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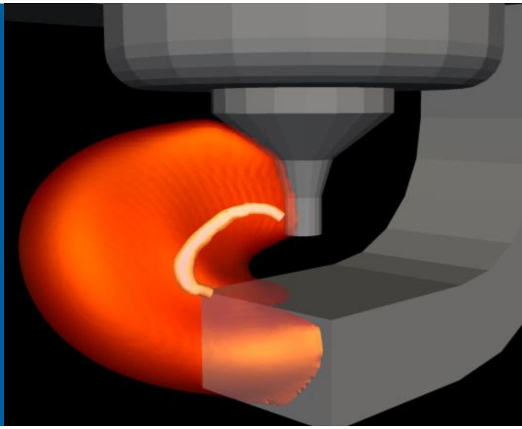
DEVELOPMENT AND VALIDATION OF SIMULATION TOOLS FOR ADVANCED IGNITION SYSTEMS



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Project ID: ACE084

2019 DOE Vehicle Technologies Office AMR
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OVERVIEW

Timeline

- Project start: FY 2017
- Project end: FY 2019
- Transitioning into the Light-Duty Combustion Consortium (FY19-24)

- Started as modeling/experiments task for the VTO Lab Call FY17
- Re-defined in FY18 as modeling only task
- Combined with ACS075 (PI: Som, ANL) at 2018 VTO AMR

Budget

- Funding in FY17: $370k
- Funding in FY18: $400k
- Funding in FY19: $400k

Barriers

- *Limited understanding* of advanced ignition mechanisms enabling high-efficiency internal combustion engines
- *Limited availability of modeling tools* to support the development of advanced ignition systems

Main Partners

- Sandia National Laboratories (SNL)
- Esgee Technologies Inc.
- Convergent Science Inc.
- Transient Plasma Systems (TPS)
- Federal Mogul (FM)
- Michigan Tech, U-Texas, U-Perugia
- USCAR (Ford, GM, FCA)
- Argonne (engine experiments)

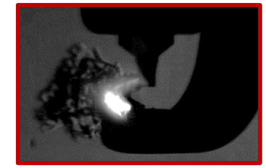
RELEVANCE AND OBJECTIVES

Limited understanding/models for advanced ignition concepts

- **Challenges for Spark-Ignition (SI) systems and models**
  - Boosted, dilute, cold-start operation impacts combustion stability
  - SI models are not predictive at severe operating conditions

  GOAL: Improve formulation & accuracy of SI models

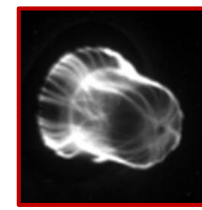
Image: MTU

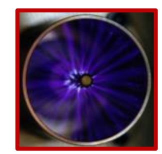


- **Strong interest in Low-Temperature Plasma (LTP) ignition**
  - OEMs develop advanced concepts with Tier I Suppliers (e.g. GBDI)
  - Improved dilution tolerance and efficiency, robust controls
  - Some advanced ignition technologies nearing production
  - Absence of LTP ignition models in engine CFD codes

  GOAL: Improve understanding, develop LTP ignition models

acs121_yun_2018_o.pdf





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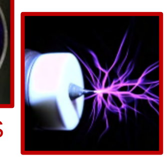


Image: BW

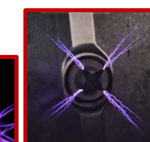
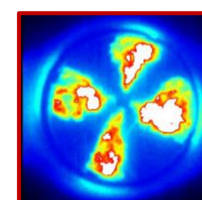


Image: FM

- **Pre-Chamber ignition (PC) is back…stronger than ever…**
  - Evaluation of passive/active PC for a wide range of engine platforms
  - Main computational challenge is for combustion modeling
  - Advanced ignition modeling required for large PC stratification/turbulence

  GOAL: Improve sub-models for PC ignition & combustion



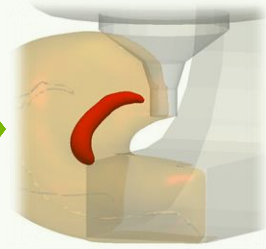
ace087_bunce_2015_o.pdf

APPROACH

* LESI = Lagrangian-Eulerian Spark-Ignition
** WSR = Well Stirred Reactor

Spark-Ignition
Eulerian Approach (energy deposition)

Q: Source Evolution

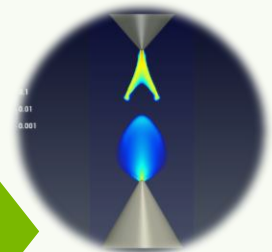


LESI* model development (CONVERGE)

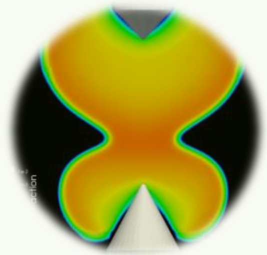
LTP Ignition
(energy + species deposition)

Q: Plasma properties and impact on ignition

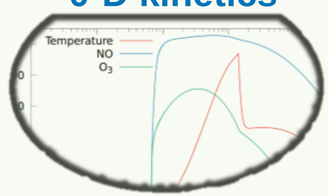
VIZGLOW



CONVERGE

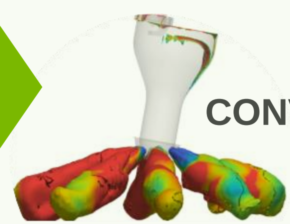


0-D kinetics



PC Ignition
(WSR or flamelet models coupled with more or less advanced ignition models)**

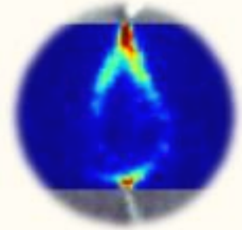
Q: Ignition & Combustion Regime



CONVERGE

VALIDATION

Isaac Ekoto (SNL, ACE006)



Toby Rockstroh (ANL, ACE134)

Image: MTU

MILESTONES FY19-20

Q1 (12/31/2018)
Evaluate real LTP ignition case with plasma and CFD solvers
{100% Complete}

Q2 (3/31/2019)
Plasma mechanisms expanded with the addition of relevant chemical species and reactions
{50% Complete}

Q3 (6/30/2019)
Expand LTP studies to advanced igniter geometries
{75% Complete}

Q4 (9/30/2019)
LESI model validation extended to different conditions
{25% Complete}

FY2020

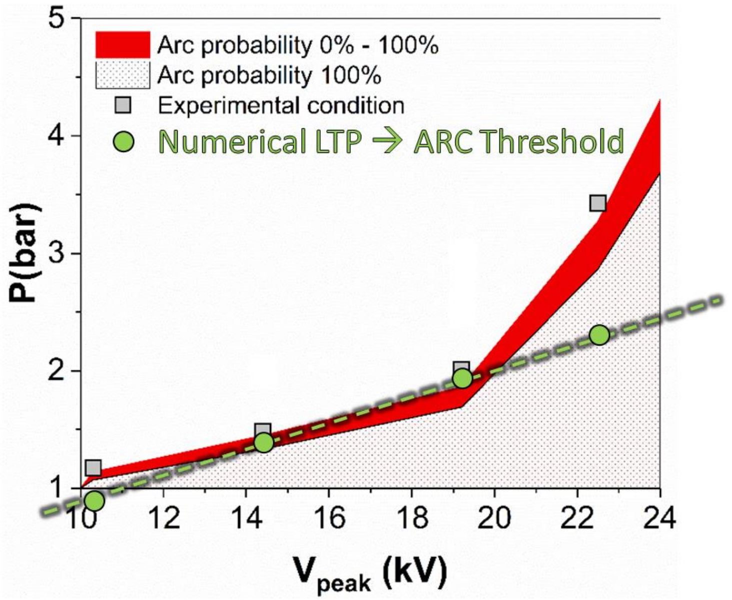
I. Build plasma/fuel reduced mechanism for CFD simulations
II. Evaluate LTP ignition models at dilute operating conditions
III. Simulate ignition for advanced compression ignition (ACI) strategies
IV. Simulate ignition processes at cold-start conditions

ACCOMPLISHMENTS FY18*

* acs075_som_2018_o.pdf

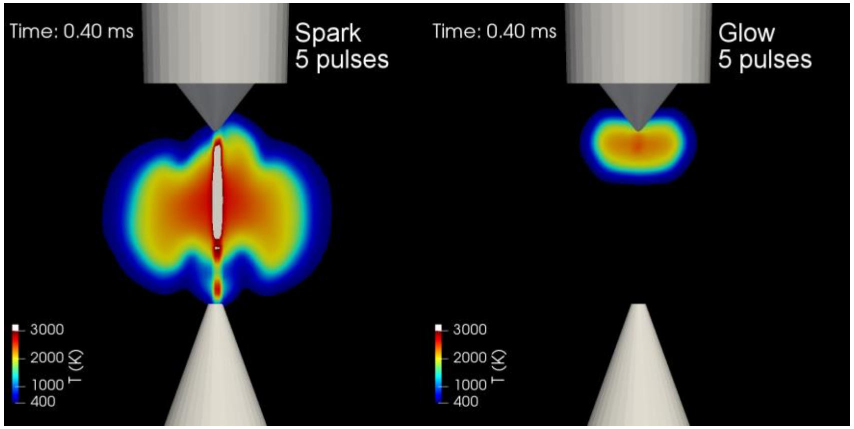
LTP solver (VIZGLOW) validated/coupled with CFD (CONVERGE)

