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

Nicholas Tsolas (Auburn University)
Fabrizio Bisetti (University of Texas at Austin)
Isaac Ekoto (Sandia National Laboratories)
Riccardo Scarcelli and **Vyaas Gururajan** (Argonne National Laboratory)

2022 DOE Vehicle Technologies Annual Merit Review | June 22, 2022

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Overview

TIMELINE:

- Project Start: January 2020
- Project End: June 2023
- Complete: ≈ 45%

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

BUDGET :

- Total project funding: $1.5M / 3yrs
  - Academic cost share: $360K
- National Labs: $300K / 3yrs
  - Sandia: $150K
  - ANL: $150K

PARTNERS:

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

*ACEC RoadMap

Relevance/Objectives

The advancement of LTP igniters requires improved predictive LTP sub-models for engine simulation tools

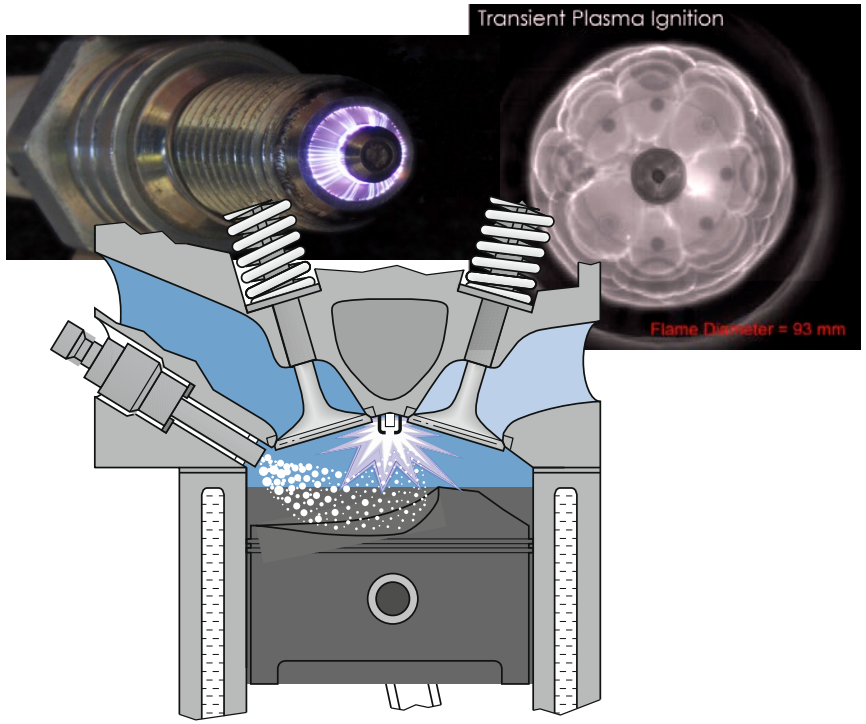
- Current models lack: (i) validated and skeletal chemical kinetic mechanisms to accurately describe the interaction of plasma-specific chemistry with neutral combustion chemistry (fuel-specific); (ii) validated exascale numerical algorithms and software to accurately model LTP ignition physics
- Project outcomes are expected to facilitate the **commercial development of drop-in LTP ignition systems** to benefit **ICE OEMs** (light-duty, heavy-duty manufactures); **Tier 1** (e.g. BorgWarner, Delphi) and **start-up** (e.g. Transient Plasma Technologies, Knite Inc.) **ignition suppliers**, and **CFD software developers** (e.g., Convergent Science Inc., Esgee Technologies)

IMPACT:

- **Advance the development of new LTP ignition technologies to enable next generation engine architectures to operate with lower emissions, improved efficiency with SACI lean and/or boosted conditions with extended EGR dilution limits.**
- **Facilitate near/long term goals to advance internal combustion engines with affordable, scalable and sustainable future fuels (e.g. methanol)**

OVERALL PROJECT OBJECTIVE:

Development of **a validated chemical kinetics model** and **benchmarked exascale software** for high-fidelity simulation of **LTP ignition of future fuels**

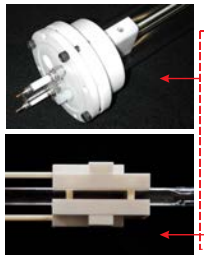


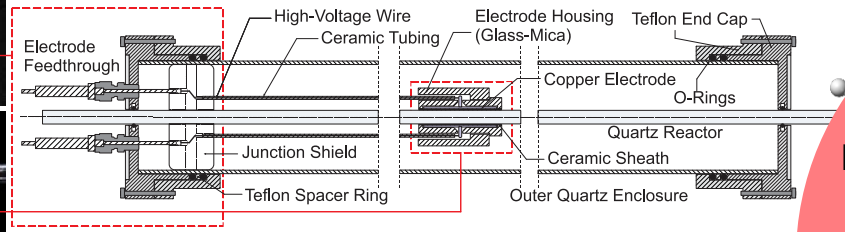
Overall Technical Approach

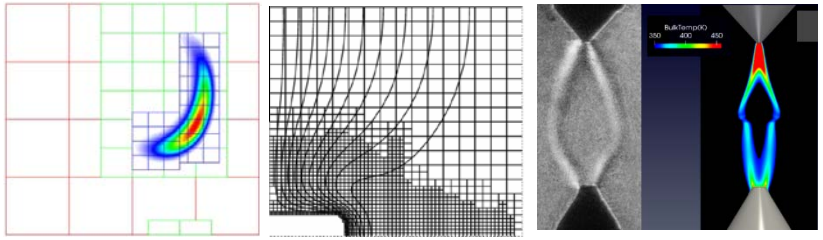
AUBURN Develop LTP Kinetic Mechanisms

- Purpose built **plasma flow reactor (PFR)** for LTP kinetic studies – ns duration pulses
- Experimental measurements/diagnostics include: GC/MS for species identification/quantification
- Utilize custom 0D plasma kinetic model for LTP-specific kinetic mechanism development

Provide LTP chemical kinetic mechanisms for LTP ignition models developed by UTexas and ANL



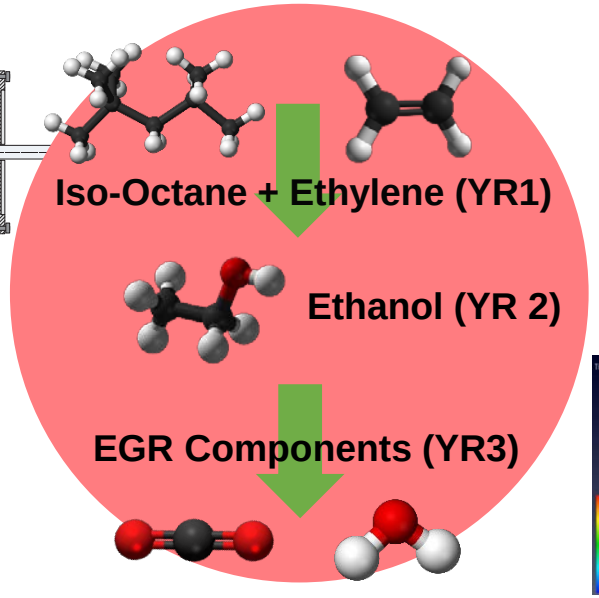




- Exascale solver **built on AMReX** featuring: hierarchy of meshes and resolution near electrodes; efficient temporal integration; ready for high-performance computing on massively-parallel DOE computers
- Development of **reduced skeletal mechanisms for LTP ignition** of future fuels

Develop new 3D unsteady LTP ignition model to meet the needs of industry

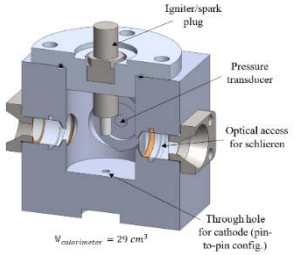
UTEXAS Develop LTP Ignition Exascale-Ready Software

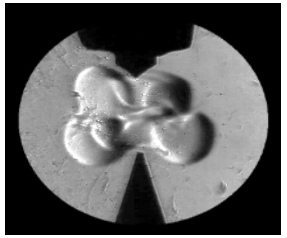


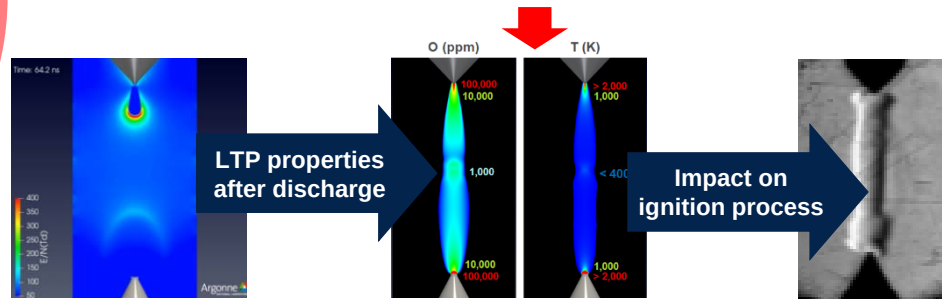
SANDIA Measure LTP Ignition Characteristics

- 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

Provide LTP ignition data to validate LTP ignition models developed by UTexas and ANL







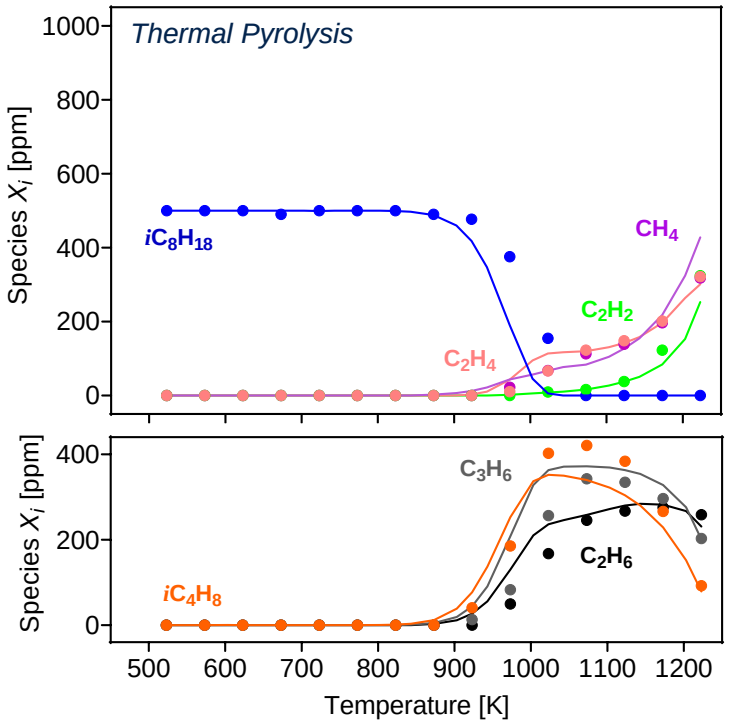
- Model **built on VizGlow (Esgee Technologies)** – commercial solver
- Validation against SNL data considers: discharge regime, gas temperature, active species
- Impact on ignition processes described by commercial solver **CONVERGE CFD** and validated against schlieren from SNL data

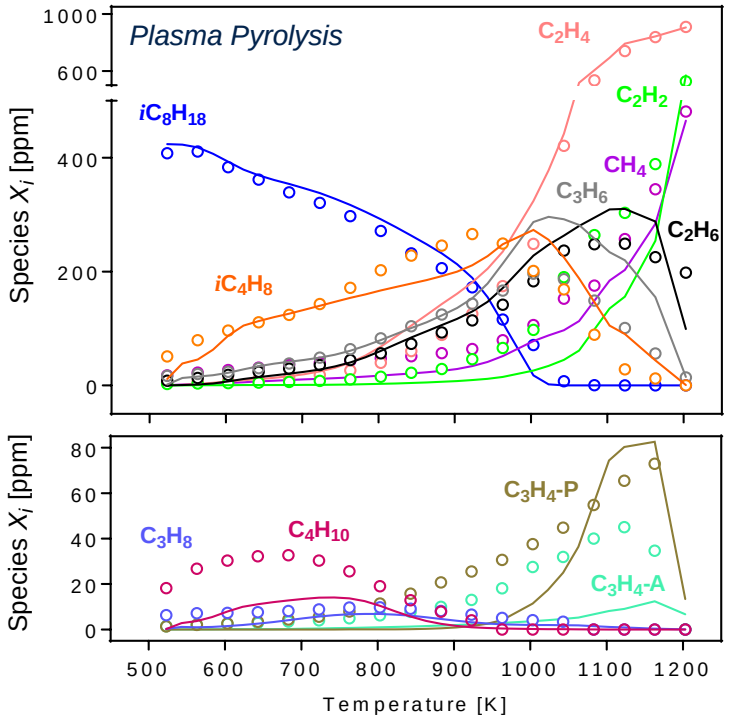
Support the development of the exascale solver at UTexas

ARGONNE Appraise Existing Commercial LTP Software

Technical Accomplishments (Auburn)

