# Enabling Low-Temperature Plasma (LTP) Ignition Technologies for Multi-Mode Engines through the Development of a Validated High-Fidelity LTP Model for Predictive Simulation Tools

Project ID: ace150


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**2020 DOE Vehicle Technologies Office Annual Merit Review | June 2, 2020**

# Overview

## TIMELINE:

- Project Start: January 2020
- Project End: December 2022
- Complete: >5%

## PARTNERS:

- University of Texas at Austin
- Sandia National Laboratories
- Argonne National Laboratories

## BUDGET:

- Total project funding: $1.5M / 3yrs
  - Academic cost share: $360K
- National Labs: $300K

## BARRIERS*:

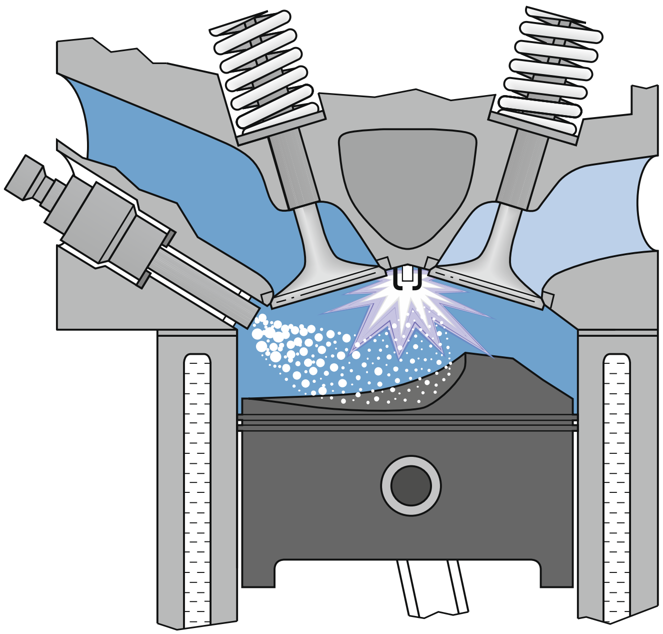
- **Robust lean-burn and EGR-diluted combustion technology and controls** needed to safeguard efficiency gains of future multi-mode engines
- **New ignition systems need to be developed - LTP igniters**
- Lack of predictive simulations tools for LTP prevents full adoption of LTP into future engine designs
- Significant deficiencies in current simulations capabilities are:
  - i. Lack of validated plasma-combustion kinetics of fuels
  - ii. Lack of validated computational methods for unsteady, 3D LTP ignition

*https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf

# Relevance

## IMPACT:

- Development of **a validated chemical kinetics model** and **benchmarked exascale software** for high-fidelity simulation of **LTP ignition of hydrocarbon/air fuels**
  - **Improve the predicative capability of current LTP sub-models for multi-mode engine simulations**
  - **Enable advanced gasoline engines to operate across the entire load-speed map, with lower emissions and improved fuel-economy**
  - **Advance the development of new LTP ignition technologies to extend SACI lean and/or EGR dilution-limits at boosted conditions**
  - **Facilitate near/long CO-OPTIMA goals to develop engines that run more efficiently on affordable, scalable, and sustainable fuels**



**LTP Enabled Multi-Mode SACI**

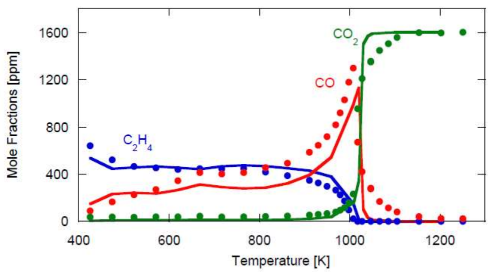
## OBJECTIVES:

