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Modelling spark-plug discharge in dry air

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ABSTRACT

This work presents a novel numerical strategy for studying the electric discharge produced by a vehicular spark plug in dry air. For such a task an axial symmetric 2D domain is used. The starting gas mixture is formed by molecular nitrogen and oxygen (8:2 ratio). The mathematical model considers heat and species diffusion and convection jointly with a discrete sub-model for energy transfer in electronic, atomic and molecular collisions. Chemical reactions between species are also included. Solutions of source terms is accomplished in the frame of ZDPlaskin, a zero-dimensional plasma modelling tool. The used plasmo-chemical kinetics model includes 53 species and 430 processes. Experimental properties from an actual spark plug discharge are introduced to the simulation. Spatio-temporal evolution of species concentrations are obtained within this model. Gas temperature evolution and species distribution is discussed and compare with available values in literature.

1. Introduction

The ignition discharge in spark plugs can be divided into three phases: the break- down, the arc discharge, and the glow discharge. The breakdown phase lasts for a few nanoseconds and the discharge voltage drops from its initial value of several kV or more to significantly lower values of a few hundred volts. For (relatively) low gas pressures around 1 bar, the arc discharge is not ignited and the glow discharge occurs immediately after the breakdown [1]. For higher pressures, the arc discharge follows the breakdown and changes into a gl ow discharge when the current decreases. Duration of the arc phase is typically of the order of 1 µs, however it depends on the pressure: the arc fraction of ignition discharges at higher pressures increases as the pressure increases, irrespective of the cathode material or gas used [2].

During the discharge process, the energy from the electric field is mostly used to heat the free electrons. Such energized electrons collide with molecules and atoms of the mixture. Then, dissociation, excitation and ionization processes take place, resulting in radicals, ions, electronically and ro-vibrationally excited species [3–5]. This low temperature plasma (LTP) comprises chemically reactive species, responsible for first oxidation steps of the fuel [6–9]. The subsequent chemical reactions leading to fuel consumption, heating of the chamber and shock waves production, depends upon the temperature and the concentration of reactive species. The relationship of the voltage applied to the spark plug with gas temperature and reactive species production is not direct. Hence, realistic numerical investigation of LTP produced in spark discharges coupled to gas phase processes are required [10].

Diagnostics of plasma produced by spark plugs have been reported in literature. Oliveira et al. presented an experimental study of a commercial spark-plug discharge in air [11]. There, electric current and voltage were measured as a function of time. Also, gas and electronic temperatures were estimated from optical emissions. In a paper by Hnatiuc and collaborators, another diagnostic for plasma produced by a spark plug was presented [12]. Similarly, gas and electronic temperatures were there estimated.

From the theoretical side, there have been large efforts to model the time evolution of LTP produced in electronic discharges. The phenomenological investigation of the application of electric discharges in gases mixtures is initiated by obtaining the energy distribution function for the electrons (EEDF) [5]. The work of Kang et al. [13] reports the influence of the loss of energy and pressure in the calculation of EEDF in nitrogen and argon mixtures. A numerical study of the ignition delay was reported by Han and Yamashita [7]. There, using zero and one-dimensional models, authors studied the effects of the strength of the reduced electric field, the discharge duration and the initial temperature on the ignition. A quasi-zero dimensional approach is used in the work of Yang et al. to study the vibrational excitation of N_2 in a nanosecond discharge in the order of few kV [14]. Electron emission

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mechanisms and determination of the electronic and vibrational temperature of the nitrogen are reported as well. A model for nanosecond discharges, with tension in the order of few kV, in gas mixtures is presented in the works of Xu et al. [15], where a simplified plasmo-chemical cycle (7 species and 9 processes) and a two-dimensional domain were considered. The heating of the mixture, species densities and the compression waves generated by the rapid heating of the mixture are also reported [15].

Concerning the numerical models for spark-plug discharges, there are some references which resolved numerically the partial differential equation system. One example is the work of Reinmann and Akram [16]. There, authors adopted a 2D model and resolved the differential equation by applying a predictor-corrector one-dimensional two-step difference operators corresponding to the time-split MacCormack scheme and a flux corrected transport as a stability criterion. Thiele et al. also conducted the discretization in space and time separately by the method of lines [10]. Space discretization was done with central finite differences. An implicit time integration methods were applied. Since the pressure wave has an important influence on the flow field in the beginning, it has to be treated accurately by the scheme. In order to cope with the steep gradients at the shock fronts, an artificial viscosity method was used, which broadens the wave but does not influence the flow-field.

More recently, Castela et al. [17] proposed a 3D direct numerical simulation (DNS) aiming at studying the impact of gas flow recirculation on the temporal evolution of species and gas temperature in the vicinity of the discharge zone. The model is implemented in a structured Direct Numerical Simulation solver with 16,8 millions grid. The spatial derivatives are computed within a 4th order centered finite-difference scheme. An 8th order filtering scheme is used for stability purposes. The code is explicit in time using a 4th order Runge–Kutta method. To capture stiff pressure waves induced by each plasma discharge, the hyper-viscosity technique developed is employed [17,18].

