High-Fidelity, Computational Modeling of Non-Equilibrium Discharges for Combustion Applications

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# High-Fidelity, Computational Modeling of Non-Equilibrium Discharges for Combustion Applications

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Standard Form 298 (Rev. 8-98)
Prepared by ANSI Bal Z39-18
Motivation

- There is significant evidence to show cold (non-equilibrium) plasma discharges have distinct advantages as combustion ignition / stabilization sources.

- At high pressures relevant to applications, cold plasmas generated by nanosecond pulsing that result in streamer like constricted discharges.

- Significant experimental difficulty in probing the structure and properties of streamers (small length scales, short time scales).

- High-fidelity computational modeling can play an important role in describing physics and chemistry in these discharges.
Cold (non-equilibrium) plasma discharge in plasma parameter space

- **Thermal plasmas (“Hot”)**
  - Most electrical energy goes into gas heating (~10,000 K)
  - All species can be characterized by the same temperature (in thermal equilibrium)

- **Non-thermal plasmas (“Cold”)**
  - Electrical power is absorbed by electrons which in turn produce radicals and ions.
  - Electrons have high temperature (~10,000 K and more)
  - Ions and Neutrals remain at lower temperature (~300-1000 K)
  - Not in thermal equilibrium (non-equilibrium plasma)

From: NRL plasma formulary
Characteristic molecular energies and electron energy loss pathways

- Rotational
- Vibration
- Dissociation
- Electronic excit.
- Ionization

$N_2:O_2:CH_4 = 8:2:1$

- Reduced electric field $E/N$ is an important parameter for plasmas ($1 \text{Td} = 10^{-17} \text{V cm}^2$)
- Note: Breakdown threshold $\sim 100 \text{Td}$ (e.g. 120 Td for air)

Ref: Starikovskiy and Alexsandrov, Prog. Energy Comb. Sci., 2013
In principle can maintain non-equilibrium by high discharge voltages (i.e. high E/n) 
   (Rate of energy gain by electrons) > (Rate of energy loss to gas heating)

However at high pressures non-equilibrium discharges are susceptible to Glow-to-Arc Transitions (GAT) 
   Discharge instabilities cause gas temperature to rise rapidly

GAT has time-scale of ~100’s ns

Can sustain non-equilibrium, by repeated pulsing on nanosecond time scales 
   First demonstration in early 2000 [Kruger et al. 2002]

Ref : Starikovskiy and Alexsandrov, Prog. Energy Comb. Sci., 2013
Nanosecond pulsing produces enhanced tail in the electron Energy Dist. Func. (EEDF)

- Power budget for nanosecond pulsed discharge is much lower than a DC discharge

Computational challenges for plasma ignition and flame spread prediction

- Multiple physical and chemical processes with vast disparity in time scales
- Complex chemistries with high degree of uncertainty
Coaxial electrode cold plasma igniter for automotive combustion applications

From: Shiraishi et al. SAE Paper 2011-01-0660
Single electrode (Corona) excitation for automotive ignition applications

RF : Freq. ~10 MHz
Voltage ~100kV

Nanosecond pulsed ignition of supersonic combustion

- 7 kV unipolar pulses
- 20 ns pulse width
- 50 kHz pulse freq.

Approach

- High fidelity multi-dimensional computational simulations of the plasma processes relevant to plasma assisted combustion
  - Self-consistent plasma
  - Multi-species
  - Multi-temperature
  - Gas-phase kinetics
  - Surface kinetics

- Plasma model + Gas dynamic model
  - Two-way gas dynamic / plasma coupling
Plasma model

- Species continuity
  \[ \frac{\partial n_k}{\partial t} + \nabla \cdot \vec{f}_k = \dot{G}_k \quad k = 1, \ldots, K_g (k \neq k_b) \]

- Ideal Gas Law
  \[ p = \sum_k n_k k_B T_k \]

- Drift-Diffusion approximation with bulk convection
  \[ \vec{f}_k \equiv n_k \vec{u}_k = -\mu_k n_k \nabla \phi - D_k \nabla n_k + n_k \vec{V} \]

- Poisson’s equation
  \[ \nabla^2 \phi = -\frac{e}{\varepsilon_0} \sum_k Z_k n_k \]

- Electron Energy Equation
  \[ \frac{\partial e_e}{\partial t} + \nabla \cdot \left( \left( \frac{5}{3} \mu_e \vec{E} + \vec{V} \right) e_e - \kappa_e \nabla e_e \right) = \left( +e \vec{f}_e \cdot \nabla \phi \right) - \frac{3}{2} k_B n_e \frac{2m_e}{m_{kb}} (T_e - T_g) \vec{v}_{k_b} + e \sum_i \Delta E_i r_i \]
Plasma model

- Gas Energy Equation
  - Ions and Neutrals have temperature $T_g$
  - $T_g$ assumed constant, or obtained by solving Gas Energy

\[
\frac{\partial}{\partial t} \sum_{k \in H} n_k h_k + \nabla \cdot \left( \sum_{k \in H} \tilde{f}_k h_k - \sum_{k \in H} \kappa_k \nabla T_g \right) = \eta_{Th} \left( -e \sum_{k \in H} \tilde{f}_k \cdot \nabla \phi \right) + \frac{3}{2} k_B n_e \frac{2m_e}{m_{kB}} (T_e - T_g) \tilde{v}_{kB} - e \sum_i \Delta E_i^g \nabla_i
\]

