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Title: Flamelet modeling of plasma and ignition process in a variational LES computational method

Author(s): Waters, Jiajia
Mahamud, Rajib
Carrington, David Bradley

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Flamelet modeling of plasma and ignition process in a variational LES computational method

Objective

The study will develop mathematical and numerical models of the turbulent ignition process that comprises plasma species interaction with turbulence and principles of ignition kernel growth or extinction based on a flamelet modeling approach.

Problem and Proposed Innovation

In the last fifty years, fuel economy in engines has grown from ~10 MPG to 30 MPG [1] and an average of 40% efficiency, resulting from engine improvements, controls systems that vary valve timing, mixture formation, and material sciences advancement. However, the question remains: how to reach over 60% efficiency or nearly 60~70 MPG in a pure gasoline direct injection vehicles. One of the needed technological advances (a very needed component) required to achieve the goal, relies on sustaining ignition at a very early stage with a very lean mixture. The ignition kernel growth is governed by energy exchange mechanisms between plasma radicals and electrons. This study aims to develop models for ignition kernel growth considering three temperatures and primary radicals that existed during the very early stages and investigating the necessary condition of ignition kernel growth or suppression in a leaner mixture. To our knowledge, at present, there is no such study presented in the literature that resolves turbulence and plasma radical interaction during the early stage of ignition. The Los Alamos Laboratory was one of the forerunners of multiscale engine combustion simulation by developing KIVA code during the 80s [2], which was further advanced by finite element based solver FEARCE, an R&D 100 award-winning software[3]. The proposed study will develop a flamelet model of plasma ignition kernel growth on FEARCE's *hp*-adaptive LES CFD platform [3-5] and investigate the criterion of ignition kernel growth at a very early stage for lean mixture conditions. FEARCE's particular form of Vreman LES is a requirement for modeling plasma kernal growth because these kernels are subject to highly unsteady turbulence, changing from nearly quiescent at onset of spark, to highly turbulent flow as the plasma kernel growth and ignition proceeds [3-5].

R&D Methods and Anticipated Results

The proposed study will develop multiscale-multiphysics models that incorporate three temperatures (neutral gas, electron, and vibrational), plasma reaction kinetics, and flow mechanism to predict the possibility of ignition kernel growth. The ignition delay time in engine combustion is generally higher than species (electron, radicals, etc.) and nonequilibrium transport time. In a comparative timescale, we may write it in the following form [6]:

$$\tau_{ignition} > \tau_{nonequilibrium} > \tau_{plasma}$$

The proposed study will also include the influence of vibrational and electronic energy transfer mechanisms during the nonequilibrium energy deposition and thermalization process during the equilibrium energy deposition (e.g. Spark) [7]. The electron-induced reaction rates, electron

species transport parameters, mobility and diffusivity, and the electron energy mobility and diffusivity and the ions and neutrals can be treated hydrodynamically in a CFD code. The initial calculation of the model is presented in Figure 2 ~ 6. The three temperatures distribution in a nonequilibrium energy deposition (e.g., microwave, nanosecond discharge, laser) and equilibrium energy deposition are shown in Figure 2, predicting a higher degree of nonequilibrium at a very early stage. The initial results suggested that the electron, vibrational, and gas temperatures quickly (~100 ns) reach a steady-state condition, which can not be captured by conventional modeling approaches. Besides, the time at which the electron temperature reaches a steady state is related to plasma lifetime and strongly relies on energy deposition rate [7]. However, the initial calculations suggested that the vibrational-translational energy exchange mechanism is much slower than the electronic-translational and electronic-vibrational process. After the plasma lifetime, the energy is continuously transferred into the translational state from the vibrational state. As a result, the vibrational-translational relaxation process primarily governs the thermalization of the process. Therefore, the nonequilibrium effect could facilitate to increase in the translation temperature (or gas temperature), even when the species densities are low, as observed in lean conditions. If the process is developed in such a method that the energy is continuously being fed into translational degrees of freedom, the condition will provide an edge to sustain ignition even for low initial energy input and a leaner mixture [8,9].

The initial results suggested that the vibrational-translation energy exchange process effectively governs the thermalization of the process, whereas the electronic-translational energy exchange process regulates the probability of ignition. The results indicated that the level of thermalization increases with initial energy deposition, as shown in Figure 4. The perturbation of the ignition kernel by the surrounding flow can significantly influence the combustion process. This trend can be studied with respect to the kinetic energy of the stress tensor in Figure 7 for a different level of energy deposition that can be characterized by a degree of ionization. The results show that the flow and the shock interaction is higher for a higher degree of initial ionization. The maximum shock-flow interaction signifies the point when flow diffuses through the kernel. The higher ionization level also indicates that the kernel will sustain for a longer time and an increasing probability of ignition. Therefore, the initial results suggest that ignition with minimum perturbation of the external flow can support ignition at any level of mixture condition.

