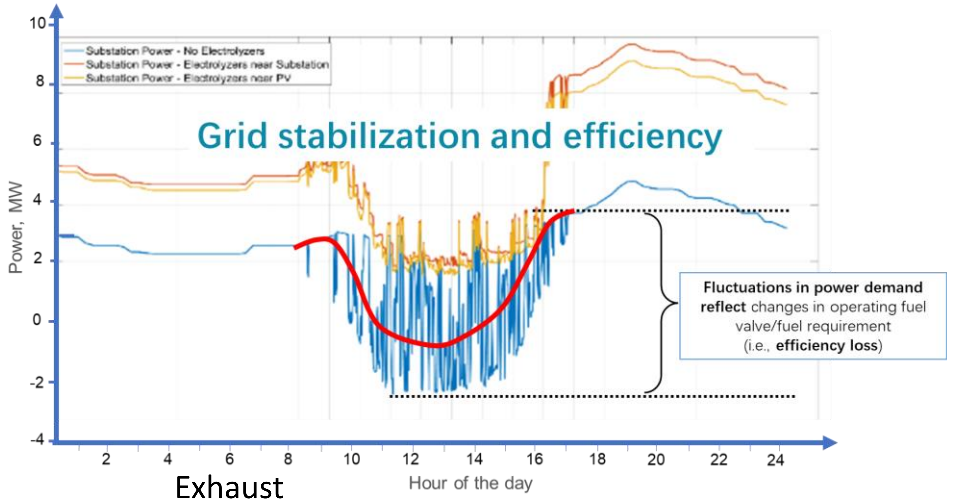


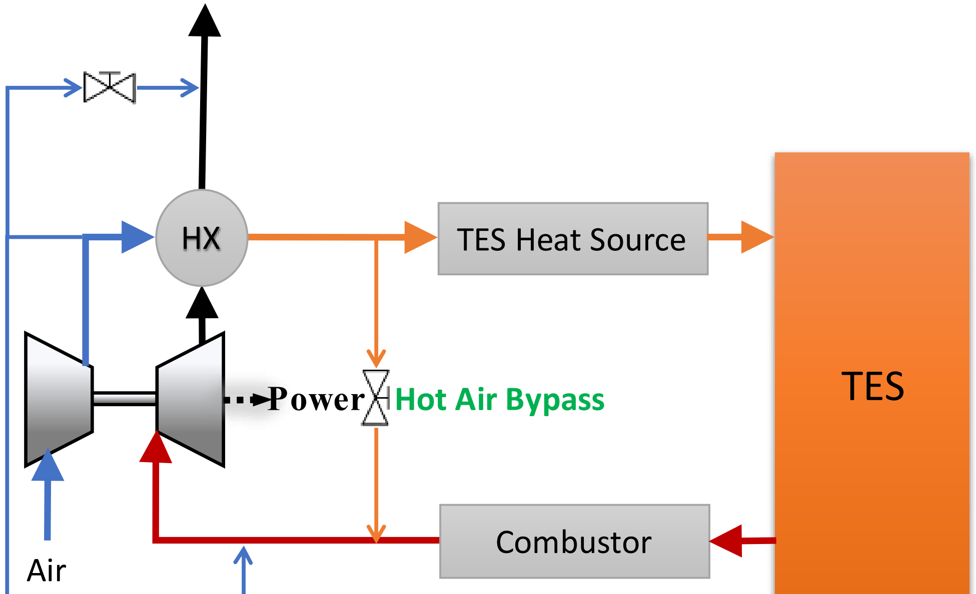
- ✓ *Cogeneration of H_2, heat, and power*
- ✓ *High H_2 partial pressure (Low capture cost)*
- ✓ *Low pressure and high efficiency*
- ✓ *Chemical capacitance in carbon capture*
- ✓ *Heat sink of fuel reforming for TIT control*
- ✓ *HX required*
- ✓ *High temperature- membrane or temp swing*
- ✓ *Anode preheat required*
- ✓ *Complicated shift reactor control*

U.S. DEPARTMENT OF ENERGY

Proof of Concept of a Thermal Energy Storage (TES) System

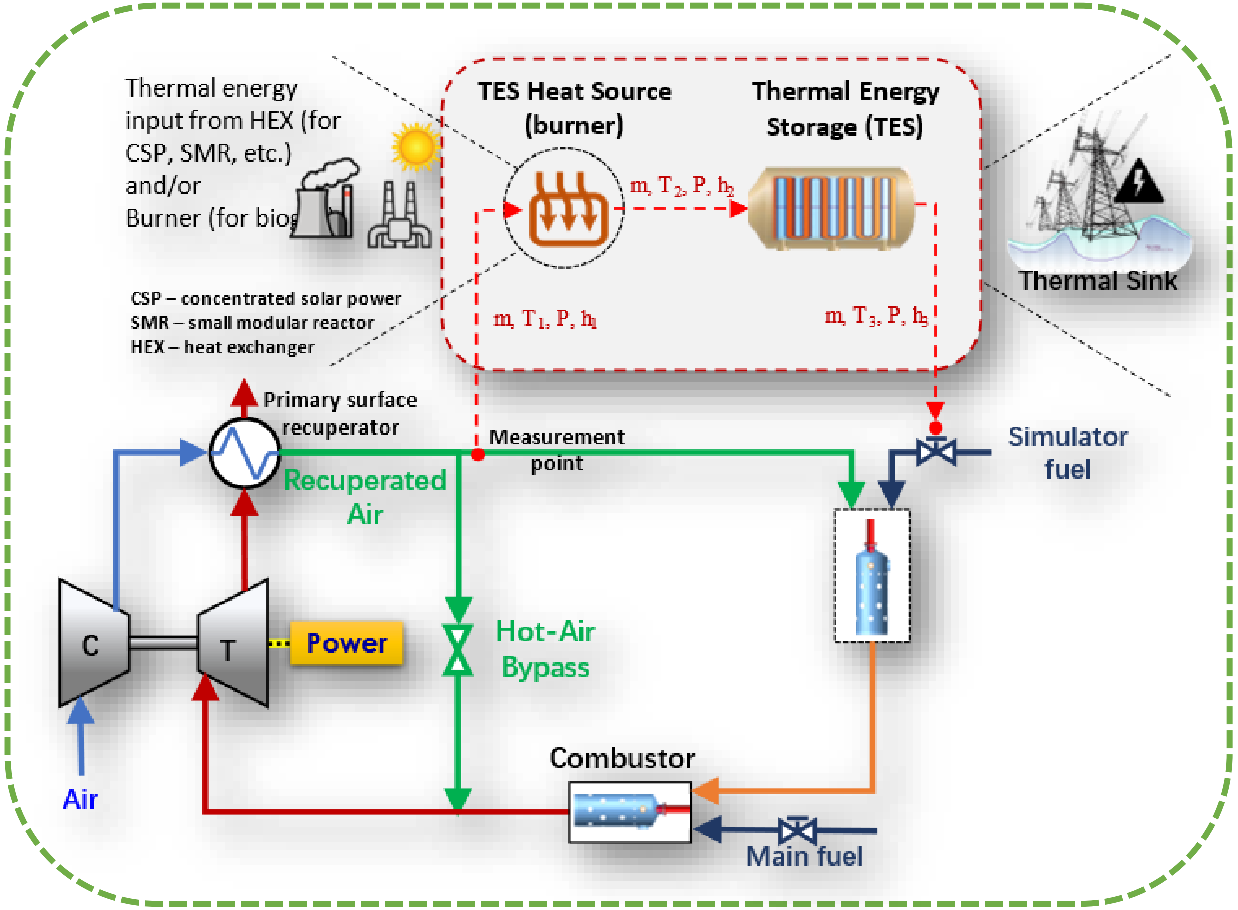
THERMAL ENERGY STORAGE CONCEPT





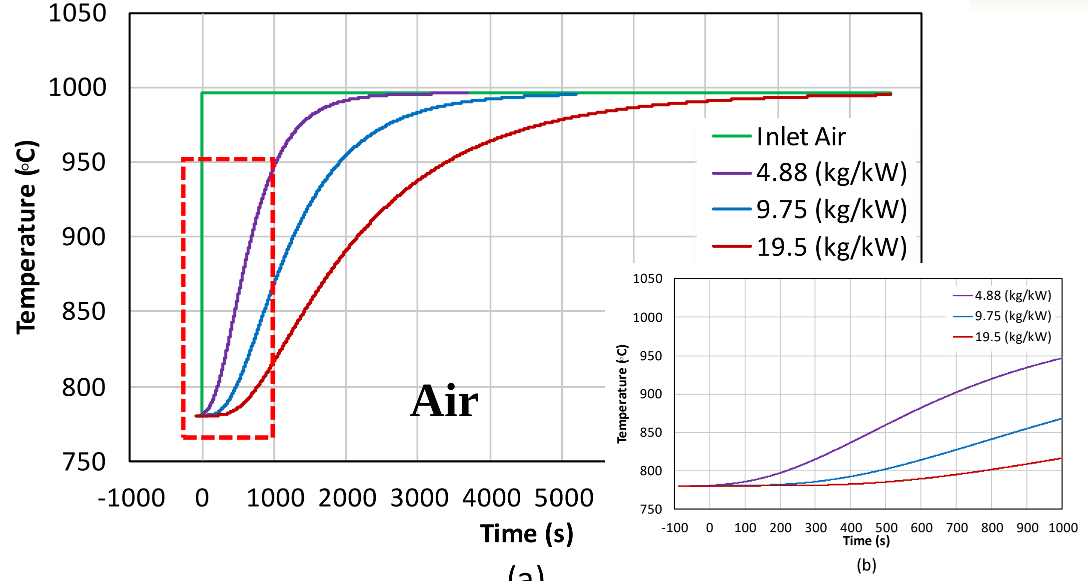
Simplified process flow of an ***integrated thermal energy storage in a recuperated gas turbine system***

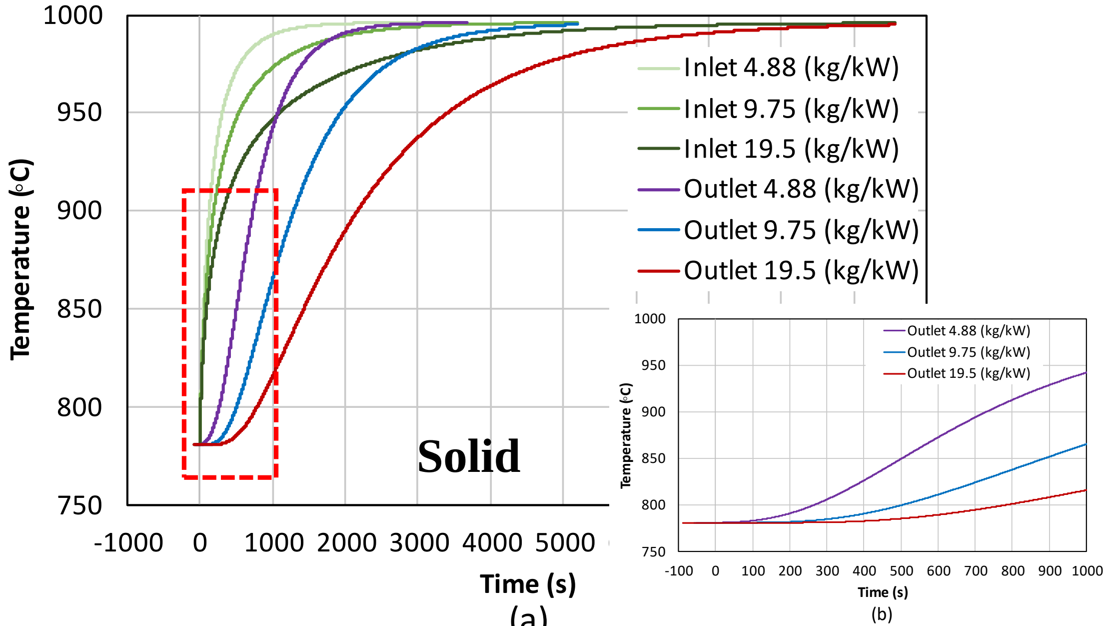
HARDWARE-BASED TEST IN HYPER



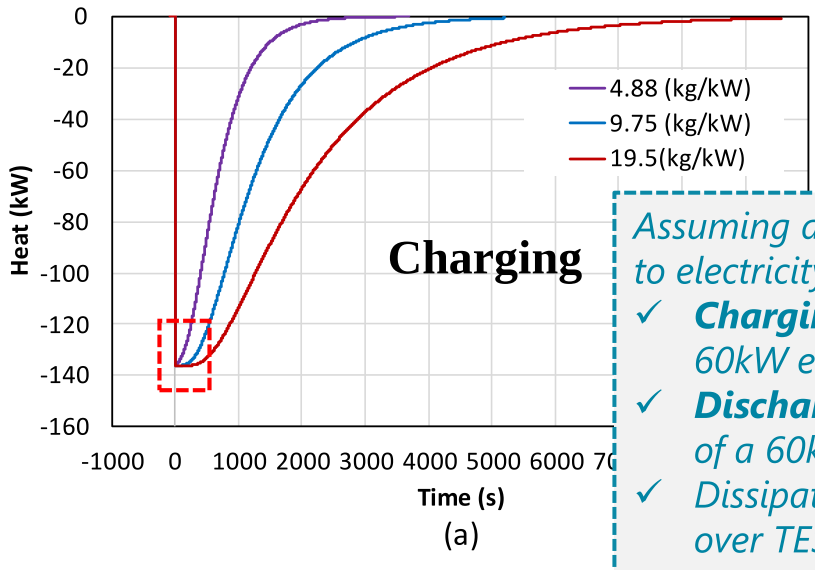
Control Strategy for TES: Air mass flow control

TEMPERATURE DYNAMICS (increase air bypass flow)



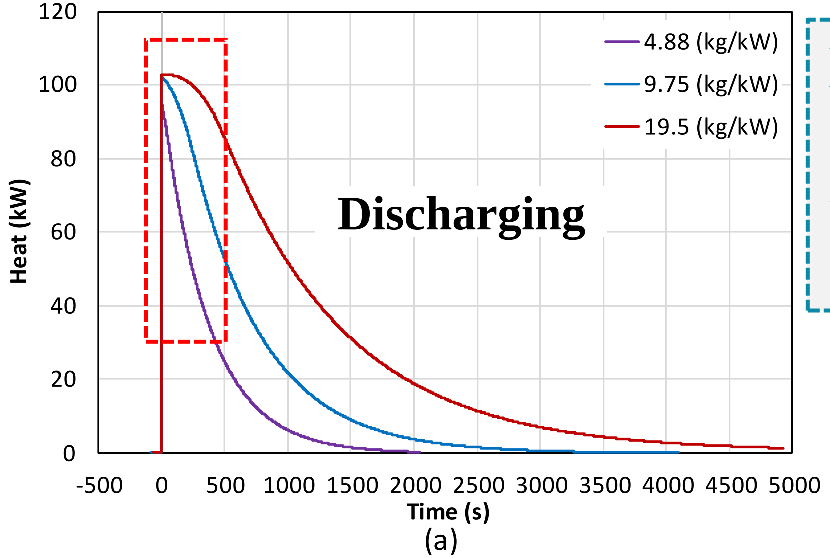


TES CAPACITY



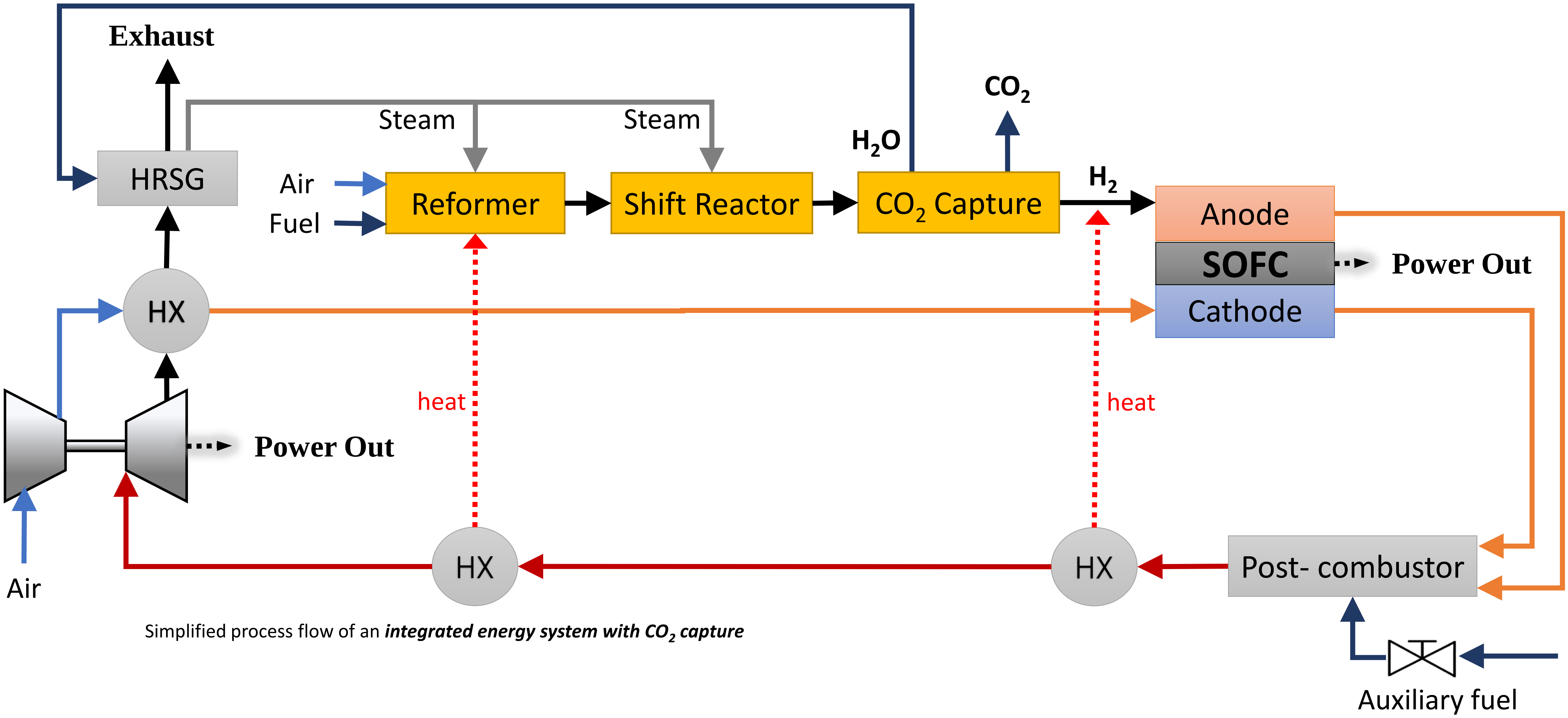
Assuming a 33% efficiency heat to electricity:

- ✓ ***Charging:** 135kW (**76%** of a 60kW electric load)*
- ✓ ***Discharging:** 103 kW (**57%** of a 60kW electric load)*
- ✓ *Dissipation rate is a function over TES size*