- If plasma model is solved with flow model, $T_g$ is obtained from Navier-Stokes solver and only source terms are calculated by Gas Energy module
Flow model (Compressible Navier-Stokes)

\[
\iiint \frac{\partial \mathbf{U}}{\partial t} dV + \iiint \mathbf{F}_{\text{inviscid}} \cdot \hat{n} dS = \iiint \mathbf{F}_{\text{viscous}} \cdot \hat{n} dS + \iiint \mathbf{S} dV
\]

\[
\mathbf{U} = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho e_t 
\end{bmatrix}, \quad \mathbf{F}_{\text{inviscid}} = \begin{bmatrix}
\rho u \\
\rho u^2 + p \\
\rho v u \\
(\rho e_t + p) u 
\end{bmatrix} \hat{i} + \begin{bmatrix}
\rho v \\
\rho v u \\
\rho v^2 + p \\
(\rho e_t + p) v 
\end{bmatrix} \hat{j}
\]

\[
\mathbf{F}_{\text{viscous}} = \begin{bmatrix}
0 \\
\tau_{xx} \\
\tau_{xy} \\
u \tau_{xx} + v \tau_{xy} - \dot{q}_x 
\end{bmatrix} \hat{i} + \begin{bmatrix}
0 \\
\tau_{yx} \\
\tau_{yy} \\
u \tau_{yx} + v \tau_{yy} - \dot{q}_y 
\end{bmatrix} \hat{j}
\]

\[
\mathbf{S} = \begin{bmatrix}
0 \\
\mathbf{f}_x \\
\mathbf{f}_y \\
S + \mathbf{f}_{ES} \cdot \mathbf{V}
\end{bmatrix}
\]
Photoionization (3-term Helmholtz equation model)

\[ \text{UV radiation} \quad (98-102.5 \text{ nm} / 12.1-12.65 \text{ eV}) \]

\[ e + N_2 \rightarrow e + N_2 + hv \]

\[ O_2 + hv \rightarrow e + O_2^+ \]

Integral Model (Zheleznyak et al 1982):

\[ S_{ph}(\vec{r}) = \iiint \frac{I(\vec{r}^i)g(R)}{4\pi R^2} dV \]

Emission function:

\[ I(\vec{r}) = \frac{P_q}{P + P_q} \xi S_i(\vec{r}) \]

Absorption function:

\[ g(R) = \frac{\exp^{-\chi_{\text{min}} P_{O_2} R} - \exp^{-\chi_{\text{max}} P_{O_2} R}}{P_{O_2} R \ln(\chi_{\text{max}}/\chi_{\text{min}})} \]

3-term expansion approach:

\[ \nabla^2 S_{ph}^j - (\lambda_j P_{O_2})^2 S_{ph}^j = -A_j P_{O_2}^2 I(\vec{r}) \quad (j = 1, 2, 3) \]

\[ S_{ph}(\vec{r}) = S_{ph}^1 + S_{ph}^2 + S_{ph}^3 \]

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<th>( A_j ) (cm(^{-1}) Torr(^{-1}))</th>
<th>( \lambda_j ) (cm(^{-1}) Torr(^{-1}))</th>
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<tr>
<td>( S_{ph}^2 )</td>
<td>0.0346</td>
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<tr>
<td>( S_{ph}^3 )</td>
<td>0.3059</td>
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  + Bourdon A, Pasko NP, Liu NY, Celestin S, Segue P and Maroude E 2007 Plasma Sources Sci. Technol. 16 656
Mathematical approach to coupling plasma and flow physics

Electrostatic Force Term (No Magnetic field):

\[ \vec{f}_{ES} = e \sum_k Z_k n_k \vec{E} \]

Gas Energy Source Term

\[ S_{T_g} = \eta_{Th} \left( -e \sum_{k \in H} \vec{f}_k \cdot \vec{\nabla} \phi \right) + \frac{3}{2} k_B n_e \frac{2 m_e}{m_{k_b}} (T_e - T_g) \vec{v}_{k,b} - e \sum_i \Delta E^g_i r_i \]
Numerical approach

- 1D, 2D, 3D
- Fully unstructured, hybrid mesh
- Finite-volume spatial discretization, backward Euler time discretization (formally 1st order in space and time)
- Flow model:
  - AUSM family of spatial discretization (2nd order accuracy through gradient reconstruction)
  - 4th order RK time integration
- Domain decomposition parallel enabled
Plasma chemistry mechanism

- Methane-air plasma chemistry mechanism
  - Species and pathways relevant to plasma time scale (~10’s ns)

- 26 Species:
  E, O, N₂, O₂, H, N₂⁺, O₂⁺, N₄⁺, O₄⁺, O₂⁺N₂, O₂⁻, O⁻, O₂(a1), O₂(b1), O₂⁺, N₂(A), N₂(B), N₂C, N₂(a1), CH₄, CH₃, CH₂, CH₄⁺, CH₃⁺, CH₂⁻, H⁻