1. Matched experiments on glow/spark regime transition
2. O atom and Temperature validated against experiments (O-TALIF measurement near the anode)
3. VIZGLOW output fed into CONVERGE source input (combination of thermal energy and species)
4. Thermal and non-thermal plasma deposition practically simulated in CONVERGE



Experimental data from Isaac Ekoto, SNL

	SIMULATIONS		EXPERIMENTS	
	O (#/m^3)	Temp (K)	O (#/m^3)	Temp (K)
14kV - 1.5bar	**0.9E^{+24}**	**770**	**1.3E^{+24}**	**779**
19kV - 2.0bar	**1.8E^{+24}**	**938**	**2.1E^{+24}**	**1094**



☑ **Expand CFD modeling capabilities to simulate non-thermal ignition**

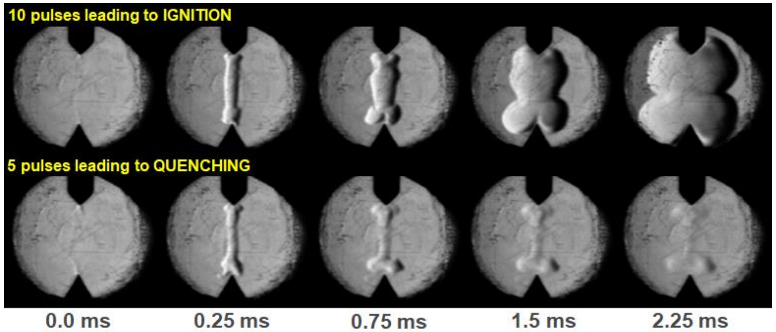
ACCOMPLISHMENTS FY19

* PRR = Pulse Repetition Rate

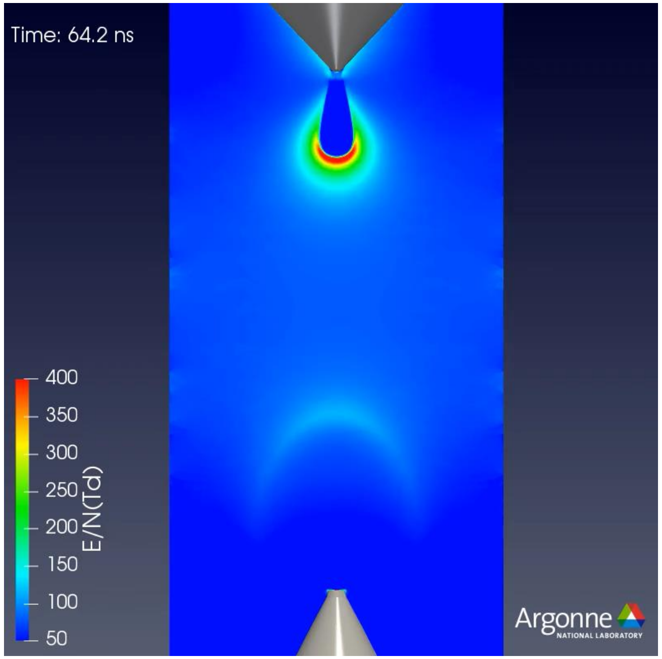
Real LTP ignition case investigated

- Ignition observed from non-thermal plasma (SNL)
- Clear impact of no. pulses on ignition/quenching
- LTP simulations performed with improved detail of the actual geometry of the two pin electrodes
- Model tuning consistent with previous validation

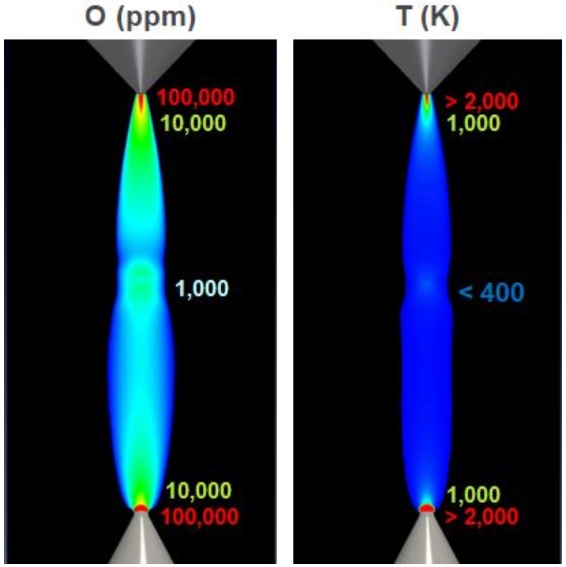
LTP ignition from P2P geometry into C_3H_8/air mixture
$\phi = 1.0$, $P_i = 1.3$ bar, $T_i = 343$ K, $V_{PEAK} = 15$ kV, PRR* = 10kHz)



Courtesy of Isaac Ekoto, SNL



LTP properties at the end of discharge



LTP simulations qualitatively/quantitatively validated against experiments

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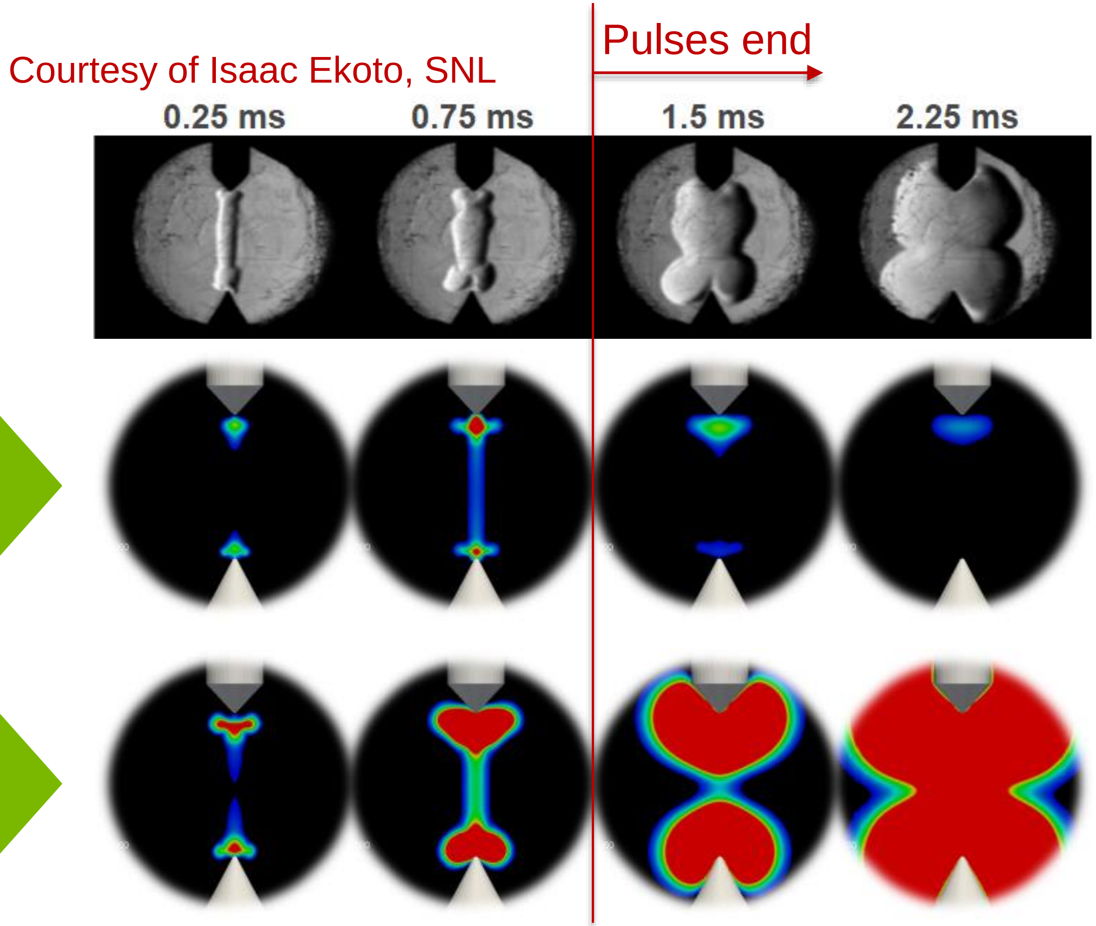
ACCOMPLISHMENTS FY19

LTP ignition simulated using CFD engine codes (CONVERGE)

- Improved source (Energy + O atom) deposition in CONVERGE CFD
- Assumption: Deposition does not change during the entire train of pulses