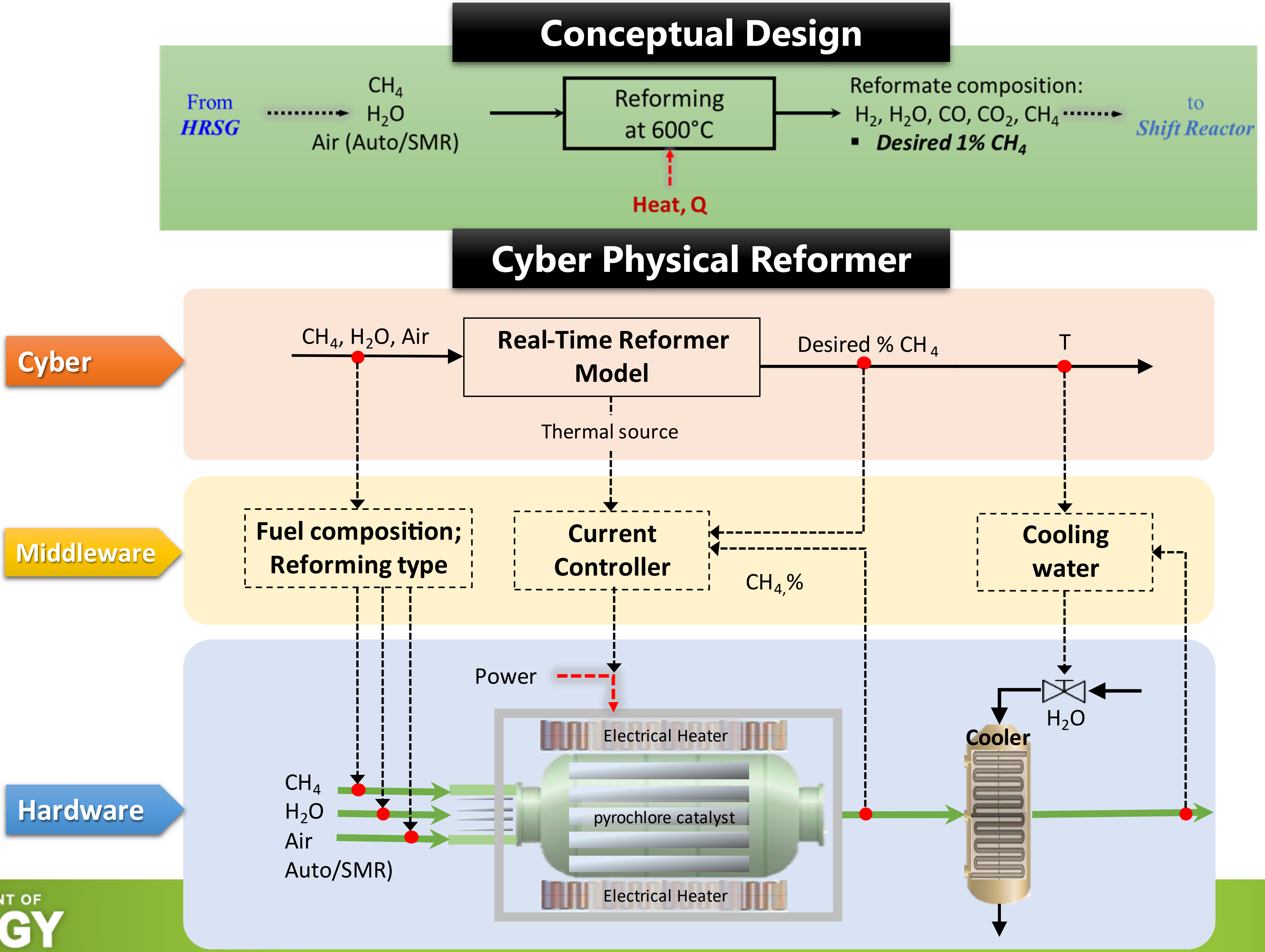
- ✓ *Dissipation rate :*
- ✓ *4minutes - using a thermal storage size of 19.5 kg/kW*
- ✓ *12 seconds with the size of 4.88 kg/kW*

IES Cycles: CO_2 Capture



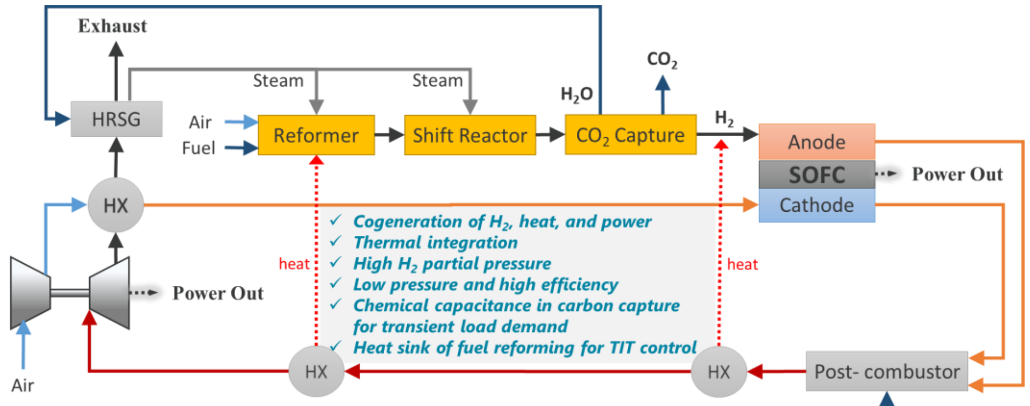
Simplified process flow of an ***integrated energy system with CO_2 capture***

CPS Conceptual Design: Reformer

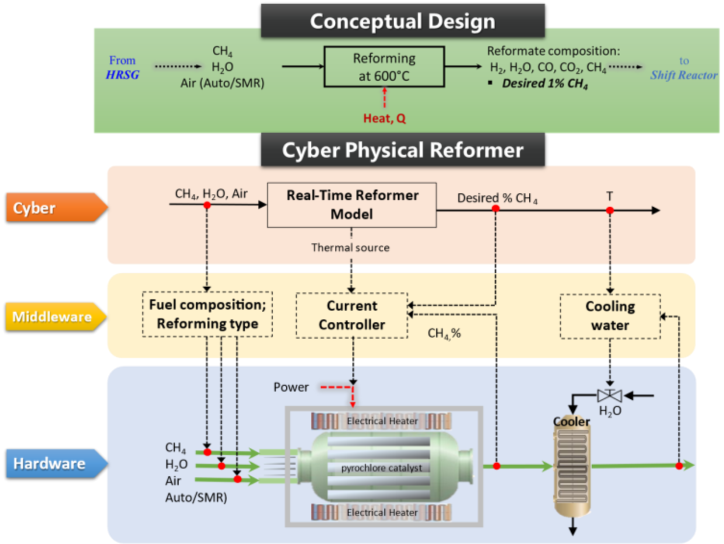


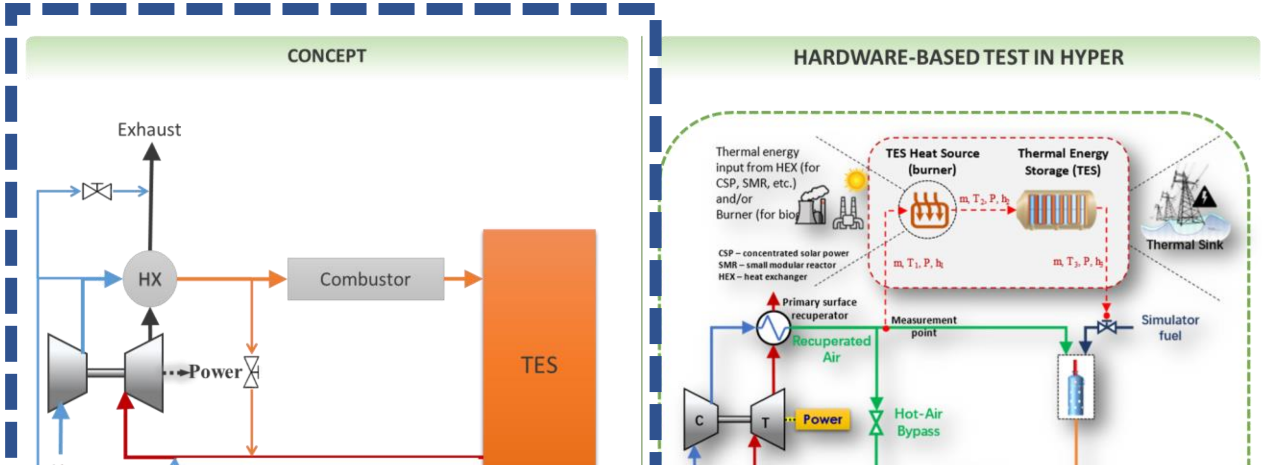
Future Direction

NATIONAL ENERGY TECHNOLOGY LABORATORY

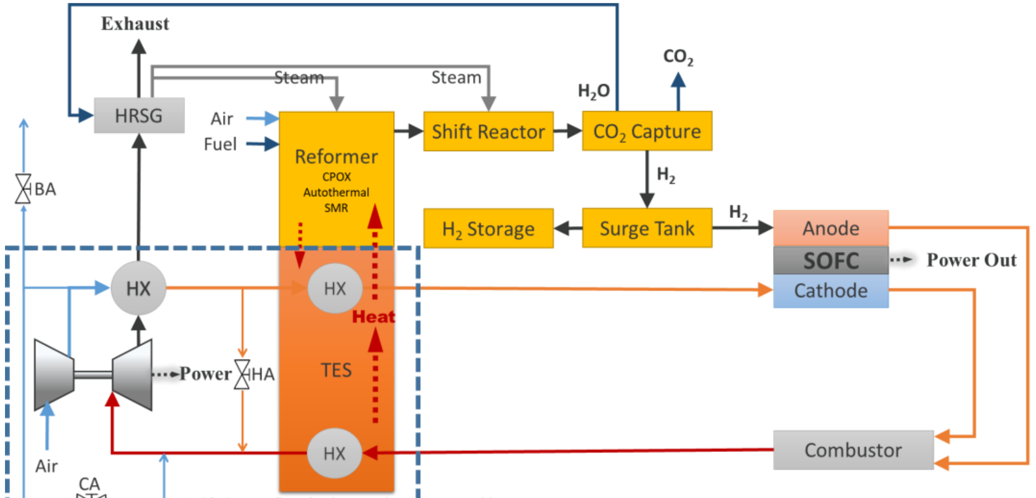


Simplified process flow of an *integrated energy system with CO_2 capture*





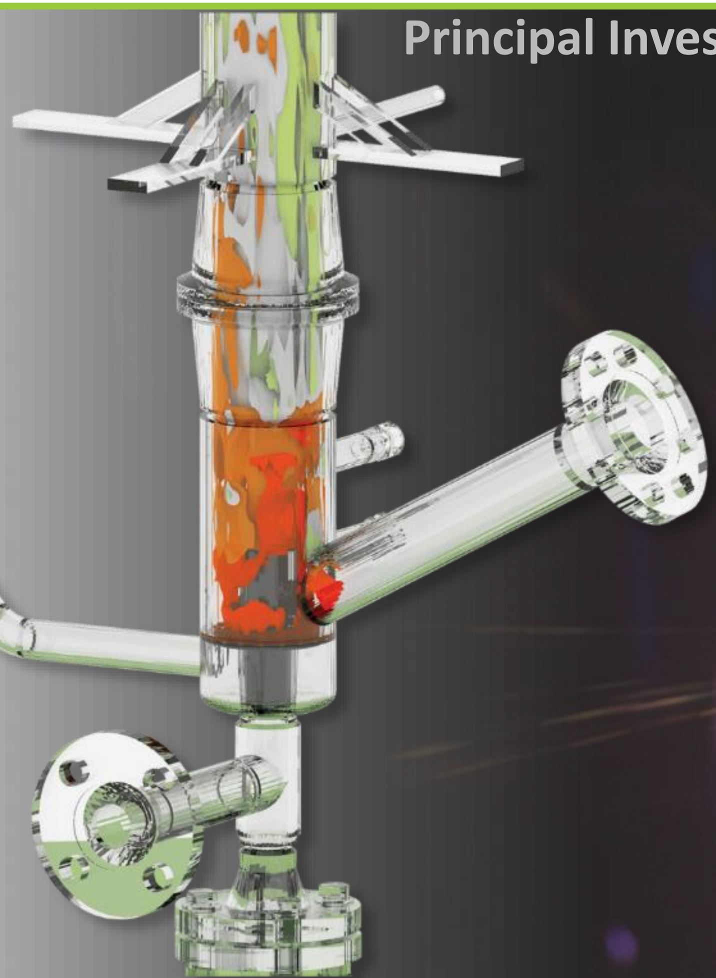
Simplified process flow of an *integrated thermal energy storage in a recuperated gas turbine system*



Simplified process flow of an *integrated energy system with CO_2 capture*

Task 53: Online System ID to Assist Power Generators During Cycling Operations

Larry Shadle
Advanced Sensors and Controls
Principal Investigator



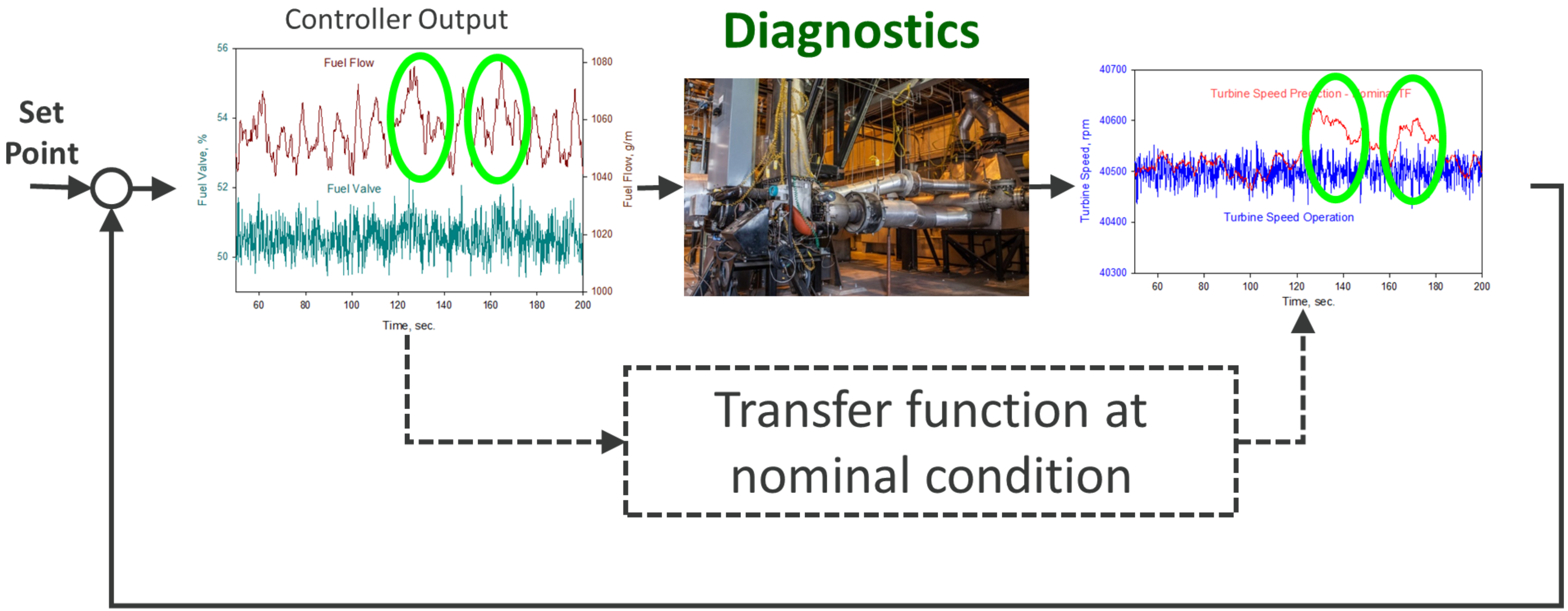
April 18, 2023

Rupen Panday, Grant Johnson, Kenneth Mark Bryden, Fernando Lima, Victor Alvez, Claudemi Nascimento

Crosscutting Research and Advanced Energy Systems Project Review Meeting
Sensor Technologies for Fossil Energy

Fault detection based upon On-line System ID

Advanced Sensors and Controls *Task 51*



Continuously Adaptive Gain Scheduling

Restrepo, B. et al., PID Control Design and Demonstration Using a Cyber-Physical Fuel Cell/Gas Turbine Hybrid System, Proceedings Power and Energy Conf, #7346, June 24-28, 2018, Lake Buena Vista, FL.

Overall Task Objectives

Objectives:

- Develop methodologies to improve system integration using online system identification
- Advance R&D on adaptive control for load following applications.

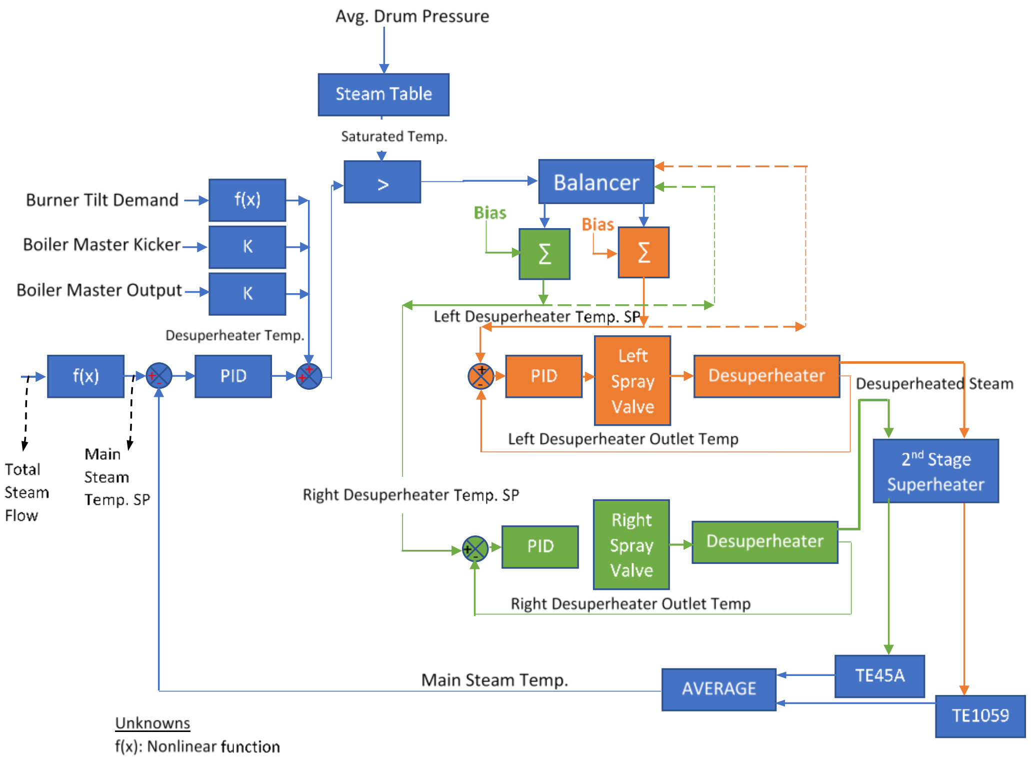
Strategy:

- Apply online system id during closed loop operations.
- Detect Operating States by monitoring input/output and computing transfer function coefficients.
- Develop algorithms to characterize plant operations and provide methods necessary to process full datasets.

