Plasma Modeling of Ignition for Combustion Simulations

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1 Abstract

Detailed ignition modeling has been traditionally left out of the combustion simulations, mainly due to its relatively small time and length scales that could not be integrated into much larger length and time scales of combustion and fluid dynamics. Although the advancements in computing power has now made possible to integrate ignition and combustion modeling, not many researchers have shown interest due to the wide scope of knowledge it needs in both plasma physics and combustion dynamics. In this paper, we are reporting a preliminary analysis of an integrated ignition+combustion model for both spark ignition (SI) and laser-induced spark ignition (LISI) combustion chambers. A common aspect of both SI and LISI is the use of equation-of-state (EOS) tables at temperatures up to 5 times higher than those assumed in most combustion codes. We report use of an atomic physics code to generate EOS tables needed for our combustion and ignition simulations.

2 Introduction

Fossil-fueled energy supply and end-use combustion systems are the cornerstone of the industrial and commercial sectors of the U.S. economy. In order to optimize the design and operation of combustion systems, a new generation of advanced design tools must be developed to provide the system designer and operator with a fundamental understanding of the interaction of key operating and design parameters. Identified as one of the grand challenge problems, combustion involves many complex phenomena including gas dynamics, chemistry, turbulence, radiative heat transfer, sprays and ignition.

Because combustion occurs at time and length scales where chemistry and turbulence interact, the combustion modeling and simulations face significant scientific challenges. Development of a computer system that can fully resolve, numerically, all aspects of the operation of a combustor may not occur in the foreseeable future. Instead, the approach proposed by the combustion community [1] involves a selective and systematic development of submodels that allow

”bootstrapping” from the microscopic regimes to the device-modeling regime. In order for this approach to be successful, new knowledge in the areas of chemistry, turbulence, materials science, mathematics, and computer science need to be discovered.

Here, we focus on development of an ignition submodel. If a reliable, and reproducible ignition is found, this will help scientists sort out effects of early ignition on combustion. This might even help studies of turbulence and turbulence-combustion interactions which are current concerns of researchers. We will limit our focus to early flame formation and its plasma characteristics.

The spatial and temporal resolutions needed to resolve the ignition source are beyond the capability of current combustion models. Ignition takes place in a very tiny space (microns) and in a quick time-frame (nanoseconds), however it has a lasting effect on what follows. Early flame formation and propagation has a vital impact on the system performance and emissions.

3 Plasma Properties of Ignition

The thermodynamic properties of hot plasma are often required in hydrodynamic and radiative energy transport of astrophysical and fusion plasmas [2]. Although the physical conditions in such cases seem to be far from those of an internal combustion engine, researchers have reported very high temperatures (up to 60,000 Kelvin) and densities during the ignition process [3]. During the spark breakdown phase, the ion density increases rapidly to values of some $10^{19} e/cm^3$ which leads to a significant energy loss for accelerated electrons due to Coulomb collisions with the ions [11]. The frequency of such collisions determines the electrical resistivity (η), which is dependent on the degree of ionization of the background gas. We know from classical transport theory that [7,10,11] conductivity (or resistivity) includes both the effects of Coulomb collisions and electron-atom collisions. The expression used is [11]

$$(1) \quad \eta = \eta_W + \eta_F$$

where η_W is (Weak) Coulomb collision, and η_F is (Full) electron-atom collision term as

$$\eta_F \equiv (5.799 \times 10^{-15}) \cdot Z(T) \cdot \ln \Lambda \cdot T^{-3/2}$$

and

$$\eta_W \equiv \frac{m_e^{1/2}}{e^2} \frac{\sigma_{ea}(T)}{\alpha(T)} T^{1/2}$$

Here, σ_{ea} is the electron-atom collision cross section, m_e is the electron mass, e is the electron charge, Z is the average ionic charge state, T is the plasma temperature, and α is the degree of ionization of the plasma. The degree of ionization is a strong dependent of the plasma temperature. When the degree of ionization falls below 0.001, the behavior of η is controlled by η_W . For α greater than 0.1, the dominant term is η_F .

Calculation of the average charge (Z), the electron-atom collision cross section (σ_{ea}), and the degree of ionization (α) is necessary for computing plasma resistivity which determines how much heat is deposited in the early ignition phase. The average charge (Z) is also needed for computing the equation-of-state (EOS)

$$P = (1 + Z)nkT,$$

which is needed to bring closure to the governing equations [4]. In most, cases, this EOS relation is sought between the specific internal energy (e), the number density (n), and the temperature (T).

We use IONMIX [12] to compute the steady-state ionization and excitation populations for a mixture of up to 10 different atomic species. The thermodynamic properties of plasma, such as the specific energy, average charge state, pressure, and heat capacity are also calculated. One can obtain the radiative absorption, emission, and scattering coefficients, however we are not using these to solve any radiation transport equations at this stage of our work.

The ionization populations for IONMIX are computed for steady-state conditions. The atomic processes considered are collisional ionization, radiative recombination, dielectronic recombination, and collisional recombination. IONMIX uses ionization potentials given at Nuclear Data Tables [12] for about 15 elements. The user must supply an ionization potential for elements outside of this range.