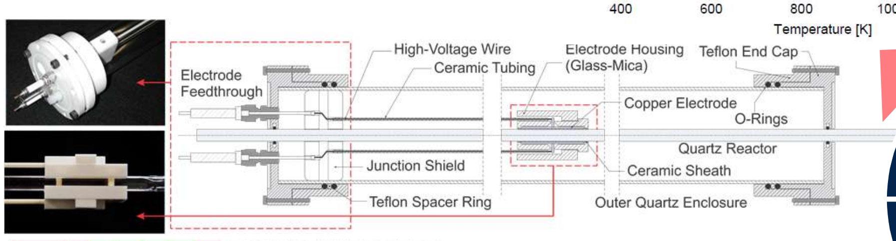
1. **(AUBURN)** Development of experimentally validated LTP-specific kinetic mechanism for relevant fuels; iso-octane, ethanol, and EGR blends
2. **(UT-AUSTIN)** Development of a validated and benchmarked massively-parallel, exascale, high-fidelity solver for the simulation of LTP discharges/ignition of hydrocarbon/air mixtures in complex geometries
3. **(SANDIA)** Experimental database of LTP ignitions of blended mixtures with iso-octane/ethanol/EGR/air at conditions relevant to the Co-Optima initiative for benchmarking and validating high-fidelity solvers and kinetic models
4. **(ARGONNE)** Appraisal of the performance and accuracy of existing LTP commercial software tools against the high-fidelity solver and plasma/combustion kinetics models and identification of areas of improvement and directions for future development

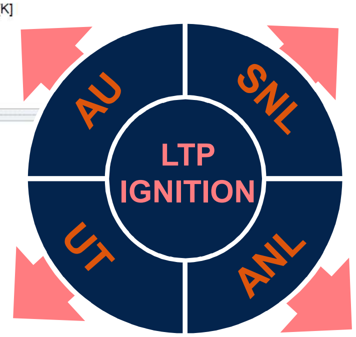
# Overall Technical Approach

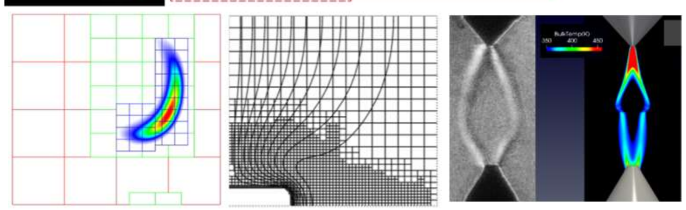
## LTP Kinetic Model Development via Plasma Flow Reactor

- Custom-built plasma flow reactor with nanosecond-duration high-voltage pulse perturbation for LTP kinetic studies
- Offline GC/MS for ex-situ diagnostics for species identification/quantification
- 0D plasma kinetic model for LTP-specific kinetic mechanism development



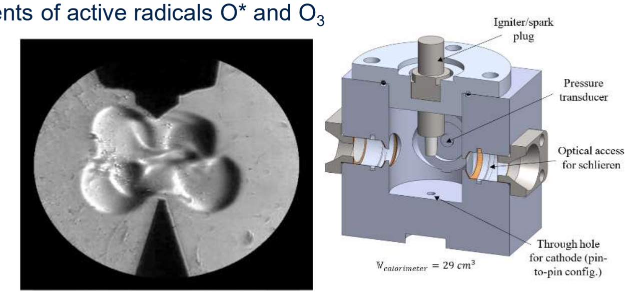



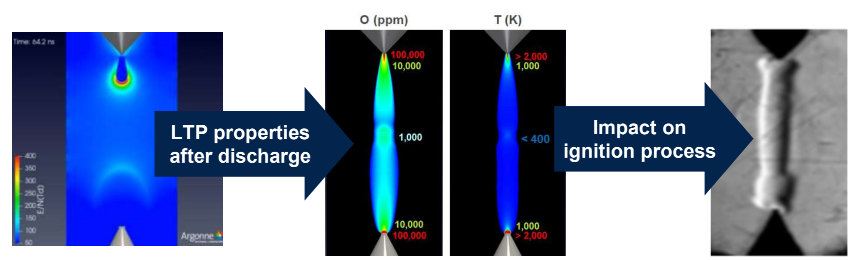
- Exascale solver build on AMReX (Lawrence Berkeley National Lab)
  - Hierarchy of meshes and resolution near electrodes
  - Efficient temporal integration
  - Ready for high-performance computing on massively-parallel DOE computers
- Development of reduced skeletal mechanisms for LTP ignition of hydrocarbon fuels

## Development of LTP Ignition Exascale-Ready AMR Software

## Measuring LTP Ignition Characteristics via Ignition Cell

- Purpose built ignition test vessel for LTP ignition studies
- Experimental measurements/diagnostics include:
  - Pressure rise calorimetry – bulk energy deposition
  - High-Speed Schlieren and OH* measurements – flame propagation measurements
  - Direct measurements of active radicals O* and $O_3$