PFR experiments and modelling of LTP pyrolysis of isooctane





- ***Thermal Pyrolysis*** described in two phases: (i) Initial decomposition (900K - 1200K) resulting in butyl-radical formation of butene, propene and ethane; (ii) Secondary decomposition of products (above 1200K) mainly forming acetylene.
- LLNL-detailed iso-octane mechanism [1] shows good agreement with experiments

- ***LTP Oxidation*** enhances fuel decomposition significantly, consuming nearly 50% of initial fuel loading by 900K – decomposition is linear with temperature, indicating the plasma effects are increasing linearly with E/N
- Developed mechanism predicts **(all major species accounted for)** experimental results of pyrolysis with very good agreement **(less than 10% deviation)** for all measured species and temperatures.
- Quenching reactions with $N_2(A)$ leads to fuel fragments, and initial H-atom density
- Neural chemistry dominates at longer time scales due to enhanced radical formation (H-atom)

$+N_2^*/e$

Recycled

$$C_8H_{18} + N_2^* \rightarrow C_8H_{17} + H \qquad H + C_8H_{18} \rightarrow C_8H_{17} + H_2$$

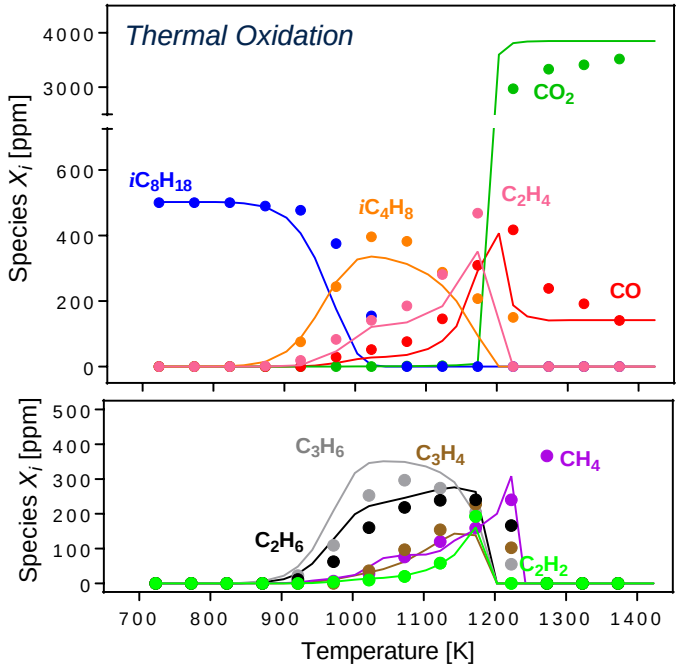
Initial times scales low H-atom density and fuel fragments

Longer times scales high H-atom density

[1] *H. J. Curran, et al. Combust. Flame 129 (2002) 253-280*

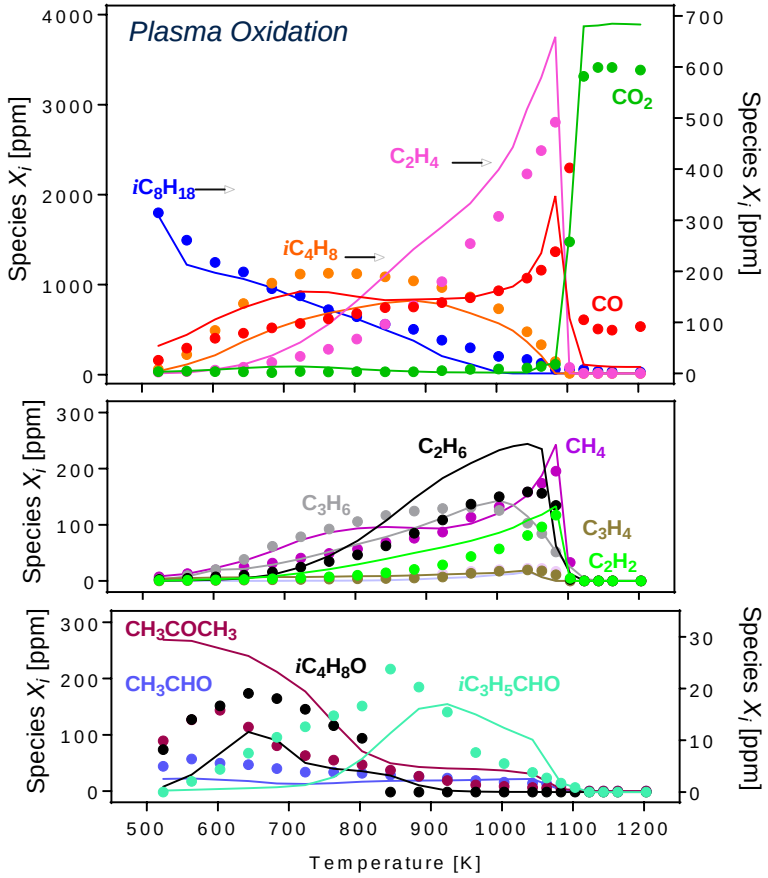
Technical Accomplishments (Auburn)

PFR experiments and modelling of LTP oxidation of isooctane



- **Thermal Oxidation** follows pyrolysis scheme decomposing to smaller fuel fragments; CO formation formed through formaldehyde oxidation; at 1200 K high-temperature chain-branching reactions lead to ignition and CO_2 production
- LLNL-detailed [1] iso-octane mechanism shows good agreement with experiments

- **LTP Oxidation** enhanced fuel consumption at low-T; 80% fuel consumption by 900 K
- Developed mechanism predicts **(more than 80% of major species)** experimental results of oxidation with very good agreement **(less than 30% deviation)** for all measured species and temperatures.
- Quenching reactions with oxygen and $N_2(A)$ leads to O-radicals; plasma pyrolysis plays secondary role
- Plasma reactions regenerate and recycles O-radicals to continue fuel decomposition from OH-attack
- Significant oxygenates formed (not seen in thermal reaction) – RO_2 chemistry being enhanced at low-T
- Ignition temperature lowered by ~100 K



$N_2^*/e + O_2 \rightarrow N_2 + \boxed{2O}$ → $O + C_8H_{18} \rightarrow C_8H_{17} + \boxed{OH}$ → $OH + C_8H_{18} \rightarrow C_8H_{17} + H_2O$ → terminates

Initial times scales
O-atom density generated by plasma

Longer times scales OH-radical attack
facilitates fuel consumption sustained by plasma generated O-atoms

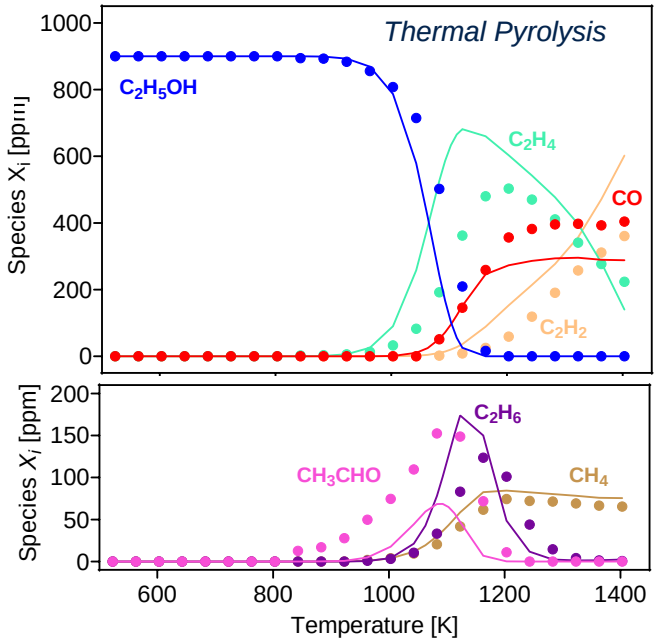
Technical Accomplishments (Auburn)

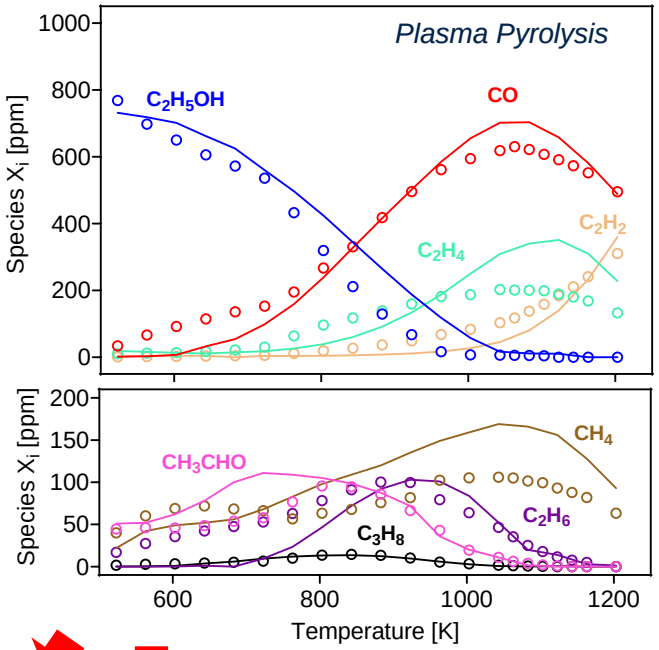
PFR experiments and modelling of LTP pyrolysis of ethanol

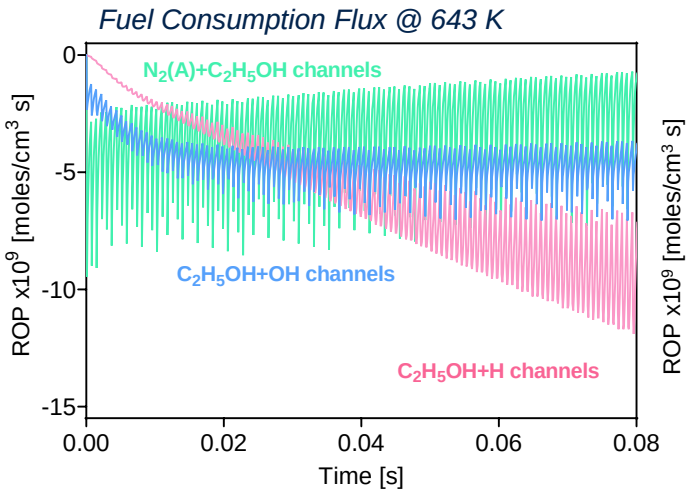
- We demonstrated significant **enhanced reactivity of pyrolysis reactions** with the effects of LTP compare to thermal reactions
- LLNL thermal mechanism demonstrates sufficient predictive capabilities for use as neutral chemistry in plasma mechanism.
- **Reaction rate and branching ratios** for $N_2(A)$ quenching reactions with fuel are tuned to replicate experimental fuel consumption profile and magnitude and speciation of intermediate species
- Developed mechanism predicts with **less than 20% deviation** all measured species for all temperatures

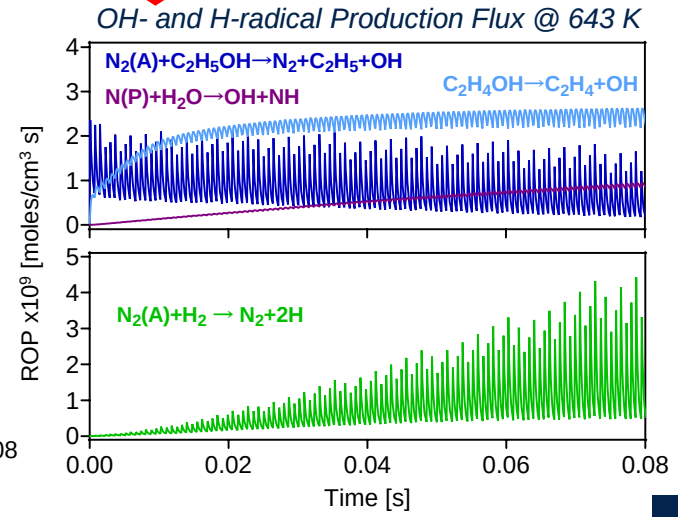
Summary of Results

- Fuel consumption controlled by plasma quenching reactions with $N_2(A)$ leading to fuel radicals
- OH- and H-radicals generated in the plasma (high-voltage pulse) cascades into the afterglow leads to further fuel consumption to enhance reactivity **(propagating reaction effect)** – time scale dependent
- **OH functional group provides OH-attack channel in pyrolysis**
- Recombination of fuel fragments (as a function of temperature) leads to the formation of intermediate species









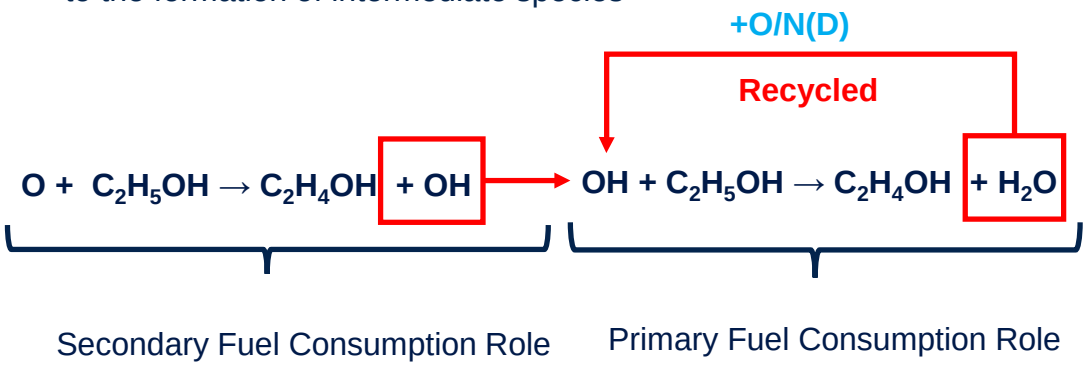
Technical Accomplishments (Auburn)