- 85 Reactions:
  1) electron impact, 2) ion-ion, 3) ion-neutral, 4) neutral-neutral
## Methane-air plasma mechanism

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<th>Rxn</th>
<th>Reaction</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>Activation energy (eV)</th>
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<td></td>
<td>BOLSIG+</td>
<td></td>
<td>4.5</td>
<td>(22)</td>
</tr>
</tbody>
</table>
# Methane-air plasma mechanism

<table>
<thead>
<tr>
<th>Rxn</th>
<th>Reaction</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>Activation energy (eV)</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>C84</td>
<td>N$_2^+$ + N$_2$ + M $\rightarrow$ N$_4^+$ + M</td>
<td>5.0e-41</td>
<td>0</td>
<td>0</td>
<td>1.0</td>
<td>(24)</td>
</tr>
<tr>
<td>C85</td>
<td>N$_2^+$ + O$_2$ $\rightarrow$ O$_2^+$ + 2N$_2$</td>
<td>2.5e-16</td>
<td>0</td>
<td>0</td>
<td>-3.51</td>
<td>(24)</td>
</tr>
<tr>
<td>C86</td>
<td>N$_2^+$ + O$_2$ $\rightarrow$ O$_2^+$ + N$_2$</td>
<td>1.04e-15</td>
<td>-0.5</td>
<td>0</td>
<td>-3.51</td>
<td>(24)</td>
</tr>
<tr>
<td>C87</td>
<td>O$_2$ + 2N$_2$ $\rightarrow$ O$_2$+N$_2$ + N$_2$</td>
<td>8.1e-30</td>
<td>-2.0</td>
<td>0</td>
<td>-</td>
<td>(24)</td>
</tr>
<tr>
<td>C88</td>
<td>O$_2$+N$_2$ + N$_2$ $\rightarrow$ O$_2^+$ + 2N$_2$</td>
<td>14.8</td>
<td>-2.0</td>
<td>0</td>
<td>2357</td>
<td>(24)</td>
</tr>
<tr>
<td>C89</td>
<td>O$_2$+N$_2$ + O$_2$ $\rightarrow$ O$_2^+$ + N$_2$</td>
<td>1.0e-15</td>
<td>0</td>
<td>0</td>
<td>-</td>
<td>(24)</td>
</tr>
<tr>
<td>C90</td>
<td>O$_2$ + O$_2$ + M $\rightarrow$ O$_4^+$ + M</td>
<td>2.03e-34</td>
<td>-3.2</td>
<td>0</td>
<td>-</td>
<td>(24)</td>
</tr>
<tr>
<td>C91</td>
<td>E + 2O$_2$ $\rightarrow$ O$_2$ + O$_2$</td>
<td>6.0e-39</td>
<td>-1.0</td>
<td>0</td>
<td>-0.43</td>
<td>(24)</td>
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<tr>
<td>C92</td>
<td>O$_2^+$ + O$_2^+$ $\rightarrow$ 3O$_2$</td>
<td>1.0e-13</td>
<td>0</td>
<td>0</td>
<td>-11.64</td>
<td>(24)</td>
</tr>
<tr>
<td>C93</td>
<td>O$_2^+$ + O$_2^+$ + M $\rightarrow$ 3O$_2$ + M</td>
<td>3.12e-31</td>
<td>-2.5</td>
<td>0</td>
<td>-11.64</td>
<td>(24)</td>
</tr>
<tr>
<td>C94</td>
<td>O$_2$ + O$_2^+$ + M $\rightarrow$ 2O$_2$ + M</td>
<td>3.12e-31</td>
<td>-2.5</td>
<td>0</td>
<td>-11.64</td>
<td>(24)</td>
</tr>
<tr>
<td>C95</td>
<td>O + O$_2^+$ $\rightarrow$ O + O$_2$</td>
<td>3.464e-12</td>
<td>-0.5</td>
<td>0</td>
<td>-10.61</td>
<td>(24)</td>
</tr>
<tr>
<td>C96</td>
<td>N$_2$A + O$_2$ $\rightarrow$ N$_2$ + 2O</td>
<td>1.7e-18</td>
<td>0</td>
<td>0</td>
<td>-1.05</td>
<td>(25)</td>
</tr>
<tr>
<td>C97</td>
<td>N$_2$A + O$_2$ $\rightarrow$ N$_2$ + O$_2$(b1)</td>
<td>7.5e-19</td>
<td>0</td>
<td>0</td>
<td>-4.54</td>
<td>(25)</td>
</tr>
<tr>
<td>C98</td>
<td>N$_2$A + N$_2$(A) $\rightarrow$ N$_2$ + N$_2$(B)</td>
<td>7.7e-17</td>
<td>0</td>
<td>0</td>
<td>-4.99</td>
<td>(25)</td>
</tr>
<tr>
<td>C99</td>
<td>N$_2$A + N$_2$(A) $\rightarrow$ N$_2$ + N$_2$(C)</td>
<td>1.6e-16</td>
<td>0</td>
<td>0</td>
<td>-1.31</td>
<td>(25)</td>
</tr>
<tr>
<td>C100</td>
<td>N$_2$(A) + N$_2$ $\rightarrow$ N$_2$ + N$_2$(B)</td>
<td>1.0e-16</td>
<td>0</td>
<td>1500</td>
<td>-0.32</td>
<td>(25)</td>
</tr>
<tr>
<td>C101</td>
<td>N$_2$(A) + O $\rightarrow$ N$_2$ + O</td>
<td>3.0e-17</td>
<td>0</td>
<td>0</td>
<td>-6.17</td>
<td>(25)</td>
</tr>
<tr>
<td>C102</td>
<td>N$_2$(B) + O$_2$ $\rightarrow$ N$_2$ + 2O</td>
<td>3.0e-16</td>
<td>0</td>
<td>0</td>
<td>-2.23</td>
<td>(25)</td>
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<tr>
<td>C103</td>
<td>N$_2$(B) + N$_2$ $\rightarrow$ N$_2$(A) + N$_2$</td>
<td>1.0e-17</td>
<td>0</td>
<td>0</td>
<td>-1.18</td>
<td>(25)</td>
</tr>