Importance for the Laboratory and the Nation

Los Alamos National Laboratory has a long history in studying and modeling of plasmas in turbulent flow as is part of many foundational efforts pursued by the national and LANL. The work is also highly relevant to sustained ignition in engines of scramjet [10] and hypersonic [11] vehicle, the crux technological advance needed for sustained hypersonic flight. In addition, the efforts as mentioned are of immense importance to reducing the impact engines have on climate change and reducing our use of and money spent on oil drilling, shipping, and refining. It is estimated that up to 4 million barrels of oil a day would be the savings of achieving the 50 mpg goal alone, which is an estimated 200 million dollar a day saving at today's prices -- quite an economic boost, let alone an immense reduction in greenhouse gases [2].

Figures

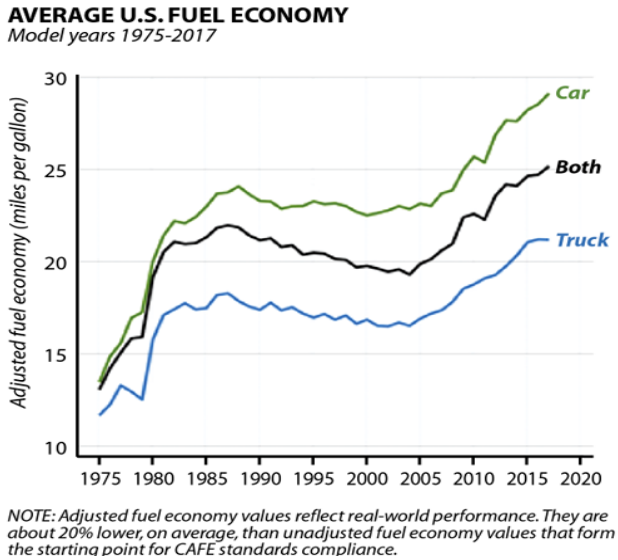
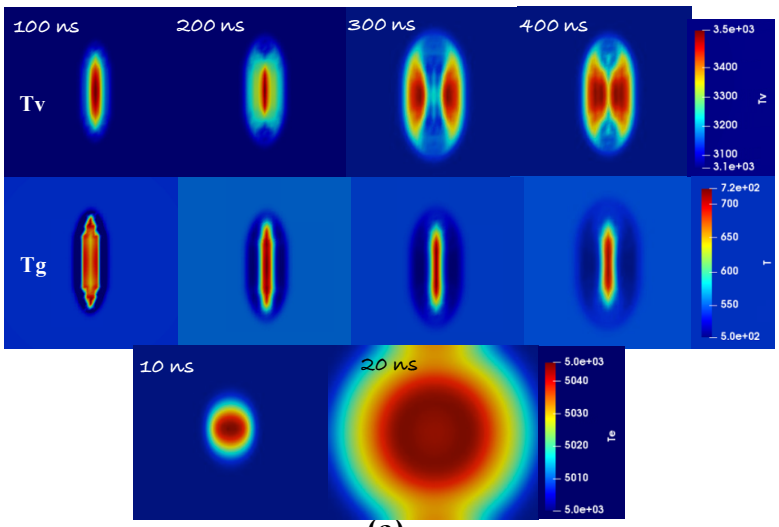
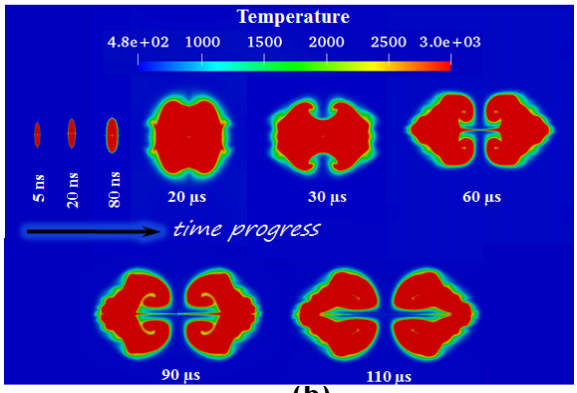


Figure 1: The average US fuel economy since the 1970s



(a)



(b)

Figure 2: (a) Spatio-temporal contours of the temperature profile (electronic, vibrational, and gas) for a low initial energy deposition case (no ignition case) (b) Spatio-temporal contours of the ignition kernel (ignition case)