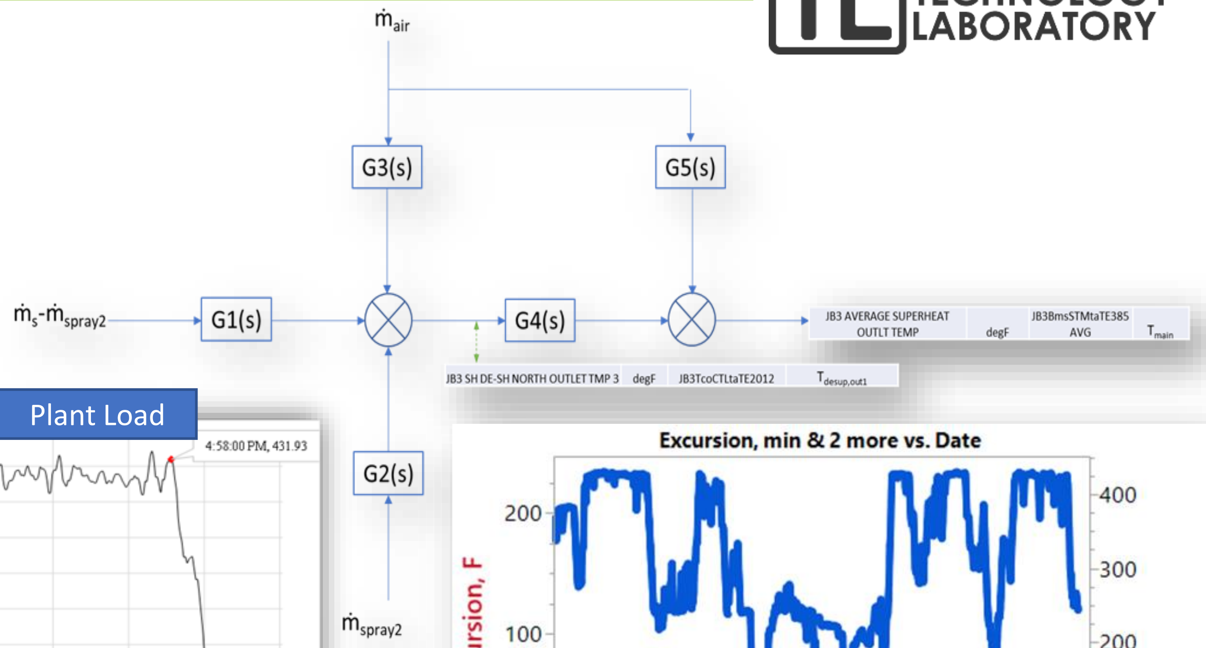
Online System Identification and Adaptive Controls

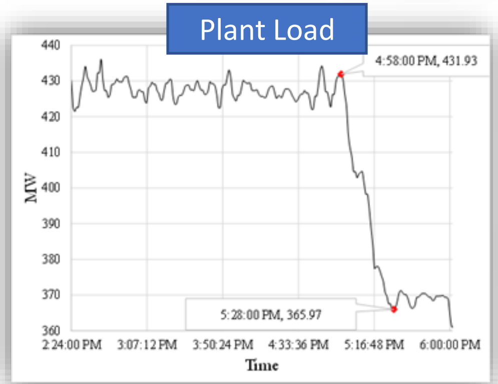
Industrial Case: Steam superheat T control

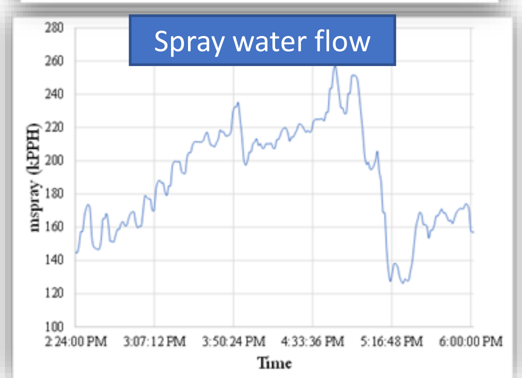
- SH-T Control tolerances critical constraint to plant operations

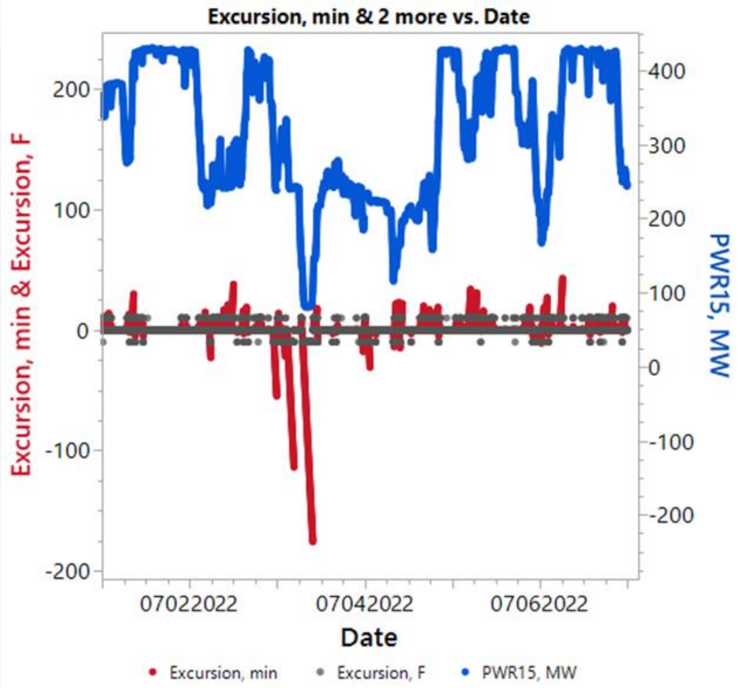


Unknowns
f(x): Nonlinear function
K: Gain
Note: Interlocks not included





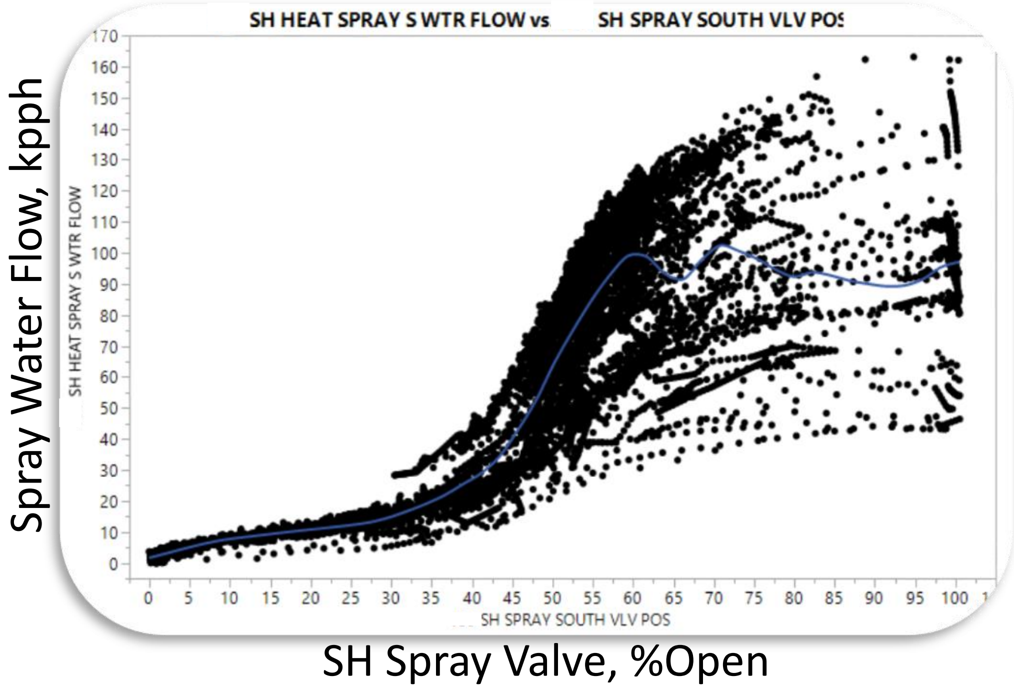


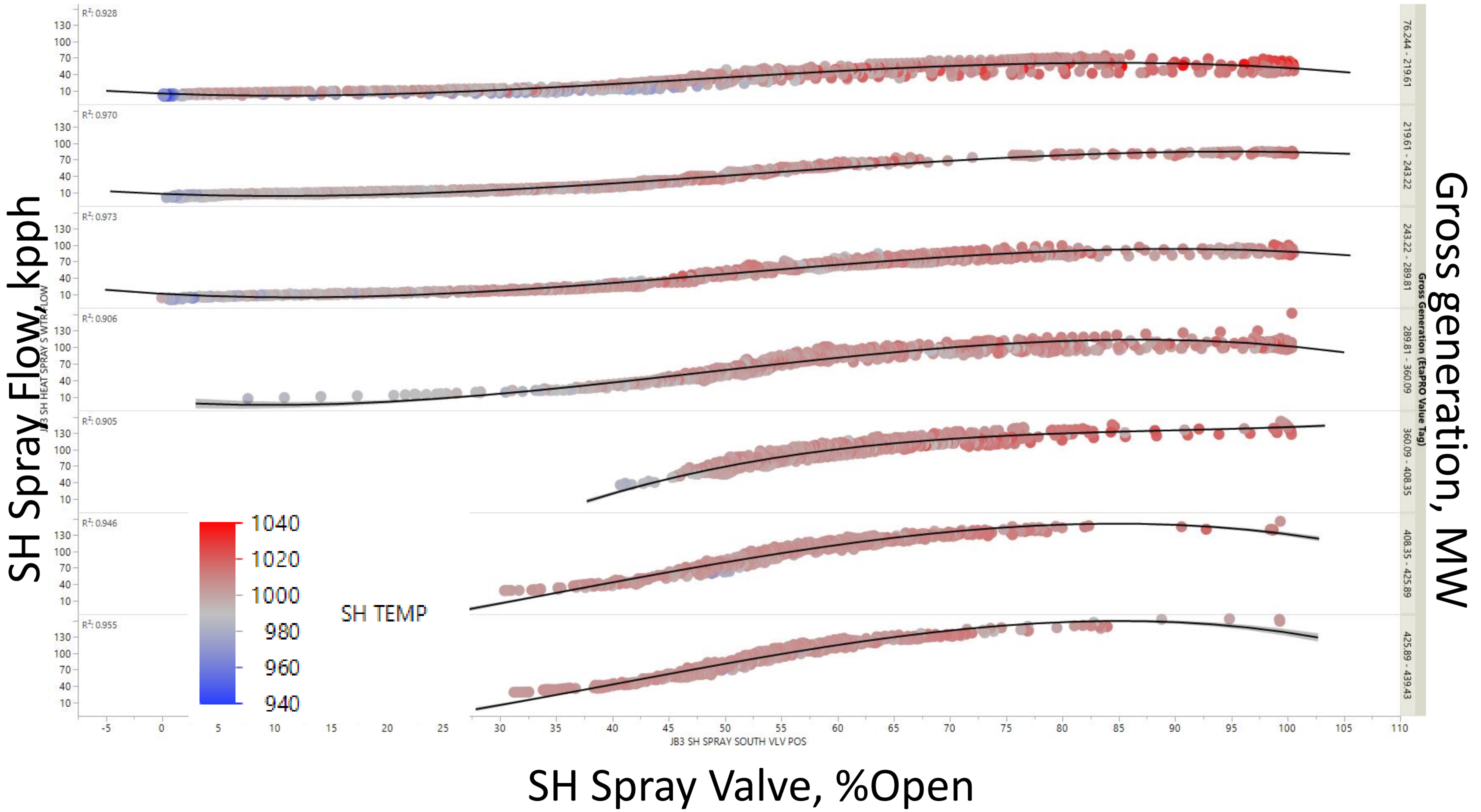


Online System Identification and Adaptive Controls

Task 53 Accomplishments

- Received and Analyzed five months of data from industrial partner
- Characterized responses and identified Control State changes with changes in Power Generated.

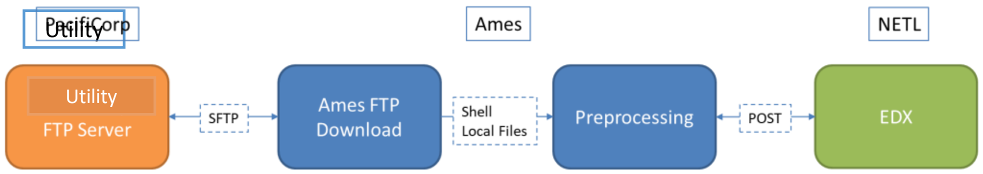




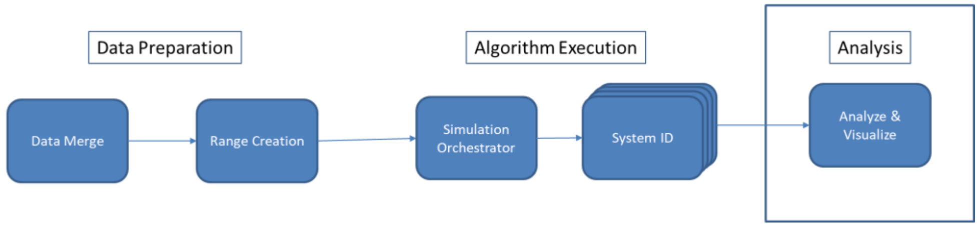
System ID Evaluation – System Operating in Closed Loop

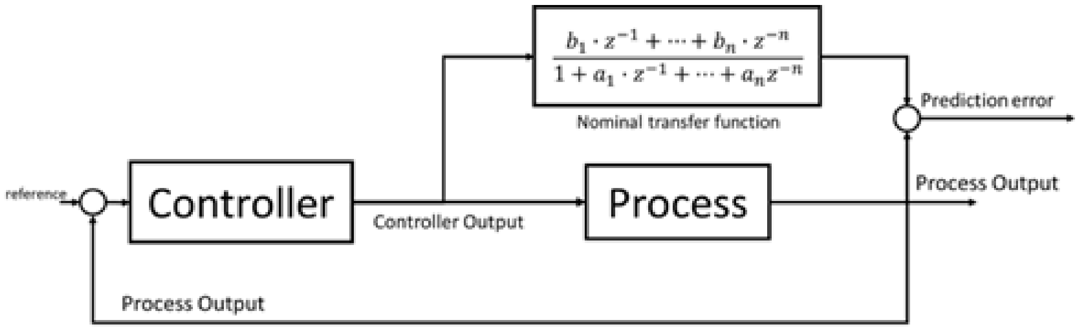
Closed loop transfer function variation from Full Load Operations

Data Pipeline

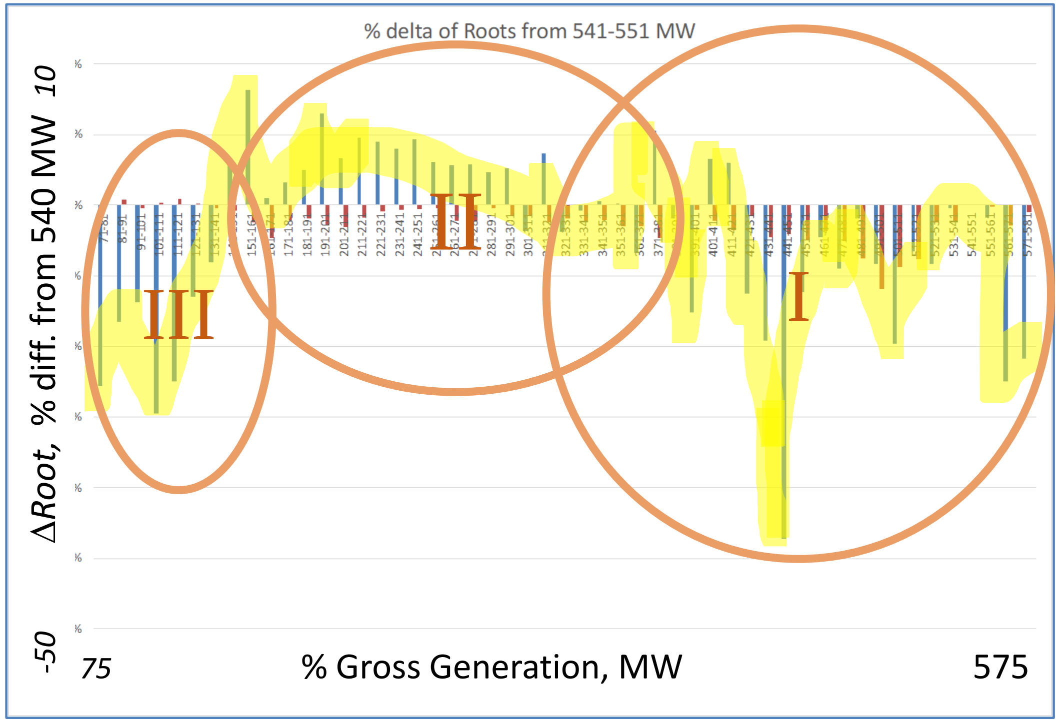


System ID Execution





- Three Different Regimes Identified
  - I- Nominal Control
  - II – Off-design Control
  - III – Limited Control



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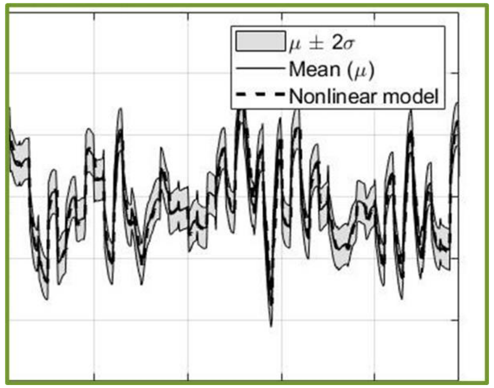
Future Direction

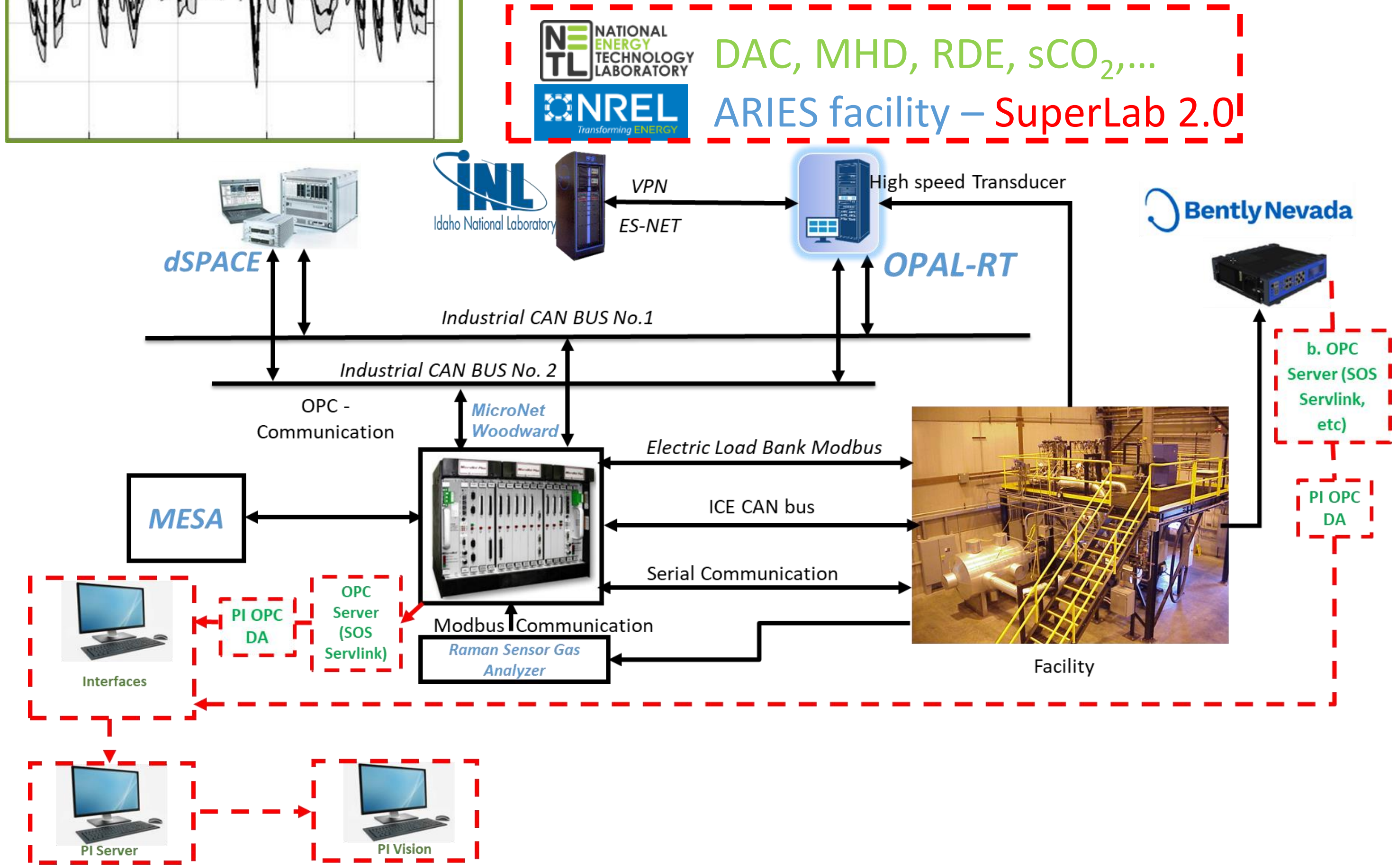
Next Steps

- Wrap up System ID analysis and present to industrial Partner
- Gaussian Process propagation
- CLOE analysis



Task 54 – Data Historian

- Set up information system to support SAMI application to Cyber Physical hybrid technologies
- Compile and synchronize info from experimental sensors & models with meta data
- Develop Roadmap for Information Integration



Acknowledgements and Disclaimer

- **This material is based upon work supported by the Department of Energy Advanced Sensors and Controls, FWP-1022427**

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Cyber-Physical Systems are Awesome!!!