<tr>
<td>C104</td>
<td>N$_2$(a1) + O$_2$ $\rightarrow$ N$_2$ + 2O</td>
<td>2.8e-17</td>
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<td>0</td>
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<tr>
<td>C105</td>
<td>N$_2$(a1) + N$_2$ $\rightarrow$ N$_2$ + N$_2$</td>
<td>2.0e-19</td>
<td>0</td>
<td>0</td>
<td>-8.4</td>
<td>(25)</td>
</tr>
<tr>
<td>C106</td>
<td>N$_2$(C) + O$_2$ $\rightarrow$ N$_2$ + 2O</td>
<td>3.0e-16</td>
<td>0</td>
<td>0</td>
<td>-5.91</td>
<td>(25)</td>
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<tr>
<td>C107</td>
<td>N$_2$(C) + N$_2$ $\rightarrow$ N$_2$(a1) + N$_2$</td>
<td>1.0e-17</td>
<td>0</td>
<td>0</td>
<td>-2.63</td>
<td>(25)</td>
</tr>
<tr>
<td>C108</td>
<td>N$_2$(C) $\rightarrow$ N$_2$(B) + hv (photon)</td>
<td>3.0</td>
<td>0</td>
<td>0</td>
<td>-</td>
<td>(25)</td>
</tr>
<tr>
<td>C109</td>
<td>N$_2$(A) + CH$_4$ $\rightarrow$ N$_2$ + CH$_4$</td>
<td>3.0e-21</td>
<td>0</td>
<td>0</td>
<td>-6.17</td>
<td>(25)</td>
</tr>
<tr>
<td>C110</td>
<td>N$_2$(B) + CH$_4$ $\rightarrow$ N$_2$(A) + CH$_4$</td>
<td>2.85e-16</td>
<td>0</td>
<td>0</td>
<td>-1.08</td>
<td>(25)</td>
</tr>
<tr>
<td>C111</td>
<td>N$_2$(B) + CH$_4$ $\rightarrow$ N$_2$ + CH$_3$ + H</td>
<td>1.5e-17</td>
<td>0</td>
<td>0</td>
<td>3.15</td>
<td>(25)</td>
</tr>
<tr>
<td>C112</td>
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<td>3.0e-16</td>
<td>0</td>
<td>0</td>
<td>2.1</td>
<td>(25)</td>
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<td>C113</td>
<td>N$_2$(C) + CH$_4$ $\rightarrow$ N$_2$ + CH$_3$ + H</td>
<td>3.0e-16</td>
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<td>(25)</td>
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<tr>
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<td>O$_2^+$ + CH$_4$ $\rightarrow$ O$_2$ + CH$_3$ + H</td>
<td>3.0e-21</td>
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<td>-</td>
<td>(25)</td>
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<tr>
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<td>1.86e-19</td>
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<td>(25)</td>
</tr>
<tr>
<td>C116</td>
<td>O$_2^+$ + O$_2$ $\rightarrow$ O$_2$(b1) + O$_2$</td>
<td>8.1e-20</td>
<td>0</td>
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<td>(25)</td>
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<td>C117</td>
<td>O$_2^+$ + O$_2$ $\rightarrow$ O$_2$ + O$_2$</td>
<td>2.3e-20</td>
<td>0</td>
<td>0</td>
<td>-4.5</td>
<td>(25)</td>
</tr>
<tr>
<td>C118</td>
<td>O$_2^+$ + O $\rightarrow$ O$_2$ + O</td>
<td>5.0e-18</td>
<td>0</td>
<td>0</td>
<td>-4.5</td>
<td>(25)</td>
</tr>
<tr>
<td>C119</td>
<td>O$_2^+$ + O $\rightarrow$ O$_2$(a1) + O</td>
<td>2.7e-18</td>
<td>0</td>
<td>0</td>
<td>-3.52</td>
<td>(25)</td>
</tr>
<tr>
<td>C120</td>
<td>O$_2^+$ + O $\rightarrow$ O$_2$(b1) + O</td>
<td>1.35e-18</td>
<td>0</td>
<td>0</td>
<td>-2.87</td>
<td>(25)</td>
</tr>
<tr>
<td>C121</td>
<td>N$_2^+$ + CH$_4$ $\rightarrow$ N$_2$ + CH$_3$ + H</td>
<td>1.3e-15</td>
<td>0</td>
<td>0</td>
<td>-</td>
<td>(25)</td>
</tr>
<tr>
<td>C122</td>
<td>CH$_4^+$ + O$_2$ $\rightarrow$ CH$_4$ + O$_2^+$</td>
<td>5.0e-16</td>
<td>0</td>
<td>0</td>
<td>-</td>
<td>(25)</td>
</tr>
<tr>
<td>C123</td>
<td>E + CH$_4^+$ $\rightarrow$ CH$_4$ + H</td>
<td>2.95e-12</td>
<td>0</td>
<td>0</td>
<td>-</td>
<td>(25)</td>
</tr>
<tr>
<td>C124</td>
<td>E + CH$_4^+$ $\rightarrow$ CH$_4$ + 2H</td>
<td>2.95e-12</td>
<td>-0.5</td>
<td>0</td>
<td>-</td>
<td>(25)</td>
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<td>C125</td>
<td>E + CH$_3^+$ $\rightarrow$ CH$_2$ + H</td>
<td>6.06e-12</td>
<td>-0.5</td>
<td>0</td>
<td>-</td>
<td>(25)</td>
</tr>
</tbody>
</table>