Apply VIZGLOW output

Increasing [O] by a factor of 10



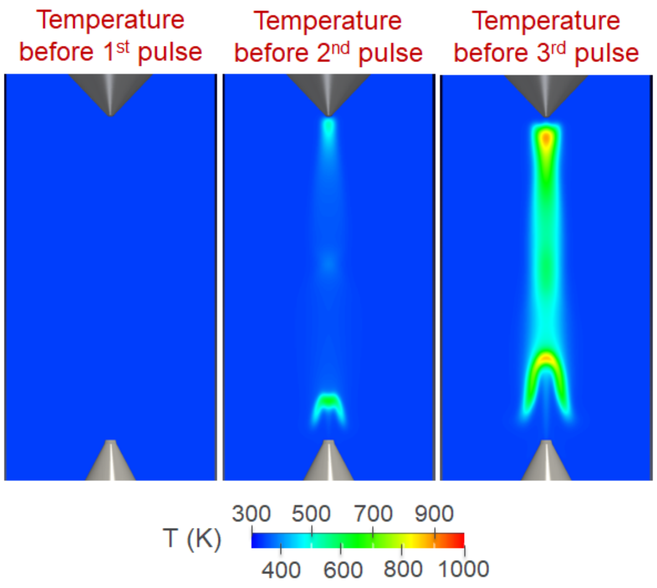
☑ **Evaluate real LTP ignition case with plasma + CFD solvers**

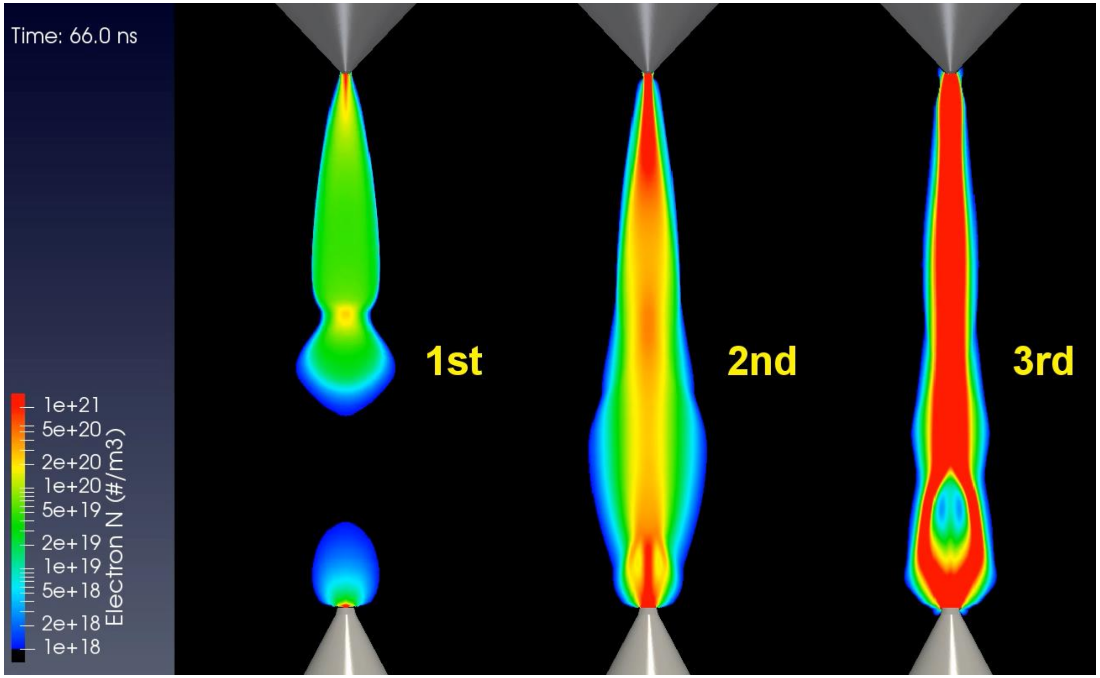
☐ **Quantitative validation → Ignition achieved only by boosting [O]**

ACCOMPLISHMENTS FY19

Multi-pulse LTP discharge simulated using VIZGLOW

- Main challenge is from the large gap in discharge (10^{-7} s) and flow (10^{-4} s) time-scales
- Inter-pulse simulations achieved by variable time-step (from 10^{-12} to 10^{-10} s). 3 pulses/week



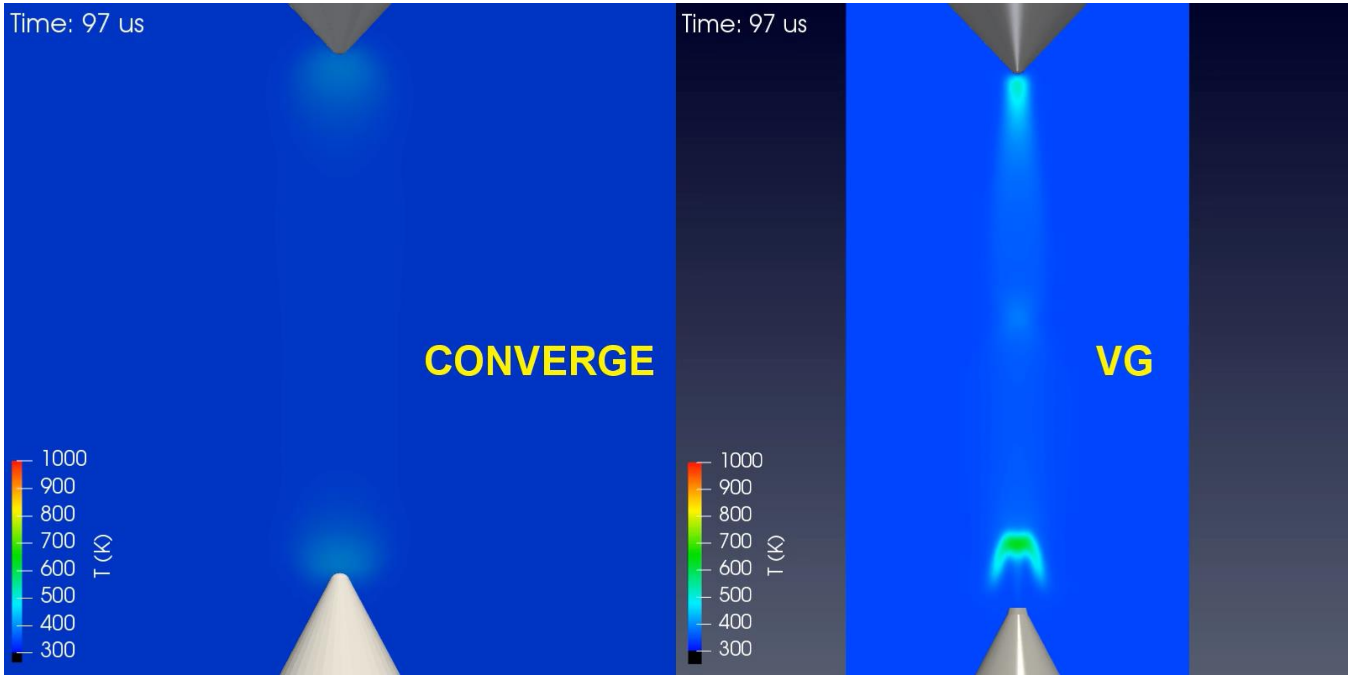


- More thermal/chemical energy will go into the gap because of larger E/N values
- How fast (this process is) depends on fluid mechanics in the after-glow phase

ACCOMPLISHMENTS FY19

Impact of fluid mechanics on LTP deposition/ignition evaluated

- CONVERGE simulations dissipate the effects of one pulse entirely before next pulse
- VIZGLOW simulations still show “hot spots” nearby the electrodes before next pulse
- Mesh size and flow solver are quite different between the two codes
- Some details (e.g. cathode geometry) not taken into account in CONVERGE