Thank You

Larry Shadle, Ph.D.
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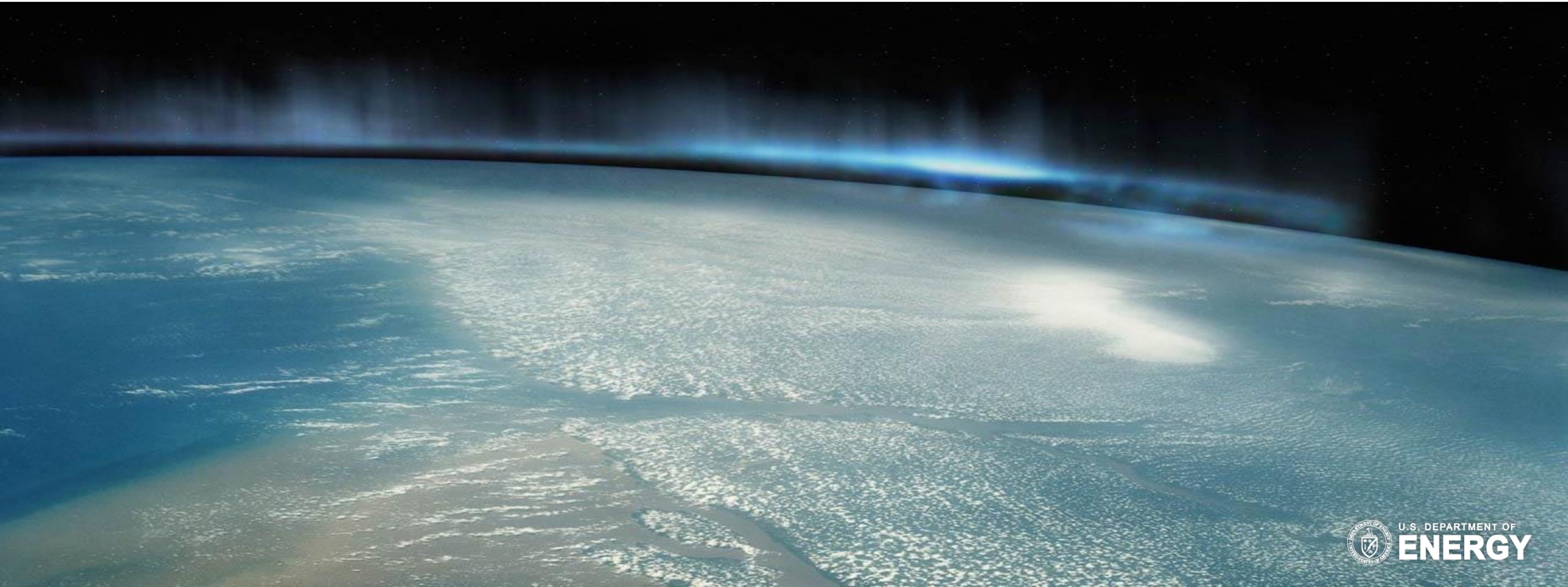
Direct Power Extraction

NETL Research & Innovation Center

Presented by Rigel Woodside, Ph.D. - Rigel.Woodside@netl.doe.gov

2023 FECM/NETL Spring R&D Project Review Meeting

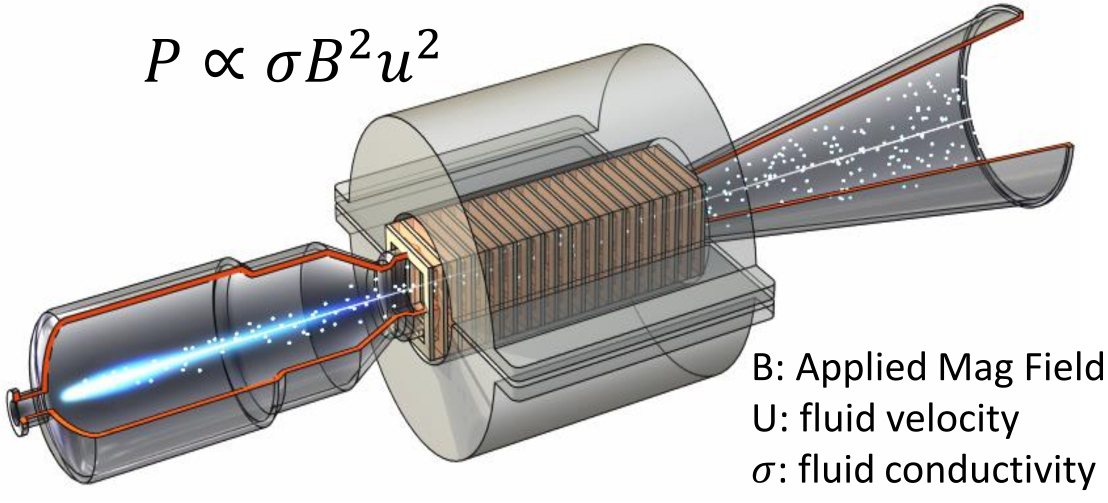


Introduction

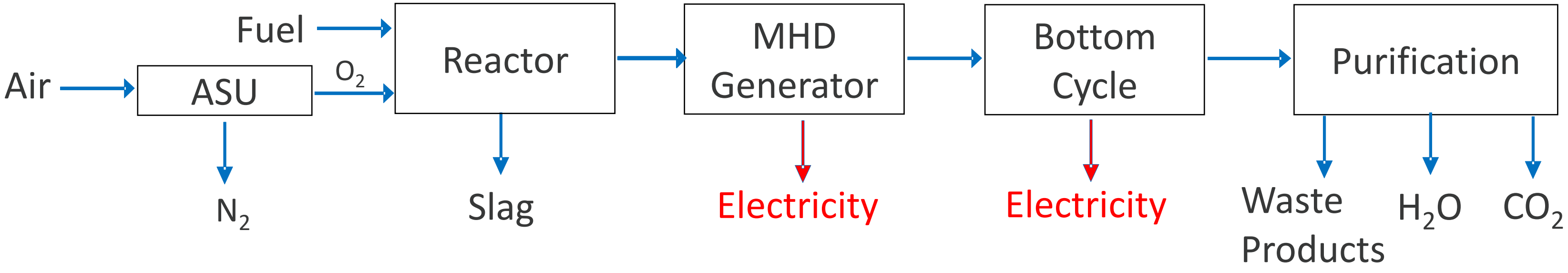
- **Why use a MHD generator?**
  - Extract power at higher temperatures then turbines
    - higher combined cycle efficiency possible (eg w/oxy-fuel and CCUS)
  - Resilient to particles as compared to turbines
    - Power production or hydrogen production from mixed sources (fossil, biomass, waste streams) with CCUS
- **Prior Efforts in Direct Power Extraction FWP**
  - TEA showed 30% COE reduction possible for oxy-coal + CCUS power system[1]
    - Unique NETL simulation codes for MHD power gen performance developed and utilized
  - Lab R&D work discovers & develops new MHD channel materials[2]
    - Potentially solving legacy issue for technology
  - MHD Gen 1 successfully built and tested at NETL[3]
    - Combustion plasma created; electrical impedance simulated and measured

MHD Power Generator

$$P \propto \sigma B^2 u^2$$



B: Applied Mag Field
U: fluid velocity
σ: fluid conductivity



<u>Project objectives</u>

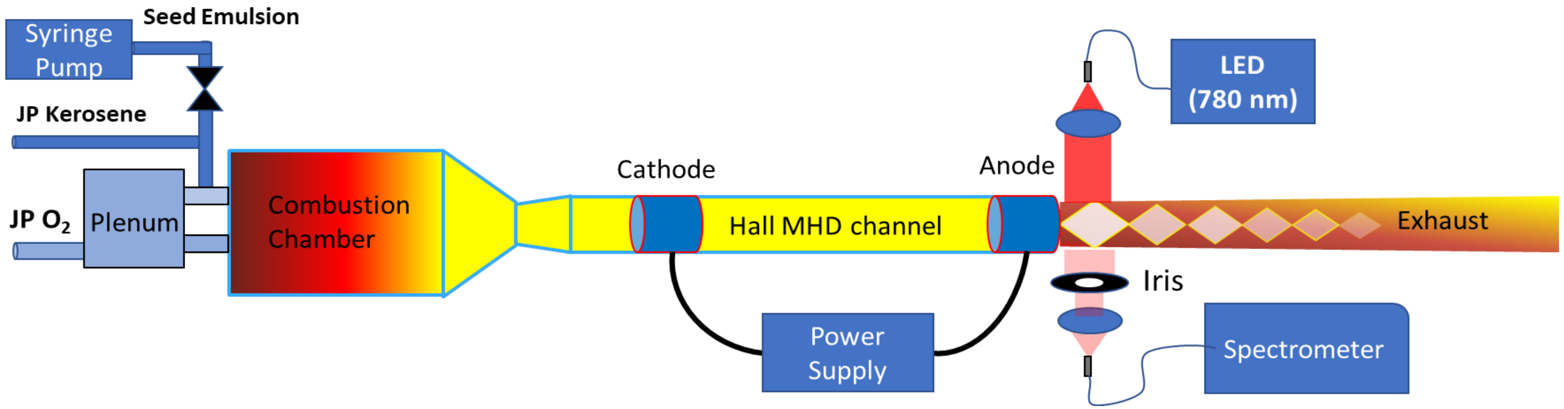
- Experimentally validate CFD simulations of MHD generator's impedance
- Calculate cost and performance of system with biomass co-firing
- Develop new ceramic channel materials

U.S. DEPARTMENT OF ENERGY

1. N. Weiland, C.R. Woodside, Charles White, Jason Mazzoccoli, "Scoping Study for Direct Power Extraction (DPE) Systems: final report", NETL technical publication DOE/NETL-2021/2751, 2021.
2. Michael S. Bowen, Kyei-Sing Kwong, Peter Hsieh, David P. Cann, C. Rigel Woodside; *"High Temperature Corrosion Stability of Ceramic Materials for Magentohydrodynamic Generators"*; 2021 ASTM International Journal on Materials Performance and Characterization
3. Lee Aspitarte, Hyoungkeun Kim, E. D. Huckaby, Mick Carter, Danylo B. Oryshchyn, Emily Davis, Clinton R. Bedick, and C. R. Woodside, Resistance Measurements of a High-velocity Oxy-fuel Powered MHD Channel, AIAA Propulsion and Energy 2020 Forum.

NETL MHD Gen 1 Lab system

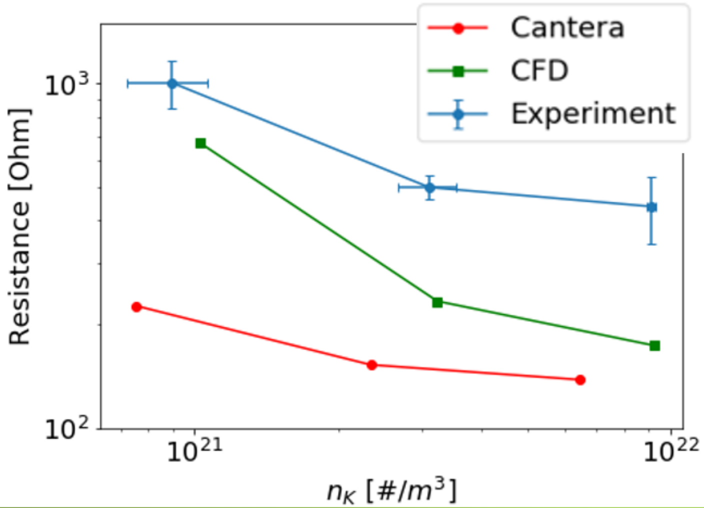
measure plasma + boundary layer impedance



NETL's MHD Gen 1 channel outside of a magnet

Emulsions used to 'seed' the fuel are being developed and tested

- Test system capable of operating over range of mass flow, equivalence ratio, and seeding rates to provide validation data points
- Initial reported simulation results not within measurement uncertainties
  - Working on improving MHD Gen hardware design (MHD Gen 2) to minimize other possible sources of error
  - Working on improving simulation methods



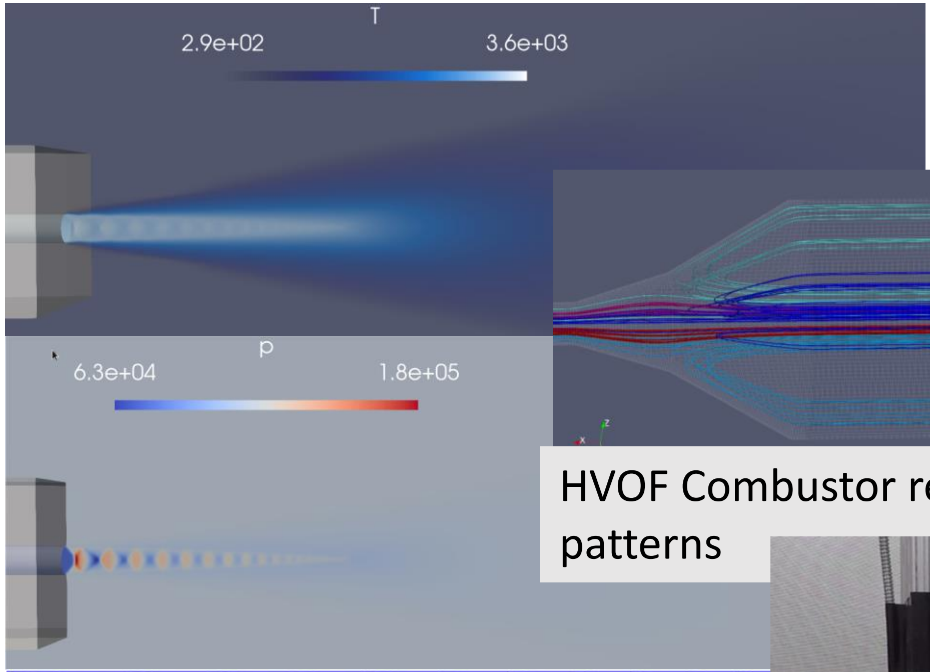
CFD Simulations

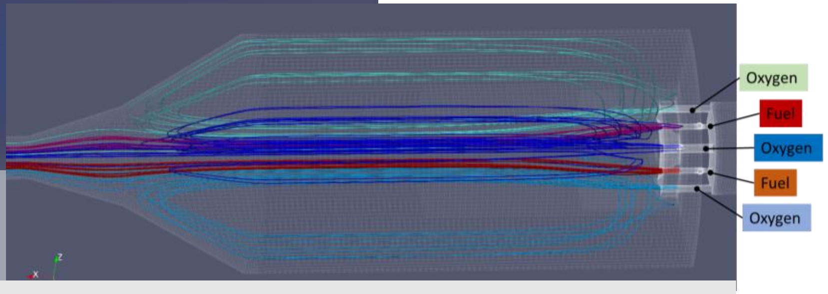
To determine generator impedance

Uncoupled CFD model w/ OpenFOAM

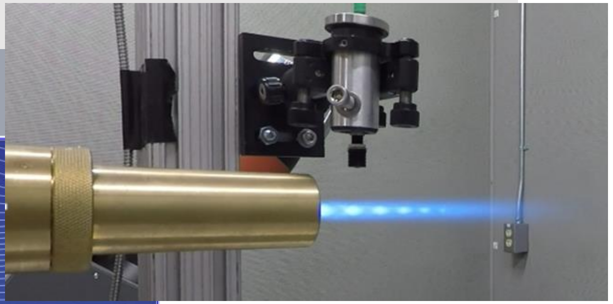
1. Solve fluid flow & thermo properties:
   - uniform mixture of combustion product of fuel, oxygen and seed, injected at combustor back plate section.
   - 2D axi-symmetric geometry
     - Convective wall heat transfer & boundary layer formation
   - finite rate chemistry for tracing the evolution of species (considers non-equilibrium chemistry)
2. Calculate resistance using conductivity model & electrostatic model
   - Electrostatics decoupled from flow
   - OpenFOAM and other tools

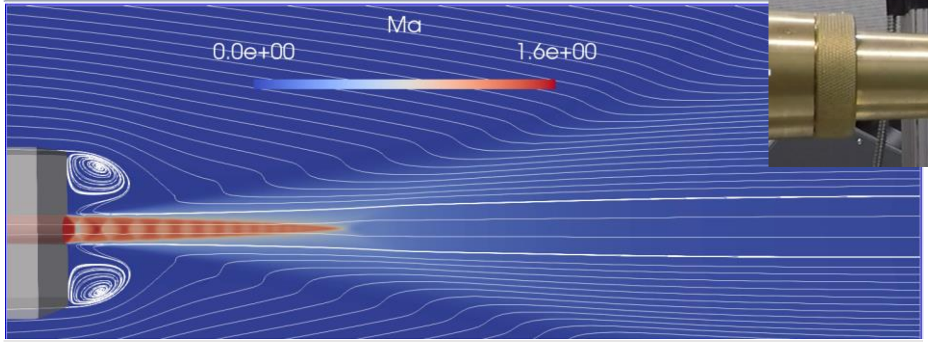
- **Additional computational capabilities**
  - 3D multiphase (liquid kerosene) w/ evap. and combustion
  - Fully coupled EM
  - Upstream kerosene-emulsion (K-seed) mixing
- **Planned work includes adding addition complexity to model including consideration of arcing**





