Fundamental Mechanisms, Predictive Modeling, and Novel Aerospace Applications of Plasma Assisted Combustion

AFOSR
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Personnel

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  - (Peter Barker)
Miles – Shneider Group
Primary Foci

- **Thrust 1. Experimental studies of nonequilibrium air-fuel plasma kinetics using advanced non-intrusive diagnostics**
  - Task 2: *Laminar Flow Reactor and Nanoparticle Studies at Low to Intermediate Temperatures (Radar REMPI and Filtered Rayleigh Scattering in flames)*
  - Task 7: *Fundamental studies on microwave enhanced combustion at atmospheric and higher pressures (Laser designated microwave driven ignition and microwave enhanced flame propagation)*

- **Thrust 3. Experimental and modeling studies of fundamental nonequilibrium discharge processes**
  - Task 10: *Characterization and Modeling of Nsec Pulsed Plasma Discharges (Modeling and Radar REMPI of nonequilibrium states)*
  - Task 11: *Experimental and Modeling Study of Plasma properties using Radar REMPI (Radar REMPI measurement of electron loss mechanism and rates and local electron number density)*
Preliminary Work

• **Radar REMPI**
  - Atomic oxygen in a flame
  - NO mole fractions in laboratory air to <10 ppb
    - Limited by natural NO concentration in NJ air (~10 ppb)
  - Electron attachment and recombination rate measurements in nitrogen, air and humid air

• **Laser Designated Microwave Driven Ignition**
  - Point ignition with 180 µJ, 200 fsec laser designator plus 50 mJ, 2 µsec microwave pulse
  - Line ignition with 600 µJ, 200 fsec laser designator plus 50 mJ, 2 µsec microwave pulse
  - > 50% ignition kernel growth rate enhancement with triple pulsed microwave
  - Multiple point ignition
Radar REMPI

- Microwave scattering from laser-induced carriers
- Microwave illuminates the ionization spot.
- Microwave scattering is collected.

Microwave/laser measurement configuration. The focused laser creates a small region of ionization and the microwaves are scattered from that region into the microwave detector.
Microwave Experimental Setup: Homodyne and Heterodyne

- Homodyne 100 GHz system.
- 100 GHz probes the plasma.
- The mixer output is proportional with the scattering amplitude, hence electron density.
- Heterodyne 100 and 90 GHz system.
- 100 GHz probes the plasma, the phase shift is measured on the 10 GHz beating signal.
- The quadrature mixer provides the X and Y components, hence we also measure the phase.

Sub-nano-second temporal resolution!
Atomic oxygen in a flame

- 2000K Methane — Air flame
- Atomic line of oxygen in flame is narrow (34 cm\(^{-1}\) limited by laser bandwidth)
- Spectral line in cold air — atomic oxygen via photolysis is 10 times broader: high temperature (50,000K) imposed by intense laser pulse.
- Radar REMPI can distinguish between flame and photolysis atomic oxygen.
Resonant signal from atomic oxygen vs. equivalence ratio

Equilibrium model – 1D chemkin
1+1 Radar REMPI in NO

- Pure NO shows longer lifetime due to electron diffusion.
- In order to measure the recombination rate we suppress diffusion by adding N₂.
- In air we can measure attachment rate.

Princeton University
NO trace Detection
(limited by background ~ 10 ppb NO in air)
Direct measurement of electron attachment in atmospheric air

Previous extrapolated estimate for 850 Torr dry air (78% N₂, 21% O₂, 1% Ar):

\[ \beta = 2 \cdot 10^{-13} \sqrt{\frac{300}{T_e(K)}} \frac{m^3}{s} \]

\[ \nu_a \approx 1.05 \cdot 10^8 \text{ s}^{-1} \]

NO in N₂ - recombination only:

\[ N(t) = \frac{N_0}{1 + \beta N_0 t} \]

gives \( \beta N_0 = 3.2 \times 10^8 \text{ s}^{-1} \)

