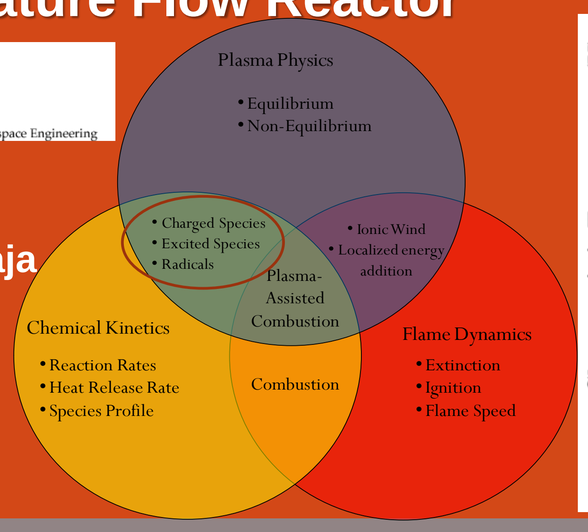
1D Numerical Investigation of Nanosecond-Pulsed Plasma Activated $C_2H_4/O_2/Ar$ Mixture in a Low Temperature Flow Reactor

Georgia Tech College of Engineering
Daniel Guggenheim School of Aerospace Engineering

Authors: **Suo Yang, Sharath Nagaraja**

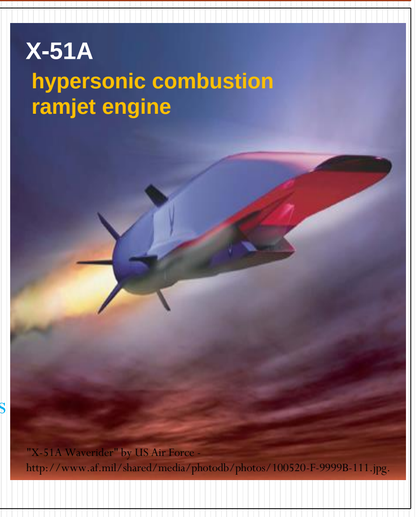
Mentors: **Wenting Sun, Vigor Yang**

Institution: **Aerospace Engineering**



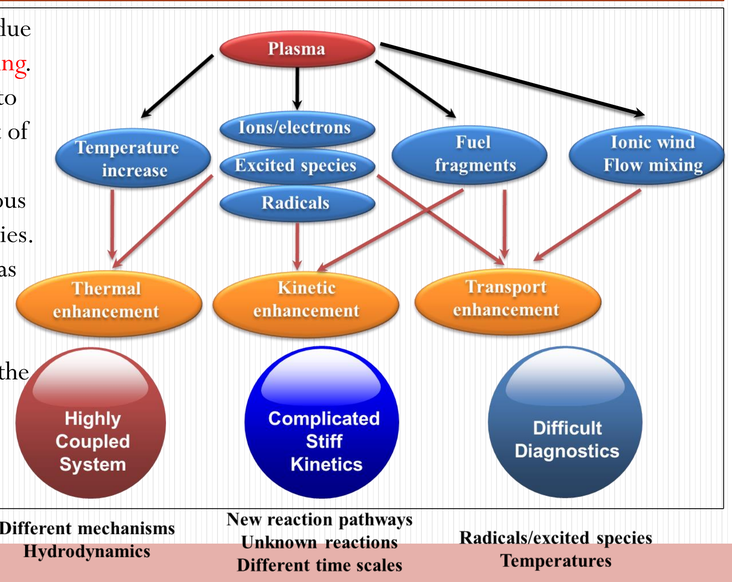
I. Motivations

- Understanding of how low temperature plasma effects ignition of hydrocarbon fuel-air mixtures remains sketchy.
- There is a need to investigate the plasma/combustion interaction mechanisms for hydrocarbon fuels using self-consistent numerical simulations.
- Ethylene (C_2H_4) is a typical hydrocarbon fuel for **scramjet/ramjet**, which is the most promising potential application of PAC, because **hypersonic air-breathing engines** require **extremely fast ignition&stabilization**.
- In previous work, simulations using a 0D kinetic model were conducted. Large discrepancies were observed in measured and predicted H_2O and CH_4 densities. In addition, ambiguities in choosing electric field and electron density also introduced significant uncertainties.