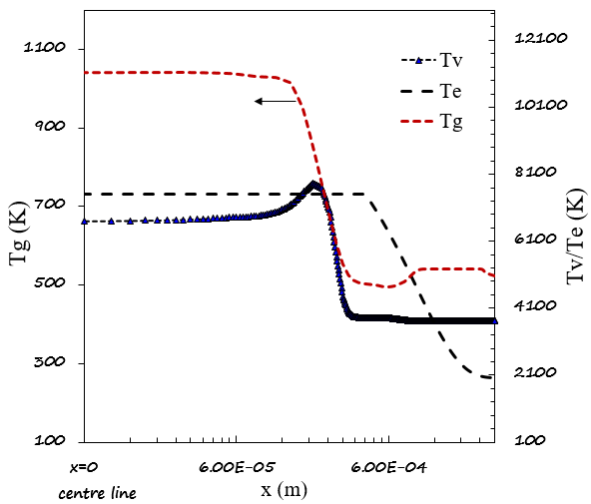


Figure 3 (a): Spatial distribution of electronic, vibrational, and translational temperatures around the core of the kernel axis

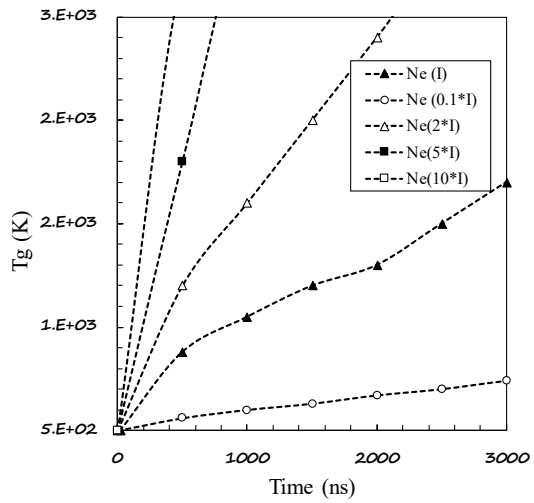


Figure 3(b): Temporal maximum gas temperature profiles for the different initial electron number densities due to the different energy deposition levels. Base condition: $N_{e,0}$ (I): 1×10^{18} (1/m^3)

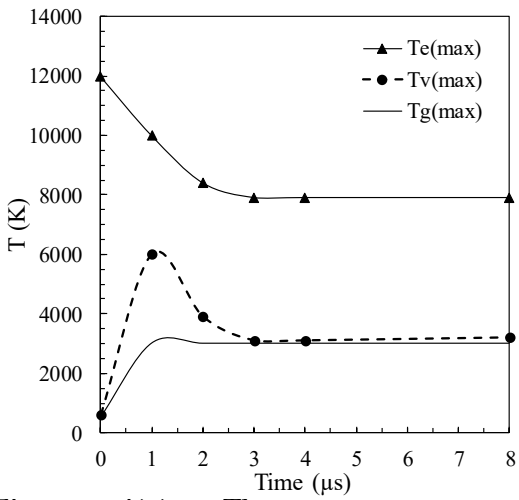


Figure 4(a): Three temperature distribution at a very early stage when the system is in the nonequilibrium stage.

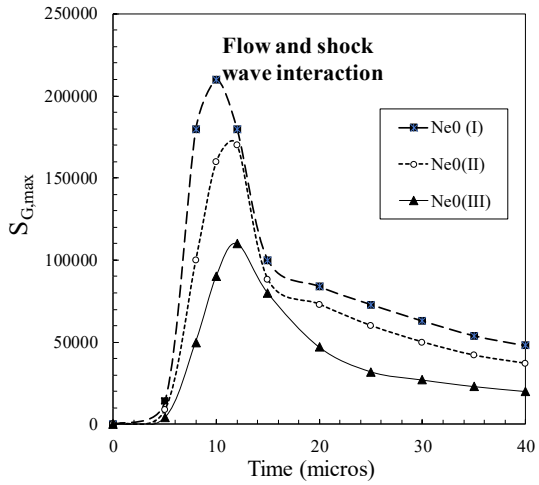


Figure 4(b): The flow kernel interaction with time under laminar flow conditions (Ne_0(I): 1×10^{18}, Ne_0(II): 2.5×10^{18}, Ne_0(III): 5×10^{18} (1/m^3))

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Glossary of Acronyms

CFD	Computational Fluid Dynamics
FEARCE	Fast, Easy, Accurate, and Robust Continuum Engineering Improving
LES	Large Eddy Simulation
MPG	Miles Per Gallon