NO in air - recombination and attachment:

\[ N(t) = \frac{N_0 e^{-\nu_a t}}{1 + \frac{\beta N_0}{\nu_a} \left(1 - e^{-\nu_a t}\right)} \]

gives \( \nu_a = 1.3 \times 10^8 \text{ s}^{-1} \)
Identifying Electron loss mechanism and rate

NO at 0.13 Torr in 1 atm. buffer (170 ppm)

- Air buffer, $dn/dt = -\beta n^2$  
  $\beta n_0 = 9.4 \times 10^7 s^{-1}$

- $N_2$ buffer, $dn/dt = -\beta n^2$  
  $\beta n_0 = 14 \times 10^7 s^{-1}$

In $N_2$: $N(t) = \frac{N_0}{1 + \beta N_0 t}$

Recombination only, not an exponential decay.

Attachment in air:

$N(t) = \frac{N_0 e^{-\nu_a t}}{1 + \frac{\beta N_0}{\nu_a} \left(1 - e^{-\nu_a t}\right)}$

$N(t) \approx \frac{N_0}{1 + \frac{\beta N_0}{\nu_a}} e^{-\nu_a t}$

Close to exponential.

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Testing NO in buffer gases

1+1 Radar REMPI in NO at 226 nm

- $N_2$ increases electron loss via recombination by suppressing diffusion
- Dry air — faster decay due to electron attachment to $O_2$
- Humid air — further increase of losses due to higher attachment rates in water
Microwave Field
- 3GHz
- 30kW peak power
- TE10 Mode
- $\lambda_{\text{guide}} = 11.2\ \text{cm}$
- $E_{\text{field}} \sim 0.1E_{\text{breakdown}}$

Laminar Premixed Flow
- $D_{\text{premixed}} = 1.9\ \text{cm}$
- $U_{\text{exit}} = 70\ \text{cm/s}$
Ps Laser-MW Evolution in Air

Laser spot evolution

Laser + MW evolution
### IGNITION: Kernel Growth Comparison

**Single and Multiple Pulse Microwave**

<table>
<thead>
<tr>
<th>Laser</th>
<th>0.0 ms</th>
<th>1.0 ms</th>
<th>1.1 ms</th>
<th>1.9 ms</th>
<th>2.0 ms</th>
<th>2.1 ms</th>
<th>2.9 ms</th>
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<tbody>
<tr>
<td>Micro-wave Pulse 1</td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
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<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
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<tr>
<td>Single Pulse Ignition</td>
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<td>Micro-wave Pulse 1</td>
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<tr>
<td>Single Pulse Ignition</td>
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<tr>
<td>Micro-wave Pulse 1</td>
<td><img src="image15.png" alt="Image" /></td>
<td><img src="image16.png" alt="Image" /></td>
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<td><img src="image18.png" alt="Image" /></td>
<td><img src="image19.png" alt="Image" /></td>
<td><img src="image20.png" alt="Image" /></td>
<td><img src="image21.png" alt="Image" /></td>
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<tr>
<td>Triple Pulse 1 msec intervals</td>
<td></td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

**Note:**
- Laser pulse intervals are 1.0 ms, 1.1 ms, 1.9 ms, 2.0 ms, 2.1 ms, and 2.9 ms.
- Images show kernel growth comparison for single and multiple pulse microwave ignition.
- Single pulse ignition shows growth at 6 mm.
- Triple pulse ignition shows growth at 6 mm.