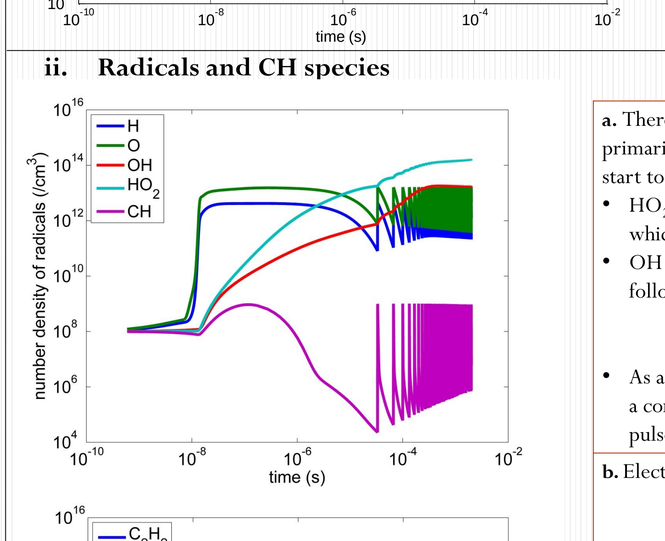
II. Problems & Difficulties

- Plasma/combustion interaction is not well-understood due to the complicated thermal, kinetic and transport coupling.
- There have been few detailed numerical studies of PAC to provide significant insights into the plasma enhancement of the combustion process.
- The multi-scale nature of PAC, however, creates enormous challenges for conducting comprehensive modeling studies.
- In simplified 0D kinetic models, the plasma discharge was assumed to be uniform. The electric field and electron density values were pre-specified. The model did not consider sheath formation, and charge accumulation on the dielectric layers. In addition, species and heat diffusion effects were ignored.



I. What is PAC (Plasma Assisted Combustion)?

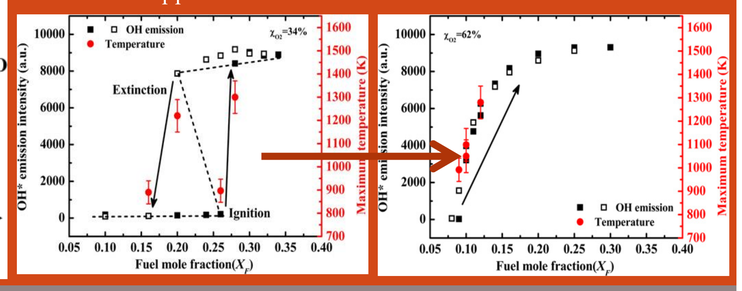
PAC modify fuel oxidation pathways through low temperature radical production (e.g. O, H and OH) instead of thermal heating.



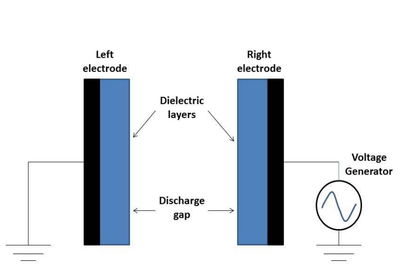
II. Non-equilibrium plasma – the way to clean and efficient combustion

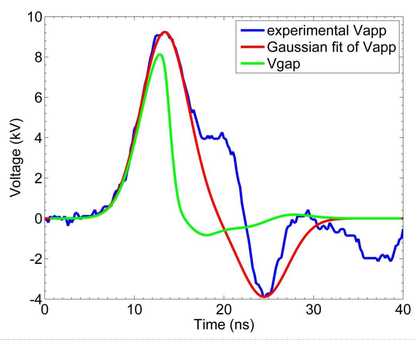
Great potential to enhance and stabilize the combustion process in **internal combustion engines, gas turbines, and scramjet/ramjet engines**:

- shorten the ignition delay times;
- extend extinction limits;
- a new ignition/extinction curve without hysteresis;
- improve flame stabilization;
- increase flame speed;
- suppress soot formation



III. Approach: 1D Numerical Modeling





- Poisson equation for electric potential:

$$\nabla \cdot (\epsilon \nabla \phi) = -e(n_+ - n_- - n_e)$$

- Electron energy equation:

$$\frac{\partial n_\epsilon}{\partial t} + \nabla \cdot J_\epsilon = \dot{Q}_\epsilon$$