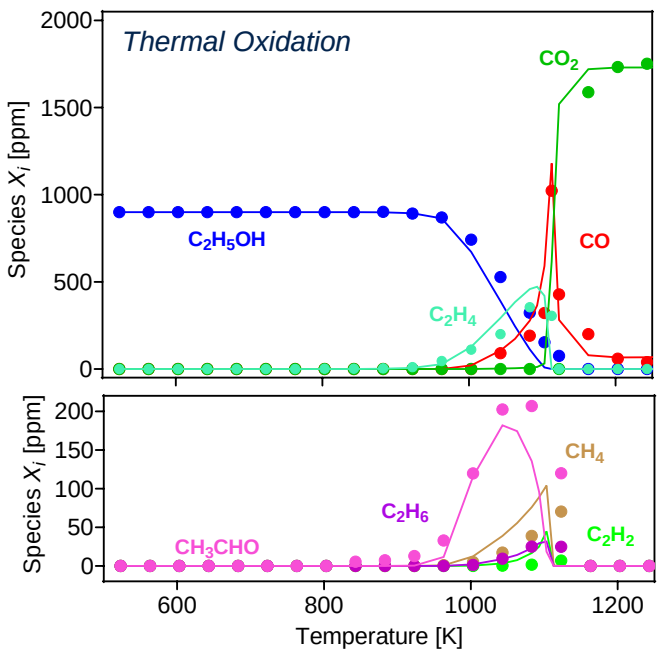
PFR experiments and modelling of LTP oxidation of ethanol

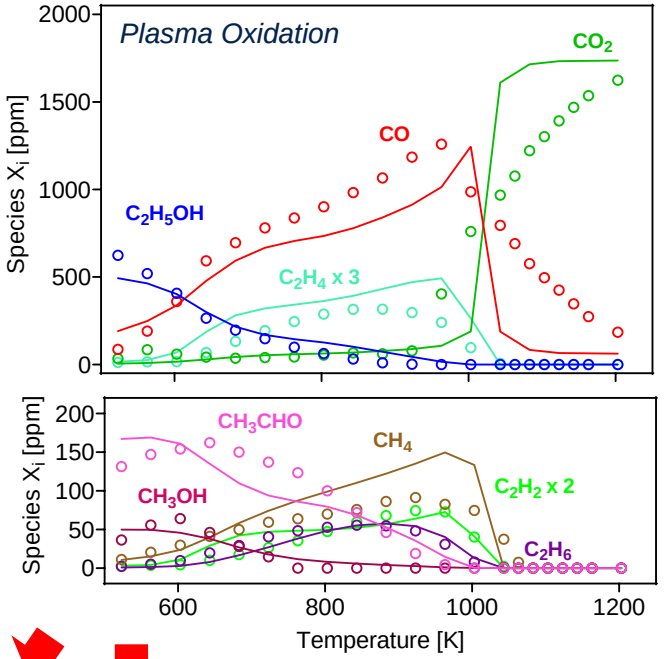
- We demonstrated significant **enhanced reactivity of oxidation reactions** with the effects of LTP compare to thermal reactions
- LLNL thermal mechanism demonstrates sufficient predictive capabilities for use as neutral chemistry in plasma mechanism.
- Developed mechanism predicts with **less than 20% deviation** all measured species for all temperatures

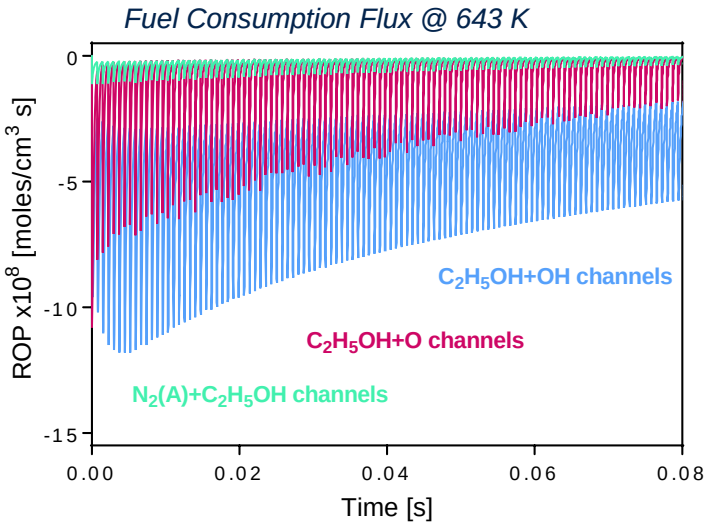
Summary of Results

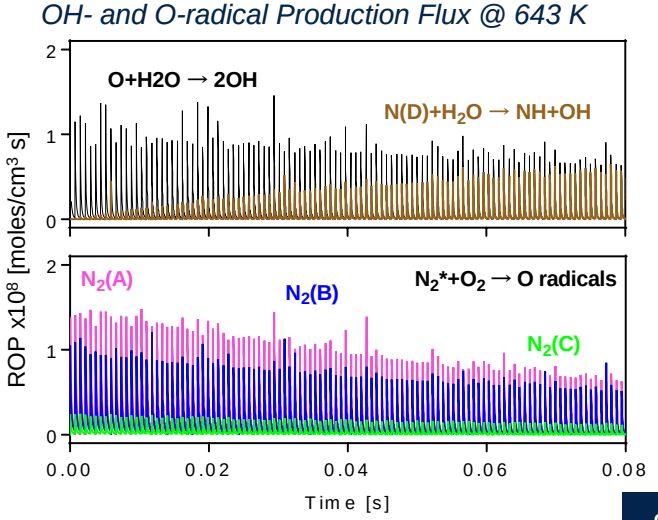
- Additional fuel consumption observed with enhanced O-radicals **(secondary role)** from plasma; direct quenching from plasma negligible
- Plasma reactions regenerate and recycles OH-radicals from H_2O to continue fuel decomposition from OH-attack **(primary role)**
- Recombination of fuel fragments (as a function of temperature) leads to the formation of intermediate species











Technical Accomplishments (UT Austin)

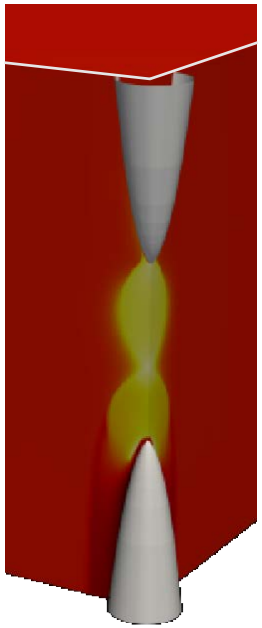
Simulating three-dimensional LTP discharges with AMReX & PeleC

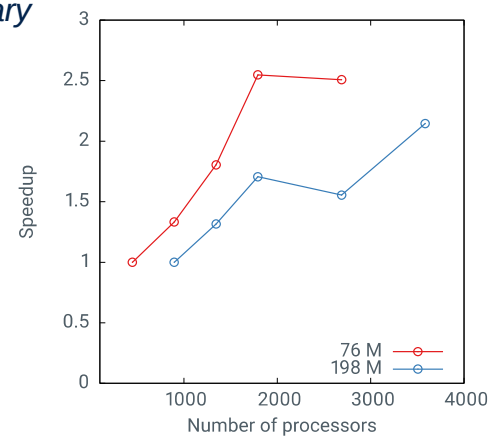
- We demonstrated a three-dimensional, unsteady massively parallel solver for the simulation of LTP discharges in reactive mixtures built on the DOE AMReX library and PeleC application

- **Demonstrated capabilities**
  - Full physical coupling between multi-component chemically reactive mixture, compressible flow, and plasma species (including excited state neutrals)
  - Three-dimensional meshes with complex-shaped electrodes
  - Automated local refinement capable of tracking streamer propagation and cathode sheaths
  - Execution up to 3,600 cores and problem sizes of 200 M cells
  - Integrated with a circuit model (collaboration with Argonne National Lab) across multiple pulses

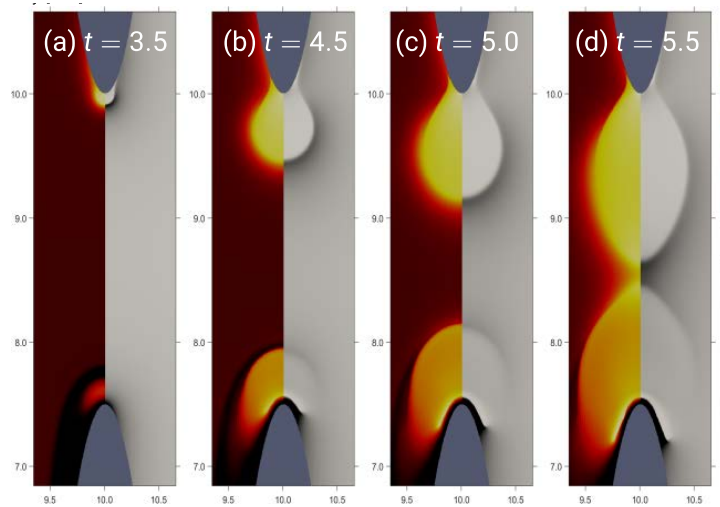
- **Preliminary results and extended capabilities**
  - Fully implicit time integration
  - Transport equation for mean electron energy
  - Scaling to O(10,000) cores

3D domains with arbitrary electrode geometries



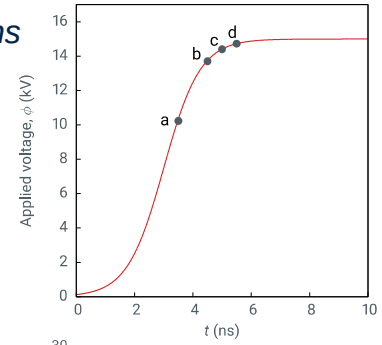


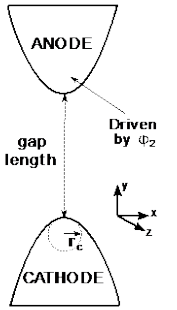
Scaling tests up to 3,600 cores performed.



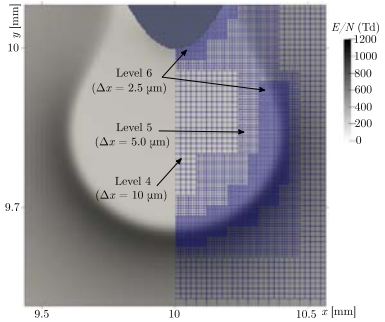
Time resolved simulations of LTP via NSD

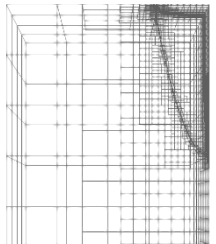
Simulations of LTP discharges at the exascale

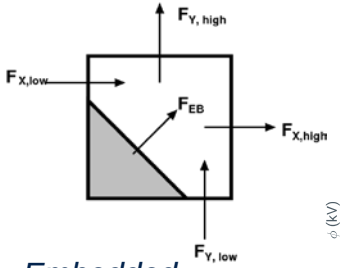




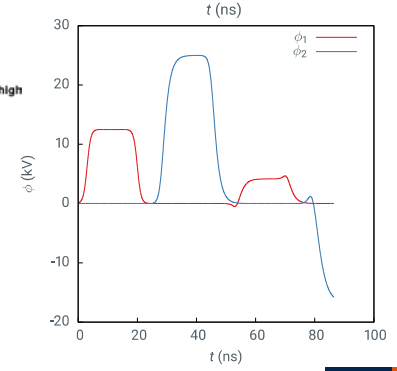
AMR grids down to O(1 um) resolution







Embedded Boundary (EB) for complex geometries



Circuit model

Technical Accomplishments (UT Austin)

High-fidelity three-dimensional unsteady simulations of LTP discharges in atmospheric air and ethylene/air

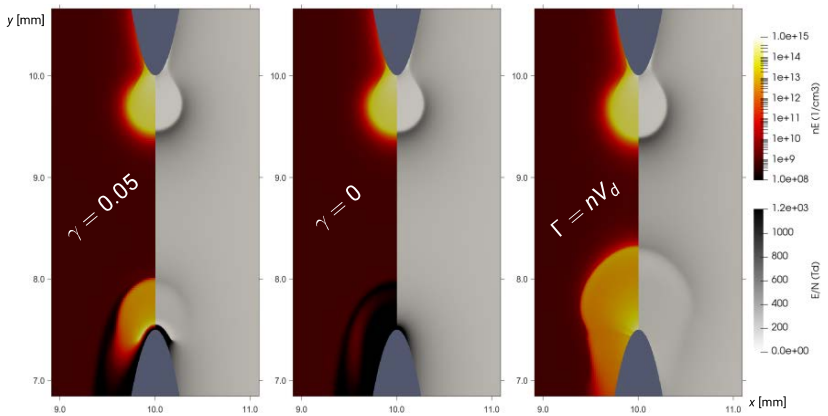
- We conducted simulations of low-temperature plasma (LTP) discharges in air and lean ethylene/air reactive mixtures

