Modeling and Simulation of Plasma-Assisted Ignition and Combustion

Vigor Yang and Sharath Nagaraja
Georgia Institute of Technology
Atlanta, GA


Nanosecond Plasma Enhanced H₂/O₂/N₂ premixed flat flame

Objectives

To understand the effects of *in situ* nanosecond plasma discharges on the structure of a lean premixed H₂/O₂/N₂ laminar flame (ϕ = 0.5, P = 25 Torr)

**OSU Experiment**

- McKenna burner low pressure (25 Torr) 1D flame
- Porous high voltage electrode 40 mm above burner, no flow-field disturbance.
- -14 kV peak voltage, 7 ns duration (FWHM) waveform with coupled energy ~3 mJ.

Plasma off

Plasma ON
Numerical Framework

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**model setup**

- High Voltage Electrode
- Voltage Pulse Generator
- Premixed Mixture
- 1D Simulation Domain
- Flame

**Governing Equations**

**Species** (charged & neutral)

\[
\frac{\partial n_k}{\partial t} + \nabla \cdot J_k = S_k
\]

**Electron Energy**

\[
\frac{\partial n_\varepsilon}{\partial t} + \nabla \cdot J_\varepsilon = S_\varepsilon ; n_\varepsilon = n_e \bar{\varepsilon}
\]

**Electric Potential**

\[
\nabla (\varepsilon \varepsilon_0 \nabla \varphi) = -e(n_+ - n_- - n_e)
\]

- also mass, momentum & energy conservation

**H₂/O₂/N₂ plasma flame kinetics**

- (42 species, 310 reactions)

H₂/O₂/N₂ plasma chemistry

(Uddi, 2009 and Popov, 2008)

+ conventional H₂-O₂ combustion kinetics

(Popov, 2008 and Konnov, 2008)

+ Low temperature NOₓ kinetics

(Takita, 2007)

- Two temperature model
- Lookup table for electron transport and rates using two-term expansion for electron Boltzmann equation (BOLSIG).
Pulsed Nanosecond Plasma and Flame Interactions

Multi-Scale Problem

- electrical breakdown
- cathode sheath formation
- electron impact dynamics

- excited species quenching
- ion recombination
- gas heating

- cumulative effects of multiple discharge pulses
- species and heat transport

Adaptive Time-Stepping

$\Delta t \sim 10^{-13} - 10^{-12} \text{ s}$  $\Delta t$ fixed at $10^{-9} \text{ s}$
OH and Temperature measurements before and after 200 nsec pulses
($\phi = 0.5$, $P = 25$ Torr, $f = 40$ kHz)

- Significant OH increase observed in the low temperature, pre-flame region.
- How important is nonequilibrium plasma kinetics?
- Is the pulsed discharge just a “fancy heating source?”

**Graphs:**

1. **OH mole fraction:**
   - 40% increase post flame
   - 500% increase in the low temperature zone

2. **Temperature (100 K):**
   - 20% increase post flame
   - 10-20% increase in the low temperature zone
• Species and temperature profiles are sensitive to the inlet conditions.
• Best match in predicted and measured temperature and OH data is obtained with inlet temperature of 345 K.
• The flame solution provides starting estimate for the pulsed discharge simulation.
Good agreement with measured and calculated current.
Peak E/N close to the burner is \( \sim 500 \) Td, allowing efficient electron impact dissociation and electronic excitation.
• high E/N downstream of the flame can be attributed to high temperatures and low number density.
• high E/N (100 - 800 Td) and high electron densities (~1e13 cm⁻³) allow for efficient radical generation by nanosecond pulses in relative low temperature region upstream of the flame.
Two plasma enhancement mechanisms

thermal

• Thermalization of ions generated in high E/N zone (> 1000 Td) increases temperature.
• Heat transfer to upstream modifies flame structure, increases O, H, OH concentrations

kinetic

• E/N in range of 100 - 1000 Td in the lower temperature zone upstream of the flame.
• O and H generated through direct electron impact/ excited species quenching move downstream and affect the flame structure.
**O and H density distribution**