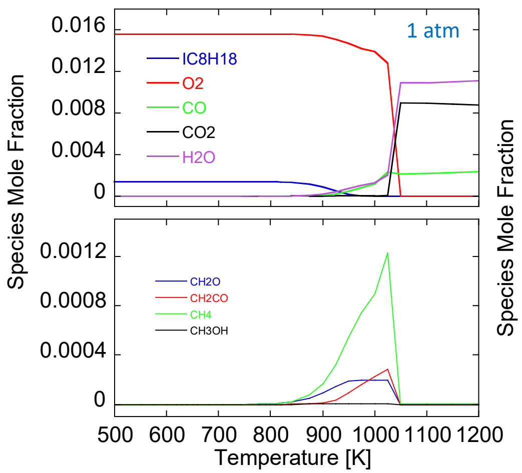



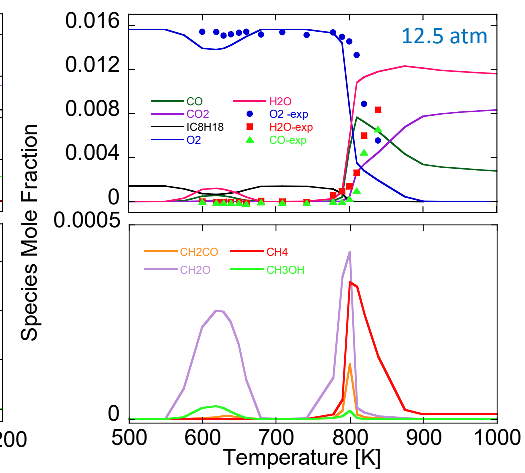

- Commercial solver use: VizGlow (Esgee Technologies)
- Validation carried out by looking at:
  - Discharge regime (glow or spark)
  - Bulk gas temperature estimates and/or active species [O, $O_3$] direct measurements
  - Impact on ignition described by CFD combustion tool (CONVERGE CFD) and validated against Schlieren from SNL

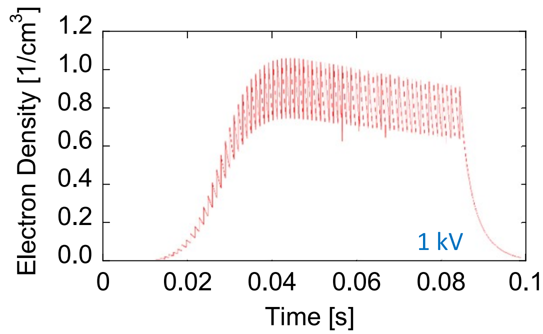
## Appraising Existing Commercial LTP Modeling Software

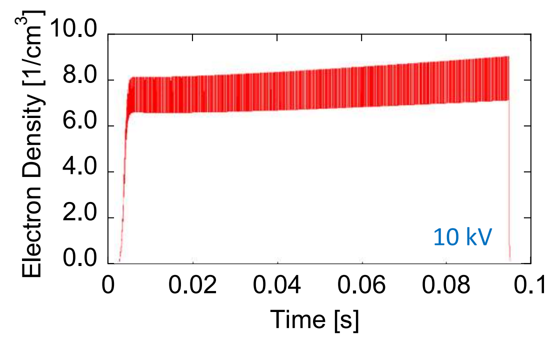
# Technical Accomplishments (Auburn)

## Parametric Modeling Studies for Thermal Mechanism and 0D Plasma Model

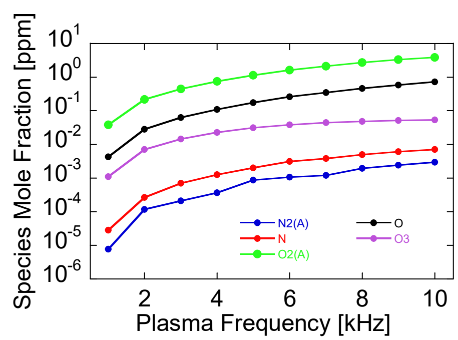



- Several iso-octane mechanisms currently being assessed, including detailed, reduced and PRFs - selection based on agreement with experimental data, and computational practicality
- High-pressure LTC kinetics provides an indication of potential reaction pathways for LTP chemistry




- Preliminary $N_2/O_2$ simulation preformed to ascertain experimental conditions
- At 1 atm pressure, plasma kinetics by, O-atom and O* excited kinetics will dominated