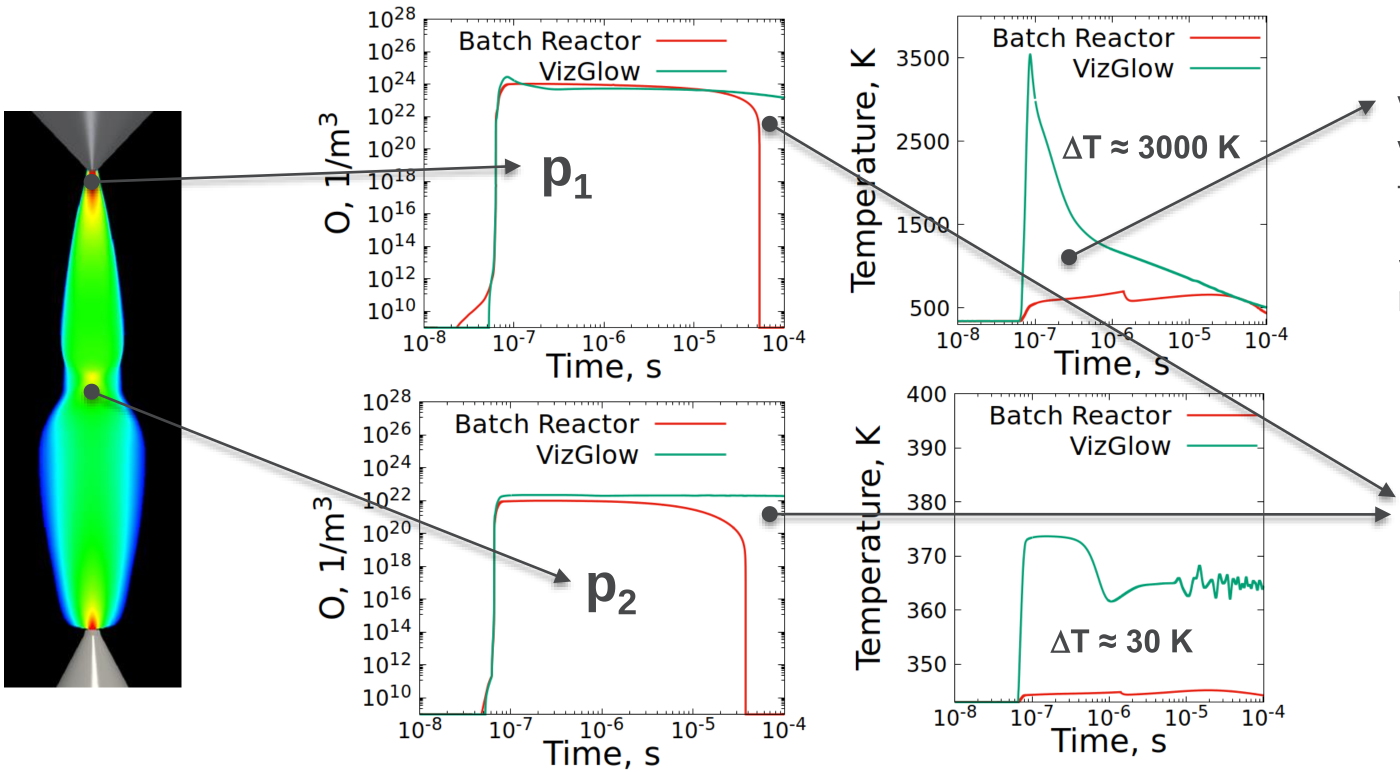


- Fluid mechanics has a significant impact on multi-pulse LTP evolution
- Validation is challenging due to the lack of data. What solver is right?

ACCOMPLISHMENTS FY19

Impact of detailed plasma kinetics evaluated in the after-glow

- Initial calculations without fuel, only air chemistry
- Electron density + E/N from VIZGLOW fed into 0-D reactor with detailed kinetics
- Good prediction of ionization wave and O (produced). Off-set in temperature calculations



Large gap due to very high Temp values predicted from VIZGLOW.

Surface chemistry might play a role

Low O decay due to the lack of recombination chemistry

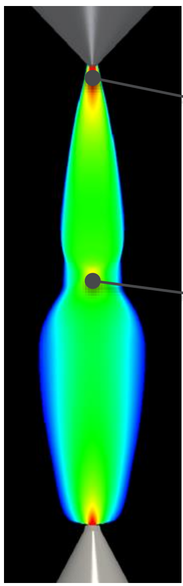
☑ **Account for detailed plasma chemistry and relevant species**

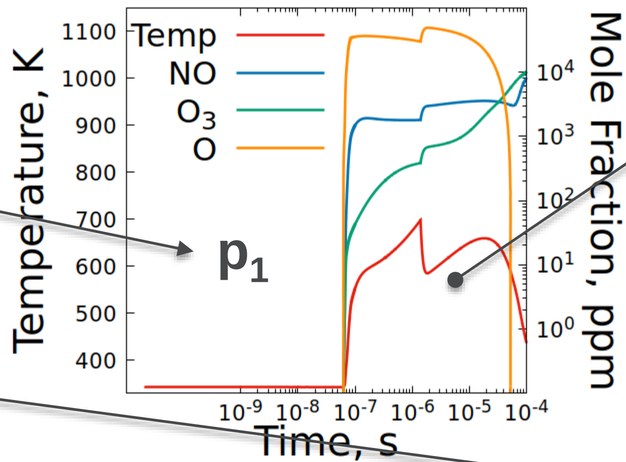
☐ **Match VIZGLOW (Big challenge. Very different mechanism size)**

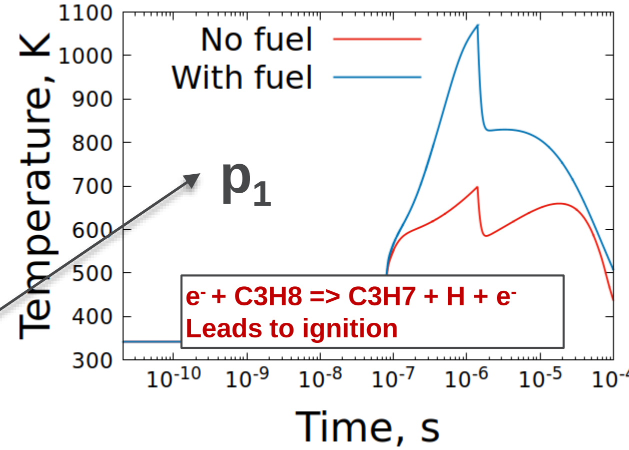
ACCOMPLISHMENTS FY19

Impact of detailed kinetics on LTP ignition evaluated

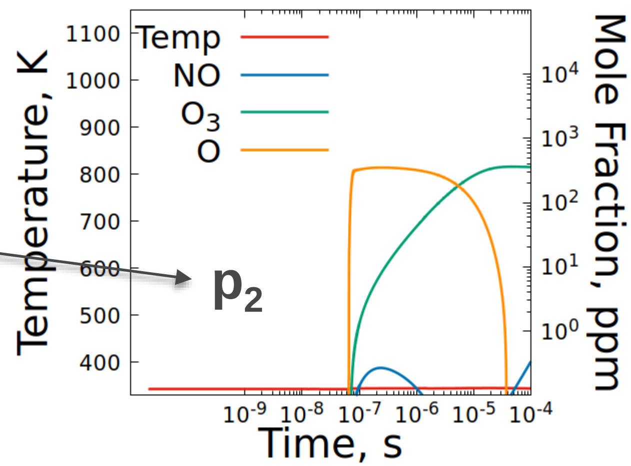
- Full chemistry accounts for species that are relevant to ignition processes, such as NO, O_3, etc.
- Fuel chemistry also interacts with plasma chemistry, promoting the formation of active fuel radicals







Generally more chemical activity in the proximity of the electrodes

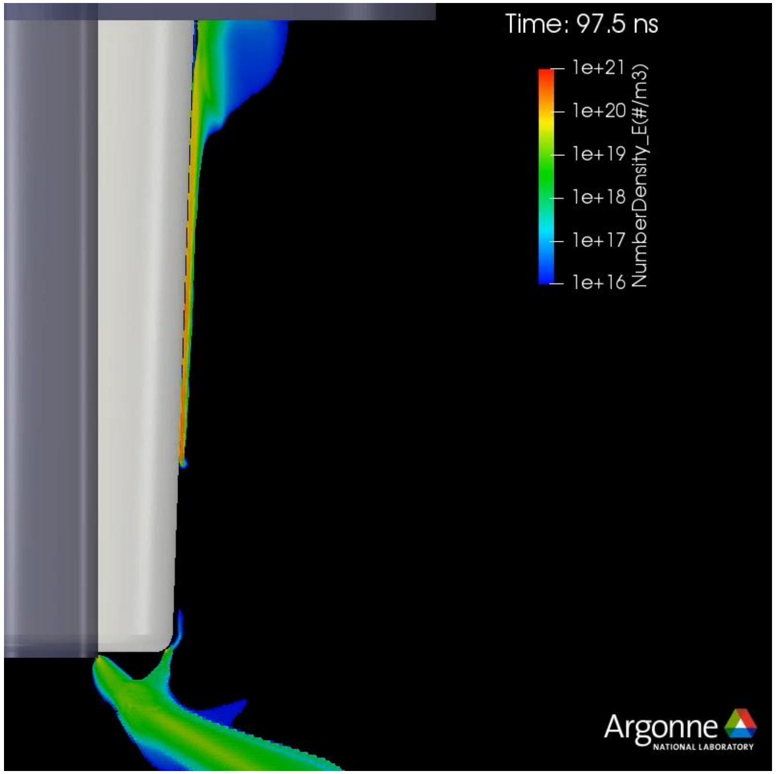


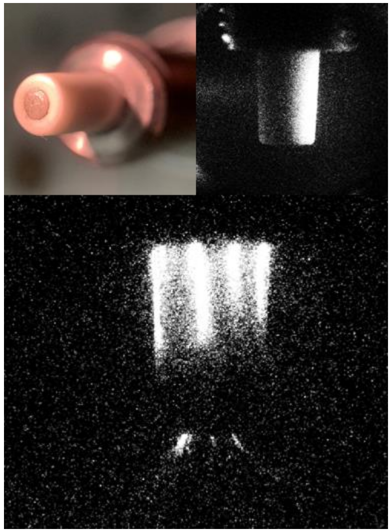
☑ **Priority established for relevant species (NO_X, O_3, Fuel radicals) to be included in plasma/fuel reduced kinetics for engine CFD simulations**