Several aspects of ignition modeling are being considered here are: the amount of energy deposition, the resistivity model, and the EOS data at high temperatures. Most of these issues are common for both SI and LISI, however the EOS data goes to the heart of our approach. The energy deposition for SI is computed through the solution of electromagnetic equations and we have presented this, at least for 1-D at an earlier publication [4]. The energy deposition for LISI is rather an estimate base on experiments [15]. All of our SI and LISI computations have been integrated as sub-models into the KIVA-3 engine combustion code [13]. To our knowledge, these SI and LISI models were first attempts to examine the influence of a computed ignition model, instead of a semi-empirical approach, on combustion output. Here, we are attempting to measure the influence of a well-expanded EOS data for both SI and LISI. Our database for chemical reactions (kinetic and equilibrium) is currently following the data available in KIVA-3. However, this database need to be expanded to higher temperatures than currently available.

4 Results

Our one-dimensional spark-ignition model described in [4] along with expanded EOS tables described here and in [12] has been integrated into the standard KIVA-3 code [6,13]. We examined the combustion output (i.e., temperature, NO_x density) against ignition energy variations. The new EOS data obtained for high temperatures via IONMIX has been used to check the variations in

combustion output. This section lists preliminary results for both SI and LSI cases.

4.1 SI

Although far from representing all spark phases in [14], the spark discharge profile taken from experimental data by [5] suffices for our initial tests involving the engine configuration in 1.

Fig. 1. Schematic of an engine.

We examine the influence of added plasma properties and equations in our simulations. These new properties include 1) computation of ignition energy source via Maxwell’s equations [4], 2) use of new EOS data from IONMIX, 3) a new resistivity model to compute spark current density. A comparison is made to a test case using the standard KIVA-3 without any such plasma properties.

These results have been obtained on a baseline engine with a spark plug centrally located at the cylinder head. Temporal and spatial data was obtained at every 5 degree crank angle for a computational mesh of approximately 5,500 elements. The engine specifications can be found in [6,13]. The enormity of the data makes visualization a necessity for scientific interpretation. The standard KIVA-3 output was converted to a format accepted by the AVS post-processing software.

We include a summary of our observations via Fig. 2 and 3 for different fuel amount and varying spark current. In these figures, we present peak values of

Fig. 2. Temperature at the ignition center

Fig. 3. NO_x density at the ignition center

temperature (T), and NO_x density at the ignition region. It is obvious that our plasma-enhanced simulations (Case B,C,D) show a more elevated peak temperature than the classic KIVA-3 run (Case A) with a simpler ignition source and limited EOS data. The difference between Case A and B (which have the same fuel amount and the same spark current) is almost seventy percent. This difference is significant enough to lead to an entirely different NO_x and fuel density profiles. We expect that a significant part of the temperature difference comes from the use of new EOS tables that enable us to move into a high temperature region rather than cutting it off at the 5,000 Kelvins as the KIVA-3 code does.

Contrary to several assumptions in previous modeling efforts, temporal and spatial variations of the spark plasma properties are important source of influence on the flame dynamics and subsequent combustion. These results justify a more comprehensive approach to account for the high temperature aspects of ignition. They also indicate that the evolution of ignition and its interaction with combustion should be taken into account.

4.2 LISI

Although experimental data from LISI clearly shows spatial and temporal variations [15], we assume a fixed energy source during the ignition window. Furthermore, the source term is $\Delta e = (P/\rho) \cdot \Delta t$, where P is the laser energy deposition rate ($ergs/s.cm^3$), ρ is the total density, and Δt is the duration of the laser pulse. Although the laser lasts only 5-10 nanoseconds, Δt here might be as low as one nanosecond. In that case, the sum of all the Δe values during the ignition window would give the total ignition source energy deposition. The use of small Δt is to prevent numerical instabilities that could arise from a high deposition rate. The laser energy deposition rate used here is $5 \times 10^{16} ergs/s.cm^3$, which deposits about a fraction of a *Joule* energy in the combustion chamber in the 5-10 nanosecond timeframe.

We examine the effect of an expanded EOS data on the combustion output. As it is in the SI case, the temperature in the combustion chamber is the most affected physical quantity. A comparison of temperature, NO_x Density, and the Fuel Density for two cases is presented in Figures 4,5, and 6. One of these two cases represents original EOS data, which is below 5,000 Kelvins. The other case is for expanded EOS data beyond 5,000 Kelvins. It seems the temperature difference between these two cases leads to a different level of fuel consumption, and NO_x production. In the expanded EOS case, the temperatures in the ignition region are allowed to rise, therefore leading to more fuel consumption and NO_x production. In the figures shown here, the NO_x density is much higher for limited EOS case in the central region due to a higher fuel density at that time compared to expanded EOS case. In the expanded EOS case, more fuel is burned earlier. The produced NO_x leaves the center of chamber. The overall NO_x production is therefore still higher for the expanded EOS case.

Since the effect of temperature is so high on fuel consumption and NO_x production, among other things, it is important that we conduct an accurate solution, particularly in the use of EOS data. If the chamber temperature is

much higher than what we believed in, then this will lead to an underestimation of pollutants and wear and tear of chamber equipment.

Fig. 4. Temperature at Crank Angle=-4.99

5 Conclusion

It is noted that temperatures in the ignition area are many times higher than those in the rest of the combustion chamber. Detailed ignition modeling is needed to enhance accuracy of combustion simulations. The equation of state (EOS) data as well as the reaction rate tables need to be updated to include temperatures up to at least 10,000 – 20,000 Kelvins. The use of an atomic physics code (IONMIX) here has been justified as there is a significant difference in results when we use an expanded EOS data. We will report further results in future publications. The ignition sub-model and the expanded EOS tables will be modularized to be used with other combustion codes.

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Fig. 5. NOx Density for LISI at Crank Angle=-4.99.

Fig. 6. Fuel Density for LISI at Crank Angle=-4.99.

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