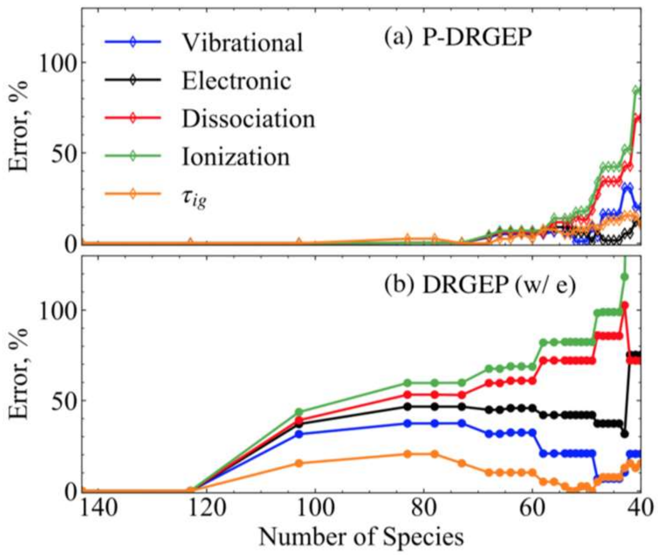
| Date | Task/ Milestone | Description | Status |
|---|---|---|---|
| FY21 Q1 | T1.1 | Perform LTP pyrolysis and oxidation experiments on iso-octane using the PFR facility | On Track |
| FY20 Q1 | T1.3 | Appraise and select thermal mechanisms for iso-octane combustion against experimental data. | Delayed Q3 |
| FY21 Q1 | T1.4 | Use PAC kinetic model to develop plasma/combustion reaction mechanism for iso-octane against experimental data. | On Track |
| FY20 Q1 | M.1 | The selection of the iso-octane thermal mechanism is complete. Selection is verified by comparing experimental pyrolysis and oxidation data to numerical results with the least error. | Delayed Q3 |

# Technical Accomplishments (UT Austin)

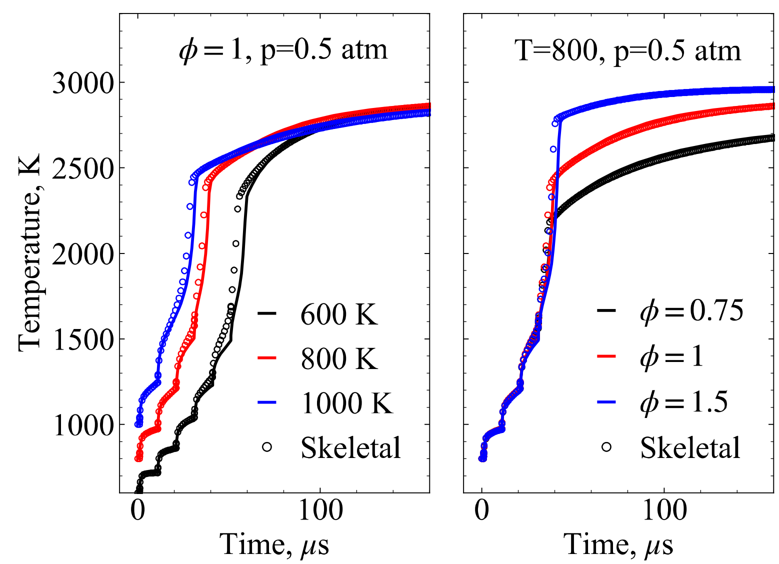
## Preliminary Benchmarking with LTP Reduced Ethylene Mechanism