- **Air LTP discharges (1 atm and 300 K)**
  - Skeletal air plasma mechanism
  - Investigated cathode sheaths and secondary electron emissions effects on streamer
  - Fine-tuned spatial and temporal resolution & identified streamer to glow transitions

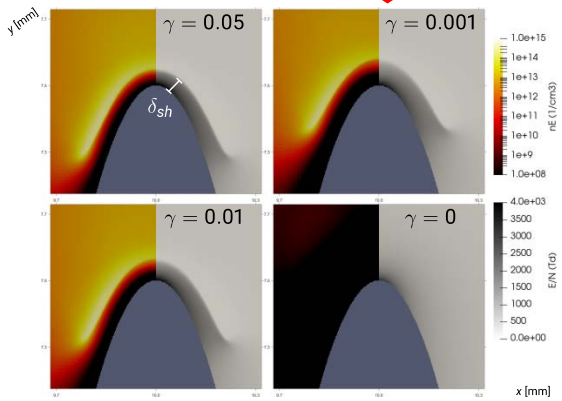
- **Ethylene/air LTP discharges (1 atm and 300 K, stoichiometric)**
  - Detailed plasma-assisted ignition mechanism used
  - 55 combustion and plasma species simulated in a three-dimensional pin-to-pin configuration
  - Local field approximation
  - Two pulses in the glow regime

- **Preliminary results**
  - Nanosecond pulsed discharges in ethylene/air
  - Single pulse (streamer regime) with circuit coupling

Effect of secondary electron emission coefficient on positive and negative streamers in air

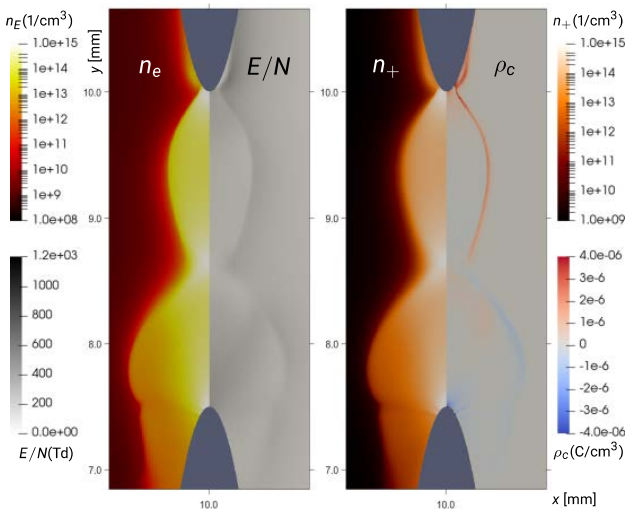


Detail of the cathode sheath and voltage drop in air

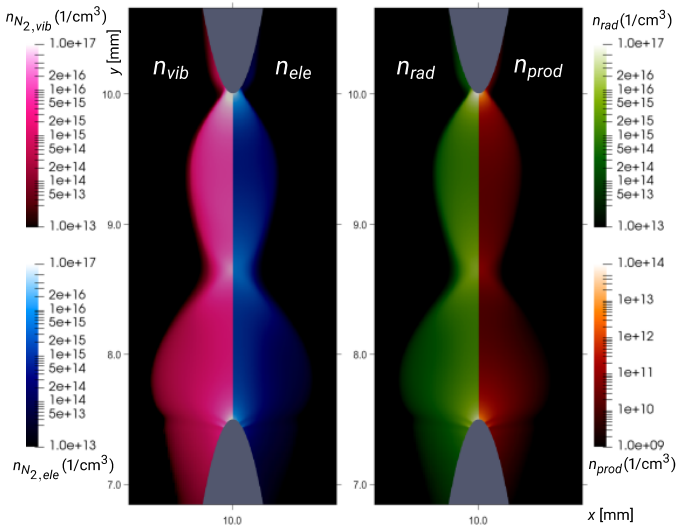


LTP discharges in air (top) and ethylene/air (bottom)

Spatial distribution of electrons, ions, space charge, and electric field after 2 pulses



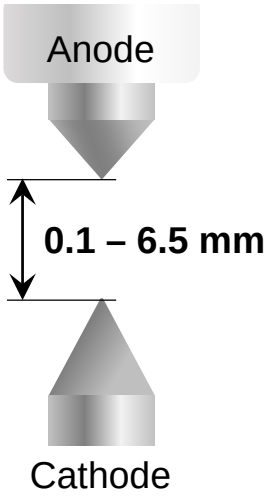
Spatial distribution of excited neutrals and combustion radicals

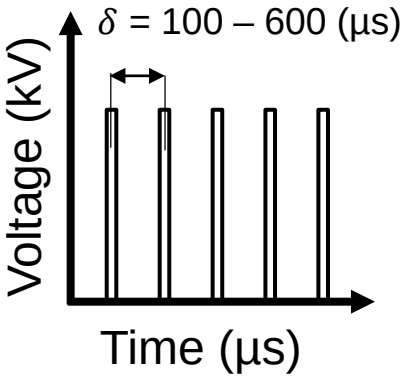


Technical Accomplishments (SNL)

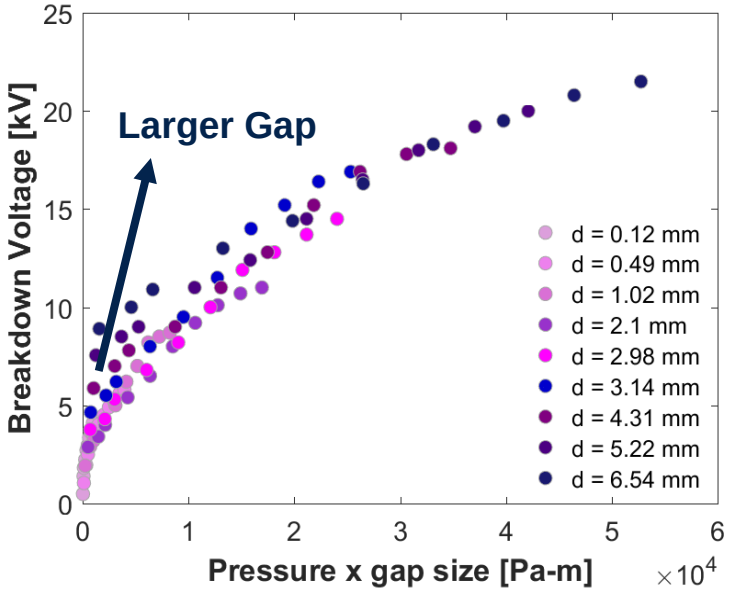
Mapping LTP transition to arc

- Single and repetitive pulse nanosecond discharges tested at range of ***voltage***, ***repetition frequencies***, and ***gap distance*** to identify transition to arc
- For single pulse operation, larger gaps extend breakdown voltage limits
- Short pulses and long distances do not allow sufficient time for ionization wave to establish



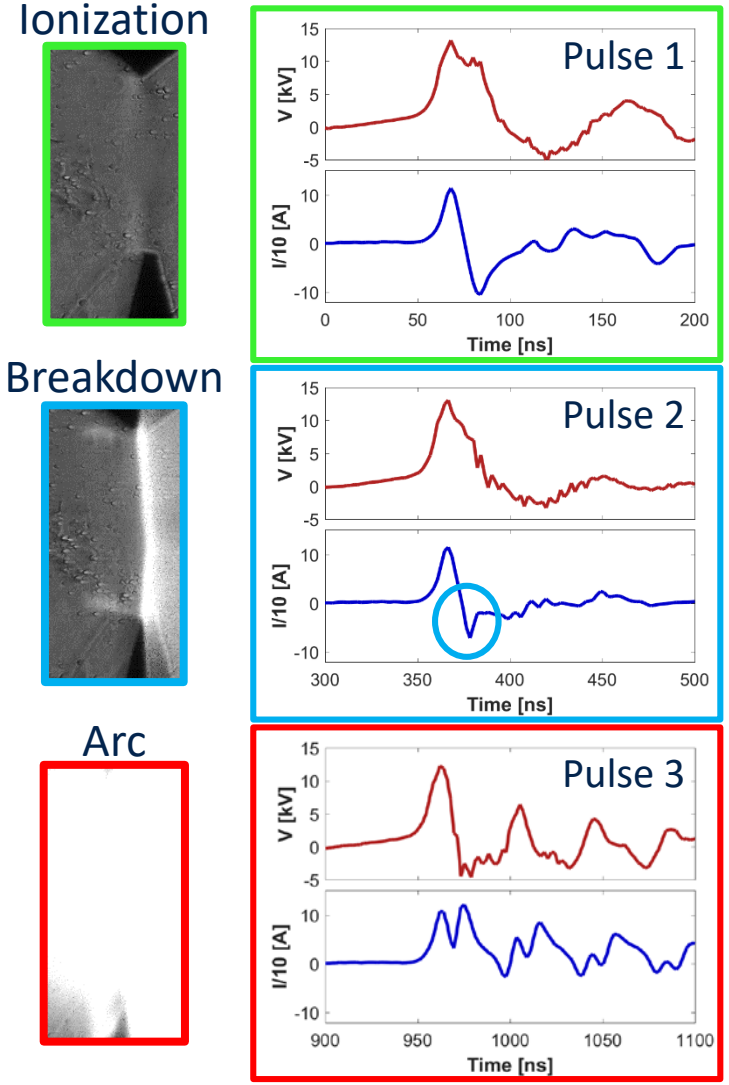


Air at 70 ℃ (Single discharge)



Repetitive pulse discharges

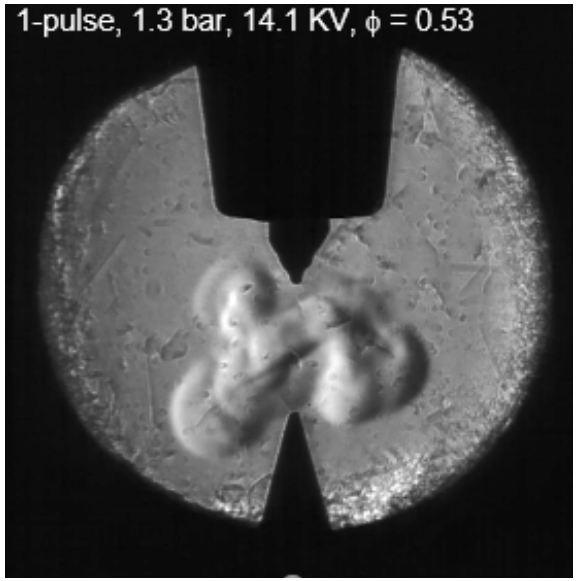
- Low voltage, multi-pulse discharges can lead to successive streamer arc transition
  - ionization → breakdown → arc
  - Inter-pulse heating from vibrational and electronic excitation that pre-conditions subsequent pulses
- Impedance changes at breakdown can be monitored by changes in reflected current to detect arc onset

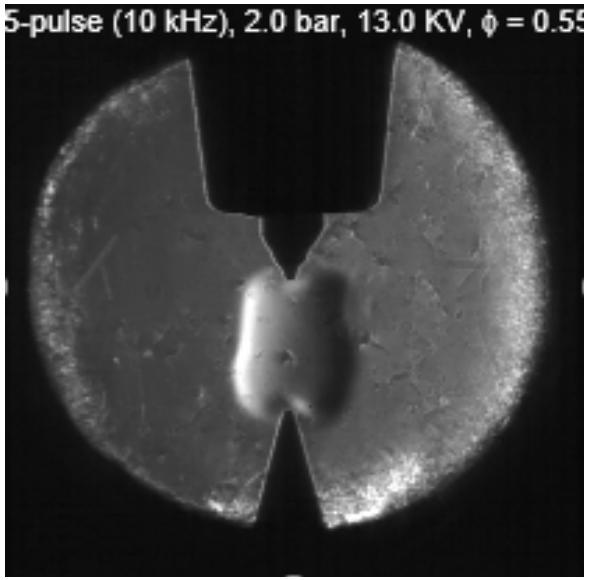


Technical Accomplishments (SNL)