- Larger concentration gradients with plasma
- Increase in reactivity closer to the burner
O, H and OH density profiles

[OH] and Temperature
w and w/o plasma

- O and H are primary radicals produced via electron impact kinetics as well as thermal pathways
- OH is a secondary radical produced from O and H

O, H and OH production and consumption pathways

(a) $N(^2\text{D}) + \text{O}_2 \rightarrow \text{O}^1\text{D} + \text{O}_2$
- $e + \text{N}_2 \rightarrow \text{O} \rightarrow \text{OH}$ (48%)
- $\text{N}_2^* + \text{O}_2 \rightarrow \text{OH}$ (63%)
- $\text{e} + \text{O}_2 \rightarrow \text{OH}$ (26%) (20%)

(b) $\text{O} + \text{H}_2/\text{HO}_2 \rightarrow \text{OH}$ (58%)
- $\text{H} + \text{O}_2/\text{HO}_2 \rightarrow \text{OH}$ (30%)
- $\text{OH} \rightarrow \text{NO} + \text{HO}_2$ (5%)
- $\text{N}_2^* + \text{H}_2 \rightarrow \text{H}$ (36%)
- $\text{e} + \text{H}_2 \rightarrow \text{H}$ (22%)
- $\text{O} + \text{H}_2 \rightarrow \text{OH}$ (30%)
Input energy averaged over a discharge pulse

Radicals and temperature profiles after 200 pulses

- only 5% of total energy is coupled in the low temperature region below 1 cm height.
- Energy coupled downstream at high E/N is expended in electron impact ionization, later into heat via ion recombination.
- the plasma kinetic effect is pronounced closer to the burner, resulting in displacement of species profiles upstream.
Summary

A novel plasma-flame facility has been developed to study the direct coupling of 1D low-pressure, $\text{H}_2/\text{O}_2/\text{N}_2$ ($\phi = 0.5$) premixed flame to nanosecond-pulsed plasma discharges.

- Temperature increased by approximately 20% at all spatial locations and OH mole fraction increased by 100-500 % in the preheat region and 40% in the post-flame gases due to the application of discharge pulses.
- Simulation results showed a significant increase in O and H densities due to plasma chemistry, with peak values increasing by a factor of 6 and a factor of 4, respectively.
- It was demonstrated that Joule heating alone cannot move the temperature and species profiles as far upstream (i.e. closer to the burner surface) as the pulsed plasma source of the same total power.

Future work will focus on techniques to increase the energy coupled in the pre-heat zone by placing the high-voltage electrode (made of tungsten for high heat resistance) closer to the flame.
Objectives

• Understand the effect of NS plasma on n-heptane-air ignition chemistry through self-consistent simulations at low temperatures.
• Investigate the effect of radical addition to the “low temperature” and “high temperature” steps of the 2-stage ignition process.

- $P_i = 160$ torr
- $T_i = 500 - 650$ K
- $f = 60$ kHz
- $\Phi = 0.5 - 1.5$
- 20 kV Gaussian pulses
- 20 ns duration
Motivation

Most of previous work in plasma assisted combustion have focused on H\(_2\) or C\(_1\)-C\(_5\) hydrocarbon fuels.

There is a lack of comparison between plasma assisted ignition of smaller and larger hydrocarbon (C\(_6\) and above) fuels.

Higher hydrocarbon fuels exhibit rich low-temperature chemistry which is weak or completely absent in the small hydrocarbon fuels.

It is of practical interest to understand how nonequilibrium plasma discharges affect the ignition kinetics of higher hydrocarbon fuels.

\[
\begin{align*}
\text{1st stage} \\
\text{R-H} & \rightarrow \text{R (H abstraction)} \\
\text{R + O}_2 & \rightarrow \text{RO}_2 \text{ (exothermic)} \\
\text{RO}_2 & \rightarrow \text{HO}_2, \text{H}_2\text{O}_2, \text{CH}_2\text{O etc.}
\end{align*}
\]

\[
\begin{align*}
\text{2nd stage} \\
\text{H}_2\text{O}_2 & \rightarrow 2\text{OH} \\
\text{CH}_2\text{O} & \rightarrow \text{CO, H}_2\text{O} \\
\text{CO} & \rightarrow \text{CO}_2
\end{align*}
\]
Numerical Framework