HVOF Combustor recirculation patterns

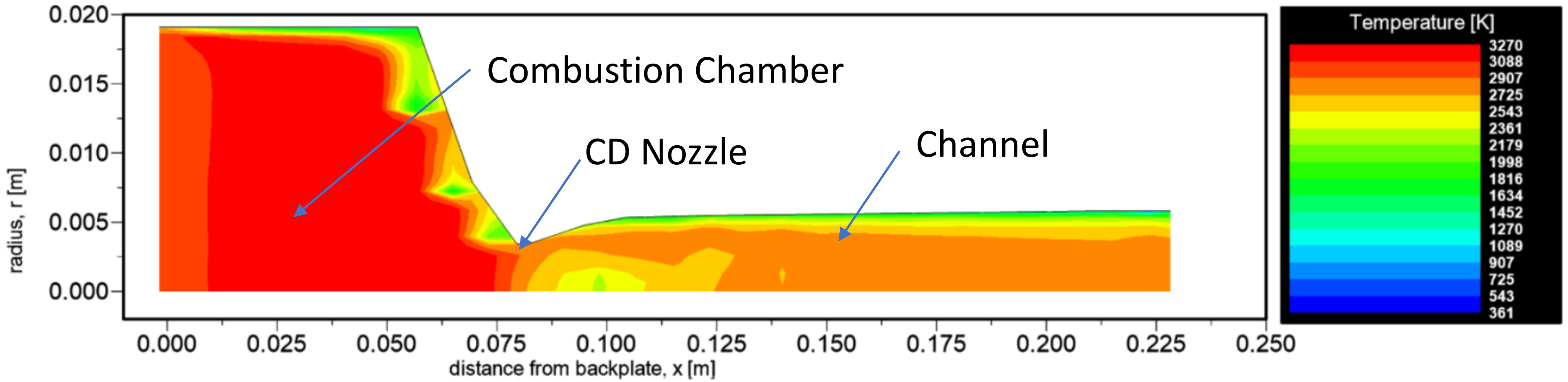


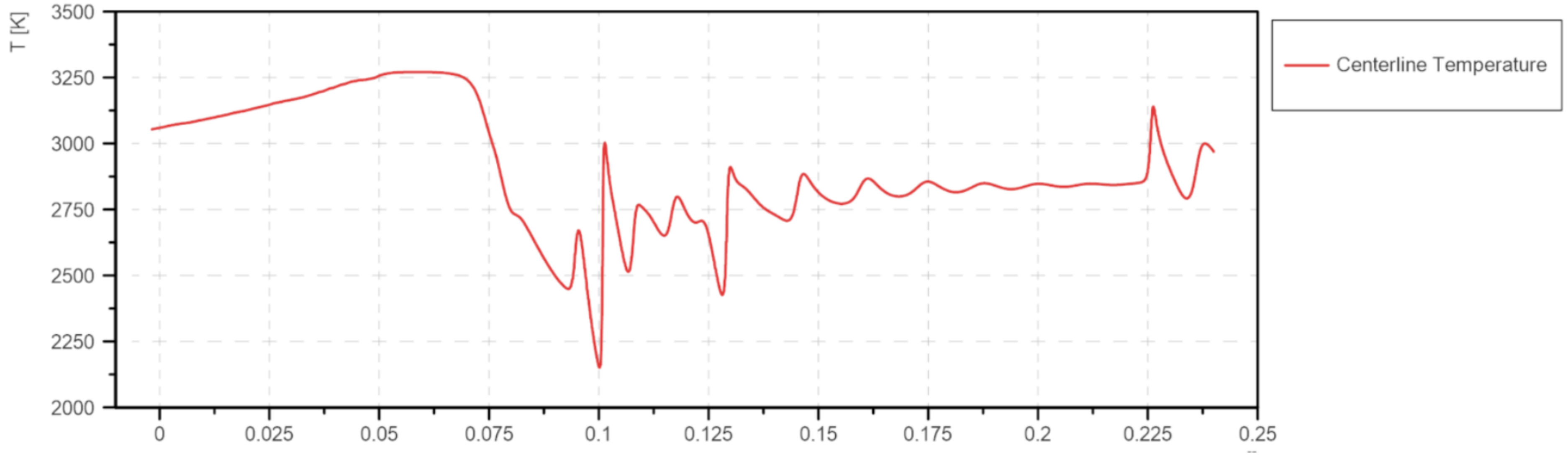


simulation of ‘free jet’ in open air at exit

CFD Simulation Results

Example Static Temperature Result

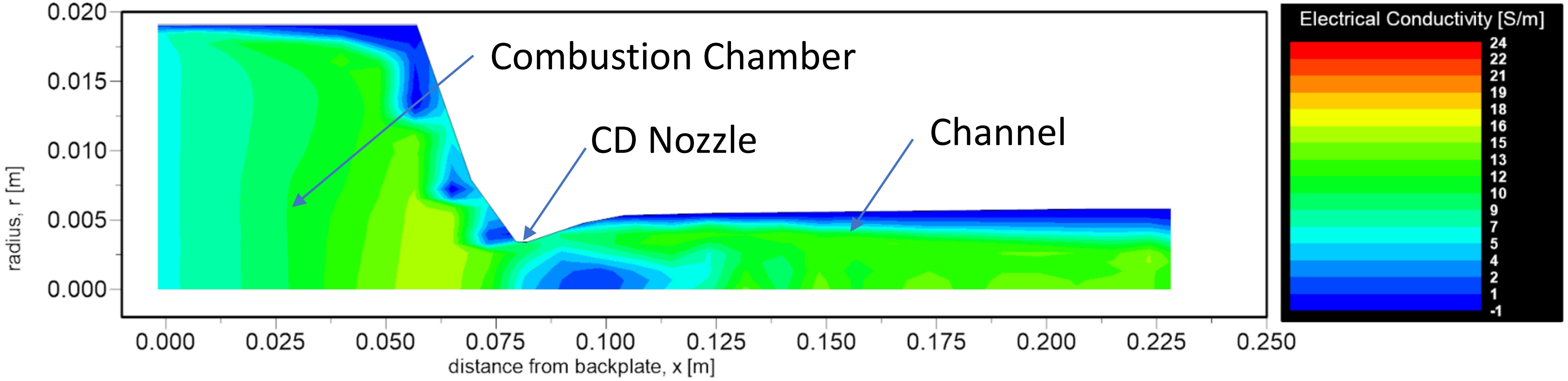


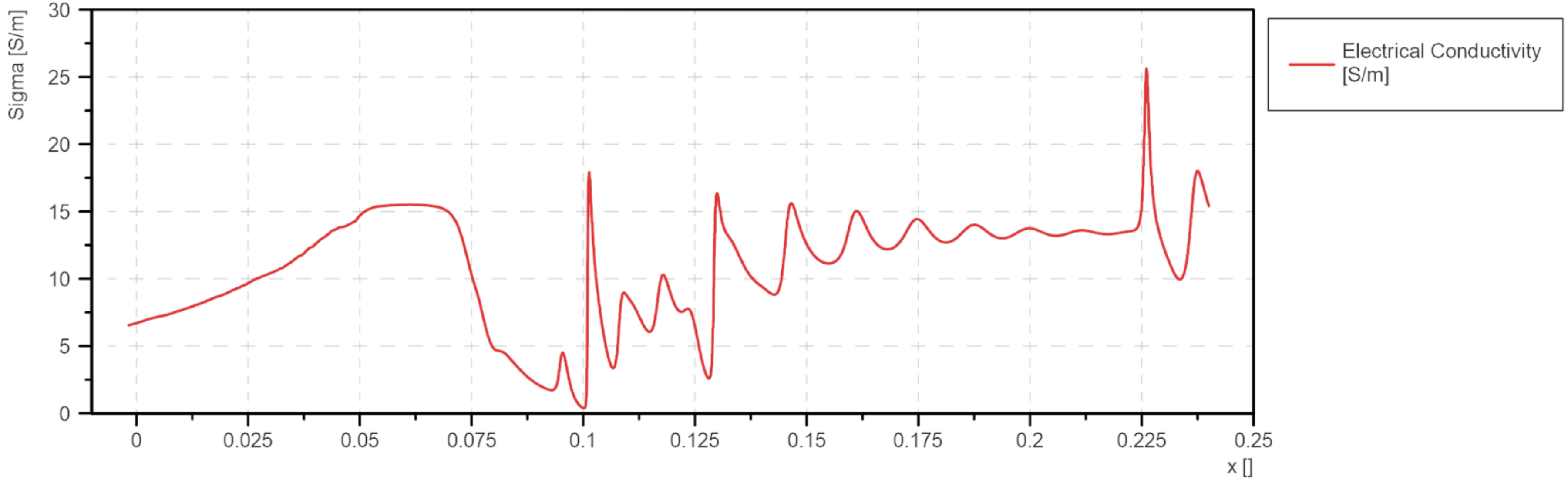


- High Temperature pressurized combustion approaches 3270K
- Expansion of gasses cools gas
- Supersonic shocks cause some T oscillation
- Cooler boundary layer observed
  - Wall T ~340K with water cooled copper wall
- Boundary layer growth apparent

CFD Simulations

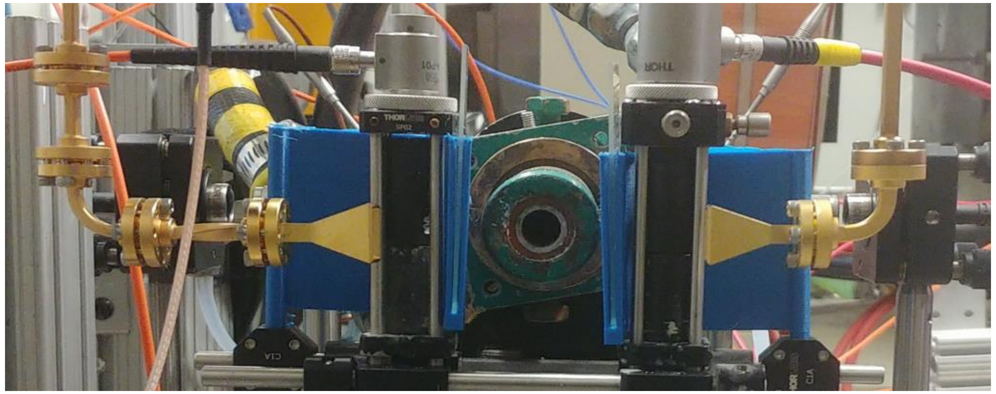
Electrical Conductivity with the Combustion Plasma





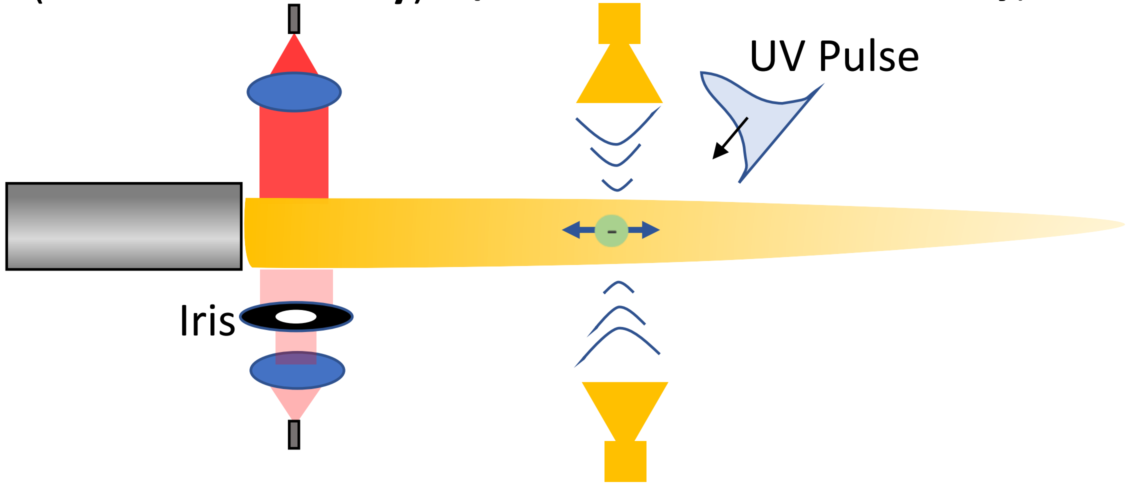
- Roughly 4 orders of magnitude greater conductivity then with no seed
  - Small addition of K_2CO_3 makes large difference
- Supersonic shock T variations lead to conductivity variation
  - And low zone downstream of CD nozzle
- Boundary layer resistance increases downstream
  - Different at cathode then anode

Plasma Diagnostics

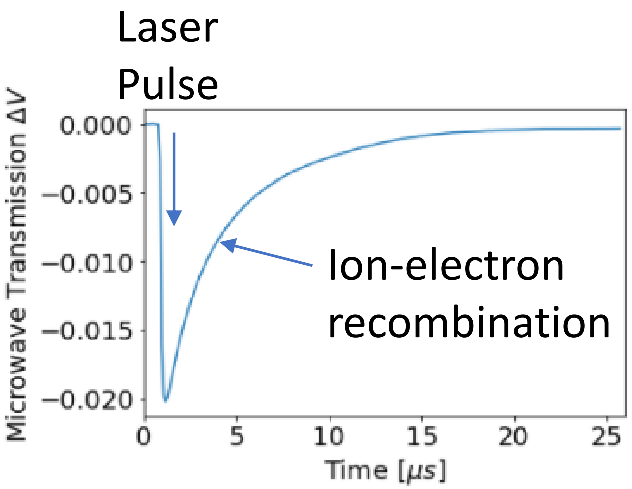


Optical Absorption (**Potassium Density**)

Microwave Scattering **(Laser-induced conductivity)**



- Optical Absorption at ~767nm used to find K concentration(#/m^3)
  - This is proxy for plasma free electron concentration and indicates seeding success
  - Measured at entrance and exit of MHD channel
- Microwave scattering at ~90 GHz used to determine electron-ion recombination rates
  - Successfully developed and demonstrated



Ion-electron recombination rates are key to assessing non-equilibrium plasma approaches

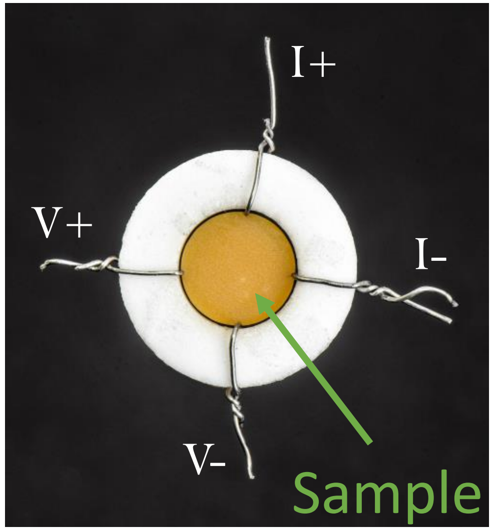
High Temp electrical measurements

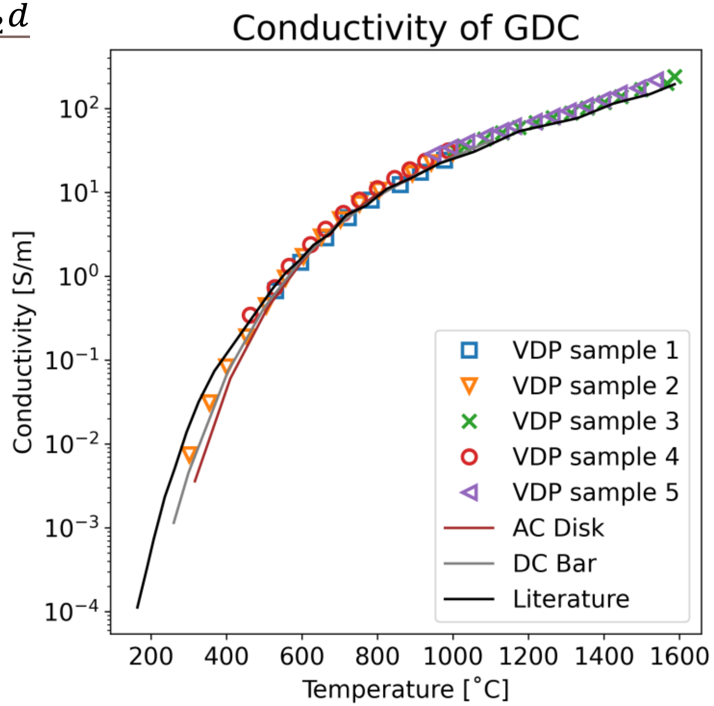
In support of EY22 Direct Extraction FWP

In collaboration with: Oregon State University College of Engineering

- **Newly developed text fixture successfully demonstrated and reported[1]**
  - Improves measurement of a material's electrical conductivity up to ~1700 °C
    - For MHD channel electrode characterization
  - Based on 4-point Van der Pauw (VDP) geometry and method[2]
  - Custom made ceramic apparatus tightly fits sample and platinum wires
    - Ceramic apparatus has lower CTE than test coupons
    - Placed in standard high temperature box or tube furnace
  - Demonstrated by testing gadolinia doped ceria (GDC)
    - Results comparable to existing techniques (DC bar and AC disk)
    - Verified high temperature from literature

$$1 = e^{-\frac{\pi R_1 d}{\rho}} + e^{-\frac{\pi R_2 d}{\rho}}$$





1. Michael S. Bowen, David Cann, C. Rigel Woodside; *"Bulk Electrical Conductivity Measurements based on 4-point Van der Pauw Geometries"* , 2023 ACerS Electronic Materials and Applications Conference, Orlando, Florida
2. L. J. van der Pauw, "A Method of Measuring Bulk Resistivity and Hall Coefficient on Lamelle of Arbitrary Shape", Philips Technical Review 20, p220-224

Acknowledgements

Lee Aspitarte, Danylo Oryshchyn, David Huckaby, Michael Bowen, David Cann, Clint Bedick, Jon Fulton

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Tasks 86 & 87 Updates

NATIONAL ENERGY TECHNOLOGY LABORATORY

Yuhua Duan

FECM Spring Project Review Meeting, Apr. 18-20, 2023

Task 86: Artificial Intelligence-Based Theoretical Approach for Screening and Design of Functional Materials for the Harsh Environment Applications

NATIONAL ENERGY TECHNOLOGY LABORATORY

Objectives:

To perform high-T gas sensing measurements, sensing materials with high stability, sensitivity and selectivity are needed. Instead of experimental trial-and-error approach, we proposed to theoretically design framework to identify good candidates from materials database.

- ❑ Temperature dependence of electronic structure (band-gap changes versus T)
- ❑ Fitting to empirical equation of band-gap changes versus T
- ❑ Developing high-T sensing database
- ❑ Performing machine learning model to determine T-dependent band-gap changes and select batter candidate materials for high-T gas sensors.

Key research team members:

- Former members: **Yu-Ning Wu, Jongwoo Park, Ting Jia**, Paul Ohodnicki, Tarak Nandi, Wissam A. Saidi
- Current members: **Jordan Chapman, Leebyn Chong**, Dan Sorescu, Jeffrey K. Wuenschell, Yueh-Lin Lee, Yuhua Duan

First-principles Simulations

NATIONAL ENERGY TECHNOLOGY LABORATORY

Temperature dependence of the electronic eigenvalues originates from the phonon population & the thermal expansion of the lattice

- **Electron-phonon coupling**
  (Major contribution)

✓ Allen-Heine-Cardona (AHC) theory
✓ Finite displacement method

$$\epsilon_{\mathbf{k}n}(T) - \epsilon_{\mathbf{k}n}(\mathbf{0}) = \frac{1}{N_{\mathbf{q}}} \sum_{\mathbf{q},\nu} \frac{a^{(2)}_{\mathbf{q}\nu;\mathbf{q}\nu}}{\omega_{\mathbf{q}\nu}} \left[\frac{1}{2} + n_{\mathrm{B}}(\omega_{\mathbf{q}\nu}, T)\right] + \cdots$$

where $\boldsymbol{q}$ and v are the phonon indices; N_q is the total number of q points that sample the first Brillouin zone (FBZ); $a^{(2)}_{\boldsymbol{qv};\boldsymbol{qv}}$ is the second-order electron-phonon coupling constant; $\omega_{\boldsymbol{qv}}$ stands for the phonon frequencies; n_B is the Bose-Einstein population of the phonons.

- **Lattice thermal expansion**
  (small contribution, could be neglected)

Quasi-harmonic approximation: map F (a) for different lattices and temperatures and fit using equation of state.

$$F(\mathbf{a}) = E_{T=0}(\mathbf{a}) + \frac{1}{2}\sum_{\mathbf{q},\lambda} \hbar\omega_{\mathbf{q},\lambda} + k_B T \sum_{\mathbf{q},\lambda} \ln\left[1 - \exp\left(-\frac{\hbar\omega_{\mathbf{q},\lambda}}{k_B T}\right)\right]$$

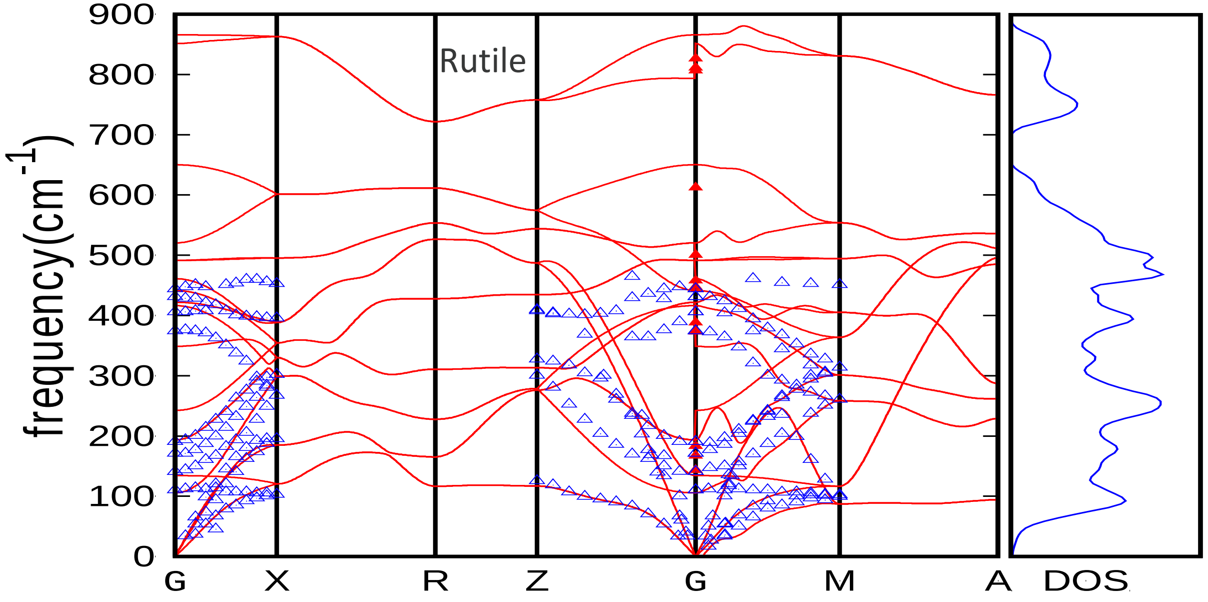
DFT Energy **Phonons**

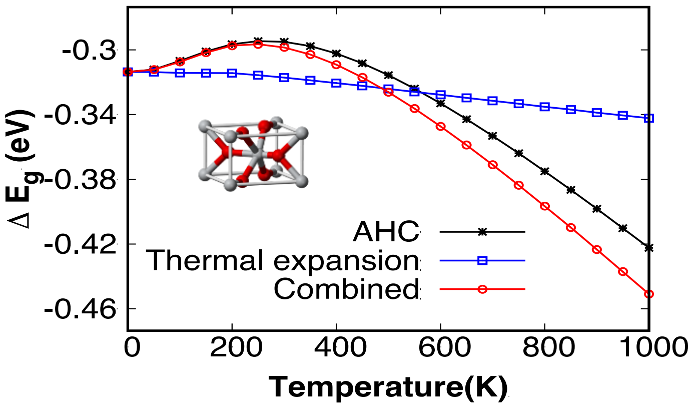
AHC Theory:

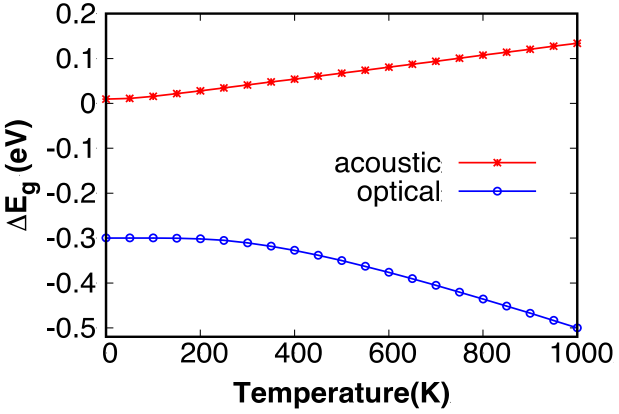
- P. B. Allen, M. Cardona, **PRB 23**(1981)1495-1505
- P. B. Allen, V. Heine, **J. Phys. C: Solid State Phys. 9**(1976)2305-2312.