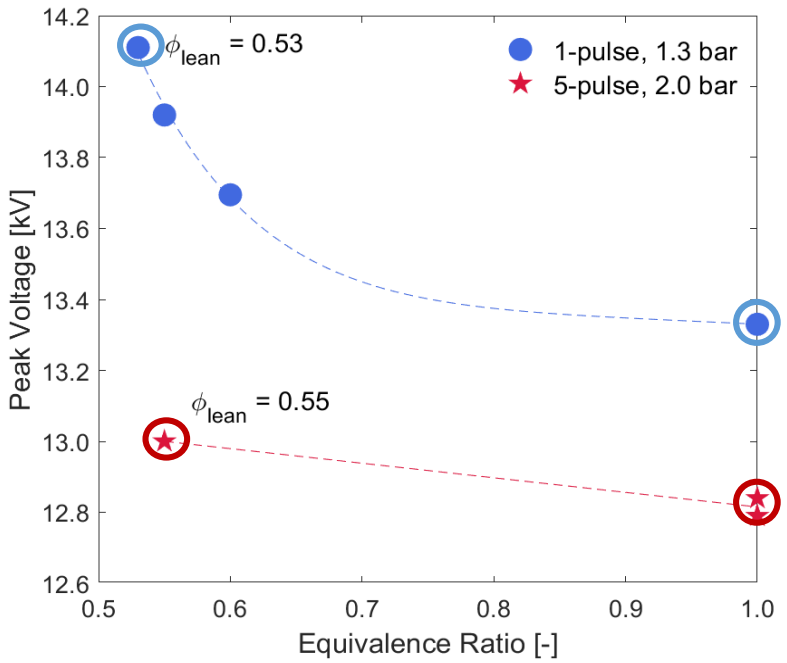
LTP Ignition

- Single and repetitive pulse nanosecond ignition of ethylene-air-EGR mixtures performed for initial pressures up to 2.0 bar.
- Narrow range of acceptable combinations in gap size, discharge voltage/number, and repetition frequency that led to successful LTP ignition.
- Leaner mixtures could accept higher discharge voltages without transition to arc.
    - Less secondary ionization from air than from the C_2H_4 fuel
    - Opposite trend for EGR dilute mixtures due to more secondary ionization from EGR constituents





Ethylene/Air, 1.3 & 2.0 bar, 343 K



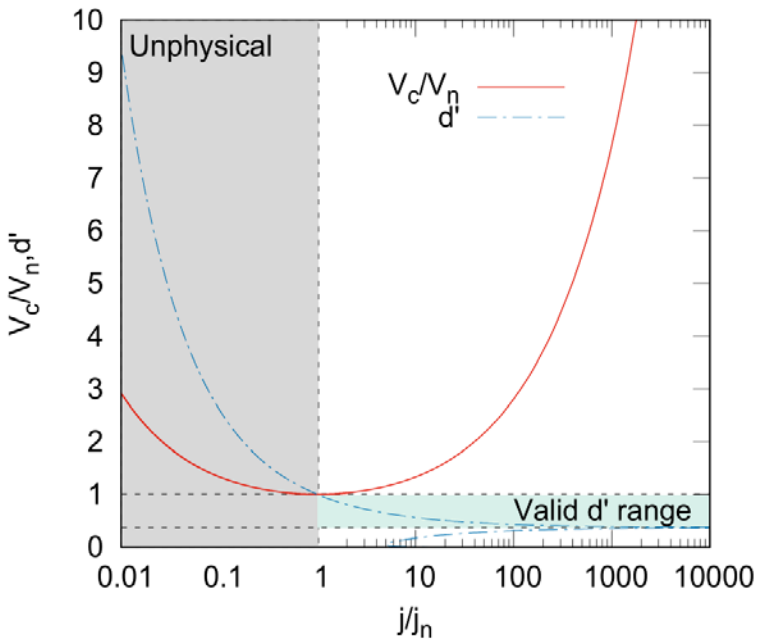
- A 3 mm electrode selected as it balances need for higher voltage with larger gaps while still producing reliable LTP ignition without arc transition.
- Single-pulse ignition possible for lower pressures (1.3 bar), while higher pressures (2.0 bar) required 5 (10 kHz) lower voltage pulses to avoid arc
    - Early pulses pre-conditioned the mixture for LTP through inter-electrode heating (i.e., lower number density within the streamer)

Technical Accomplishments (ANL)

Circuit-Plasma Coupling

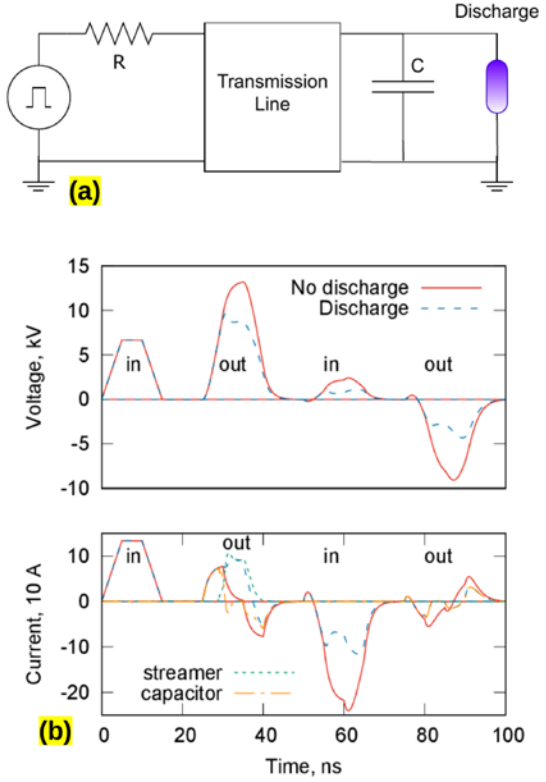
- A circuit-to-cylinder model was developed [2] to aid in drawing inferences about streamer discharges from experiments and simulations.
- Streamer breakdown, streamer velocity, plasma density evolution, radical production, cathode fall, circuit current, and transmission line losses are all considered in the model.

The cathode fall model addresses numerical difficulties when streamers bridge the gap due to very small thicknesses (d').



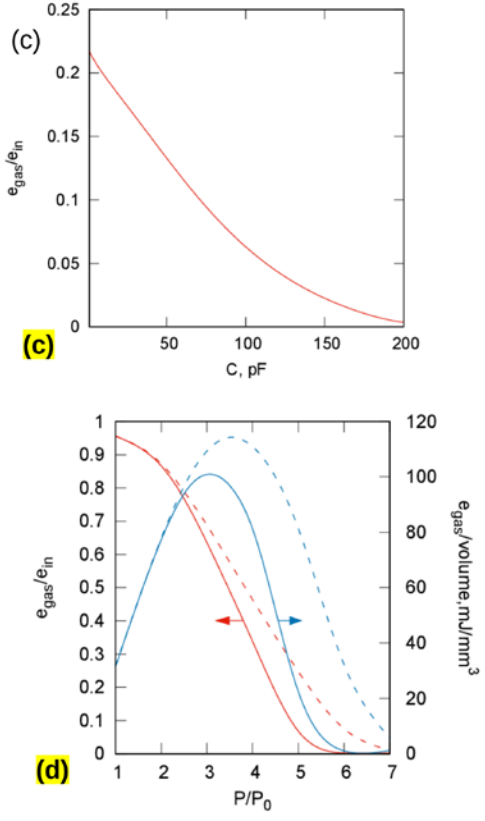
This circuit model is being used by the U-Texas group to reconcile boundary conditions between simulations and experiments.

Full characterization of nano-second pulsed circuit using transmission lines



Can determine exactly how much power is delivered to gas per pulse

Sensitivity of energy delivery to circuit parameters have been quantified

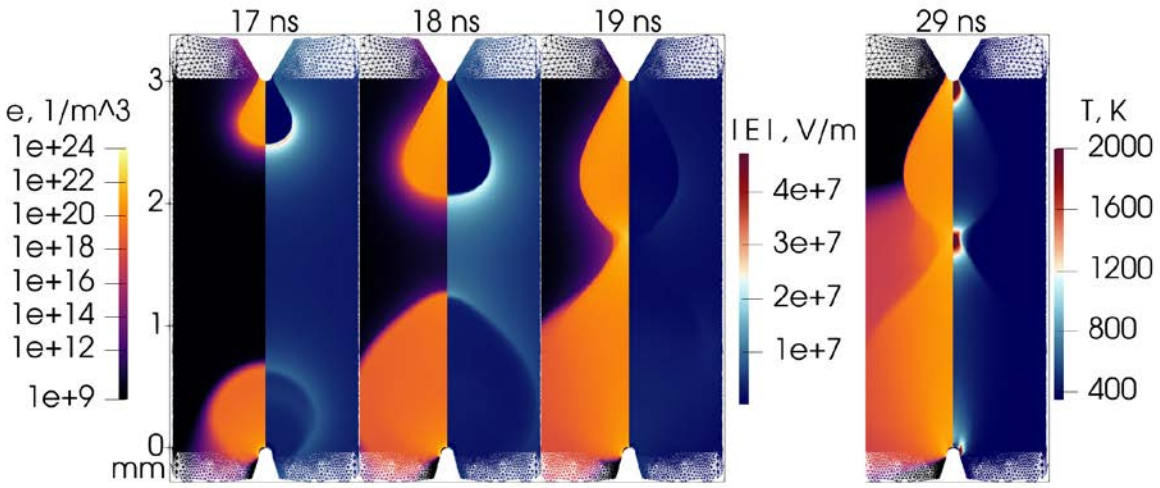


Circuit + discharge simulations show interesting optimal points for discharges in ICEs

[2] *Gururajan, V., & Scarcelli, R. (2022). A nanosecond pulsed discharge circuit model for engine applications. Journal of Physics D: Applied Physics, 55(15), 155205.*

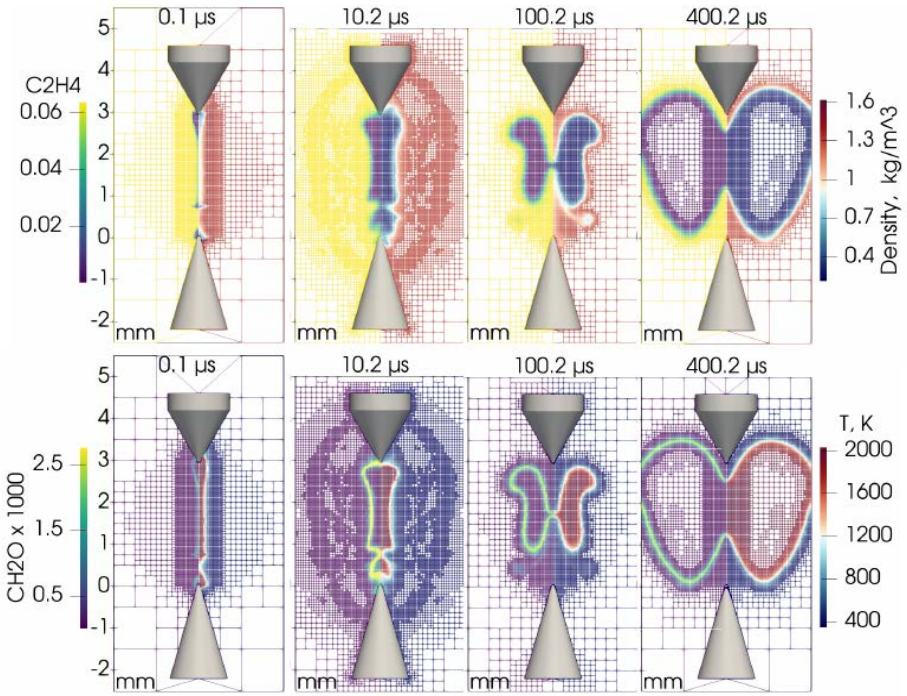
Technical Accomplishments (ANL)

Simulating LTP discharges with VizGlow and LTP ignition with CONVERGE CFD

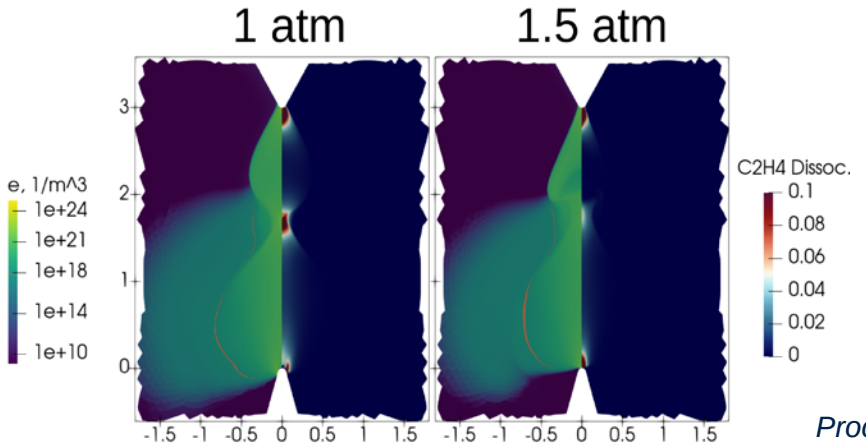


VizGlow → CONVERGE

Discharge model [2]



- Previous work [3] simulated detailed discharges and ignition of C_2H_4 assuming no fuel dissociation, i.e., only O radicals and temperature increase were considered to lead to ignition.
- Recently implemented fuel dissociation reactions in VizGlow (i.e., $C_2H_4 + e^- \rightarrow C_2H_3 + H + e^-$).
- Current focus is on adding iso-octane/ethanol kinetics in VizGlow.



- Highest dissociation occurs near anode and cathode tips.
- Streamer collision also leads to dissociation at low enough pressures.