Governing Equations

Species (charged & neutral)
\[ \frac{\partial n_k}{\partial t} + \nabla \cdot J_k = S_k \]

Electron Energy
\[ \frac{\partial n_\varepsilon}{\partial t} + \nabla \cdot J_\varepsilon = S_\varepsilon; n_\varepsilon = n_e \bar{\varepsilon} \]

Electric Potential
\[ \nabla \cdot (\varepsilon \varepsilon_0 \nabla \varphi) = -e(n_+ - n_- - n_e) \]

… also mass, momentum & energy conservation

Model details

- Plasma fluid equations with detailed kinetics
- two temperature model
- lookup table for electron transport and rates using two-term expansion for electron Boltzmann equation (BOLSIG)

nC7H16-air kinetics (154 species)

C7H16/N2/O2 combustion
(LLNL reduced mech)

+ C7H16/N2/O2 plasma chemistry
(Popov, 2008, Uddi, 2009, and
Alexandrov, 2010)

+ Low temperature NOx kinetics
(Takita, 2007)

*C7H16 (electron impact and with excited species) reaction rates estimated from C3H8 based plasma reactions.
E/N in range of 100 - 500 Td allows for efficient generation of radicals.
O is the most dominant radical species generated by the plasma burst, with peak concentrations near the boundaries.
As seen later, this small pool of plasma generated radicals have a significant impact on low temperature ignition chemistry.
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Plasma kinetic effects on 1st ignition stage
(\(\phi = 1.0, P = 160\) Torr, \(f = 60\) kHz)

“self-acceleration” of low temperature chemistry

- Addition of small amount of radicals accelerates the H abstraction step
- \(RO_2\) produces more radicals which accelerate the whole process further.
the plasma enhancement of the 1st stage is identical in each case, suggesting that the addition of radicals has a strong impact on the initiation time, irrespective of the equivalence ratio.

- Application of NS pulses at start has no noticeable effect on the 2nd stage ignition delay times.
With increase in initial temperature, the initiation time decreases but the induction period increases.

- at a higher initial temperature (above 650 K), the initiation time is negligible compared to the ignition delay.
- application of nanosecond discharge pulses at the beginning has negligible impact for temperatures above 600 K.
Staggered application of discharge pulses

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“staggered” application of NS pulses

- only a few NS pulses sufficient to rapidly trigger 1st stage temperature rise
- NS pulses are applied after the 1st stage to reduce the overall ignition delay

• inclusion of NOX catalytic reactions change the predictions by ~5% because of new OH generation pathways

\[
\begin{align*}
\text{NO} + \text{HO}_2 & \rightarrow \text{NO}_2 + \text{OH} \\
\text{NO} + \text{CH}_3\text{O}_2 & \rightarrow \text{NO}_2 + \text{CH}_2\text{O} + \text{OH}
\end{align*}
\]
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Summary

Effect of nanosecond plasma on two-stage ignition of n-heptane

• first theoretical study to explore the impact of non-equilibrium plasma on the low temperature chemistry of a heavy fuel.
• plasma generated radicals significantly accelerate the H abstraction from fuel molecules and create a “self-accelerating” chemistry loop, reducing first stage ignition delay by a factor of 10.
• the second stage of the ignition process is not sensitive to radical addition by the plasma, but is sensitive to the heating rate.
• A staggered application of voltage pulses suggested be most optimal.

Few plasma pulses to generate small pool of radicals

• Large number of pulses to increase temperature.
• need not be nanosecond pulses!
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**objectives**

- understand flow dynamics and combustion of twin H₂ jets injected into supersonic O₂ crossflow
- investigate the effect of nanosecond plasma on ignition and flame holding in supersonic turbulent flow environment.