**Cluster ion formation**

**Charge exchange**

**Attachment**

**Ion-ion recombination**

**Neutral reactions**

**Dissociative charge exchange**

**Dissociative recombination**
Electron impact reaction rate coefficient computed using off-line Boltzmann solver

- Bolsig+ (Hagelaar and Pitchford, 2005)

\[
\begin{align*}
k &= k(E/N) \\
T_e &= T_e(E/N)
\end{align*}
\]

\[k = k(T_e)\] (Recovers non-local aspects of electron energy transport)

Coaxial electrode Nanosecond Pulsed Plasma (NSP)

Reference:
Coaxial electrode NSP discharge

- Describe initial plasma kernel formation stage
  - ~ 10's ns of physical time

- Experimental observations
  - Unbranched streamers propagate from inner high-voltage electrode to outer ground electrode
  - Streamer dia (sub-mm)
  - Brighter discharge near inner electrode
  - Flame spreads from inner electrode to outer ground electrode


Coaxial electrode NSP discharge simulation conditions

- Simulation conditions:
  - 10 atmospheres
  - 700 K fixed gas temperature
  - 40 kV applied voltage ($E/n \sim 143$ Td)
  - Lean A/F ratio (40:1 air/methane)
Coaxial electrode NSP plasma simulation domain

- Simulation domain: sector of circle
  - 20 deg. sector angle
  - Characteristic size for single streamer propagation
  - Roughness element on inner electrode to pin location of streamer

60,000 cells

24 processor partition
Sensitivity to roughness element configuration

Conditions: $P=10 \text{ atm}$, $T_{\text{gas}}=700 \text{ K}$, 40 kV, 40:1 A/F ratio (lean)

- Verified insensitivity to roughness element configuration
- Verified characteristic sector angle for single streamer
Time evolution of electron density and temperature for coaxial electrode NSP

Conditions: \( P=10 \ \text{atm}, \ T_{\text{gas}}=700 \ \text{K}, \ 40 \ \text{kV}, \ 40:1 \ \text{A/F ratio (lean)} \)

- 2 ns induction time (defined: time to reach threshold of \( 10^{19} \ \text{m}^{-3} \))
- Streamers bridge electrode gap in about 10 ns
- \( N_e(\text{peak}) \sim 10^{21} \ \text{m}^{-3} , \ T_e(\text{head}) \sim 4\text{eV}, \ T_e(\text{body}) \sim 1\text{eV} \)
- Secondary streamer (electron attachment luminosity? Self-sustaining?)
Reduced electric field profiles along axis of coaxial electrode NSP

Conditions: \( P=10 \text{ atm}, T_{\text{gas}}=700 \text{ K}, 40 \text{ kV}, 40:1 \text{ A/F ratio (lean)} \)

- Recall breakdown \( E/n \) about 120 Td (for air)
- Head of streamer has significant over-voltages (\( \sim 500 \text{ Td} \)) \( \rightarrow \) high \( T_e \)
- Body of streamer has no sustaining E-field (\( E/n \sim 10 \text{ Td} \)) \( \rightarrow \) low \( T_e \)
- Secondary streamer formation at end of pulse with \( E/n \sim 200 \text{ Td} \)
Species yields for coaxial electrode NSP (volume-averaged at 9.5 ns)

Conditions: $P=10$ atm, $T_{\text{gas}}=700$ K, 40 kV, 40:1 A/F ratio (lean)

- Charged species ($\sim 10^{20}$ m$^{-3}$)
- Dominant radical O ($\sim 10^{22}$ m$^{-3}$)
Time evolution of radical densities and for coaxial electrode NSP

Conditions: $P=10$ atm, $T_{gas}=700$ K, $40$ kV, $40:1$ A/F ratio (lean)

- Secondary streamer has significant impact on overall radical yield
O radical distribution in coaxial electrode NSP at end of transient