*Princeton University*
Multi-point ignition

- Two 7mJ seed laser spots
- 75 mJ MW pulse
- $\phi = 0.7; \ U_{\text{exit}} = 70 \text{ cm/s}$
- 3 ms after initial seed laser pulse
- Flame kernel indicates ignition
200 Femtosecond Seed – 180 μJ

10 us 100 us 500 us 1000 us

6 mm
200 Femtosecond Seed – 600 μJ

10 us

100 us

500 us

1000 us

6 mm
Ignition of Methane/Air Mixtures

- **Seed ionization pulse**
  7mJ; 200 ps, 780 nm
- **MW heating pulse**
  50mJ; 2 μs, 3GHz

### Observed Minimum Seed Laser Energies

<table>
<thead>
<tr>
<th>$\lambda_{\text{seed}}$ [nm]</th>
<th>$\varphi$</th>
<th>$f$ [m]</th>
<th>$E_{\text{laser}}$ [mJ]</th>
<th>$E_{\text{MW}}$ [mJ]</th>
</tr>
</thead>
<tbody>
<tr>
<td>800 (200 fs)</td>
<td>0.8</td>
<td>0.06</td>
<td>0.2</td>
<td>50</td>
</tr>
<tr>
<td>780</td>
<td>0.8</td>
<td>0.06</td>
<td>3</td>
<td>50</td>
</tr>
<tr>
<td>780</td>
<td>0.8</td>
<td>0.10</td>
<td>7</td>
<td>50</td>
</tr>
<tr>
<td>780</td>
<td>0.7</td>
<td>0.10</td>
<td>7, 7</td>
<td>75</td>
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<tr>
<td>390</td>
<td>0.8</td>
<td>0.10</td>
<td>1.5</td>
<td>50</td>
</tr>
</tbody>
</table>
Fundamental Mechanisms, Predictive Modeling, and Novel Aerospace Applications of Plasma Assisted Combustion

Yiguang Ju

AFOSR MURI Kick off meeting

The Ohio State University
Nov 4, 2009

Team members:
Wenting Sun, Sanghee Won, Mruthunjaya Uddi

Collaborators:
Interactional: Fei Qi, University of Science and Tech. China
AFRL collaborators: Campbell Carter, Timothy Ombrello, Skip Williams
Ju’s Group Primary Research Focus

Thrust 1. The effects of kinetic and transport of plasma assisted ignition
- Task 1: Experimental measurements of minimum ignition energies using a spherical bomb with different electrode geometries
- Task 2: Experimental measurements of ignition/extinction limits by using counterflow flames

Thrust 2. Intermediate Species Measurements at Elevated Pressures by Using a Plasma Assisted Jet Stirred Reactor with Molecular Beam Sampling
- Task 1: Development of plasma assisted a jet stirred reactor
- Task 2: Measurements of intermediate species of fuel oxidation

Thrust 3. Mechanism Reduction and Dynamic Multi-time Scale Modeling of Detailed Plasma-Flame Chemistry
- Task 1: Development of dynamic multi-timescale modeling
- Task 2: Simulations of unsteady ignition and extinction of plasma discharge with detailed kinetic mechanisms
Research Task Description, Methods, and Preliminary Results
Thrust 1. The effects of kinetic and transport of plasma assisted ignition

- Task 1: Experimental measurements of minimum ignition energies using a spherical bomb with different electrode geometries.
Experimental methods
Thrust 1. The effects of kinetic and transport of plasma assisted ignition

- Task 2: Experimental measurements of ignition/extinction limits by using counterflow flame w/wo non-equilibrium plasma discharge
Thrust 1. The effects of kinetic and transport of plasma assisted ignition

- Task 2: Experimental measurements of ignition/extinction limits by using counterflow flame w/wo non-equilibrium plasma discharge

LIF: OH, NO, CH2O
TALIF: O, H

Nanosecond pulser: Carter
Thrust 2: High pressure JSR and MBMS experimental methods of intermediate species measurements

High pressure, high temperature chamber

Preheated air

Fuel

Mixing

DBD discharge

Jet stirred reactor

1\textsuperscript{st} Turbo pump

10^{-4}\textsuperscript{Torr}

Quartz nozzle

0.1-5\textsuperscript{atm}

$10^{-6}$ Torr

2\textsuperscript{nd} Turbo pump

Mass analyzer

Charged ion separation

Laser beam

MBMS analysis
Three stage molecular beaming sample for high pressure
Equipment installation (EFRC program)