- Species continuity equations for all charged and neutral species:

$$\frac{\partial n_k}{\partial t} + \nabla \cdot J_k = \dot{\omega}_k$$

- The transport of energy and species is calculated by the drift (mobility)-diffusion model.
- Mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0$$

- Momentum conservation equation:

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + F_i^{EHD}$$

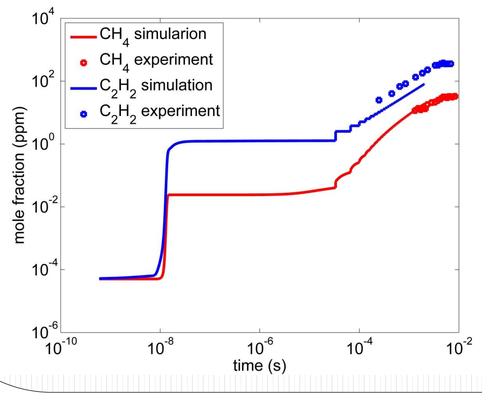
- Energy conservation equation:

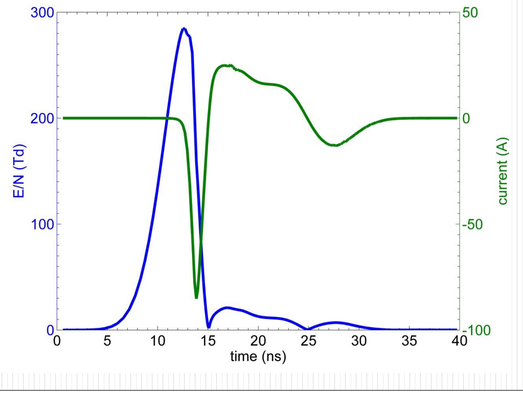
$$\frac{\partial \rho E}{\partial t} + \frac{\partial [(\rho E + p) u_i]}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} + \dot{Q}^{JH}$$

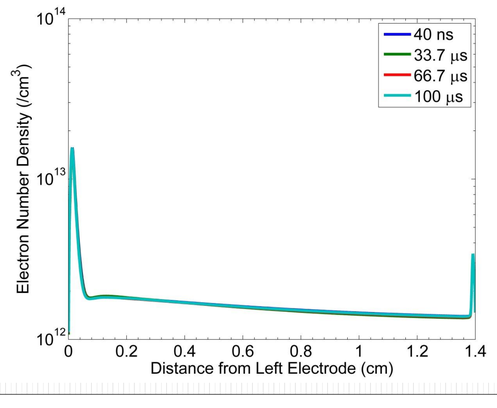
- The electron reaction rate and transport coefficients are fitted as functions of electron energy calculated by BOLSIG[1], and renewed at every time step via interpolation.

- The plasma combustion chemistry mechanism used in the present work is assembled by combining USC Mech II[2] kinetics dataset with Ar and O_2 plasma reactions taken from ZDPlasKin[3] database.
- To tackle the **multi-scale** nature of the problem, **adaptive time-stepping** is implemented with small time-steps (10^{-13} - 10^{-12} s) during each voltage pulse, and larger time-steps (10^{-10} s) in the gap between two consecutive pulses.