**Improved**

**Conventional**




**Predicated Temperature During LTP Ignition**

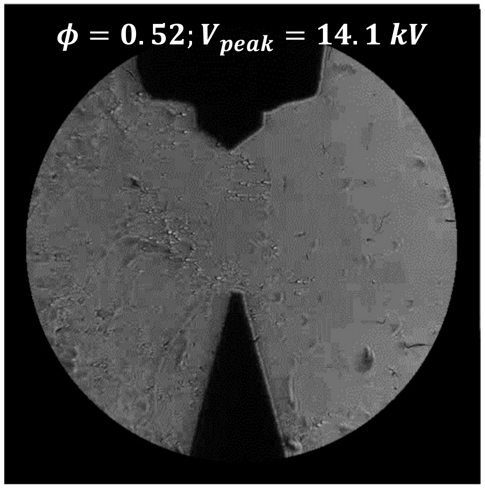


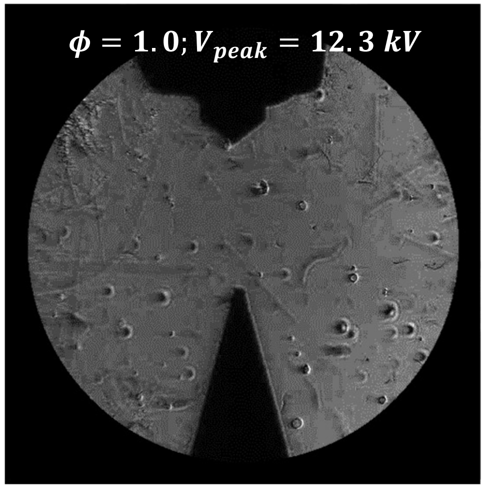

- Extension of DGREP to plasma kinetics with P. Pepiot (Cornell U)
- Ethylene/air plasma/combustion kinetics
- Reduction from 140 to 50 species

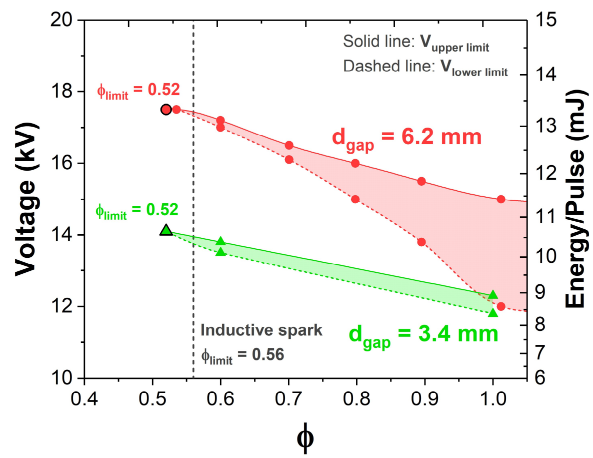
| Date | Task/ Milestone | Description | Status |
|---|---|---|---|
| FY20 Q3 | T1.5 | Extend available DGREP framework to DRGEP-2T to address plasma kinetics | On Track |
| FY20 Q4 | T1.6 | Formulation of a skeletal mechanism for ethylene/air plasma/combustion via the DGREP-2T reduction methodology. | On Track |
| FY20 Q3 | T1.8 | Assembly of mathematical models and closures. | On Track |
| FY20 Q3 | M.3 | Software for skeletal reduction of detailed plasma/combustion kinetics mechanism is complete. Software is distributed with validation suite. | On Track |

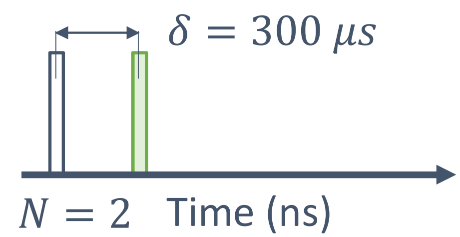
# Technical Accomplishments (SNL)

## Parametric LTP Ignition Mapping – Initial Propane/Air Studies




| $\phi$ | 1 |
|---|---|
| **Fuel** | Propane |
| **# of pulses, N** | 2 |
| **Dwell, $\delta$** | 300 $\mu s$ |
| $V_{peak}$ | 12.3 kV |
| **P** | 1.3 bar |

- Pin-to-Pin NRPD ignition points identified for different gap sizes and pulse strategies
- Lean ignition limits were extended due to a combination of larger ignition volumes and reduced electrode heat losses due to the larger gaps