ACCOMPLISHMENTS FY19

SNL groundless barrier discharge igniter (GBDI) simulated

- SNL version has exposed electrode. Plug metal thread and calorimeter walls behave as the missing ground
- Streamers propagating along the dielectric surface. Streamers into air aiming at the calorimeter walls





Courtesy of Isaac Ekoto, SNL

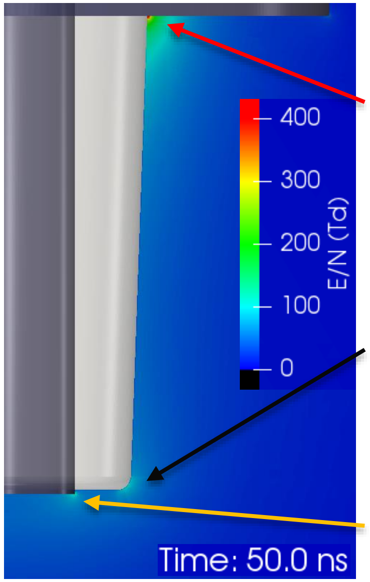
- <u>We qualitatively match images from SNL</u>
- Main challenge from the large simulation domain and complex geometry
  - Requires advanced mesh handling
  - Streamers-into-air <u>not</u> very accurate

☑ **Expand LTP studies to advanced igniter geometries**

ACCOMPLISHMENTS FY19

LTP properties from GBDI evaluated

- While streamers-into-air calculations are not very accurate, streamers might reach the walls and led to arcing
  - Arcing observed experimentally!
- Streamer emissions might happen from exposed electrode or even from the dielectric surface (if curvature is high)
- Enclosed electrode and low curvature (like the GM version) prevent streamer-into-air propagation and eliminate arcing

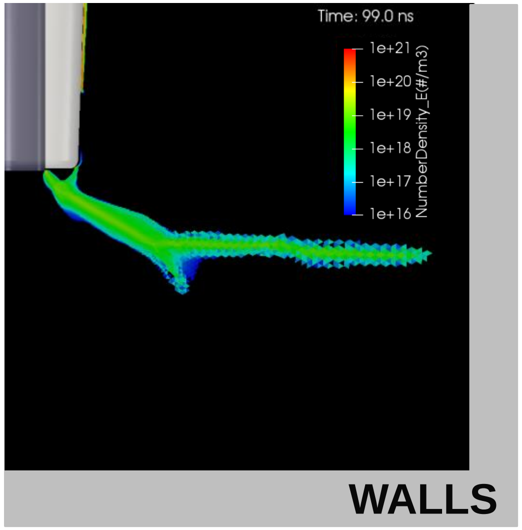


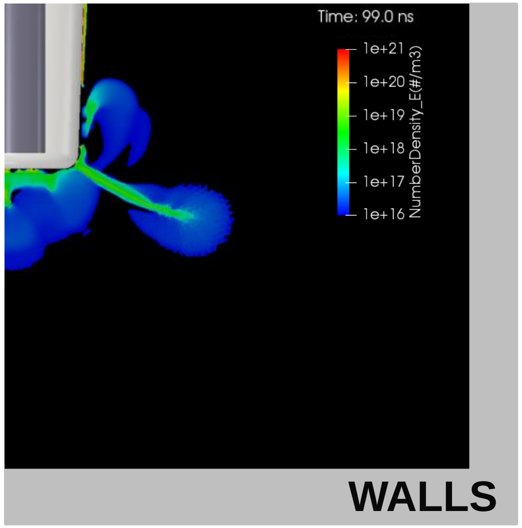
Highest Field between barrier and ground

Large Field also along the dielectric, can turn into a streamer

2nd highest Field from the exposed electrode

Fully-covered electrode reduces streamer-into-air penetration and prevents arcing





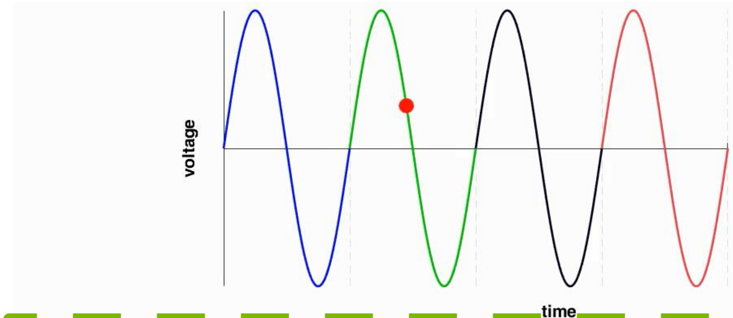
The LTP igniter geometry can be optimized to achieve highest efficiency

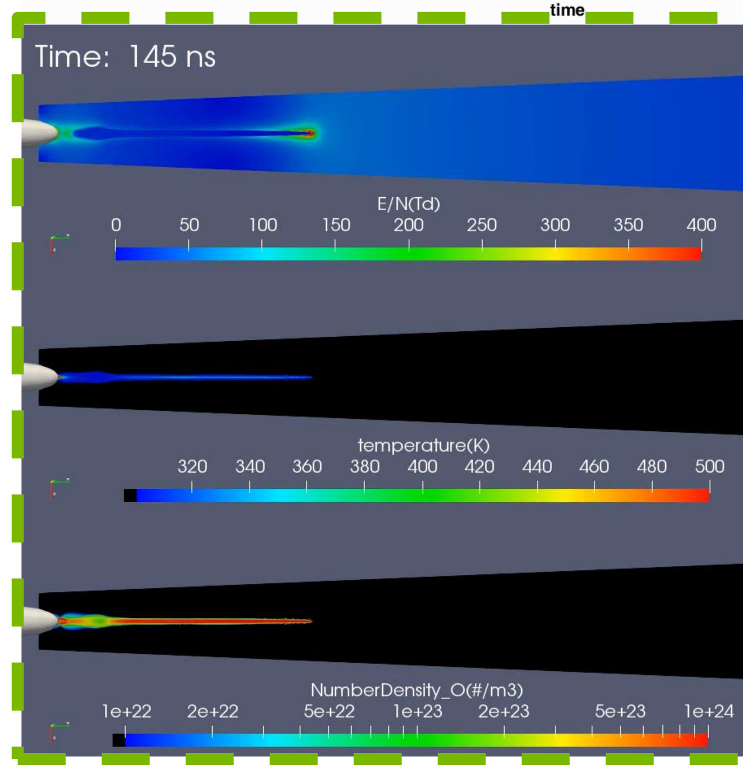
ACCOMPLISHMENTS FY19

* RF = Radio-Frequency

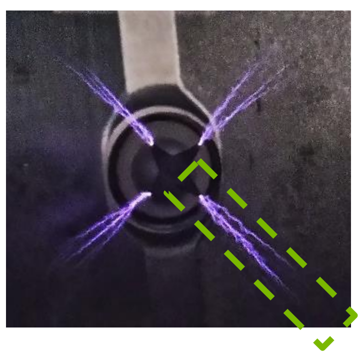
FM corona igniter simulated

- In collaboration with FM and U-Perugia, Italy
- Similar to a pin-to-plane geometry
- Main technical challenge from the RF* signal. Requires low time-steps for a long time
- Initial demonstration for 10x faster frequency to evaluate streamer evolution
- Very fast streamer propagation from 2nd cycle
  - Expansion likely not captured (flow solver)
  - 10x faster limits expansion further





Courtesy of
Federal Mogul (FM) &
University of Perugia



☑ **Expand LTP studies to advanced igniter geometries**

☐ **Validation missing (simulations in progress, challenges identified)**

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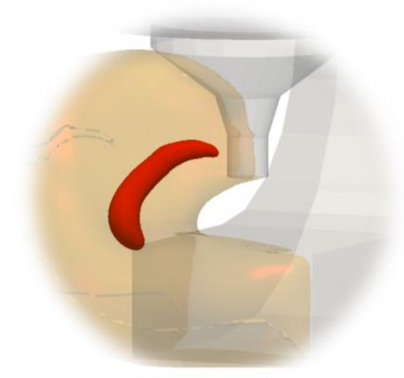
ACCOMPLISHMENTS FY19

Progress made on conventional/advanced SI modeling

Lagrangian-Eulerian Spark-Ignition (LESI) Model

- Software copyright approved by DOE (SF-18-030)
- ASME 2018 paper selected for journal (GTP-19-1137)
- Interest from industry to have LESI available in CONVERGE
- CRADA with FCA planned for further validation and development



Pre-chamber (PC) ignition in SNL optical vessel

- Experiments led by Isaac Ekoto (SNL, ACE006) with focus on SI/LTP ignition in the PC
- CFD model complete. Simulations started simultaneously with experiments. Parametric studies of T/p/ϕ and location of the spark

Pre-chamber (PC) ignition in ANL metal engine

- Experiments led by Toby Rockstroh (ANL, ACE134) with PC used for multi-mode (SI/ACI) operation
- CFD model complete. Simulations (passive PC) qualitatively match experimental trends

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RESPONSE TO REVIEWER COMMENTS

2017 VTO AMR review – Avg Score = 3.28

- …the PI may need to collaborate with the LLNL algorithm investigators…

✓ More tight collaboration with LLNL investigators, concerning solver speedup as well as LTP kinetics, is being planned for the FY19-24 Light-Duty Combustion Consortium

- …questioned if the proposed work will have an impact in removing barriers to high-dilution engines…

✓ The barrier addressed by the project are limited understanding and no predictive models for advanced ignition systems. This barrier impacts engine efficiency and emissions

2018 VTO AMR review – Avg Score = 3.50 (ACS075, Presenter: S. Som)

- "…Further development and validation over a variety of conditions are needed by the LESI model.."