Comstock Time of flight (TOF) MB system: RTOF210: Mass resolution up to 5000

Li and Qi, ACR, 2009
Thrust 3. Mechanism Reduction and Dynamic Multi-time Scale Modeling of Detailed Plasma-Flame Chemistry

- Task 1: Development of dynamic multi-timescale modeling approach
- Task 2: Simulations of unsteady ignition and extinction of plasma discharge with detailed kinetic mechanisms

Total computation time \( \propto K^3 \)

\( t_{\text{Chem}} \approx 80\% t_{\text{total}} \)

The Basic Idea of Multi-Time Scale Method: timescale changes!

\[ Y_k = K_k e^{\frac{t}{\tau_k}} \]

Diagram of multi time scale scheme

\( \Delta t_F \) is the time step of the fastest group, \( \Delta t_M \) is the time step of the medial group, and \( \Delta t_S \) is the time step of the slowest group.
Validation by homogeneous ignition

n-decane/Air 121 species (M. Chaos, IJCK, 2007)

Temperature and species profiles

Ignition delay time for n-decane-air
## Computation efficiency vs. Mechanism size

<table>
<thead>
<tr>
<th>No.</th>
<th>Mechanism</th>
<th>Base Time Step(s)</th>
<th>Initial Pressure (atm)</th>
<th>Initial Temperature (K)</th>
<th>RTOL</th>
<th>ATOL</th>
<th>CPU Time(s)</th>
<th>CPU Time Saving</th>
</tr>
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<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>VODE</td>
<td>MTS</td>
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<tr>
<td>a1</td>
<td>H₂</td>
<td>1.0E-6</td>
<td>1</td>
<td>1200</td>
<td>1.0E-4</td>
<td>1.0E-13</td>
<td>0.28</td>
<td>0.13</td>
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<tr>
<td>a2</td>
<td>H₂</td>
<td>1.0E-7</td>
<td>1</td>
<td>1200</td>
<td>1.0E-4</td>
<td>1.0E-13</td>
<td>2.58</td>
<td>1.31</td>
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<tr>
<td>a3</td>
<td>H₂</td>
<td>1.0E-8</td>
<td>1</td>
<td>1200</td>
<td>1.0E-4</td>
<td>1.0E-13</td>
<td>24.9</td>
<td>7.56</td>
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<tr>
<td>a4</td>
<td>H₂</td>
<td>1.0E-9</td>
<td>1</td>
<td>1200</td>
<td>1.0E-4</td>
<td>1.0E-13</td>
<td>260</td>
<td>18.4</td>
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<tr>
<td>b1</td>
<td>CH₄</td>
<td>1.0E-6</td>
<td>1</td>
<td>1400</td>
<td>1.0E-4</td>
<td>1.0E-13</td>
<td>123</td>
<td>25</td>
</tr>
<tr>
<td>b2</td>
<td>CH₄</td>
<td>1.0E-7</td>
<td>1</td>
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<td>1.0E-4</td>
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<td>1269</td>
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</tr>
<tr>
<td>b3</td>
<td>CH₄</td>
<td>1.0E-8</td>
<td>1</td>
<td>1400</td>
<td>1.0E-4</td>
<td>1.0E-13</td>
<td>14639</td>
<td>1029</td>
</tr>
<tr>
<td>c1</td>
<td>C₁₀H₂₂</td>
<td>1.0E-6</td>
<td>1</td>
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<tr>
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<td>125</td>
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<td>c3</td>
<td>C₁₀H₂₂</td>
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<td>1</td>
<td>1400</td>
<td>1.0E-4</td>
<td>1.0E-13</td>
<td>7609</td>
<td>1049</td>
</tr>
</tbody>
</table>
A path flux analysis method for model reduction

$T_0=1200 \text{ K}$

The diagrams show the number of species in the skeletal mechanism at 1 atm and 20 atm, with lines representing different methods: detail, DRG, and PFA. The x-axis represents the number of species, and the y-axis represents the path flux $\tau_{sg}$.
Modeling of flame front trajectories of spherical propagating flames using MTS