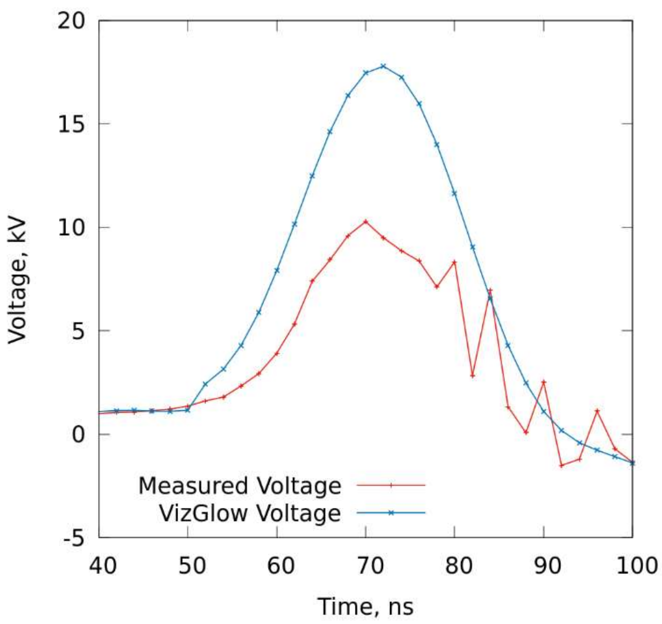
| Date | Task/ Milestone | Description | Status |
|---|---|---|---|
| FY20 Q2 | T1.10 | Ignition limit mapping - parametric studies ethylene/air | Delayed Q3 |
| FY20 Q2 | T1.11 | Qualitative O-atom luminosity measurements ethylene/air | Delayed Q3 |
| FY20 Q2 | T1.12 | LTP discharge calorimetry measurements ethylene/air | Delayed Q3 |
| FY20 Q2 | M.2 | LTP ignition experiments for Phase 1 in static cell and ignition vessel are complete | Delayed Q3 |
| FY21 Q4 | T1.13 | Flame growth rate measurements - ethylene/air | On Track |
| FY21 Q4 | T1.14 | OH* imaging for flame kernel distribution - ethylene/air | On Track |

# Technical Accomplishments (ANL)

## Boundaries and Kinetics Identified for LTP Simulations using VizGlow

### Boundary Conditions:

- Improved circuit calculations take into account for real components and transmission line losses.
- Leveraged collaboration:
  - Sandia National Laboratories (PACE program)
  - Transient Plasma Systems (HPC4Mfg program)
- Raw Voltage/Current data from Sandia experiments was post-processed to obtain realistic values of the connection Voltage




### Plasma kinetics

- Typical VizGlow LTP discharge simulations carried out in $O_2/N_2$ (18 species, 64 reactions)
- Reduced iso-octane/air/diluent mechanism identified (≈50 species, ≈300 reactions) that could be run in VizGlow
- Reduced mechanism for ethylene/air (54 species, 236 reactions) provided by UT/Cornell (Bellemans, Pepiot, Bisetti, et al., PCI 2020)

| Date | Task/ Milestone | Description | Status |
|---|---|---|---|
| FY21 Q2 | T1.15 | LTP discharge simulations in ethylene/air | On Track |

# Summary

**IMPACT:**

- Advance predictive modeling capabilities in support of the development of LTP ignition technologies to enable novel multi-mode engine concepts

**APPROACH:**

- Multi-lab team, combing prior experience of academia and leveraging technical expertise of national labs

**TECHNICAL ACCOMPLISHMENTS:**

- Modeling initiatives have started to evaluate selection of thermal mechanisms and parametric studies of plasma kinetics in air using 0D model – experimental studies to compliment models studies DELAYED
- Ethylene kinetic mechanism reduced for high-fidelity modeling
- Parametric LTP ignition studies have started for propane/air – continuation of experimental studies to have been DELAYED
- Boundary conditions and potential kinetic mechanism identified to appraise performance of LTP ignition simulation using commercial VizGlow software

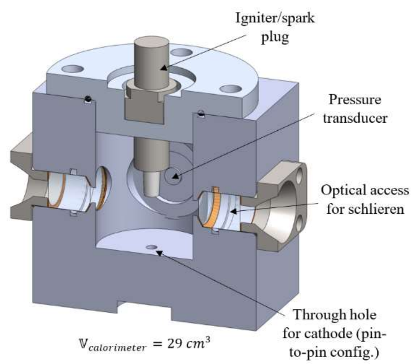
**PROJECT STATUS:**

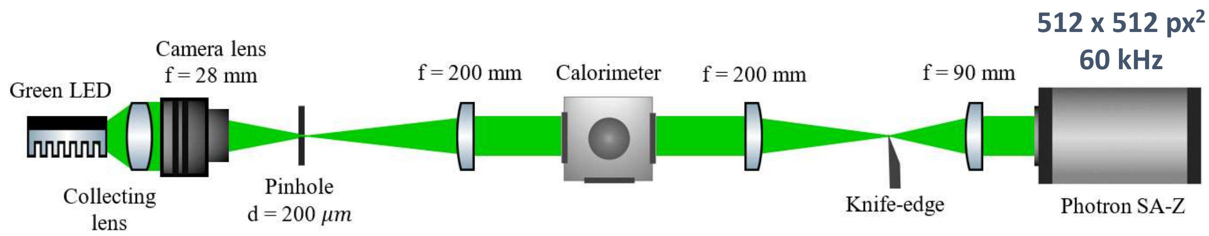
- All modeling initiatives are on track and continuing, experimental initiative delayed and set to resume