✓ This is being planned for the remainder of the fiscal year. SI model improvement will also be one of the focus areas for the FY19-24 Light-Duty Combustion Consortium

- "…many sophisticated models are used…It might be possible to devise simpler models to explore the detailed processes such that engineers can use them an effective tool"

✓ This is the approach we are initially following for LTP ignition modeling in CFD codes

COLLABORATION AND COORDINATION

Sandia National Laboratories on low-temperature plasma (LTP) and non-conventional ignition diagnostics

DOE Labs

Michigan Technological University (SI optical diagnostics).

University of Texas at Austin (non-equilibrium plasma modeling)

Academia

Esgee Technologies Inc. (non-equilibrium plasma modeling and LTP ignition).

Convergent Science Inc. (SI modeling).

Software Vendors

Transient Plasma Systems (nanosecond pulsed discharge systems)

- HPC4Mfg Award to optimize NPD discharge

Small Business

Interest/input/guidance from OEMs

- FCA, Toyota, etc. reached out about LESI model
- GM, Ford. etc. reached out about LTP/PC ignition

Large Industry

New: University of Perugia & Federal Mogul (Corona ignition modeling)

Tier I Supplier

REMAINING CHALLENGES AND BARRIERS

* LES = Large Eddy Simulations

- **Still considerable effort required to bridge the gap between fundamentals of LTP ignition and engine CFD simulations**
  - Plasma chemistry plays a key role in LTP ignition processes
  - Role of fluid dynamics is not secondary
  - Large turbulence/chemistry interaction and separation of timescales
- **Improvement required for thermal plasma ignition as well**
  - Non-predictive ignition models coupled with low fidelity combustion models
  - Combustion stability studies require higher fidelity approach (LES* at least)
  - Severe conditions (e.g. cold start) pose an additional challenge to models
- **Pushing modeling effort beyond conventional boundaries**
  - Ignition models that predict SI as well as assisted-CI combustion (e.g. O_3 generators)
  - Combustion models that capture multiple combustion regimes (e.g. pre-chamber)

PROPOSED FUTURE WORK (FY19-24)

* DNS = Direct Numerical Simulations
** CCV = Cycle-to-cycle variation

- **Continue to build understanding and models for LTP ignition**
  - Leverage improved plasma/fuel kinetics → Collaboration with LLNL
  - More validation at lean and dilute conditions
  - Improve fluid mechanics (plasma solvers) and boundary conditions (CFD solvers)

- **Improve predictions from SI calculations**
  - Improve and expand state-of-the art models. Couple with thermal plasma solvers.
  - Conduct extensive validation. Interact with DNS*. Evaluate cold-start and CCV**.

- **Expand model application to SACI, LTP-ACI, PC-ACI calculations**
  - Impact of thermal/non-thermal plasma and turbulent jets on auto-ignition chemistry
  - Evaluate coupling between advanced ignition and combustion modeling

Any proposed future work is subject to change based on funding levels

SUMMARY

Development and Validation of Simulation Tools for Advanced Ignition Systems

Relevance

- Limited understanding and modeling tools for advanced ignition concepts that have shown potential to improve combustion stability and engine efficiency

Approach

- State of the art models expanded for advanced ignition concepts by leveraging high-fidelity plasma simulations and validated against optical diagnostics and engine data

Technical accomplishments (1/2)

- Real LTP ignition case investigated using detailed plasma and engine CFD solvers
- Impact of multi-pulse discharge and induced fluid mechanics on LTP ignition evaluated
- Plasma evolution in the after-glow and impact on ignition processes evaluated with detailed plasma and fuel kinetics

Technical accomplishments (2/2)

- LTP studies expanded to simulate advanced LTP igniter geometries (GBDI, Corona) that are being evaluated by industry
- Research plan defined and simulations initiated for conventional/advanced thermal plasma ignition

Remaining barriers

- Large gap between ignition fundamental and multi-dimensional engine CFD simulations
- Well known technologies (e.g. SI) also need improved models to capture ignition physics
- Scarce modeling efforts on advanced engine strategies leveraging ignition systems

Future work

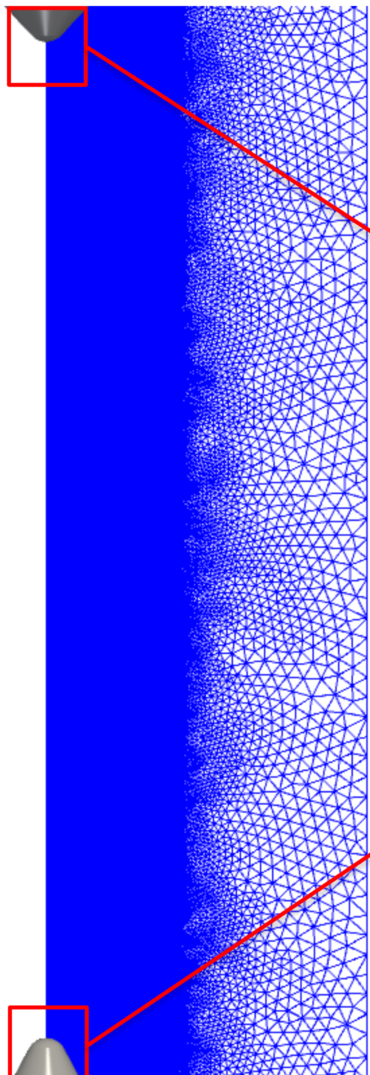
- Improve understanding & models for LTP ignition
- Continue to develop predictive SI models
- Simulate ignition for advanced engine concepts

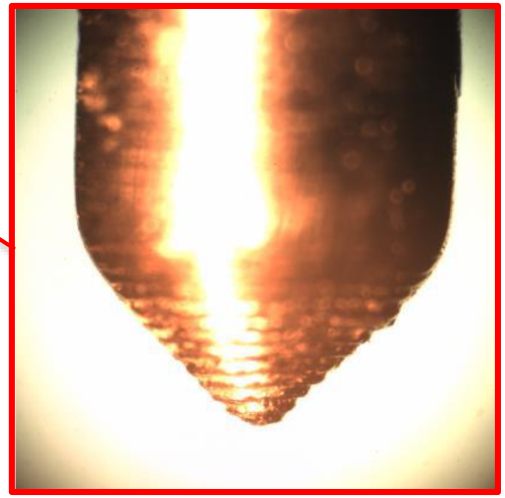
BACKUP SLIDES

TECHNICAL BACKUP SLIDES

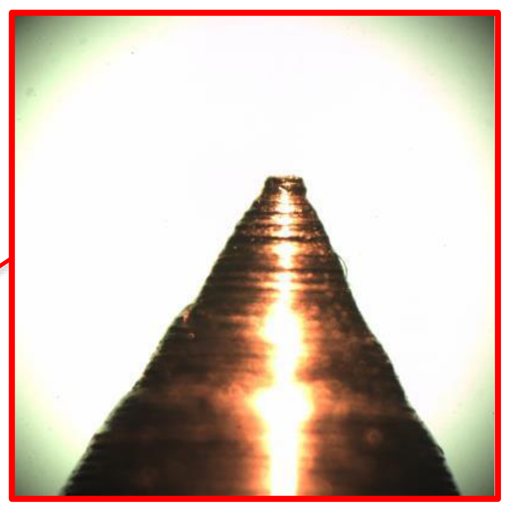
* Scarcelli, R., et al., 2018
Plasma Sources Sci. Technol.