- Significant non-uniformity in O radical distribution
  - $\sim 10^{23} \text{ m}^{-3}$ at inner electrode
  - Consequence of secondary streamer

- O radical concentration is evidence for experimentally observed flame spread profile?
Corona ignition – point to plane at infinity

Reference:
Corona igniter

- Simulation conditions:
  - 10 atmospheres
  - 700 K fixed gas temperature
  - 115 kV applied voltage
  - Lean A/F ratio (40:1 air/methane)
Transient evolution of electron density

Conditions:  P=10 atm, T_{gas}=700 K,  115 kV, 40:1 A/F ratio (lean)

- Peak electron densities in streamer head (~10^{21} m^{-3})
- Electron attachment in body
Reduced electric field profiles along axis of coaxial electrode NSP

Conditions:  \( P=10 \) atm, \( T_{\text{gas}}=700 \) K, 115 kV, 40:1 A/F ratio (lean)

- Recall breakdown \( E/n \) about 120 Td (for air)
- Head of streamer has significant over-voltages (~ 500 Td) \( \rightarrow \) high \( T_e \)
- Body of streamer has no sustaining E-field (\( E/n \sim 10 \) Td) \( \rightarrow \) low \( T_e \)
- No secondary streamer formation
Species yields for single electrode geometry (volume-averaged at 30 ns)

Conditions: $P=10$ atm, $T_{\text{gas}}=700$ K, 115 kV, 40:1 A/F ratio (lean)

- Charged species ($\sim 10^{20}$ m$^{-3}$)
- Dominant radical O ($\sim 10^{22}$ m$^{-3}$)
Comparison of species yields for Corona and Coaxial electrode geometries
Time evolution of radical densities and for coaxial electrode NSP

Baseline Conditions: $P=10$ atm, $T_{gas}=700$ K, 40 kV, 40:1 A/F ratio (lean)

O radical density at 30 ns
Corona RF excitation
Problem statement for Corona RF excited plasma igniter

Conditions: $P=10$ atm, $T_{\text{gas}}=700$ K, 40:1 A/F ratio (lean),
$+90\text{kV} \rightarrow -80\text{kV} \rightarrow +80\text{kV}$ pulse train (10 ns each)

RF excitation:
Freq. $\sim 10$ MHz
Voltage $\sim 100\text{kV}$

Air dielectric (10,000 cells)
Plasma (32680 cells)
Simulation strategy for multi-pulse excitation

Actual and Assumed Waveforms for a 10 MHz pulse
(check attached spreadsheet)
Discharge structure dependence on excitation polarity

- Thin streamers for positive excitation with low over-voltages
- Voluminous glow-like discharge for negative excitation with low over-voltages
- Streamers for high over-voltages (positive and negative excitation)

Electron density evolution for excitation pulse train

Conditions: P=10 atm, T_{gas}=700 K, 40:1 A/F ratio (lean), +90kV → -80kV → +80kV pulse train (10 ns each)
Radical density evolution at end of each pulse

**O radical density**

- End of 1st Pulse
- End of 2nd Pulse
- End of 3rd Pulse

**O₃ density**

- End of 1st Pulse
- End of 2nd Pulse
- End of 3rd Pulse
Nanosecond pulsed ignition of supersonic combustion

Reference:
Nanosecond pulsed ignition of supersonic combustion

- 7 kV unipolar pulses
- 20 ns pulse width
- 50 kHz pulse freq.

Chemical reaction mechanism

H₂-O₂ sub-mechanism:

16 Species
  e, O⁺, O₂⁺, O₄⁺, O⁻, O₂⁻, H⁺, H₂⁺, O, H, OH, O₂, H₂, O(1D), O₂(a¹Δ₉), O₂(b¹Σ₉⁺)

Assumptions:

- Rotational energy immediately heats bulk gas
- Vibrational energy convected out of simulation domain
Geometry, mesh, and operating conditions

Plasma Mesh
- 8000 cells

0.2 mm electrode

Trapezoidal Pulse
- 10 ns pulse
- 2.5 ns rise/fall time
- 6 kV peak
Unperturbed steady flow

Laminar boundary layer with lower background number density

Flat-plate leading edge shock
Electrostatic potential and electron density transients
Charged and radical species yields at end of pulse

IONS

**O₂⁺** and **O₂⁻** dominant positive and negative charge carriers

RADICALS

**O** dominant radical
Gas dynamic response to nanosecond pulsed discharge
Effect of flow field on discharge dynamics

- Lower background number density in boundary layer $\rightarrow$ higher E/N
- Confinement of streamer to within the boundary layer
- Flow carries radicals downstream over micro/millisecond timescales
A note on parallel computing for these class of problems

80,000 APPJ mesh for 500 iterations on Lonestar machine at Texas Advanced Computing Center (TACC)

- Problems with large two-dimensional meshes and large chemistries scales well to a few 100 processors, cutting simulation times from ~weeks to ~ 1 day. However further improvement in speed up improvement is limited by algorithmic bottlenecks (specifically the Poisson’s eqn).
- New “parallel friendly” discretization approaches to the Poisson’s eqn. are required
Summary

- High fidelity simulations of cold plasma (streamer) discharges at high pressure relevant to real application are demonstrated
  - Self-consistent plasma physics, multi-species, multi-temperature, gas chemistry, surface chemistry, gas dynamics
  - Computationally expensive and needs large-scale parallel computing to make simulations feasible

- Simulations provide insights into discharge physics and chemistry and coupling with gas-dynamics

- Extension to large scale problems with high-performance computing requires a rework of established computational plasma modeling approaches
End of Presentation
Plasma kernel formation with active radicals is not a sufficient condition for ignition

- Cold plasma generated radicals are accompanied with no additional gas heating
- Do radicals accelerate combustion (chain initiation and branching) reactions for ignition
- Finally are conditions suitable for flame spread

Question: Does the cold radical kernel grow in time or quench?