Developed a scheme to utilize plasma kinetics mechanism in VizGlow → CONVERGE workflow.

[3] *Gururajan, V., Scarcelli, R., Biswas, S., & Ekoto, I. (2021, October). CFD Modeling of Low Temperature Ignition Processes From a Nanosecond Pulsed Discharge at Quiescent Conditions. ICEF (Vol. 85512, p. V001T06A010). ASME.*

Milestones

MILESTONE	PI	DESCRIPTION	STATUS
M.1	Tsolas	**Iso-octane Thermal Mechanism Selection Complete** *Completion of **TASKS 1.1 and 1.3** resulted in the selection of a detailed kinetic mechanism for iso-octane that predicated experimental results with very good agreement for pressures at 0.5 atm and temperatures ranging from 300 -1300 K. Model is capable of predicting both major and minor species with less than 2% error.*	**COMPLETE**
M.2	Ekoto	***Phase I LTP Ignition Experiments Complete*** *Completion of **TASKS 3.1 to 3.5** have demonstrated the LTP ignition in ethylene/air reactive mixtures are possible. Experimental data from these studies has been distributed to co-PIs to validate and benchmark high-fidelity models to be developed.*	**COMPLETE**
M.3	Bisetti	**Software for Skeletal Reduction of Detailed Plasma/Combustion Kinetics Mechanism** *Completion of **TASKS 2.1 to 2.3** resulted in a reduced kinetic mechanism that that describes LTP combustion of ethylene/air mixtures with reduced computational cost. Software is distributed with validation suite.*	**COMPLETE**
M.4	Tsolas	**Ethanol Thermal Mechanism Selection Complete** *Completion of **TASKS 1.2 and 1.6** resulted in the selection of a detailed kinetic mechanism for ethanol that predicated experimental results with very good agreement for pressures at 0.5 atm and temperatures ranging from 300 -1300 K. Model is capable of predicting both major and minor species with less than 2% error.*	**COMPLETE**
M.5	Bisetti/Tsolas	**Mechanism reduction – Skeletal Mechanism for Iso-Octane/Air plasmas** *Formulation of a skeletal mechanism for iso-octane/air plasma/combustion via the DGREP-2T reduction methodology implemented in (T2.3)*	**In Progress – On Track**
M.6	Bisetti/Scarcelli	**LTP Ignition Solver – AMReX Library Implementation** *Software for skeletal reduction of detailed plasma/combustion kinetics mechanism is complete (T2.6) Software is distributed with validation suite.*	**COMPLETE**
GO/NO-GO	Tsolas	**LTP Ethanol Fuel Consumption Rate Predicted** *Completion of **TASK 1.7** demonstrated that mechanism development efforts predict plasma-assisted pyrolysis and oxidation ethanol experimental results with relatively good agreement. LTP fuel consumption is predicted with less than 60% deviation and more that 50% of major species are accounted for.*	**COMPLETE**

Response to Reviewer Comments

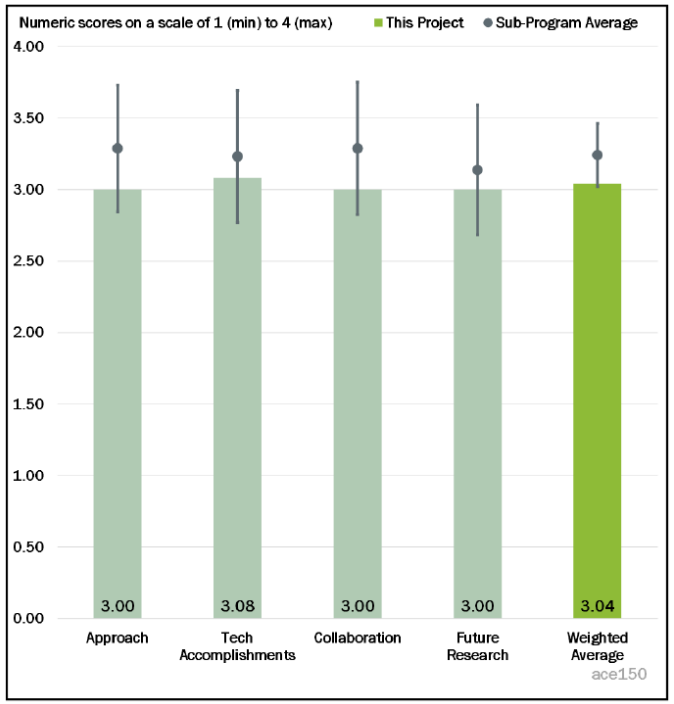
APPROACH

- ***"It is not clear how the four efforts in this work are interconnected...it would be beneficial to communicate these connections to show how the four efforts ultimately are integrated..."***
  - LTP kinetics studies to construct PAC mechanisms (Auburn) and measure LTP ignition events (Sandia) used to benchmark high-fidelity simulation results from developed computational tools (UT Austin and ANL) …. see ***Overall Technical Approach***
- ***"It is unclear why the team needs both an exascale solver based on AMReX and VizGlow. Can one solver be chosen to avoid proliferation and development of different solvers?"***
- ***"...[Are] VizGlow and AMR software work duplicative…VizGlow has some inherent issues..."***
- ***"…The direct linkage of the work being conducted at the UTexas and ANL is unclear. How do these modeling efforts overlap with each other?"***
  - The goal of the project is to develop the exa-scale code at University of Texas. The support role from Argonne has a bi-fold goal: 1) provide a benchmark for the exa-scale code (VizGlow can be thought as state-of-the-art multi-dimensional plasma modeling tool used by industry), and 2) leverage improvements in plasma kinetics to expand the VizGlow applications to a larger range of fuels and operating conditions.
  - Activities at UTexas and ANL are complementary, synergistic, and integrated. ANL simulations aid the development of the AMReX discharge solver and provide a benchmark for the performance of the exa-scale code being developed. On the other hand, ANL fuel/air discharges employed skeletal plasma/combustion mechanisms developed by UTexas.
- ***"...The reviewer's fear was that AMReX is developed for this project, but then this tool is not transferred or used by OEMs actually designing engines..."***
  - The primary goal of this DOE-funded project is to develop predictive modeling tools for plasma ignition. AMReX is the right candidate to succeed in this task. On the other hand, the development of high-order predictive modeling tools can be also leveraged to guide the development and improvement of commercial tools that are routinely used by industry (VizGlow being just one example).
- ***"...The approach is missing an industry collaborator or potential manufacturer..."***
  - The team is in contact with Convergent Science, a CFD company. They expressed interest in incorporating our newly developed numerical approaches to the simulation of plasma discharges into one of their flagship solvers for reactive flow. PIs also have working collaborations with industry partners supported by other projects to facilitate the develop of LTP igniters...see ***Collaborators and Coordinators***
- ***"...[What] overall status of plasma ignition and what other barriers besides simulation exist. For example, are these systems in use and what is the record of success?..."***
  - Developing actual LTP igniters is outside the scope of this project, however, collaborations with LTP igniter manufactures have demonstrated that drop-in LTP igniters and associated hardware are possible and have been tested. Projects supported by DoE SBIRs

PROPOSED FUTURE WORK

- ***"…it could be instructive to understand what a complex fuel breaks down into …characterization and speciation of complex fuels experimentally might inform the experiments and modeling of the simpler fuels in this work…"***
  - Mechanism developed approach's hierarchical perspective, little is known about simple fuel chemistry past work restricted to Ar systems and small fuels, complex fuels are based on surrogate fuel components – i.e. straight chain, branched, carbon number, and oxygenates
- ***"…see more details about the future tasks, their barriers, and alternate pathways…"***
  - Addressed in the present version of the presentation.

Scores from 2020 AMR (ace150)



Collaborators and Coordinators

- **Connections to other DOE projects**
  - **DE-SC0013824:** SBIR Phase IIB, Low-energy nanosecond pulsed ignition system
    PI: Dan Singleton (Transient Plasma Systems Inc.)
  - **HPC4Mfg (Round 5):** Modeling of Non-equilibrium Plasma for Automotive Applications
    PIs: Riccardo Scarcelli (ANL) and Dan Singleton (Transient Plasma Systems Inc.)

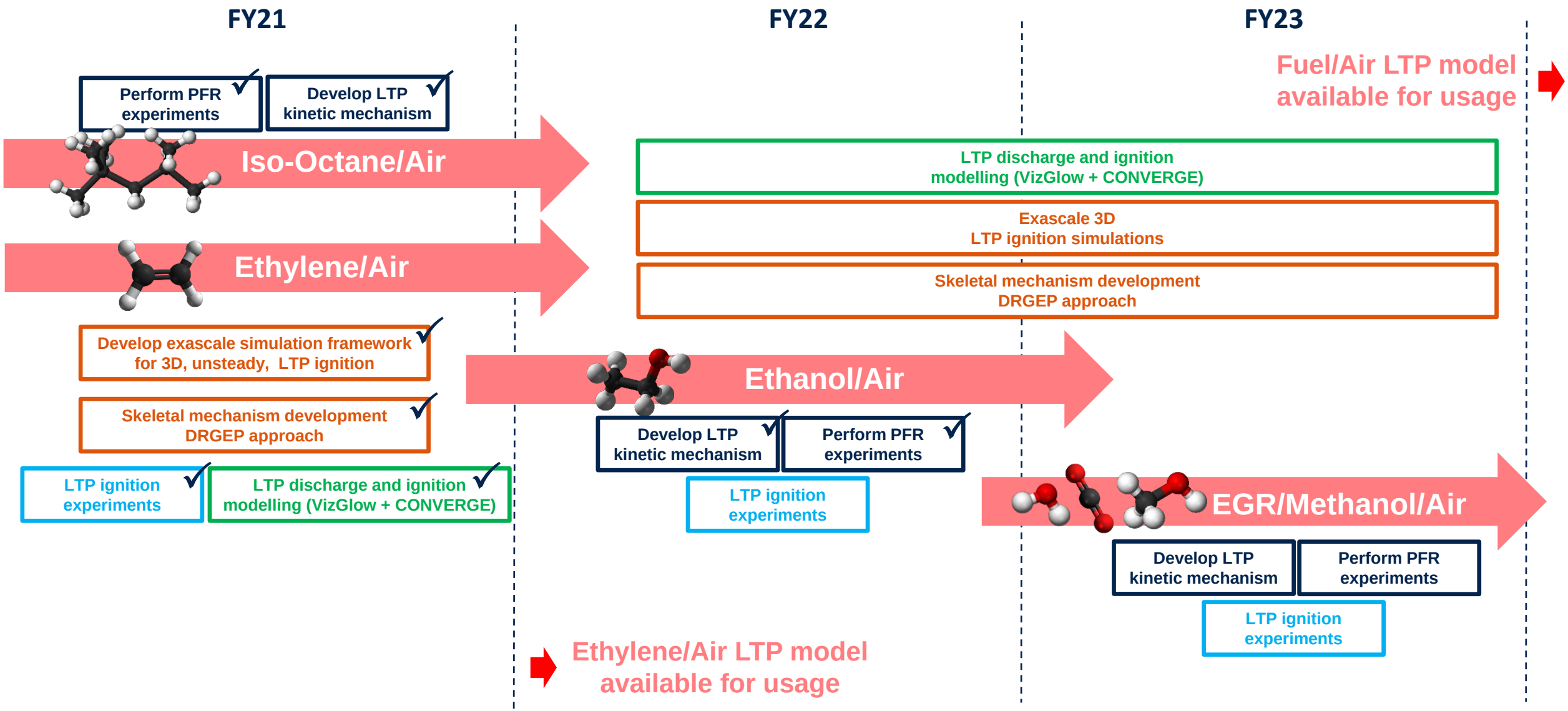
- **External Collaborations**
  - ***Transient Plasma Systems Inc.***: Plasma igniter development and testing
  - ***Prof. Perrine Pepiot, Cornell U***: Skeletal mechanism development for plasma assisted ignition
  - ***Dr. Marc Day, NREL****:* Integration of exascale solver for plasma-assisted ignition simulations into AMReX

Remaining Challenges and Barriers

- **Development of plasma-specific kinetic mechanisms of fuels:**
  - **Challenge 1:** Past PAC kinetics and ignition work solely focused hydrocarbon based fuels – simple fuels; need to transition focus on future sustainable oxygenated fuels - i.e. methanol
  - **Challenge 2:** Fuel structure implicitly controls enhanced reactivity of LTP ignition; need better understanding of implications of blended reactive mixtures – oxygenates/hydrocarbons and EGR blended components
  - **Challenge 3:** Skeletal mechanism development for iso-octane/air plasma-assisted ignition proved more challenging than expected; need to develop and implement novel “isomer lumping” strategy that incorporates plasma effects on low temperature chain branching.

- **Development of LTP ignition computational tools:**
  - **Challenge 4:** The semi-implicit time integration of the evolution of the plasma and reactive mixture in between pulses is computationally demanding, limiting the lowest repetition rates that can be realistically simulated to about 10 MHz, which is higher than the pulse rate in experiments.

Proposed Future Work



Summary

Development of validated chemical kinetics mechanisms and benchmarked exascale software for high-fidelity simulation of LTP ignition of future fuels

Relevance:

- The project addresses the lack of validated and benchmarked LTP-specific kinetic mechanisms of fuels and exascale-ready software to accurately simulate 3D, unsteady, LTP ignition phenomena.

