DEVELOPMENT AND VALIDATION OF SIMULATION TOOLS FOR ADVANCED IGNITION SYSTEMS

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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)
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

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

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
APPROACH

**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**

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

Image: MTU

Isaac Ekoto
(SNL, ACE006)

Toby Rockstroh
(ANL, ACE134)

Image: Isaac Ekoto
(SNL, ACE006)
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*

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

Expand CFD modeling capabilities to simulate non-thermal ignition

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**Experimental data from Isaac Ekoto, SNL**

<table>
<thead>
<tr>
<th>SIMULATIONS</th>
<th>EXPERIMENTS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>O (#/m^3)</td>
</tr>
<tr>
<td>14kV - 1.5bar</td>
<td>0.9E+24</td>
</tr>
<tr>
<td>19kV - 2.0bar</td>
<td>1.8E+24</td>
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</tbody>
</table>
ACCOMPLISHMENTS FY19

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 $\text{C}_3\text{H}_8$/air mixture $\phi = 1.0$, $P_i = 1.3$ bar, $T_i = 343$ K, $V_{\text{PEAK}} = 15$ kV, $\text{PRR}^* = 10\text{kHz}$

LTP properties at the end of discharge

LTP simulations qualitatively/quantitatively validated against experiments

* PRR = Pulse Repetition Rate

Courtesy of Isaac Ekoto, SNL
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]

Courtesy of Isaac Ekoto, SNL
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

**Diagram**

- 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, O₃, etc.
- Fuel chemistry also interacts with plasma chemistry, promoting the formation of active fuel radicals

\[ \text{e}^- + \text{C}_3\text{H}_8 \rightarrow \text{C}_3\text{H}_7 + \text{H} + \text{e}^- \]

Leads to ignition

- Priority established for relevant species (NOₓ, O₃, Fuel radicals) to be included in plasma/fuel reduced kinetics for engine CFD simulations

Generally more chemical activity in the proximity of the electrodes
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

![Image of streamers](Courtesy of Isaac Ekoto, SNL)

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

The LTP igniter geometry can be optimized to achieve highest efficiency
ACCOMPLISHMENTS FY19

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

![Stream of images]

Courtesy of Federal Mogul (FM) & University of Perugia

☑ Expand LTP studies to advanced igniter geometries
☐ Validation missing (simulations in progress, challenges identified)
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/\(\phi\) 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
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

Michigan Technological University (SI optical diagnostics).
University of Texas at Austin (non-equilibrium plasma modeling)

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

Transient Plasma Systems (nanosecond pulsed discharge systems)
  - HPC4Mfg Award to optimize NPD discharge

Interest/input/guidance from OEMs
  - FCA, Toyota, etc. reached out about LESI model
  - GM, Ford. etc. reached out about LTP/PC ignition

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

Tier I Supplier
REMAINING CHALLENGES AND BARRIERS

- 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. O₃ generators)
  - Combustion models that capture multiple combustion regimes (e.g. pre-chamber)

* LES = Large Eddy Simulations
PROPOSED FUTURE WORK (FY19-24)

■ **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

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

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

- O₂-N₂ 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)


Courtesy of Isaac Ekoto, SNL
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 \( \mu \text{m} \) along insulator
- Coarse mesh elsewhere (up to 150 \( \mu \text{m} \), 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)
RF corona setup in VIZGLOW

- O₂-N₂ plasma chemistry for high pressure applications with 18 species: E, O₂, O₂*, O₂a1, O₂b1, O₂⁺, O₂−, O, O⁺, O₄⁺, O₂+N₂, N₂, N₂a1, N₂A, N₂B, N₂C, N₂⁺, N₄⁺ (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
- \( T = 343 \text{K}, \ p = 1.3 \text{ bar}, \ \phi = 1.0 \)
- 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
- \( T = 500 \text{K}, \ p = 5 \text{ bar}, \ \phi = 1.0 \) (Sandia vessel)
- 1500 rpm, nIMEP 3.2 bar, \( \phi = 1 \) (Argonne single-cylinder)
- Base 1.0 mm, AMR 0.5 mm, Embedding 0.125 mm
- Ignition by thermal energy deposition (spherical source, 50 mJ)
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