Implementation in ABINIT:
G. Antonius, S. Ponce, P. Boulanger, M. Cite, X. Gonze, **PRL 112**(2014)215501

TiO_2: a case study



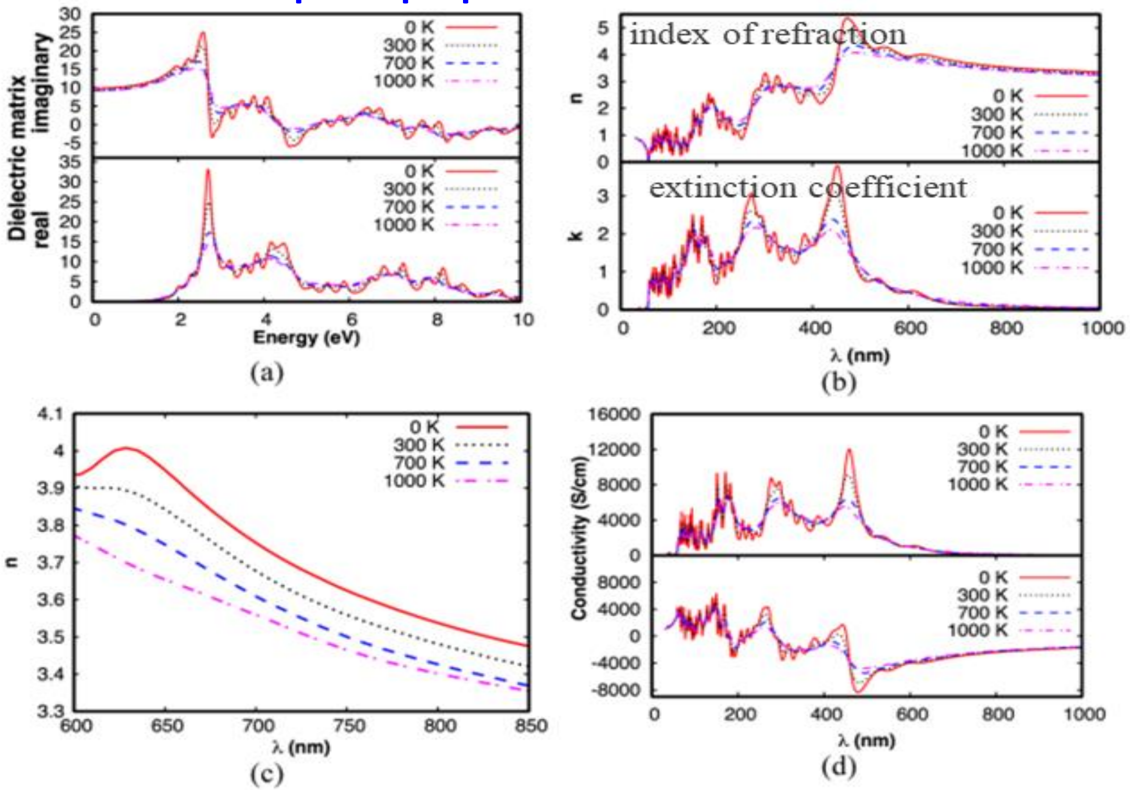




Y.-N. Wu, *et al*, **J. Phys. Chem. C 122**(2018)22642-49.

Y.-N. Wu, *et al*, **J. Phys: Condens. Matter 32**(2020)405705

Optical properties



Main conclusions:

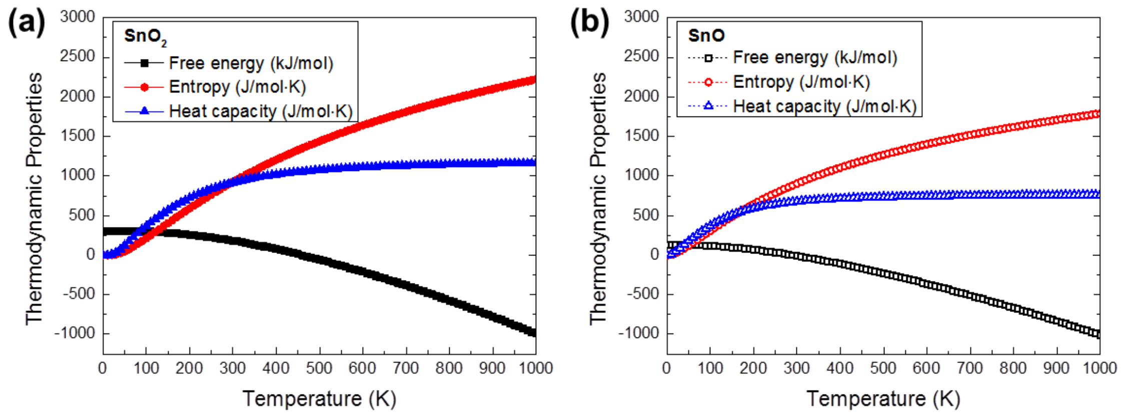
- Band-gap decrease with increase T
- Optical branches contribute such decrease
- El-ph coupling is the major contribution to band-gap narrowing over thermal expansion
- Optical properties are smoother with T increase

SnO_x: Temperature Electronic Structure

NATIONAL ENERGY TECHNOLOGY LABORATORY

Populating temperature dependence properties in SnO_x

- **Phonon properties: thermodynamic stability of materials**
  - ➢ Free energy decreases with temperature
  - ➢ Entropy and heat capacity approach zero at 0 K



- **Fully simulated $E_g = f(T)$: analytical O'Donnell model fitting**

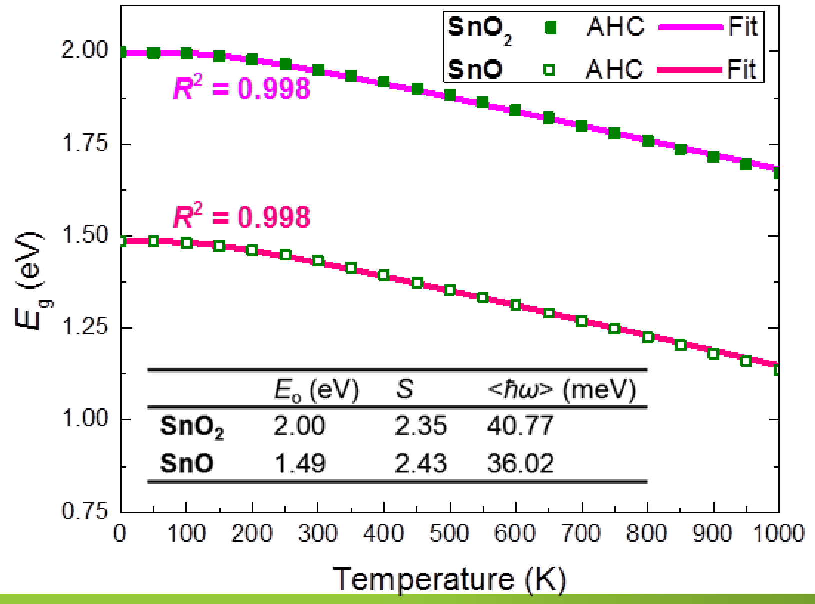
$$E_g = E_0 - S < \hbar\omega > \left[\coth\left(\frac{< \hbar\omega >}{2k_B T}\right) - 1\right]$$

- K. P. O'Donnell, X. Chen, **APL 58**(1991)2924-26**.**

E_0: zero-T band-gap

S: electron-phonon coupling constant

<ħω>: average phonon energy



- Close *S* and <*ħω*> parameters conform to comparative behavior of band gap shifts in SnO_2 and SnO

J. Park, *et al*, **J. Phys. Chem. C 125**(2021)22231-38.

MO_x: Temperature Electronic Structure

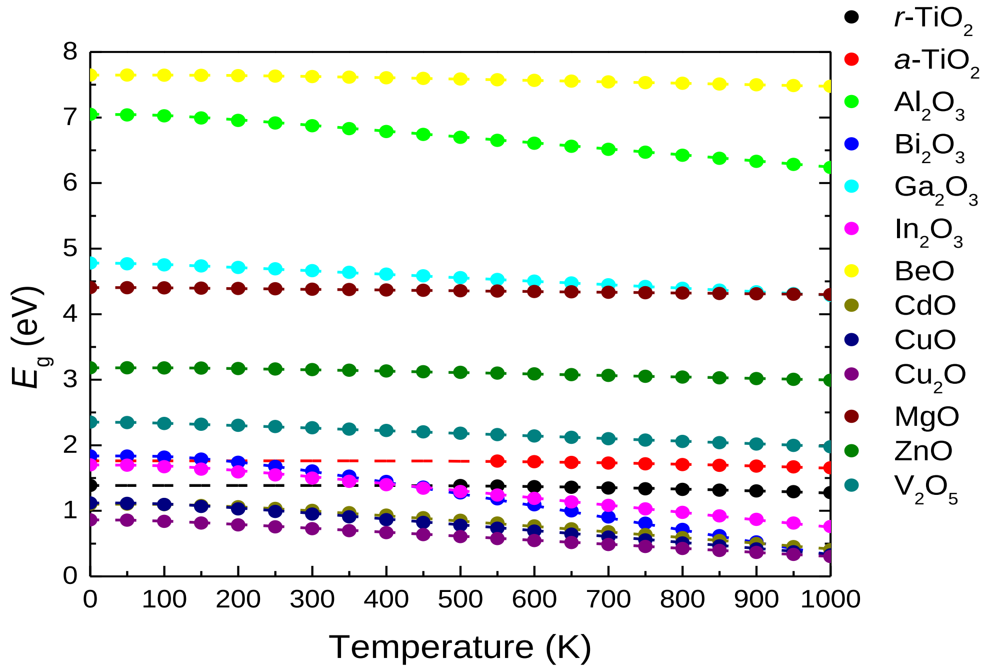
NATIONAL ENERGY TECHNOLOGY LABORATORY

Establishing materials database for temperature dependence band gaps

- Sub-set: finite temperature band gap known materials from literatures
- Fully simulated $E_g = E_{o,DFT} + \Delta E_{g,AHC} = f(T)$ rationalized with analytical O'Donnell equation

$$E_g = E_0 - S < \hbar\omega > \left[\coth\left(\frac{< \hbar\omega >}{2k_B T}\right) - 1\right]$$

- K. P. O'Donnell, X. Chen, **APL 58**(1991)2924-26.



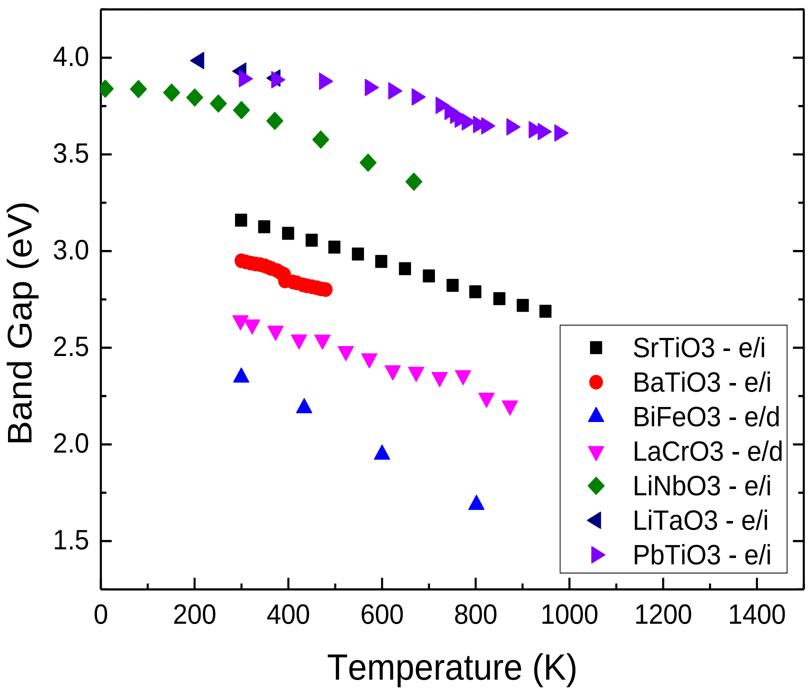
	E_o (eV)	S	<$\hbar\omega$> (meV)	R^2
r-TiO_2	1.39	3.80	244.0	0.982 *
a-TiO_2	1.76	3.94	253.0	0.989 *
Al_2O_3	7.05	5.40	25.00	0.999
Bi_2O_3	1.84	11.20	40.77	0.999
Ga_2O_3	4.78	3.10	14.70	0.999
In_2O_3	1.70	6.59	30.11	0.998
BeO	7.65	1.36	51.00	0.999
CdO	1.10	5.14	43.12	0.999
CuO	1.12	5.31	26.45	0.998
Cu_2O	0.86	3.61	18.29	0.999
MgO	4.45	0.66	11.21	0.998
ZnO	1.79	1.36	37.18	0.999
V_2O_5	2.35	2.33	13.00	0.999

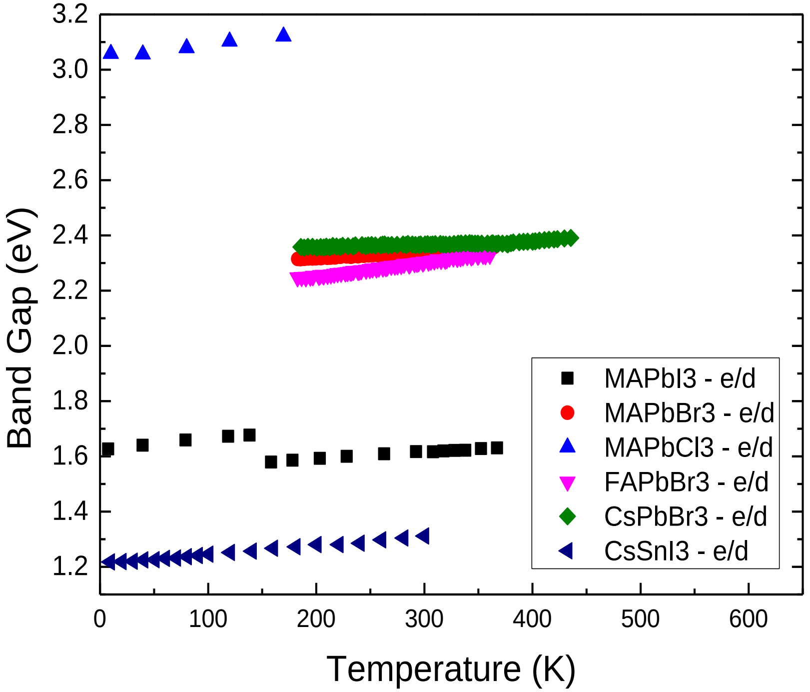
* Discard non-monotonic regime $T < 400$ K

Perovskites: Temperature dependence properties

Perovskites: ABO_3 oxides and metal halide perovskites (MHP)

- Data from literatures: either experiment (e) or simulation (s), either direct (d) or indirect (i) band gap

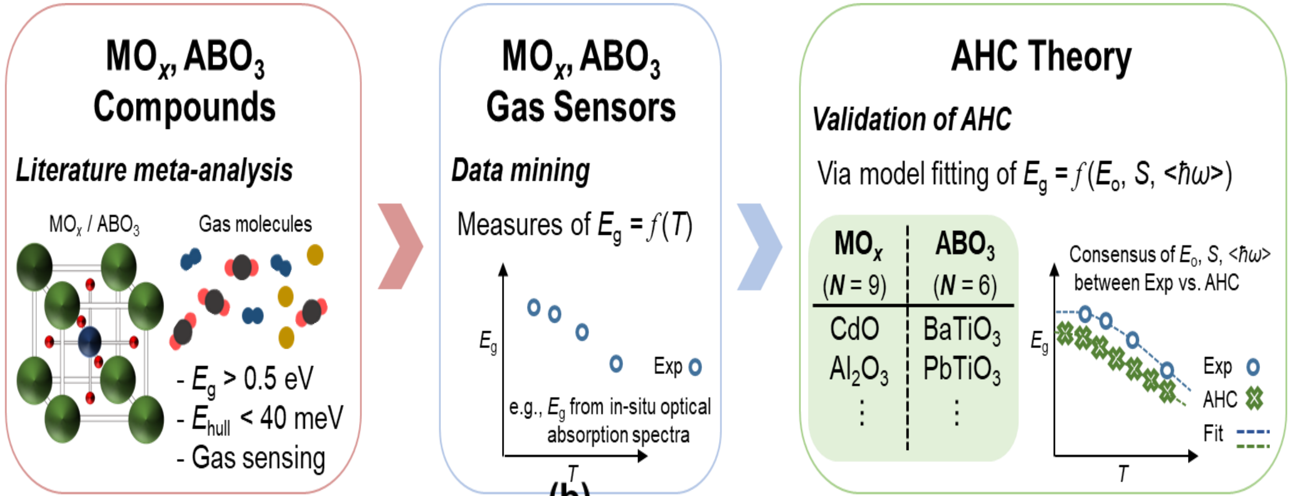


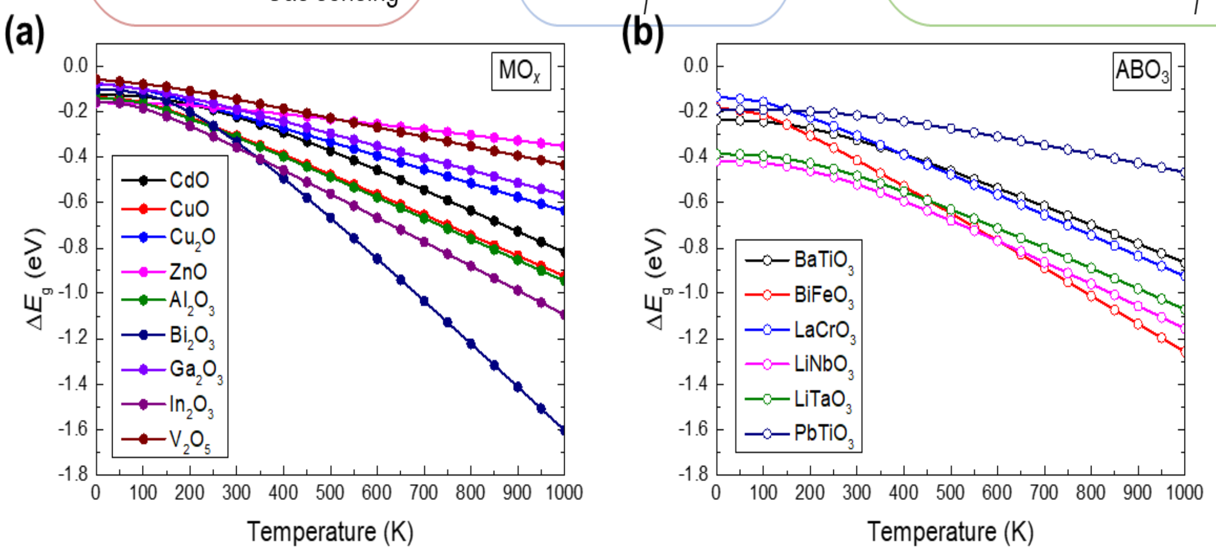


1	MAPbI3	orthorhombic	Pnma
2	MAPbBr3	monoclinic	Pm
3	MAPbCl3	monoclinic	Pm
4	FAPbI3	orthorhombic	Pmm2
5	FAPbBr3	monoclinic	Pm
6	FAPbCl3	orthorhombic	Pmm2
7	CsPbI3	orthorhombic	Pnma
8	CsPbBr3	orthorhombic	Pnma
9	CsPbCl3	orthorhombic	Amm2
10	MASnI3	orthorhombic	Pnma
11	MASnBr3	orthorhombic	Pnma
12	MASnCl3	orthorhombic	Pnma
13	FASnI3	orthorhombic	Amm2
14	FASnBr3	orthorhombic	Pnma
15	FASnCl3	orthorhombic	Pnma
16	CsSnI3	orthorhombic	Pnma
17	CsSnBr3	cubic	Pm3m
18	CsSnCl3	monoclinic	P2_1/c

- ➢ Perovskite oxides: E_g closing tendency mainly discussed with electron-phonon coupling contribution
- ➢ Metal halide perovskites: E_g opening tendency mainly discussed with thermal expansion contribution

Relationship between AHC versus empirical prediction

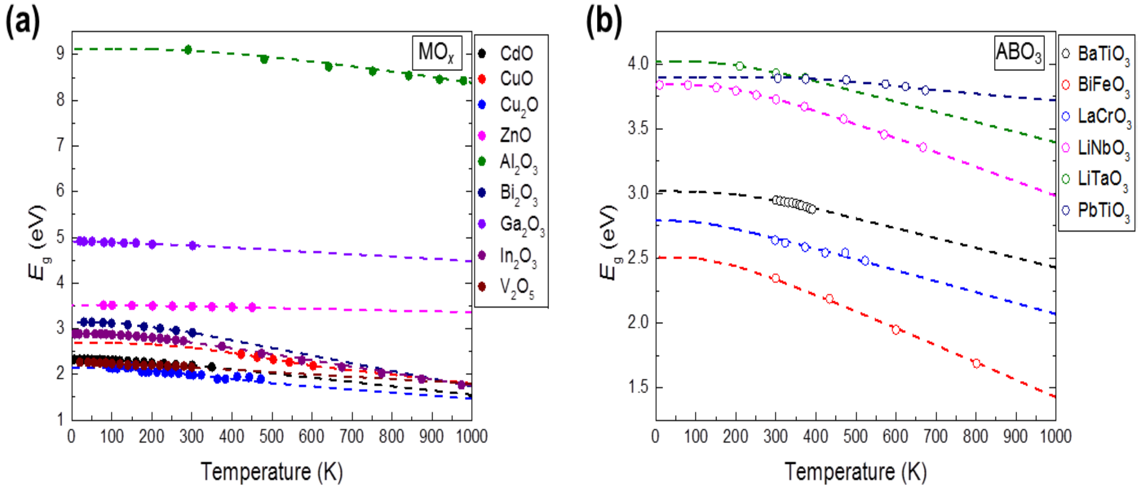




Calculated band-gap ($\Delta E_g(T)$) by AHC theory via a nonadiabatic zero-point-motion renormalization

O’Donnell analytical equation:

$$E_g = E_0 - S < \hbar\omega > \left[\coth\left(\frac{< \hbar\omega >}{2k_B T}\right) - 1\right]$$



$E_g(T)$ variation estimated by experimental data (symbols) fitted with O’Donnell model (dashed lines).