Approach:

- Multi-institutional approach consisting of PFR experimental/numerical kinetic mechanism development, LTP ignition measurements, development and simulation of 3D LTP discharges with AMReX and PeleC, and benchmarking against existing commercial solvers - VizGlow and CONVERGE CFD.

FY22 Technical Accomplishments (1/2):

- Plasma-assisted pyrolysis and oxidation experiments performed to numerically develop LTP-specific iso-octane and ethanol kinetic mechanisms
- Developed 3D LTP discharge model with AMReX & PeleC
- Advanced skeletal mechanism development utilizing novel DRGEP approach
- Simulated high-fidelity three-dimensional unsteady LTP discharges in atmospheric air and ethylene/air
- Single and repetitive pulses LTP ignition mapping experiments to identify LTP ignition regimes in air and reactive mixtures of ethylene/air

FY22 Technical Accomplishments (2/2):

- Developed circuit-plasma coupling model to reconcile boundary conditions between LTP ignition experiments and simulations.
- Simulated ethylene/air LTP discharges utilizing commercial solvers to benchmark developed software

Remaining Barriers:

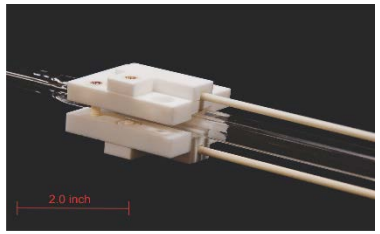
- LTP chemical reactivity highly dependent on mixture components; need to focus on sustainable future fuels and EGR components
- Skeletal mechanism development requires implementation of novel lumping strategies to capture reactivity enhancement at low-temperature conditions
- Time integration of chemistry in between pulses is computationally demanding; not feasible computationally to pulse at less that 10 MHz

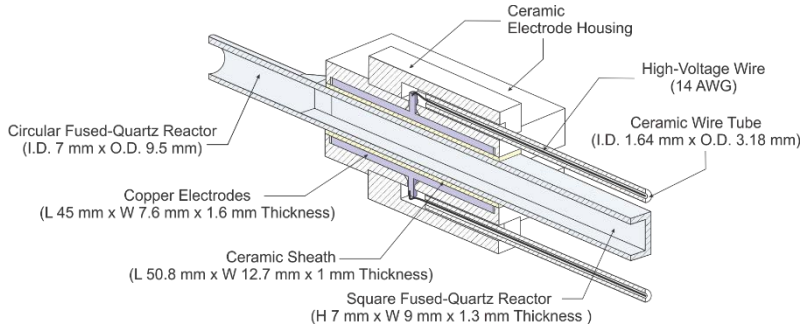
Future Work:

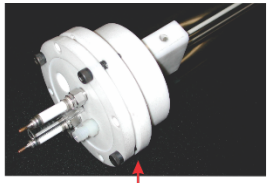
- Focus kinetic mechanism development on EGR blends and oxygenates – i.e. methanol
- Incorporate the inclusion of turbulence, turbulent mixing and mixing stratification into numerical framework
- Address skeletal mechanism lumping strategies

TECHNICAL BACKUP SLIDES

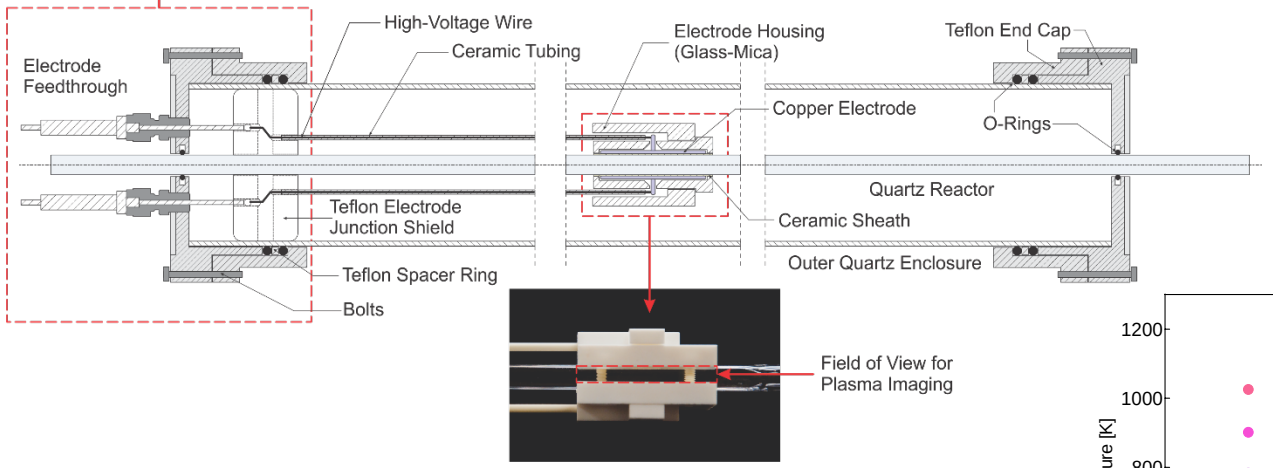
Technical Backup Slide



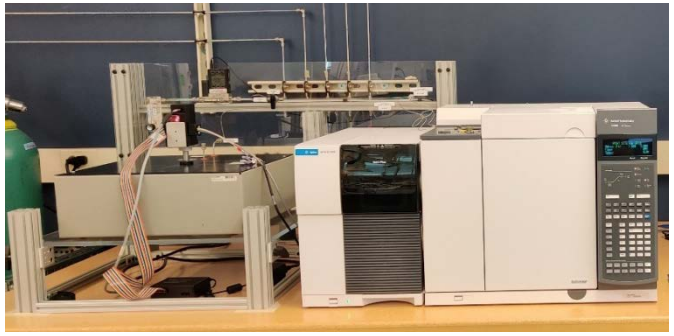


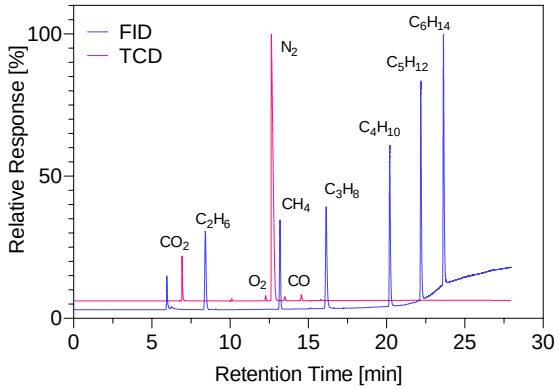


Plane-to-plane electrode orientation around quartz and ceramic dielectrics



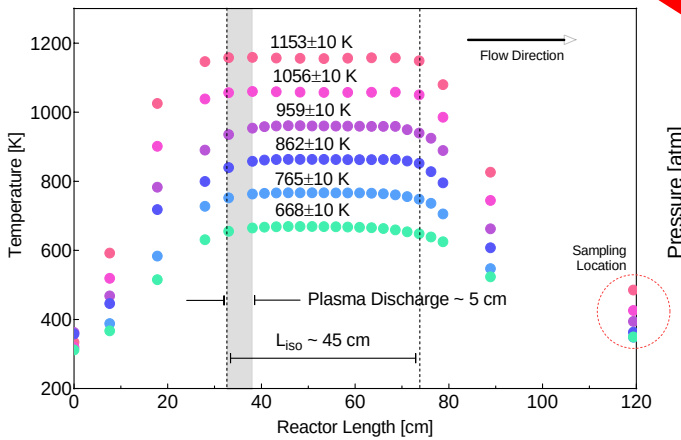
The **plasma discharge assembly** is housed in a quartz tube (58mm I.D.) with Teflon end caps

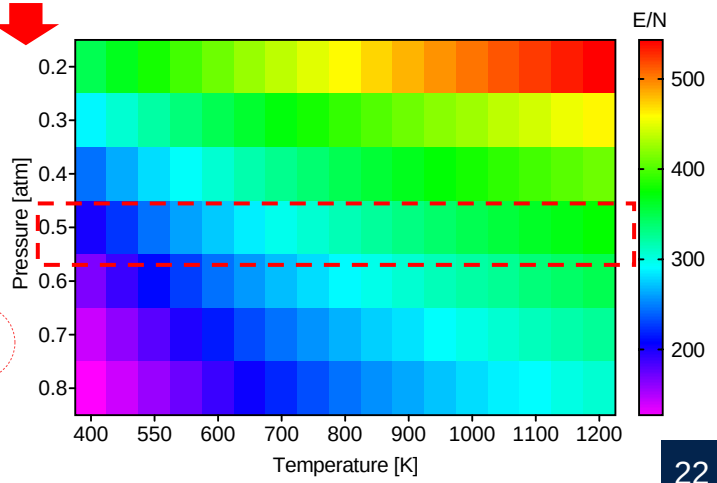




Exhaust products from PFR collected via **multi-position valve with sample loops** - product species analysis performed using and **GC/MS** equipped with FID and TCD detectors, capable of detecting hydrocarbons, oxygenates, and permeant gases

PFR heating is achieved using a **three-zone tube furnace** providing isothermal reaction zone for kinetic studies; ns-duration high-voltage (20kV) pulses (~100ns) at 0.5 atm provide a range of E/n to studied plasma effects

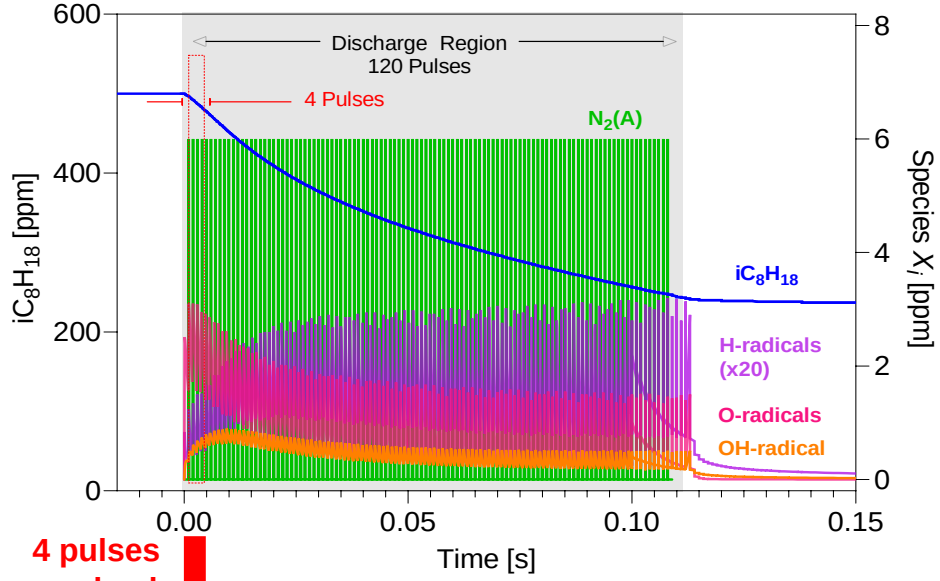




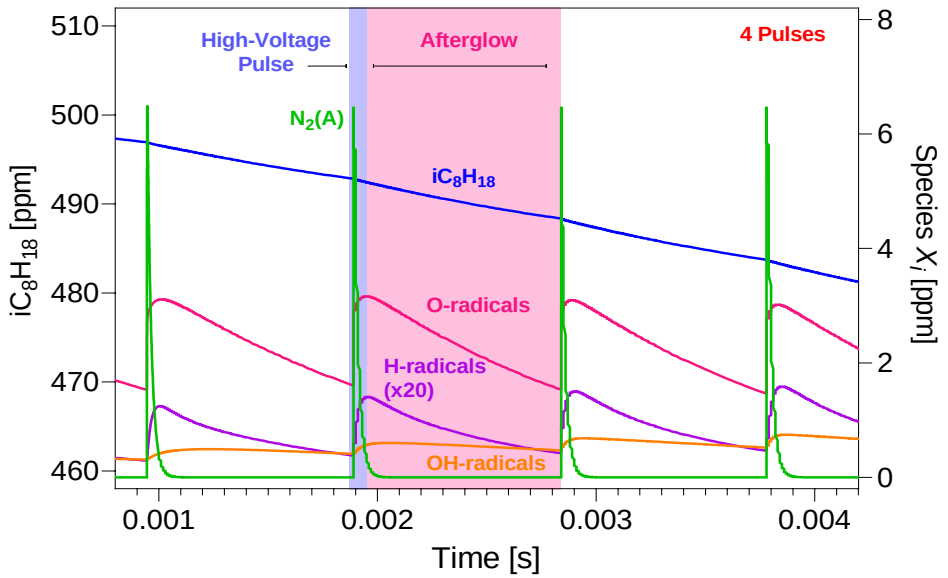
PFR Experimental Details

Technical Backup Slide

Temporal Evolution of Plasma and Neutral Species



4 pulses resolved



0D Plasma Kinetic Model Architecture

SENKIN (CHEMKIN)

CALCULATES: evolution of chemical species and rate of production assuming plug flow characteristics at constant P conditions