Same as classic ignition kernel problem, except here kernel is a cold radical region, rather than hot gas region
Solve reactive gas dynamics problem assuming an initial radical kernel
- 1D Axisymmetric transient problem
- 1 mm kernel size (~ multiple overlapping streamer widths)
- No additional gas heating from plasma
- 10 atm, 1500 K, lean mixture with EGR (A/F 20:1 + 50 % EGR)
- 1 % of O radicals (consistent with yield from streamer)

Chemistry Mechanism: DRM22 with 22 species and 105 reactions

Reactive Flow model:
- VizGlow (without plasma calculations) coupled to Compressible Navier-Stokes solver (VizFlow)
Other approaches may be considered for automotive combustion ignition applications

- Principle requirements:
  - Extended plasma kernel size
  - High radical yield
  - Low loss (volumetric; far away from surfaces)
Sub-critical microwave excitation with external plasma initiation is a possibility

- Coax-fed microwave can provide a volume filling excitation field
- External plasma initiation can be used to keep microwave E-field subcritical
Microwave excitation concept is not new for automotive ignition applications

- Igniter erosion concerns with Ikeda concept can potentially be overcome with coax-fed microwave
High-fidelity modeling capability available to simulate microwave plasmas with VizGlow

Fig. 1. Schematics of the RLSA for the microwave plasma system.

Characteristics of large-diameter plasma using a radial-line slot antenna

C. Tian, Y. T. Nozawa, K. Ishibashi, H. Kamayama, and T. Morimoto
Tokyo Electron Ltd., TBS Broadcast Center, 3-6 Akasaka 5-Chome, Tokyo 107-8481, Japan

Presentation of non-equilibrium plasma physics relevant to automotive ignition applications

- Nano-second pulsed plasma are efficient way to generate non-equilibrium plasmas at high pressures
- HSP, DBD, RFEIS devices leverage this concept in different ways

High-fidelity simulation studies of HSP presented

- Streamers produce copious amounts of radicals (particularly O radicals)
- Radicals are concentrated at inner electrode possibly explaining the dynamics of flame spread from these ignition sources

Showed initial studies of long time scale processes in ignition

- Plasma radical kernel $\rightarrow$ local combustion initiation $\rightarrow$ gas dynamic relaxation $\rightarrow$ flame spread

Extended volumetric radical kernel possible with subcritical microwave + NSP ignition
Trends in automotive combustion engines are driving need for new ignition sources

- Improved engine efficiencies and stringent emission norms are driving new technologies in automotive combustion devices

- Improved efficiencies achievable through 1) increased compression ratios in IC engines and 2) lean combustion

 Lean combustion →
  - Increase in efficiency (power/fuel rate)
  - Decrease in flame temperature → low NOx

 Enabling technologies
  - Direct injection (no air intake throttling losses) → just in time combustion
  - Lean with Exhaust Gas Recirculation (EGR) → low flame temp → lower NOx

 Technological challenges
  - Lean combustion (with EGR) → ignitability issue is key problem

Starikovskiy and Alexsandrov, Prog. Energy Comb. Sci., 2013
Conventional spark plug based IC engine ignition

- Combustion ignition via highly constricted/localized spark
- Spark is a thermal plasma with very high sensible temperatures (~ 1000’s K) -- lifetime/reliability
- Chemical initiators for combustion not the same as in a cold plasma
- Limited control on plasma yield
Nanosecond pulsed and Dielectric Barrier plasma-based ignition

Conventional spark plug

Nanosecond Pulsed

Dielectric barrier

1200 rpm, A/F=15.1(Φ=1.0), ADV: 20 deg.BTDC, iso-octane

Shiraishi and Urushira, SAE_2011-01-0660
Variety of plasma actuator concepts exist for volumetric and surface flow control

Meyer et al. AIAA J. (2005) OSU

Shin et al., AIAA J. (2007)

Kalra et al., Expt. Fluids, (2011)


Computational issues in the modeling of air plasma interactions with flows

- Extremely high degree of time disparity in component physics

- Spatial stiffness due to discharge structure

**Sheaths**

**Electronegative plasma**
Photoionization (3-term Helmholtz equation model)

Integral Model (Zheleznyak et al 1982):

\[ I(\vec{r}) = \frac{P_q}{P + P_q} \xi S_i(\vec{r}) \]

\[ g(R) = \frac{\exp^{-\chi_{\text{min}}P_{O_2}R} - \exp^{-\chi_{\text{max}}P_{O_2}R}}{P_{O_2} R \ln(\chi_{\text{max}}/\chi_{\text{min}})} \]