- J. Park*, et al*, **ACS Appl. Mater. Interfaces, 13**(2021)17717-25.
- Y.-N. Wu*, et al*, **Phys. Chem. Lett. 11**(2020) 2518-23.
- J. Park, *et al*, **Phys. Chem. Chem. Phys**. **22**(2020)27163-72.
- J. Park, *et al*, **Chem. Mater. 34**(2022)6108-15

Parity plots of O'Donnell fitting parameters

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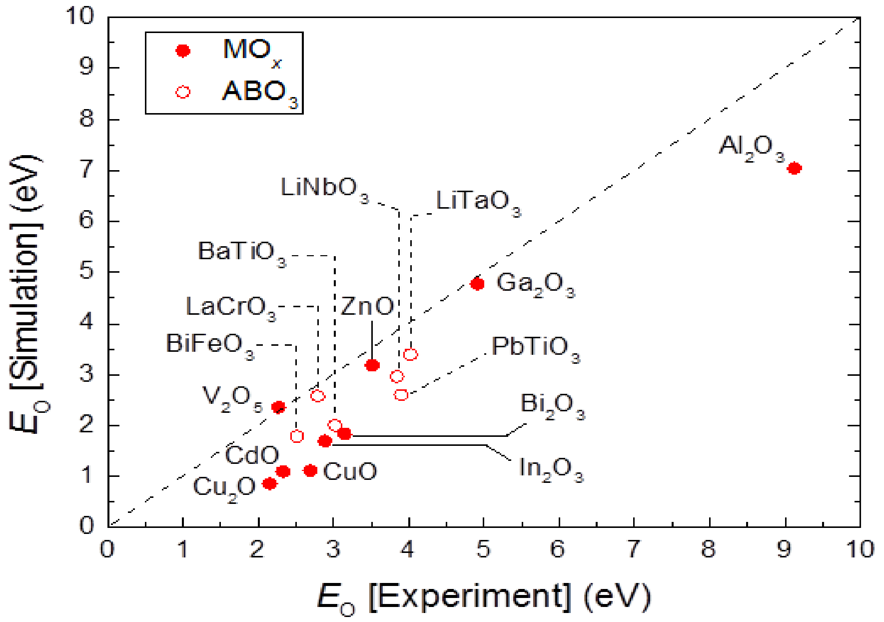
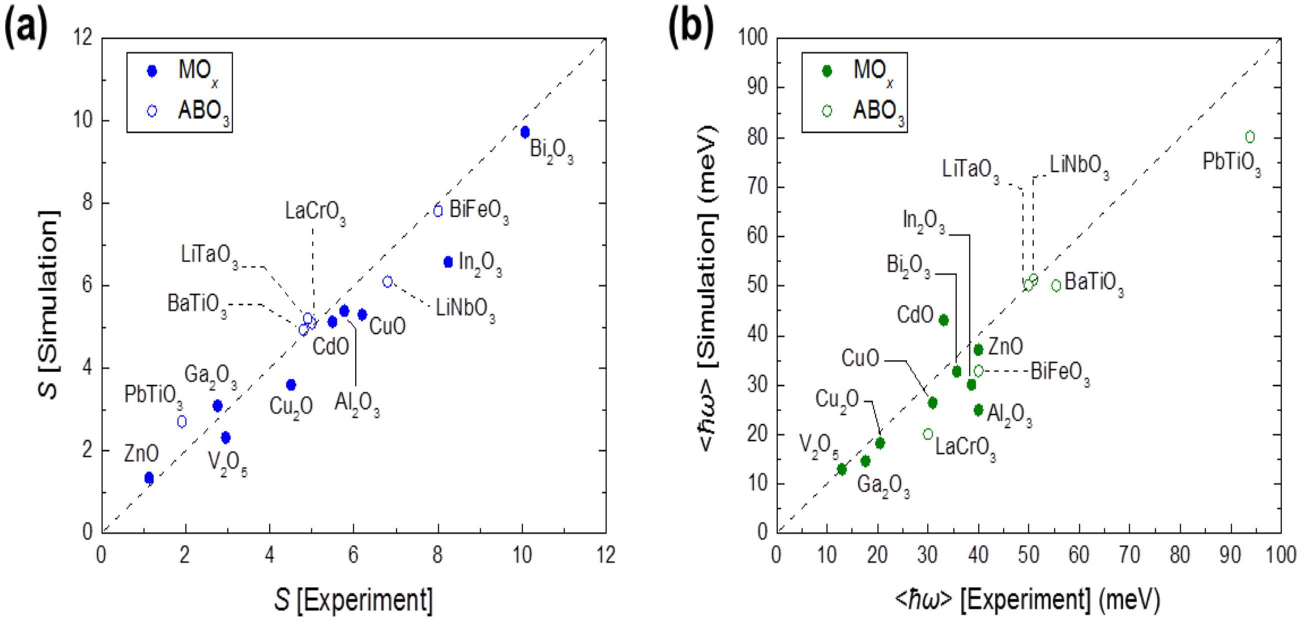
O'Donnell analytical equation:

$$E_g = E_0 - S < \hbar\omega > \left[\coth\left(\frac{< \hbar\omega >}{2k_B T}\right) - 1\right]$$





- The O'Donnell model could be represented the temperature dependence of band gap change well through the three parameters.
- To determine/fit these parameters can be done beyond DFT calculations.

- J. Park, *et al*, **Chem. Mater. 34**(2022)6108-15

- T. Nandi, *et al*, (2023)under preparation

Accomplishment--Journal publications (17)

NATIONAL ENERGY TECHNOLOGY LABORATORY

- J. Park *et al.*, **Phys. Chem. Chem. Phys. 22**(2020) 27163-72; **ACS Appl. Mater. Interfaces 13**(2021) 17717-25; **J. Phys. Chem. C 125**(2021) 22231-38; **126**(2022)8832-38; **Chem. Mater. 34**(2022)6108-15
- Y.-N. Wu *et al.*, **J. Phys. Chem. C 122**(2018) 22642-49; **J. Phys. Chem. Lett. 11**(2020) 2518-23; **J. Phys. Condens. Matter 32**(2020) 405705.
- T. Jia *et al.*, **RSC Adv. 7**(2017) 38798-804; **Phys. Chem. Chem. Phys. 22**(2020) 16721-26; **Applied Energy 281** (2021)116040; **J. Phys. Chem. C 125**(2021) 12374-81; **126**(2022)11421-25
- Y. Duan *et al.*, **J. Solid State Chem. 256**(2017) 239-251.
- S. Nations, *et al.*, **RSC Adv. 11**(2021) 22264-72; **Mater. Adv. 3**(2022)3897-3905; **Nanomaterials 13**(2023)276

For more details, please visit our poster.

EY23 Further Work

- ❑ Extend the oxides & perovskites database
- ❑ Using Machine Learning technique to determine temperature dependence of solid materials by predicting the parameters of O'Donnell model and optical properties
- ❑ Study gas sensing properties of the materials in the database
- ❑ Predict best candidates for high-temperature gas sensors.

Task 87: Quantum Sensing for Energy Applications

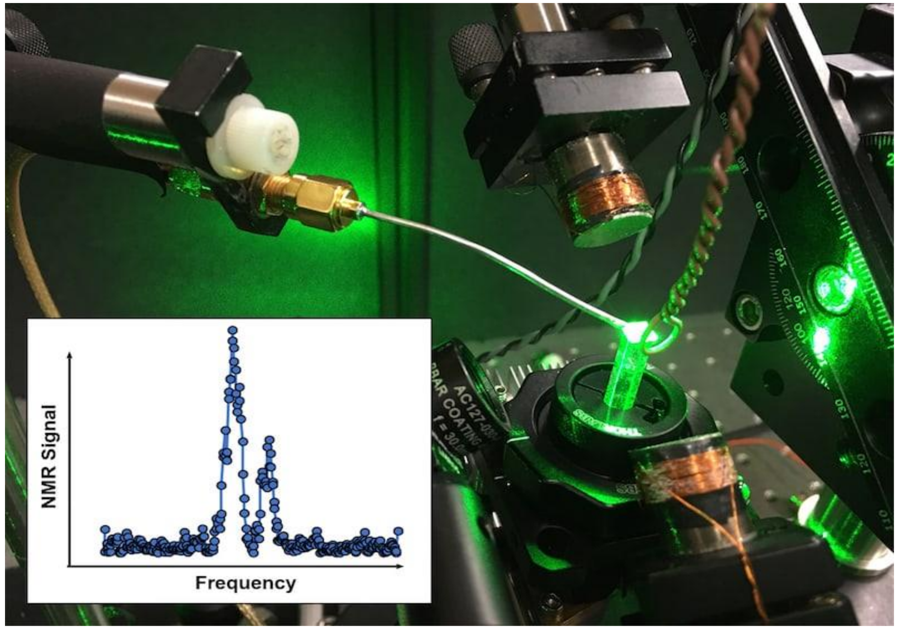
What is Quantum Sensing?

Quantum sensor utilizes properties of quantum mechanics, *such as quantum entanglement, quantum interference (superposition), and quantum state squeezing*, to optimize precision and beat current limits in sensor technology.

In solid-state physics, a quantum sensor is a quantum device that responds to a stimulus. Usually this refers to a sensor that, which has quantized energy levels, uses quantum coherence to measure a physical quantity, or uses entanglement to improve measurements beyond what can be done with classical sensors. There are 4 criteria for solid-state quantum sensors:

1) The system has to have discrete, resolvable energy levels.
2) You can initialize the sensor and you can perform readout (turn on and get answer).
3) You can coherently manipulate the sensor.
4) The sensor interacts with a physical quantity and has some response to that quantity.

- C. L. Degan, et al, **Rev. Mod. Phys. 89**(3)(2017)035002.



Diamond quantum sensor breaks new record

First experimental demonstration of NMR spectroscopy with full chemical specificity at the scale of a single biological cell

D. R. Glenn, et al, **Nature 555**(2018)351-354.

Task 87: Quantum Sensing for Energy Applications

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Objectives:

To use quantum sensing materials, quantum optics, and quantum sensing methodologies for realizing unprecedented performance in advanced sensing instrumentation for high priority FECM applications, such as detecting rare earth element, CO_2 capture & utilization, energy infrastructure, etc.

Theoretical approach

- Explore the electronic, magnetic, and optical properties of nitrogen vacancy (NV) defective nanodiamonds (NDs) as quantum sensor materials.
- Responses to the externally applied strain.
- Responses to the externally applied magnetic field.
- NV center sensing behaviors with different surface doping.

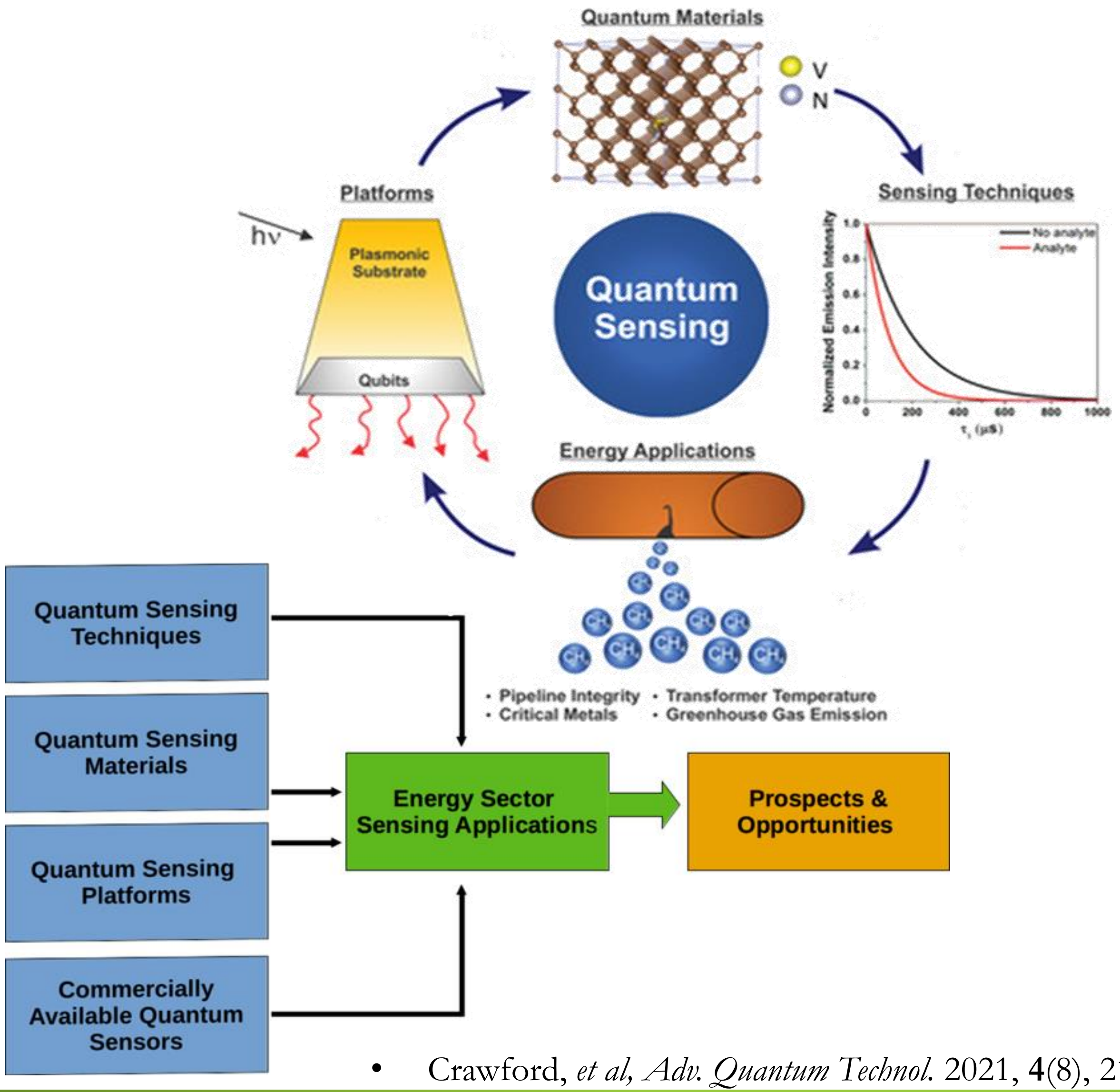
Experimental approach

- Set up Optically Detected Magnetic Resonance (ODMR) experiments.
- ODMR characterization: to characterize optical/spin properties, effects of magnetic field/strain orientation on coupling of the Hamiltonian eigenstates and selection rules.
- Spin relaxometry measurement: To correlate theoretical results with the experimental observations at a level of single and multiple NV centers.
- Develop quantum-classical hybrid optical fiber sensor network for CCUS field applications.

Key research team members:

- Former members: **Roman Shugayev**, Ping Lu, Paul Ohodnicki
- Current members: **Hari Paudel, Gary lander, Scott Crawford**, Jeffrey K. Wuenschell, Michael Buric, Yuhua Duan

Accomplishments—literature review



REVIEW

ADVANCED QUANTUM TECHNOLOGIES
www.advquantumtech.com

Quantum Sensing for Energy Applications: Review and Perspective

*Scott E. Crawford, Roman A. Shugayev, Hari P. Paudel, Ping Lu, Madhava Syamlal, Paul R. Ohodnicki, Benjamin Chorpening, Randall Gentry, and Yuhua Duan**

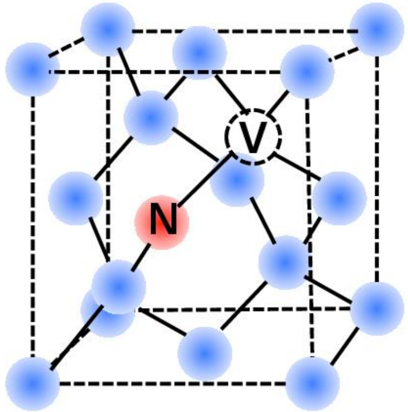
Table 1 Potential Applications of Quantum Sensing in Fossil Energy Areas

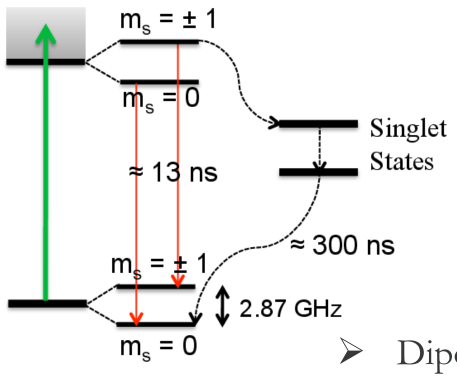
Fossil Energy Area	Sensing Application
CO_2 Utilization and Coal Beneficiation	Rapid, sensitive detection of CO_2 emission and leaks, detection high value metals from coal and coal utilization byproducts
Upstream Oil & Gas	Quantum gravimeters for the detection of oil/gas deposits
Midstream Oil & Gas	Monitoring pipeline integrity during transport and storage
Downstream Oil & Gas	Monitoring CO_2 emission during consumption
Carbon capture and storage	Rapid, sensitive detection of CO_2 emission and leaks
Coal Mining and Recovery	Sensing of critical metal elements from coal and coal utilizatio byproducts, gravimeters for coal exploration, coal mine safety
Electricity Generation	Sensors monitoring electromagnetic fields
Electricity Transmission and Distribution	Monitoring temperature in transformers
Nuclear Physics & Energy	Monitoring national nuclear security, superconducting quantum interference devices (SQUIDs)

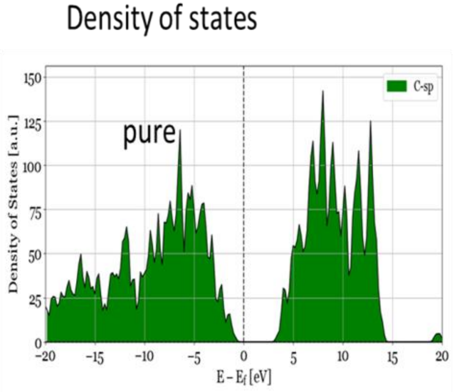
- Crawford, *et al, Adv. Quantum Technol.* 2021, **4**(8), 210049.