Pin-to-pin (P2P) case setup in VIZGLOW

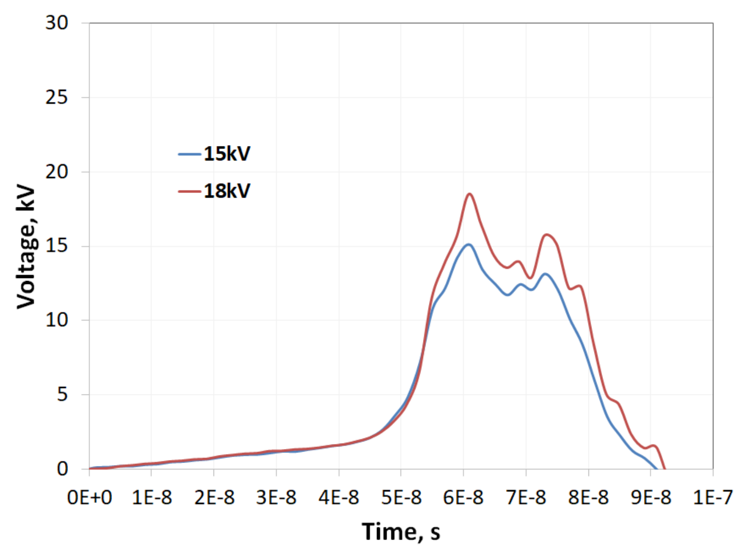




Courtesy of Isaac Ekoto, SNL

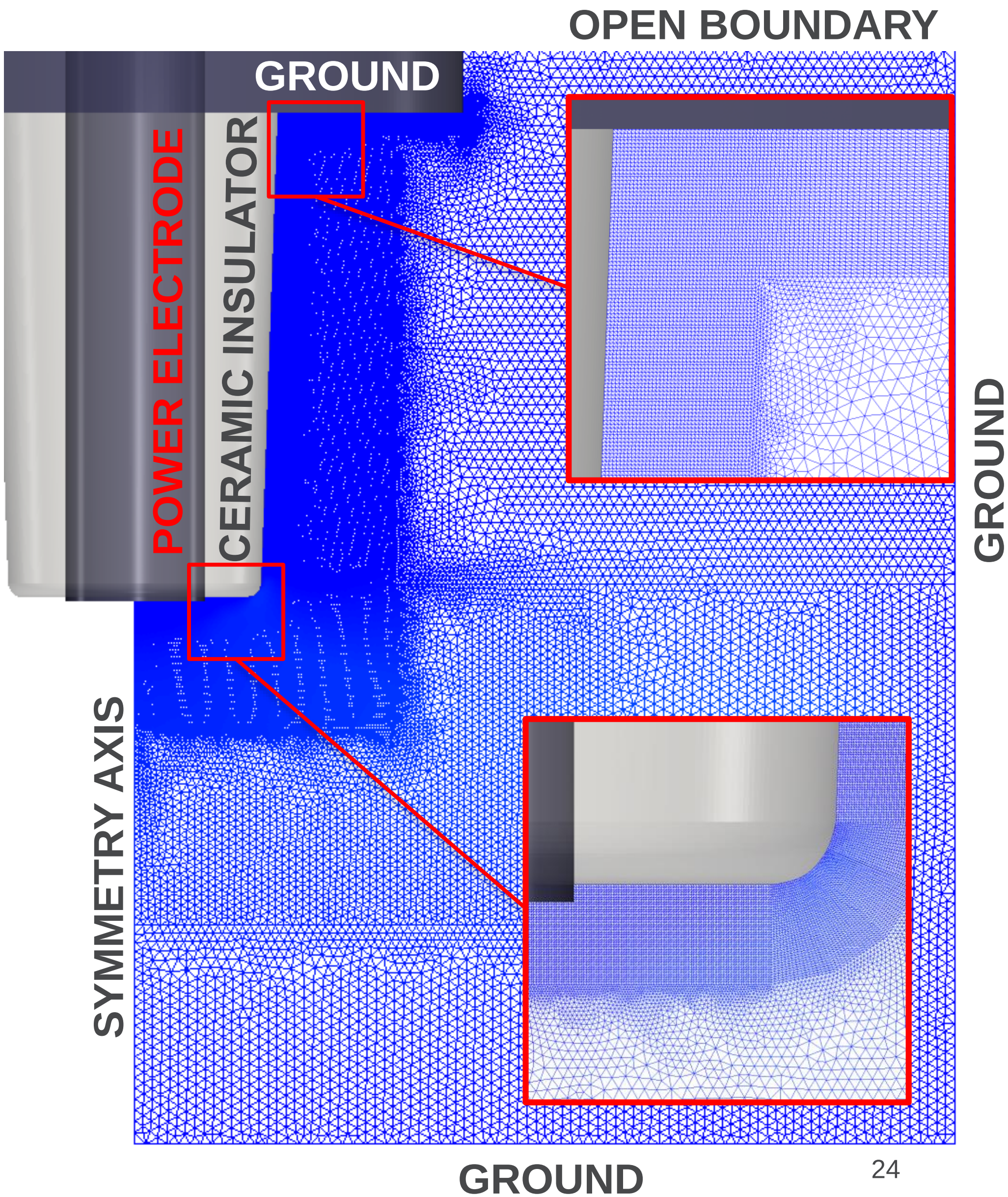


- O_2-N_2 mechanism, 18 species, 64 reactions*
- Pressure = 1.3 bar, Temp = 343 K
- Gap = 6.23 mm, MIN mesh size = 10 μm
- 80,000 cells total
- Model calibration to match experiments
- Extensive study on real electrode geometry effects
- 15kv and 18kv pulse simulated, no ringing
- Flow is solved (Navier-Stokes equations)

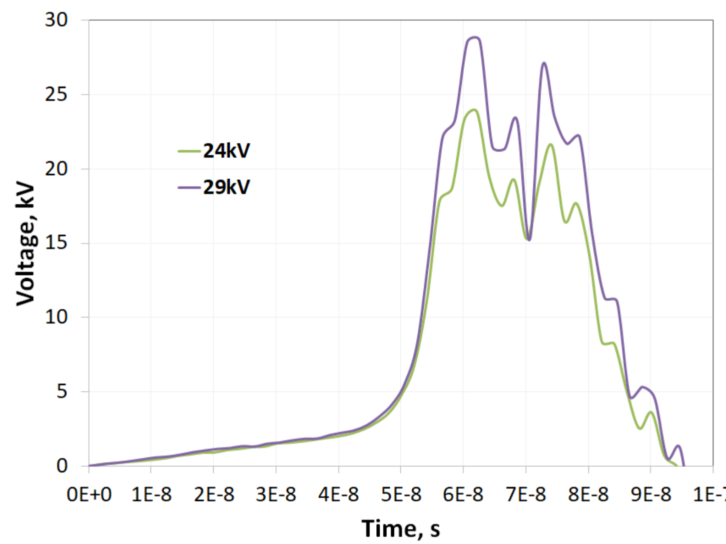


TECHNICAL BACKUP SLIDES

GBDI case setup in VIZGLOW



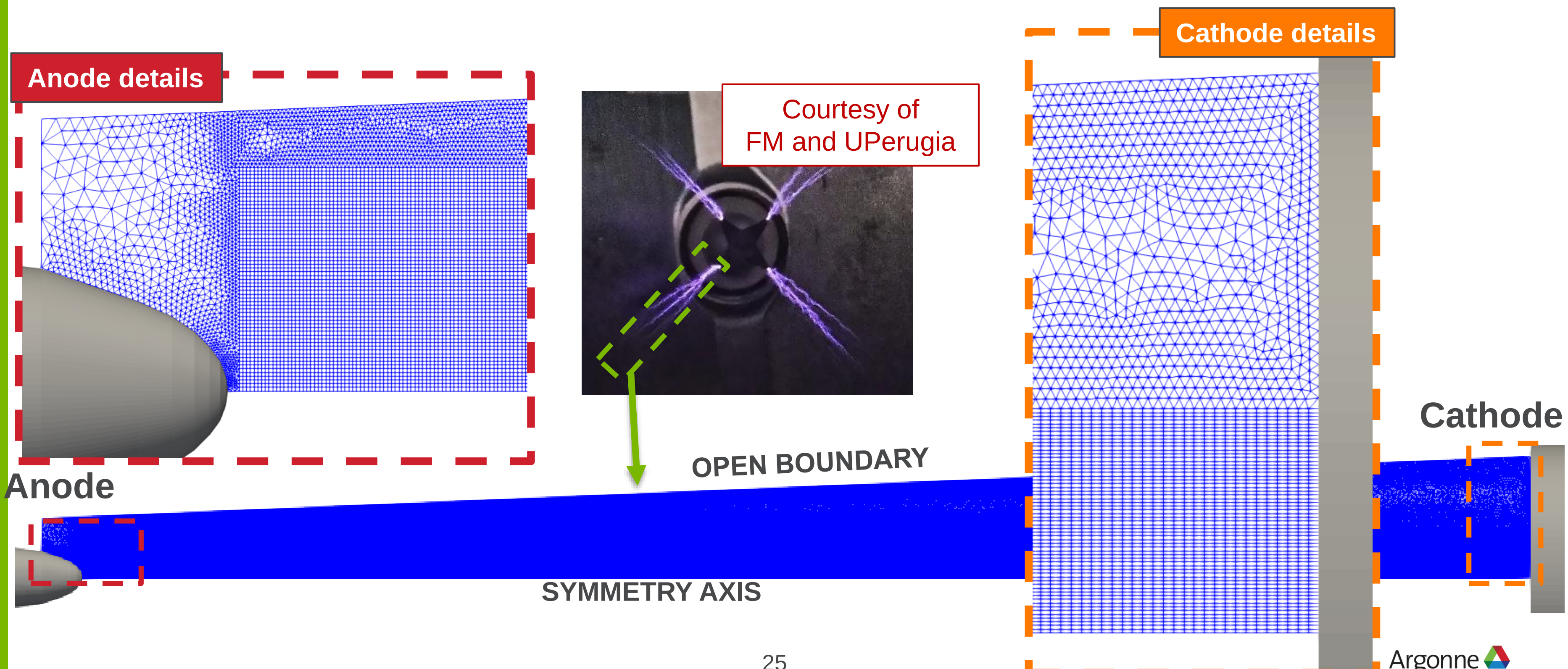
- Pressure = 1.3 bar, Temp = 343 K
- Larger analysis domain (full calorimeter) would lead to much higher cell count than P2P case
- MIN mesh size = 10 μm along insulator
- Coarse mesh elsewhere (up to 150 μm, limited accuracy for streamers in air)
- 160,000 cells total
- Extensive study on real insulator geometry and electrode protrusion
- Flow is solved (Navier-Stokes equations)