+

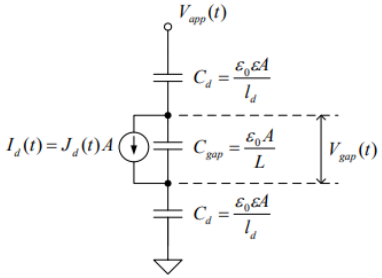
ZDPlasKIN (Boltzmann Solver)

CALCULATES: electron-impact reaction rates using collisional cross-section inputs

+

Circuit Module (E/N and DBD)

CALCULATES: temporal evolution of reduced electric field in DBD during high-voltage pulse assuming electric charge conservation



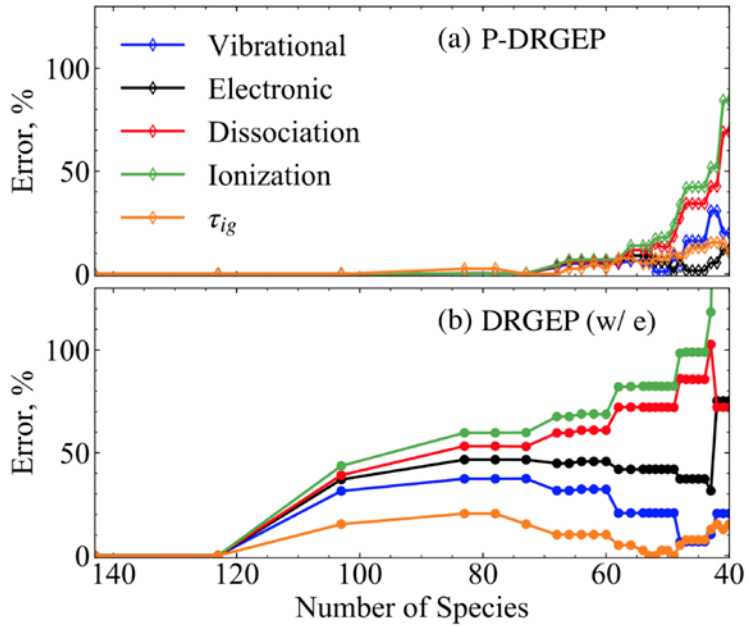
PAC Chemical Reaction Mechanism

- Electron-impact reactions (Van Gaens et al.-2013, Kossyi et al.-1992)
- Electronically excited/ionized species (Van Gaens et al.-2013, Kossyi et al.-1992, Popov-2011, Adamovich et al. – 2014, Tsolas - 2015)
- Neutral/Thermal chemistry: iC8H18 and C2H5OH Mechanism (Curran-LLNL - 2002), O_3 chemistry (Bromly et al.-1996)

Technical Backup Slide

Details on AMReX and PeleC & Kinetics Mechanism

- The detailed kinetics mechanism for discharges in air/ethylene mixtures consists of the Konnov combustion mechanism [2] combined with the detailed air plasma mechanism of Eckert [3]
- The detailed combined mechanism for LTP ignition of ethylene/air is reduced to a 53 species reduced mechanism via DRG-EP-P [4] in a manner that retains accuracy for discharges



Plasma species in mechanism

P-DRGEP ($N_s = 53$)
$N_2(v_1)$, $N_2(v_2)$, $N_2(v_3)$ $N_2(v_4)$, $N_2(v_5)$, $N_2(v_6)$, $N_2(a^3\Sigma)$, $N_2(w^3\Delta)$, $N_2(c^3\Pi)$, N2($b^3\Pi$), $O(^1D)$, $O_2(a^1\Delta)$, $O_2(b^1\Sigma)$, N_2^+, O_2^+

Integration Algorithm

Algorithm 1 PeleC advancement framework

```
procedure ADVANCE
    while t < t_out do
        E^n = −∇φ^n
        S_ph = S_ph(u^n)
        S* = AD(u^n, E^n)
        u* = u^n + Δt(S* + ω_r)
        S^{n+1} = AD(u*, E^n)
        u** = (1/2)(u^n + u*) + (Δt/2)(S^{n+1} + ω_r)
        F_AD = (1/Δt)(u** − u^n) − ω_r
        ω_r = ω_r(u^n, F_AD, S_ph)
        u^{n+1} = u^n + Δt(F_AD + ω_r)
    end while
end procedure
```

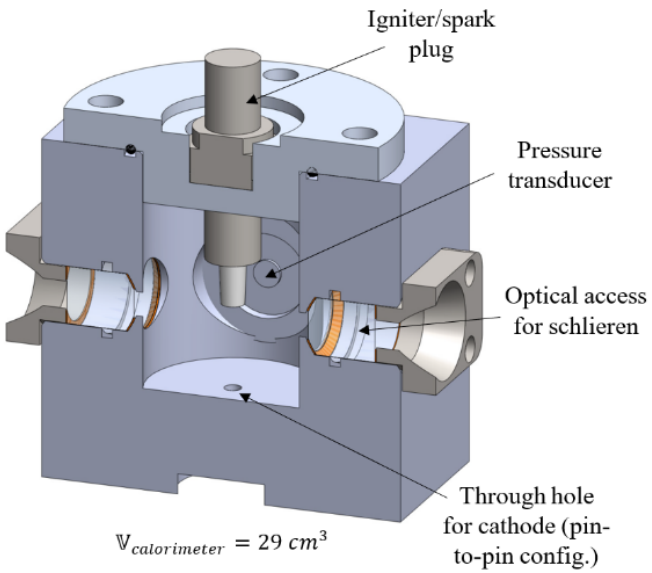
- AMReX[1] is used as the Adaptive Mesh Refinement (AMR) library [1]
- The LTP solver is built by extending the existing AMReX application PeleC, which is a compressible reactive Navier-Stokes solver, to include transport of charged species and voltage potential
- Adaptive Mesh Refinement is employed with a minimum cell size of 2.5 μm and 6 refinement levels are used
- The local "mean field approximation" is used to relate the ionization rates to the local reduced electric field strength
- Electrodes are incorporated with an embedded boundary (EB) method
- Time integration is performed with an explicit approach, embedded in the existing method of lines

[1] https://amrex-codes.github.io/amrex/
[2] Konnov, Combust. Flame 156 (11) (2009) 2093-2105
[3] Z. Eckert, N. Tsolas, K. Togai, A. Chernukho, R.A. Yetter, I.V. Adamovich, J. Phys. D Appl. Phys. 51 (37) (2018) 374002.
[4] A. Bellemans, N. Kincaid and N. Deak et al., Proc. Combust. Institut. 38 (2021) 6631–6639

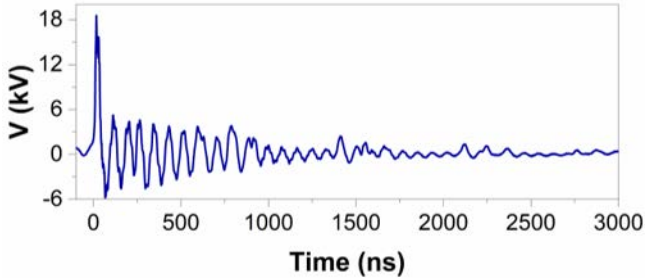
Technical Backup Slide

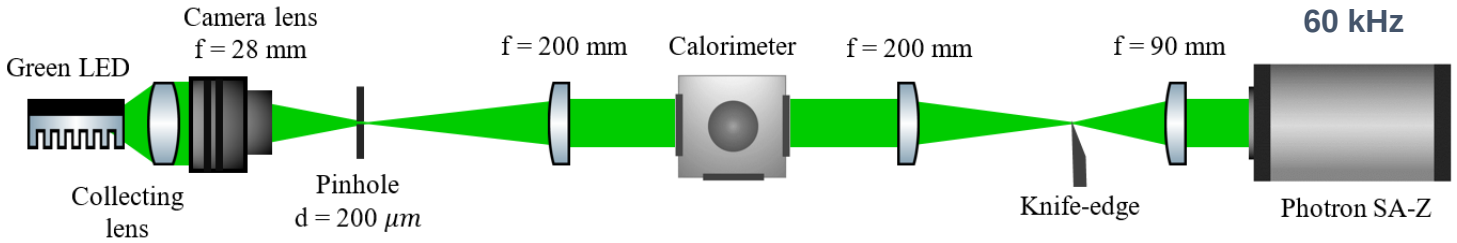
LTP Ignition Experimental Details

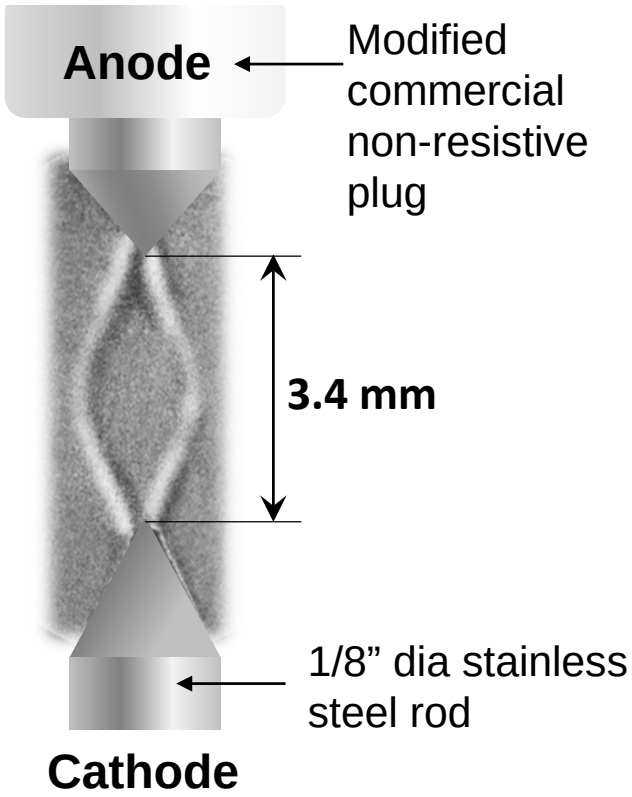
Optical Ignition Calorimeter



Transient Plasma Systems Inc.







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

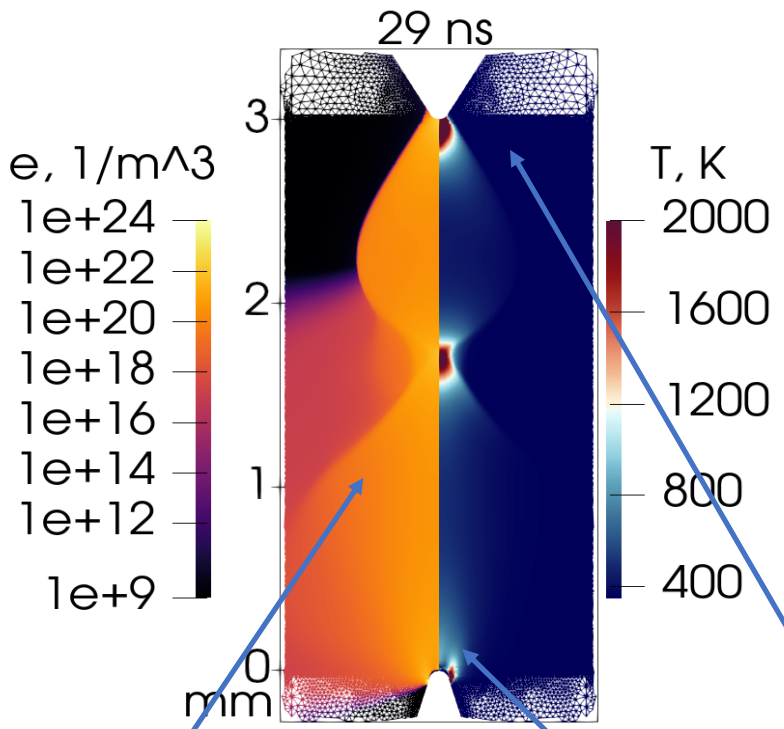
Pin-to-Pin (P2P)

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

Technical Backup Slide

Details on VizGlow and CONVERGE CFD Commercial Software

Only fast gas heating due to LTP discharge considered.



Time variation
(20 ns square pulse for this study)

$$S_{LTP} = AB(t)\left(f(x,y,z) + g(x,y)(h_a(z) + h_c(z))\right)$$

$$E_{LTP} = \int dx \int dy \int dz \int dt S_{LTP}$$

- VizGlow [1] was used to study streamers at various conditions and eventually develop S_{LTP} .
- S_{LTP} was then coded as a User Defined Function used in the CFD suite CONVERGE [2].
- Adaptive Mesh Refinement was employed with a minimum cell size of 31.25 μm (flame thicknesses in this study varied from 280 to 480 μm).
- No turbulence model was invoked: simulations correspond to quiescent starting conditions (**1.3 atm and 343 K**).
- The chemical mechanism used was Stanford's FFCM [3].
- Electrode meshing was carried out using the Constructive Solid Geometry Tool sdf [4].

[1] www.esgeetech.com
[2] https://convergecfd.com
[3] https://web.stanford.edu/group/haiwanglab/FFCM1/
[4] https://github.com/fogleman/sdf