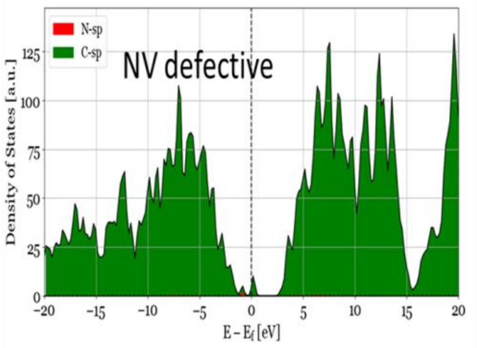
Accomplishments—Theoretical modeling

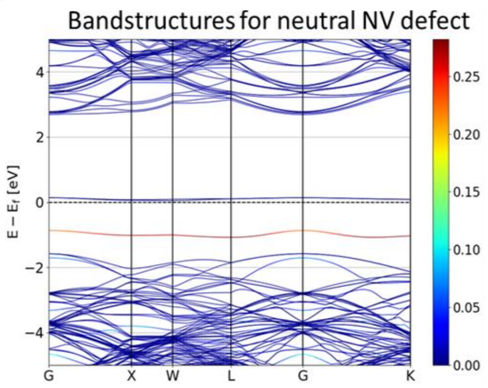
The nitrogen-vacancy (NV) center in nanodiamond (ND) is a good quantum sensor because its electron spin can be manipulated at room-T by external fields, resulting in sharp resonances which related to quantum entanglement.. We perform ab-initio density functional theory (DFT) calculations to investigate the bulk and surface properties of the N and NV defective bulk and diamond surfaces.

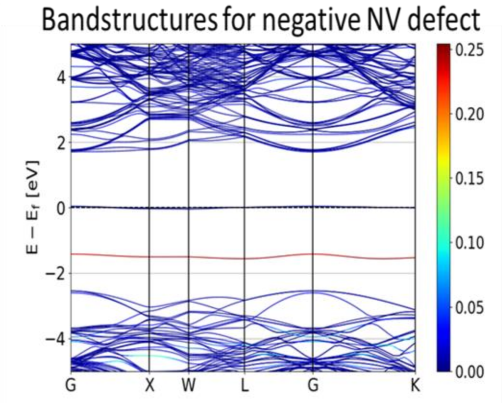


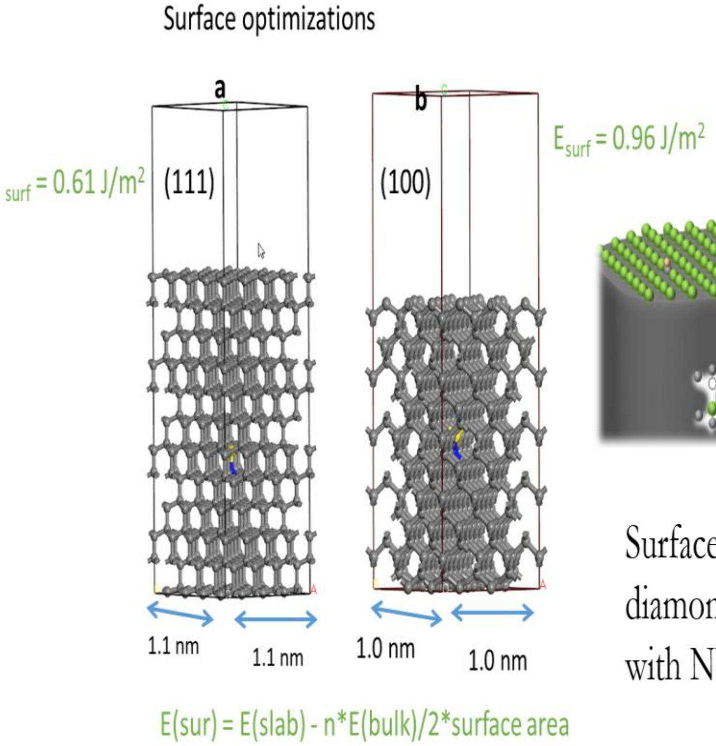


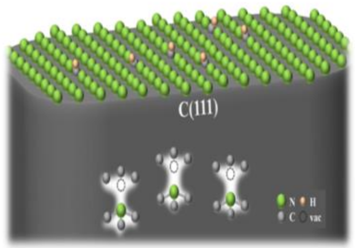












Surface model for nano-diamond with NV center

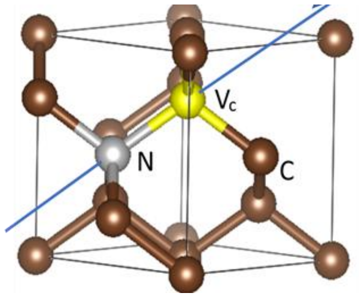
- Dipole is along NV axis
- Majority of charge is concentered around the three C atoms around the defect

Accomplishments—Theoretical modeling

We further investigated the effect of external stress on the electronic properties of nitrogen vacancy center in nanodiamond for sensing applications.

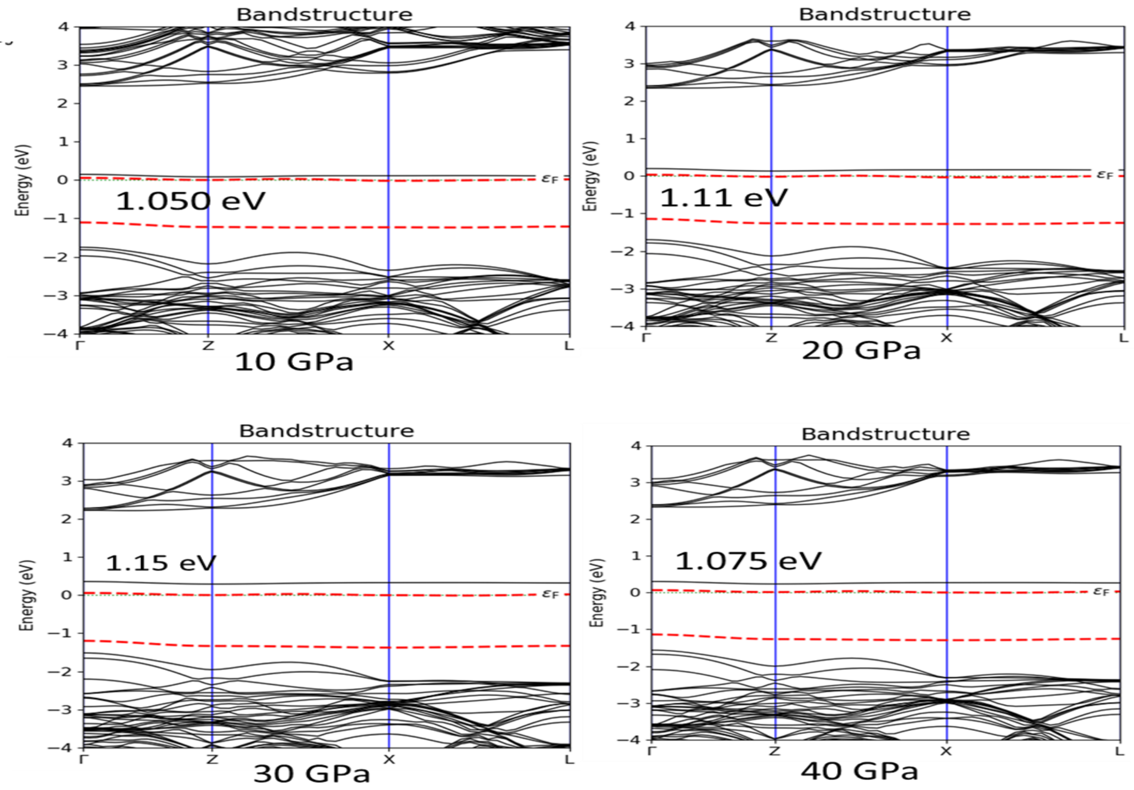
$$\hat{H}_{gs} = D_{gs}\left[\hat{S}_z^2 - S(S+1)/3\right] + A_{gs}^{\parallel}\hat{S}_z\hat{I}_z + A_{gs}^{\perp}\left[\hat{S}_x\hat{I}_x + \hat{S}_y\hat{I}_y\right] + P_{gs}\left[\hat{I}_z^2 - I(I+1)/3\right]$$

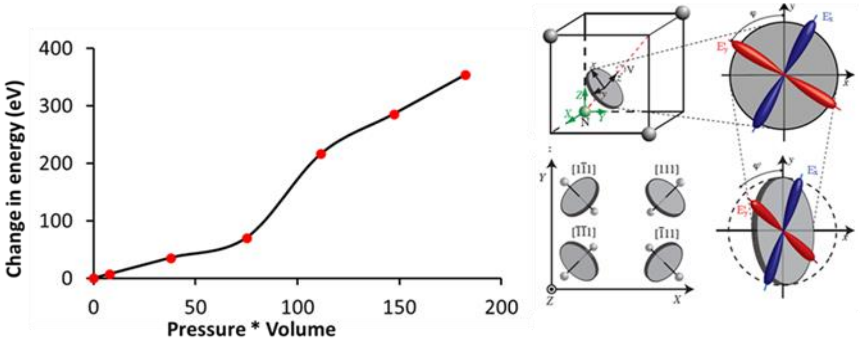
$$\textit{Pressure sensitivity}: \ \eta_{gs} = \frac{1}{2\pi\frac{dD(p)}{dp}K\sqrt{T_2^*}}$$



Spin splitting energy required to get pressure sensitivity

$$\Delta = \alpha \pm \sqrt{\beta^2 + \gamma^2}$$





(a) Calculated change in PV vs change in energy of ground state NV center, (b) Orientations of different surfaces of NV center

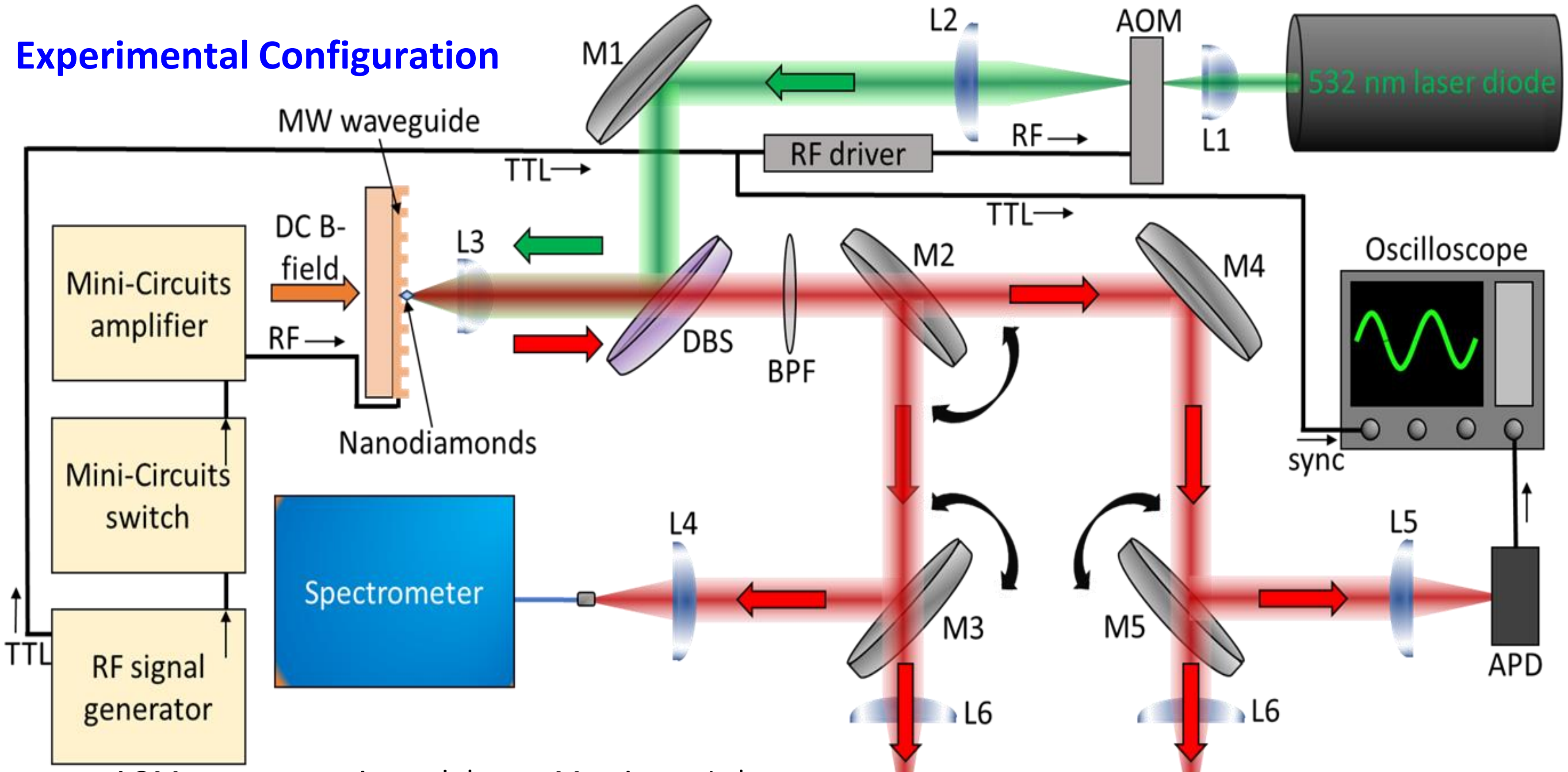
- With increasing the external stress, the band energy splitting is increased linearly. The spin splitting parameter also varies as the diagonal components of the stress tensor increases.
- The change in the sensing behavior under axially applied stress can be quantified.
- Provide an avenue for possibility of sensing stress at elevated environmental conditions

- H. Paudel, et al, (2023) under preparation.

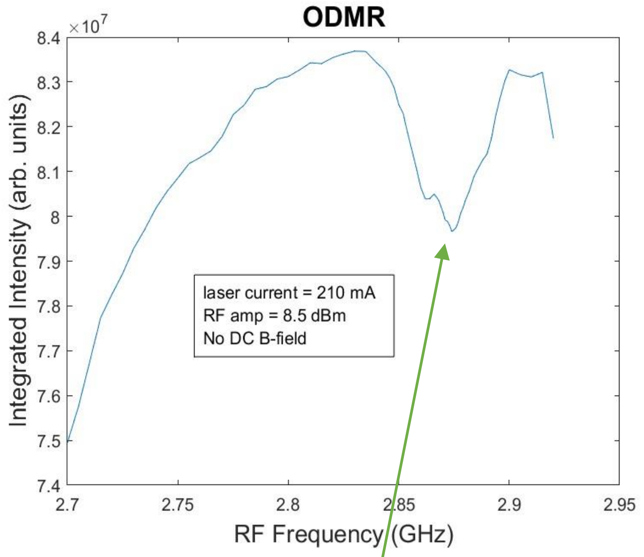
Accomplishment--Experimental

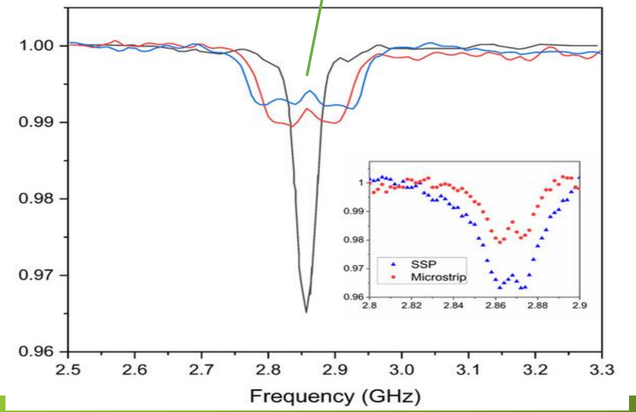
Set up an enhanced optically-detected magnetic resonance (ODMR) and spin relaxometry platform

Experimental Configuration



AOM: acousto-optic modulator; M: mirror; L: lens;
DBS: dichroic beam splitter; BS: beam splitter;
APD: avalanche photodiode; BPF: bandpass filter





Accomplishments—Publications & Presentations

NATIONAL ENERGY TECHNOLOGY LABORATORY

Publications (7):

1) S. E. Crawford, R. A. Shugayev, H. P. Paudel, P. Lu, M. Syamlal, P. R. Ohodnicki, R. Gentry, *Y. Duan*, "*Quantum information science: review and perspective for energy applications*", **Advanced Quantum Technologies**, **4**(2021)2100049.

2) R. Shugayev, S. Crawford, J. Baltrus, N. Diemler, J. Ellis, K.-J. Kim, "*Synthesis and quantum metrology of metal-organic framework-coated fluorescent nanodiamonds containing nitrogen vacancy centers*", **Chem. Mater.** **33**(16)(2021)6365–6373**.**

3) R. Shugayev, J. Devkota, S. Crawford, P. Lu, M. Buric "*Giant microwave spontaneous emission enhancements in planar aperture waveguide structures*", **Adv. Quantum Technol. 4**(6)(2021)2000151

4) R. Shugayev, P. Lu, Y. Duan, M. Buric, "*Hong-Ou-Mandel sensing via superradiant coupling of discrete fluorescent emitters*" **AVS Quantum Science,** **4**(2022)034402**.**

5) H. P. Paudel, M. Syamlal, S. E. Crawford, Y.-L. Lee, R. A. Shugayev, P. Lu, P. R. Ohodnicki, D. Mollot, Y. Duan, "*Quantum computing and simulations for energy applications: review and perspective*", **ACS Engineering Au**, **2**(3) (2022)151-196**.**

6) H. P. Paudel, S. E. Crawford, M. Leuenberger, R. A. Shugayev, Y.-L. Lee, M. Syamlal, P. R. Ohodnicki, P. Lu, D. Mollot, Y. Duan, "*Quantum Networking for Energy Applications: Review and Perspective*", **Adv. Quantum technol.** (2023) submitted

7) H. P. Paudel, G. Lander, S. E. Crawford, Y. Duan, "*Effect of external stress on the electronic properties of nitrogen vacancy center in nanodiamond for sensing applications: a first principles density function theory study*", N**anomaterials**, (2023) to be submitted

Presentations (6):

1) R. Shugayev, P. Lu, Y. Duan, "*Near field Hong-Ou-Mandel sensing via superradiant coupling of discrete fluorescent emitters*", **Quantum Technologies for Critical Energy Infrastructure summit(QuTCISS), ORNL,** Jan.14-15, 2021

2) P. R. Ohodnicki, K. Chen, G. Dutt, E. Stewart (PIT), L. Kiani, M. Messerly, R. Mellors (LLNL), S. Crawford, J. Devkota, Y. Duan (NETL), J. Gopinath (Univ. Colorado at Boulder), "*Robust Quantum Sensing and Distributed Analytics for Critical Energy Infrastructure*", **Quantum Technologies for Critical Infrastructure Security Summit (QuTCISS)**, https://qutciss.ornl.gov, ORNL, Jan.14-15, 2021

3) H. P. Paudel, S. E. Crawford, R. A. Shugayev, Y.-L. Lee, M. Syamlal, P. Lu, P. R. Ohodnicki, Darren Mollot, Y. Duan, "*Quantum Information Science for Energy Sector Applications*", **TechConnect World Innovation Conference and Expo**, June 13-15, 2022, Washington, DC

4) S. E. Crawford, H. P. Paudel, Y.-L. Lee, Y. Duan, "*Overview of Quantum Information Science Research at NETL*", **PQI2022**, Sept. 13-15, 2022, Pittsburgh, PA.

5) H. P. Paudel, S. E. Crawford, Gary, Lander, Y. Duan, "*Electronic and optical properties of NV center in diamond for sensing applications: first-principles density functional theory and experimental approach*", **APS March Meeting**, Mar.05-10, 2023, Las Vegas, Nevada.

6) S Crawford, R. Shugayev, G. Lander, H. Paudel, ***Y. Duan***, J. Baltrus, N. Diemler, J. Ellis, K. Kim, P. Cvetic, "*Controlled Encapsulation of Nanodiamond Qubits by Metal-Organic Frameworks: Towards Enhanced Quantum Sensing*", **TechConnect World Innovation Conference & Expo,** June 19-21, 2013, Washington DC

For more details, please visit our poster.

EY23 Work

- Complete model of nitrogen vacancy (NV) center sensing behaviors in regard to stress sensing.
- Set up experiments to conduct optically-detected magnetic resonance (ODMR) measurements using NV centers in nanodiamonds (NDs) on CO_2 conversion applications.
- Conduct technology review and evaluate commercially available solutions and provide an in-depth survey of hybrid quantum-classical sensing networks with a target for energy infrastructure applications.
- Demonstrate the effect of an external magnetic field in NV centers in NDs

Questions & Discussion

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