TECHNICAL BACKUP SLIDES

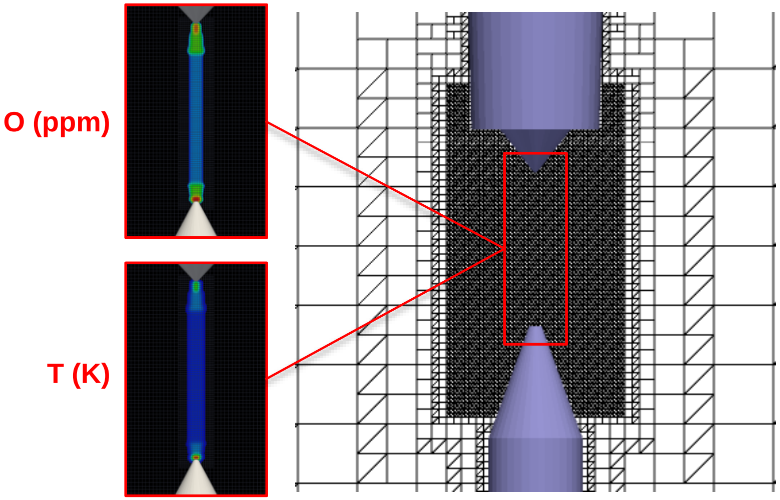
RF corona setup in VIZGLOW

- O2-N2 plasma chemistry for high pressure applications with 18 species: E, O_2, O_2*, O_2a1, O_2b1, O_2^+, O_2^-, O, O^-, O_4^+, O2+N2, N_2, N_2a1, N_2A, N_2B, N_2C, N_2^+, N_4^+ (**common chemistry used in all our VIZGLOW calculations** shown here)
- Flow is solved (Navier-Stokes equations)
- 18 mm gap between rounded electrode tip and plane ground
- Mixture: 20.9% O2, 79.1% N2 @ 300 K, 1.3 abs bar
- **RF sinusoidal voltage profile applied to the anode**; cathode is grounded
- Mixed quad/tri mesh with 10 μm min size
- Quad cells in the center gap
- Total cell count ~107,000



TECHNICAL BACKUP SLIDES

CONVERGE simulations setup



LTP ignition in SNL calorimeter

- RANS modeling (RNG k-ε)
- SAGE solver (well stirred reactor + multi-zone)
  - GRI MECH 3.0
- T = 343K, p = 1.3 bar, ϕ = 1.0
- Base 2.0 mm, AMR 0.25 mm, Embedding 0.0625 mm
- Total cell count = 350k-550k (increase due to AMR)
- Combined energy/O deposition from VIZGLOW

PC ignition in SNL optical vessel and ANL single-cylinder engine

- RANS modeling (RNG k-ε)
- SAGE solver (well stirred reactor + multi-zone)
  - Aramco Mechanism 1.3 (253 species, 1542 reactions) for C_3H_8
  - Co-Optima mechanism (122 species, 647 reactions) for Alkylate
- T = 500K, p = 5 bar, ϕ = 1.0 (Sandia vessel)
- 1500 rpm, nIMEP 3.2 bar, ϕ =1 (Argonne single-cylinder)
- Base 1.0 mm, AMR 0.5 mm, Embedding 0.125 mm
- Ignition by thermal energy deposition (spherical source, 50 mJ)

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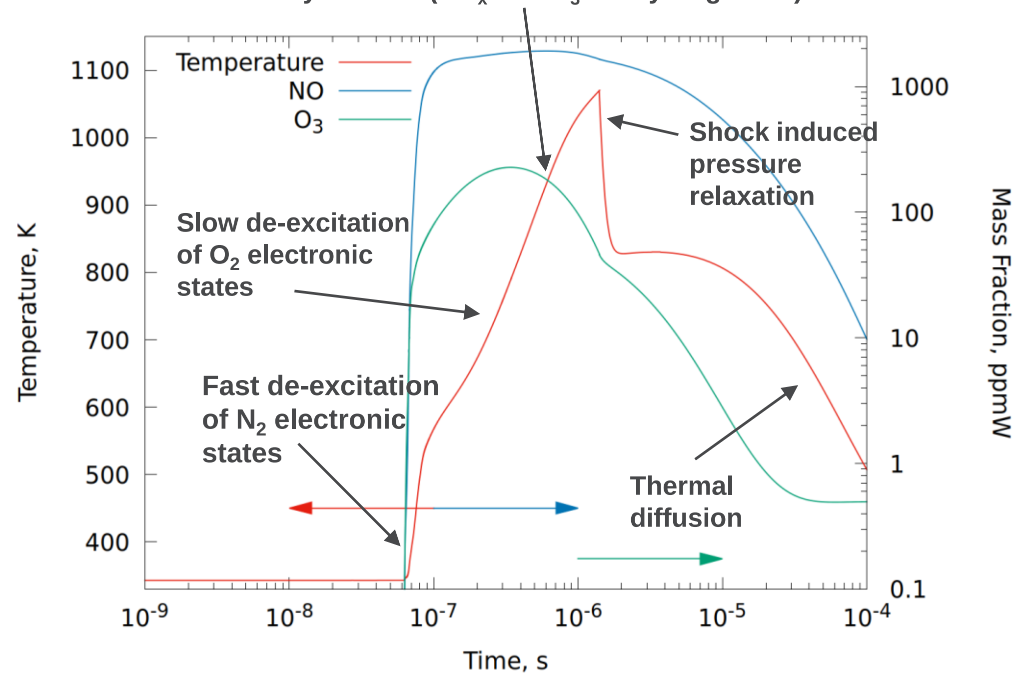
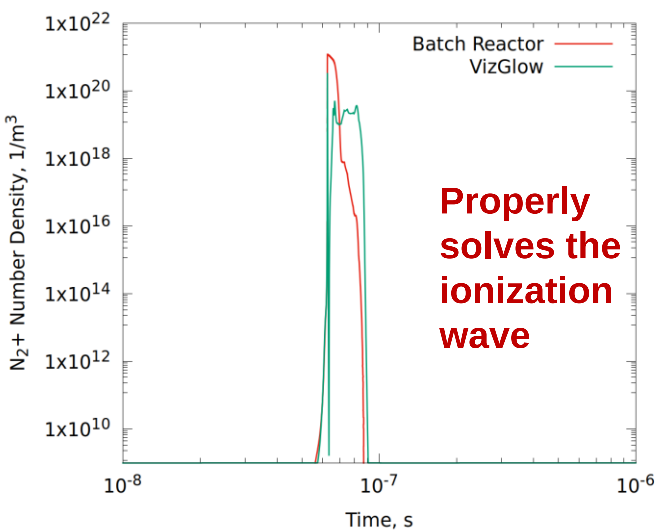
TECHNICAL BACKUP SLIDES

Batch reactor detailed chemistry calculations

- **CANTERA** to calculate thermodynamics and ground state kinetics
- **BOLOS** for the rates of electron impact reactions
- **libMATH** to evaluate other non-Arrhenius rate forms (like Vib.-Trans. Relaxation)
- **SUNDIALS' CVODE** for time integration
- **BASILISK** framework for cylindrical/ spherical shock wave computations





- Full non-equilibrium electron kinetics*
- Pressure relaxation due to gas dynamics
- Heat losses due to diffusion
- Streamer derived electron densities

** Adamovich, et.al., Philosophical Transactions of the Royal Society A 373.2048 (2015).*
** Rasmussen, et al., International Journal of Chemical Kinetics 40, no. 8 (2008): 454-480.*
** Chemical-Kinetic Mechanisms for Combustion Applications (http://combustion.ucsd.edu).*