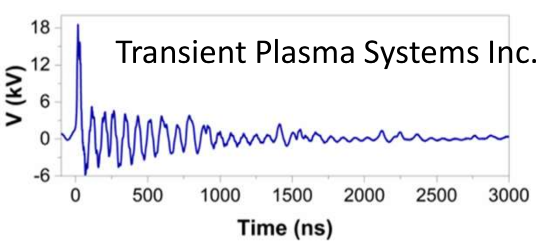
# Technical Back-Up Slides

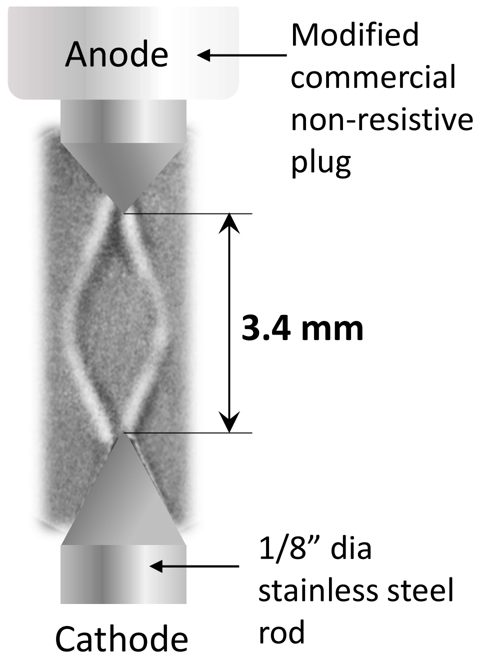
# Technical Back-Up Slide (SNL)

## Optical Ignition Calorimeter



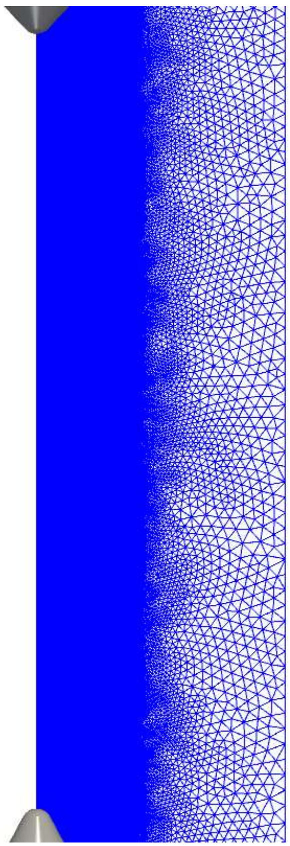

**Schlieren Imaging**
- Discharge volume
- Channel temperature (with calorimetry)
- Flame kernel growth

**Experimental Conditions**
- Propane/air
- $\phi = 0.52 - 1.0$
- EGR 0 – 34%
- Voltage 8 – 14.1 kV
- Pressure 1.3 – 4 bar

**Pin-to-Pin (P2P)**
- Strong electric fields at electrode tips
- Concentrated pulse energy and wide gap lowers flame kernel heat loss
- ***Ignition primarily thermally driven?***

# Technical Back-Up Slide (ANL)

## Pin-to-Pin (P2P) case setup in VizGlow



**SETUP VALIDATED AGAINST EXPERIMENTAL DATA FROM SNL**

- 2-D axis-symmetric (preferred) or 2-D planar simulations.
- Computational time-step = $1\text{x}10^{-14} – 1\text{x}10^{-12}$
- Pressure range = 1-5 bar, Temperature = 343 K
- Voltage range = 5-30 kV, pulse repetition rate 5-20 kHz
- Gap size = 3-6 mm
- Minimum mesh size = 2-10 mm, 40,000-400,000 total cell count.
- Coarser mesh case run on ≈ 100 CPUs. Finer meshes scale up to ≈ 500 CPUs
- <u>Boundary conditions needed: applied voltage profile</u>
- Model calibration through Electron collision frequency to match experiments
- Extensive study on real electrode geometry effects on streamer discharge
- Flow solver coupled with Poisson equations