A theoretical framework to study spatial and temporal evolution of a non-equilibrium plasma was presented by Nagaraja et al. [19]. There, electric field equations are simultaneously solved with a plasmo-chemical model. In these works, the studied non-equilibrium plasma were produced by high voltage (of the order of few kVs) nano-seconds pulsed discharges. Yet, to produce a discharge in vehicular spark-plug, 5–15 kV are usually applied during few milliseconds to the electrodes [20]; i.e., rather different conditions than those used in the mentioned simulations. Furthermore, considering the total energy deposited in the gas mixture during a spark-plug like discharge, the isobaric approximation is not appropriate [13,21]. Thus, a realistic model for such a process requires considering gas dynamics coupled to the plasmo-chemical problem. Such a coupling in previous theoretical studies [10,17,18] has follow simplifications motivated mostly by the computational cost. Also remarkable, is the scarcity of literature studying the evolution of a single discharge up to few milliseconds.

The aim of this work is to present a 2D theoretical and numerical framework to model the spatio-temporal evolution of the plasma produced in a spark-plug discharge coupling plasma kinetics to continuum fluid dynamics. Temporal profile of the reduced electric field (E/N), electronic density (n_e) and electronic temperature (T_e) are fixed to values mimicking experimental results from optical and electrical diagnostics of a spark-plug in air [11]. Conservation equations for mass and energy for the fluid are combined with Boltzmann equation for the electronic energy distribution function (EEDF) [22,23]. Splitting operators are used to tackle with the non-linearity of the source term and the differential equations for the fluid. Cylindrical coordinates are used due to the imposed axial symmetry of the problem. As mentioned elsewhere [17,18], strategies coupling the LTP equations with fluid models are computationally expensive; hence, a domain decomposition with a message passing interface (MPI) is used for multiprocessors parallelization of the calculations.

2. Theoretical framework

Methodological assumptions and physical considerations to model the title problem are here presented.

2.1. Electronic collisions

To describe the energy distribution of the electrons in the mixture, the electronic Boltzmann equation is used:

$$\frac{\partial f}{\partial t} + \vec{v}\cdot\nabla f - \frac{e}{m}\vec{E}\cdot\nabla_V f = C[f] \tag{1}$$

There, f is the electronic energy distribution function (EEDF), $\vec{v}$ is the electronic speed vector, $\vec{E}$ is the electric field, $C[f]$ accounts for changes in f due to the collisions with the species. e and m are the electron charge and mass, respectively. In this work, such a equation is solved following a steady state two terms approximation expansion reported elsewhere [24]. Cross sections for electronic collisions were obtained from Lxcat database [25]. The electron Boltzmann equation is coupled to an state specific kinetic model describing the concentration of vibrationally and electronically excited states of the $N_2 - O_2$ mixture [26]. These excited species can create structures in EEDF through the action of super-elastic collisions at low E/N values [27,28]. Yet, once the electronic temperature is parametrically introduced (see later), these modifications in EEDF are not expected to play a significant role in our model.

The electric power deposited to the gas, can be written as [26]:

$$\dot{E}_{ext} = eN_e\nu_e E \tag{2}$$

with N_e being the number of electrons in the unitary volume and ν_e the electron velocity. Such power is accordingly redistributed as [26]:

$$\dot{E}_{ext} = \dot{E}_{elc} + \dot{E}_{gas} + \dot{E}_{chem} \tag{3}$$

where $\dot{E}_{elc}$ stands for the translational power of the electrons, $\dot{E}_{gas}$ is the molecular species translational counterpart and $\dot{E}_{chem}$ is the released/absorbed power in chemical processes.

Each of these terms is represented by:

- $\dot{E}_{elc} = \frac{3}{2}\frac{d(N_eT_e)}{dt}$
- $\dot{E}_{gas} = \frac{1}{\gamma-1}\frac{d(NT_{gas})}{dt}$
- $\dot{E}_{chem} = \sum_i Q_i\frac{dN_i}{dt}$

which are related by the equation [26]

$$\frac{1}{\gamma-1}\frac{d(NT_{gas})}{dt} = eN_e\nu_e E - \frac{3}{2}\frac{d(N_eT_e)}{dt} - \sum_i Q_i\frac{dN_i}{dt} \tag{4}$$

being T_e the electronic temperature, γ, N and T_{gas} the gas adiabatic coefficient, density (in cm^{-3}) and temperature respectively, Q_i is the released/absorbed energy of the ith chemical processes and N_i the concentration of the ith species in the mixture. Notice inelastic and super-elastic collisions are also included in $\dot{E}_{ext}$ with positive or negative threshold energies, correspondingly.

2.2. Mathematical formalization of the model

The mathematical model is demanded to account for macroscopic and microscopic phenomena considered in electrical discharge in gases. Thus, is necessary to include the effects of collisions at the molecular level i.e., changes in internal energy and