IV. Model Validation: Compare Numerical Modeling and Experiments

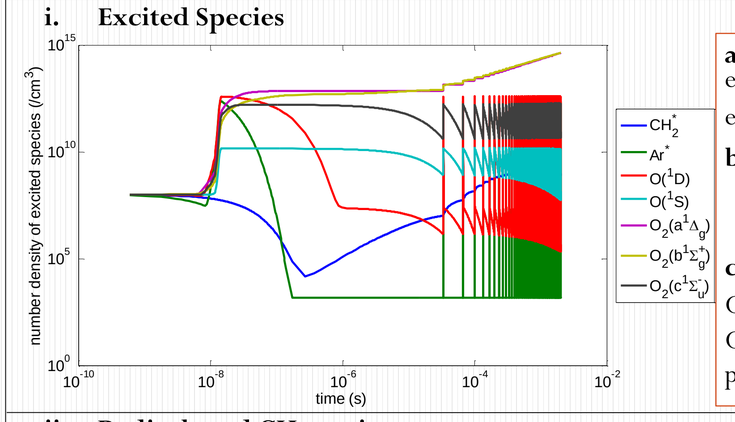






V. Results, Analysis & Conclusion

i. Excited Species



Analysis & Conclusion

a. Electron Impact Excitation Reactions

$e + O_2 = e + O + O(^1D)$

$e + O_2 = e + O_2(a^1\Delta_g, b^1\Sigma_g^+, c^1\Sigma_u^-)$

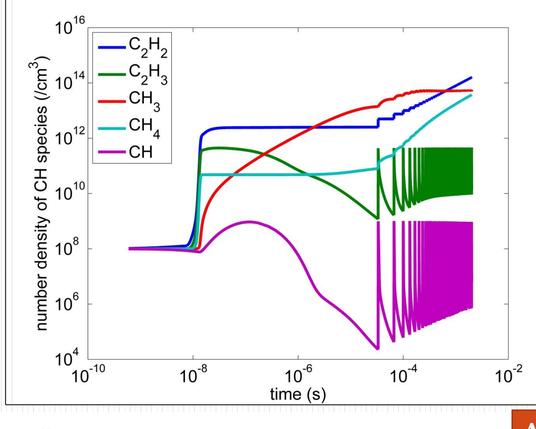
b. Quenching Reactions

$O(^1D) + Ar = Ar + O$; $O(^1S) + O_2 = O + O + O$

$O_2(c^1\Sigma_u^-) + O_2 = O_2(b^1\Sigma_g^+) + O_2(b^1\Sigma_g^+)$

c. Globally, concentrations of CH_2^*, $O_2(a^1\Delta_g)$ and $O_2(b^1\Sigma_g^+)$ keep accumulating, while those of Ar^*, $O(^1D)$, $O(^1S)$ and $O_2(c^1\Sigma_u^-)$ only oscillate periodically.

ii. Radicals and CH species



Analysis & Conclusion

a. There is a sharp increase for H and O in the time interval of 10 - 15 ns primarily due to the fast electron impact reactions, while OH and HO_2 only start to increase gradually.

- HO_2 is formed from three-body recombination of H with O_2 molecules, which is fast at the present low temperature conditions.
- OH is produced from HO_2 reacting with O and H atoms through the following reactions:

$$O + HO_2 = OH + O_2$$
$$H + HO_2 = OH + OH$$

- As a consequence, we observe a gradual decay in O and H densities, whereas a continuous accumulation of OH and HO_2 during the gap between two pulses.

b. Electron impact reactions:

$$e + C_2H_4 = e + C_2H_2 + H_2$$
$$e + C_2H_4 = e + C_2H_2 + H + H$$
$$e + C_2H_4 = e + C_2H_3 + H$$
$$e + C_2H_4 = e + C + CH_4$$
$$e + C_2H_4^+ = CH_3 + CH$$

- CH_3 only gradually increases because it is generated by electron/$C_2H_4^+$ recombination, which is limited by the formation of $C_2H_4^+$, rather than direct electron impact reaction.
- After the breakdown, C_2H_2 and CH_4 densities remain constant until further increase in the next pulse. CH_3 densities continue to rise due to further accumulation of $C_2H_4^+$.
- On the other hand, C_2H_3 radicals are rapidly consumed to form C_2H_2, CH_3 and CH_4 or CH_2CHO during the gap between two pulses.
- Overall, C_2H_2 and CH_4 keep increasing with the number of pulses, while CH and C_2H_3 only periodically change from one pulse to the next pulse.

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Reference:

[1] Hagelaar, G. J. M. and Pitchford, L. C. "Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models," Plasma Sources Sci. Technol. Vol. 14, No. 4, 2005, pp. 722-733.

[2] Wang, H., You, X., Joshi, A. V., Davis, S. G., Laskin, A., Egolfopoulos, F., and Law, C. K. http://Ignis.Usc.Edu/Usc_Mech_Ii.Htm.

[3] S. Pancheshnyi, B. Eismann, G.J.M. Hagelaar, L.C. Pitchford, Computer code ZDPlasKin, http://www.zdplaskin.laplace.univ-tlse.fr (University of Toulouse, LAPLACE, CNRS-UPS-INP, Toulouse, France, 2008).