**operating conditions**

Mach number: 2.0  
Stagnation enthalpy: 2 MJ/kg  
Static pressure: 16 kPa  
Static temperature: 1250 K  
Momentum ratio (upstream jet): 3.5  
Momentum ratio (downstream jet): 9.0

**model configuration (front view)**

**simulation details**

- 40 million grid points  
- 768 blocks/processors  
- near wall resolution: 32 µm  
- near injector resolution: 60 µm
LES of Plasma Ignition of Transverse $H_2$ jets injected into supersonic $O_2$ cross-flow

Numerical Framework

- Favre average filtered mass, momentum, energy and species equations.
- the conservation equations are solved using a central scheme with artificial dissipation.
- Gradient diffusion assumption based on eddy viscosity hypothesis is used to calculate the sub grid scale transport terms.
- SGS terms for turbulence chemistry interactions are neglected

Inlet conditions

- inlet velocities at the fuel injectors are calculated from the specified jet momentum ratios.
- white noise fluctuations are superimposed on inlet mean velocities to provide turbulent inflow conditions.

Reduced Order Plasma Model

- a narrow cubical region of 6 mm length, 2 mm width, 2mm breadth is assumed to the discharge domain in the present configuration.
- the E/N and the electron density are fixed at 300 Td and $10^{14} \text{ cm}^{-3}$ in the plasma domain.

$H_2/O_2$ plasma combustion chemistry

9 species, 78 reactions

- the kinetics scheme includes $H_2$, $O_2$, $H_2O$, $HO_2$, $H_2O_2$, $O$, $H$, $OH$ and $O(1D)$.
- electron impact dissociation reactions of $H_2$ to give H, and dissociation of $O_2$ to give O and $O(1D)$ are considered.
- the electron based reaction rates are calculated using a pre-generated BOLSIG library as a function of E/N.

![Diagram of Plasma Domain with Upstream $H_2$ injector, Discharge Electrodes, and Plasma Domain at 60°]
Flow Structures

Vorticity Magnitude

Shadowgraph

Density Gradients
Effect of Plasma on O atom Distribution

without plasma discharge, \( t = 85 \mu s \)

with plasma discharge, \( t = 85 \mu s \)

Plasma O atom production
Effect of Plasma on OH Distribution

without plasma discharge

\[ t = 85 \mu s \]

O and OH density around the 2\textsuperscript{nd} jet is distributed in a wider region with the plasma.

This suggests the flame zone is enlarged by more than 50\% with the plasma pulses.
- H$_2$O distributions with plasma clearly shows that the presence of a more intense, larger flame zone with nanosecond plasma radical addition.
- An intense burning zone is observed in a semi circular region upstream of the 2$^\text{nd}$ jet.
Large Eddy Simulation of H\textsubscript{2} Jets injected into supersonic O\textsubscript{2} Crossflow is performed.

Ignition and Flameholding are studied with and without assistance from pulsed, nanosecond discharges.

A reduced order model is employed to describe the plasma discharge development. A 10×2×3 mm\textsuperscript{3} cubic region is assumed to be the plasma domain. E/N and electron density is prescribed beforehand in the plasma region.

Two distinct flames are seen with/without discharge. First weaker flame is found downstream of the 1st H\textsubscript{2} injector. The intermediates/combustion products from this region ignite the fuel coming in from 2nd H\textsubscript{2} injector, and create a larger flame downstream.

Key plasma effect observed is the production of O atoms via electron impact dissociation of O\textsubscript{2} molecules.

O atoms generated by the discharge increase the width of the 1st flame. As a consequence a larger quantity of partial burnt gases convect downstream and enhance the ignition around the 2nd H\textsubscript{2} jet.
THANK YOU
Mixing occurs primarily in the vortical structures upstream and downstream of the jet.

Interaction of bow shock with boundary layer results in the recirculating region upstream of the jet seen at $x/D = 12$. 
- High temperatures seen in the boundary region between the jets is due to combustion heat release
- Elevated temperatures can also be observed along the jet shear layer where cold fuel is ignited when it comes in contact with the hot oxidizer stream.
Low momentum ratio of first jet results in much of injected fuel to spread within the boundary layer region.
Lack of coherent vortex structures along the jet shear layer maybe due to numerical issues.
Mixing occurs in the large counter-rotating vortex structures downstream of the 2nd jet.