Luque et al* proposed approximating \( g(R)/P_{O_2} \) using two exponentials functions and expanded by Bourdon et al+ to three terms

\[ S_{ph}(\vec{r}) = S_{ph}^1 + S_{ph}^2 + S_{ph}^3 \]

\[ S_{ph}^j = \iiint \frac{I(\vec{r})}{4\pi R^2} A_j P_{O_2}^2 \exp^{-\lambda_j P_{O_2}^2} \]

The integrals are solutions to three Helmholtz equations:

\[ \nabla^2 S_{ph}^j - (\lambda_j P_{O_2})^2 S_{ph}^j = -A_j P_{O_2}^2 I(\vec{r}) \quad (j = 1, 2, 3) \]

+ Bourdon A, Pasko NP, Liu NY, Celestin S, Segue P and Maroude E 2007 Plasma Sources Sci. Technol. 16 656

\[
\begin{array}{|c|c|c|}
\hline
 & \lambda_j \text{ (cm}^{-1} \text{ Torr}^{-1}) & \lambda_j \text{ (cm}^{-1} \text{ Torr}^{-1}) \\
\hline
S_{ph}^1 & 0.0067 & 0.0447 \\
S_{ph}^2 & 0.0346 & 0.1121 \\
S_{ph}^3 & 0.3059 & 0.5994 \\
\hline
\end{array}
\]
Plasma chemistry mechanism used in studies

- Plasma Chemistry mechanism relevant to plasma time scale (~10’s ns)

- Methane-air mixtures
  - 26 Species:
    - E, O, N₂, O₂, H, N₂⁺, O₂⁺, N₄⁺, O₄⁺,
    - O₂⁺N₂, O₂⁻, O⁻, O₂(a1), O₂(b1), O₂*, N₂(A)
    - N₂(B), N₂C, N₂(a1), CH₄, CH₃, CH₂, CH₄⁺,
    - CH₃⁺, CH₂⁻, H⁻
  - 85 Reactions:
    - 1) electron impact, 2) ion-ion, 3) electron neutral, 4) neutral-neutral

- Methane-air with EGR mixtures
  - 39 Species:
    - E, O, N₂, O₂, H, N₂⁺, O₂⁺, N₄⁺, O₄⁺,
    - O₂⁺N₂, O₂⁻, O⁻, O₂(a1), O₂(b1), O₂*, N₂(A)
    - N₂(B), N₂C, N₂(a1), CH₄, CH₃, CH₂, CH₄⁺,
    - CH₄⁺, CH₃⁺, CH₂⁻, H⁻,
    - H₂O, H₂O⁺, H₂, H⁺, H₂⁻, OH, OH⁺, OH⁻, O⁺,
    - CO₂, CO₂⁺, CO⁻, O₃
  - 110 Reactions:
    - 1) electron impact, 2) ion-ion, 3) electron neutral, 4) neutral-neutral
    - Additional: CO₂, H₂O and O₃ reactions
Comparison of baseline and With EGR cases for HSP discharge streamer

- Baseline (lean A/F = 40:1)
- With EGR (A/F = 20:1 + 50% exhaust)

![Graph showing comparison]

- Propagation speeds higher with EGR
- Electron density slightly higher with EGR
Radical densities for baseline and With EGR cases for HSP discharge streamer

- No significant changes in radical densities for case with EGR
Case 1: Pulse train of $-90\text{kV} \rightarrow +90\text{kV} \rightarrow -90\text{kV}$ (gas temperature 700K)

Pulse Durations:

1$^{\text{st}}$ pulse: 7 ns
2$^{\text{nd}}$ pulse: 7 ns
3$^{\text{rd}}$ pulse: 7 ns
Evolution of Number Density of Electrons
Evolution of Number Density of O radicals
Evolution of Electron Temperature (K)
Evolution of Reduced Electric Field (E/N)
O Radical Number Density at End of Different Pulses

![Graph showing O Radical Number Density at End of Different Pulses](image)

- **End of 1st Pulse**
- **End of 2nd Pulse**
- **End of 3rd Pulse**

**Axes:**
- **Y-axis:** Number Density of O (#/m³)
- **X-axis:** Axial Distance (m)
O3 Radical Number Density at End of Different Pulses

- **End of 1st Pulse**
- **End of 2nd Pulse**
- **End of 3rd Pulse**
Voltage Amplitude Comparison
Voltage: Streamer Propagation

Higher voltages result in stronger Electric Field

Streamers propagate further as voltage increases
Voltage : Thermal Effects

Stronger Electric fields result in greater ion Joule heating
Conclusions

• O radicals dominant species in plasma (~0.5% peak mole fraction)

• Ion Joule heating dominates gas temperature increase and results in blast waves

• Increasing Voltage increases peak densities, gas heating and volume of plasma formed

• Chemistry (electropositive vs electronegative plasma) affects –
  - Streamer propagation distance/speed
  - Region of plasma formation (inside/outside boundary layer)
  - Intensity of gas heating for different polarities

• Anodic pulses appear more efficient for supersonic combustion
  - Radicals produced over greater volume
  - Less power lost to heat (for O₂-H₂)