



Modelling the impact of non-equilibrium discharges on reactive mixtures for simulations of plasma-assisted ignition in turbulent flows



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ABSTRACT

This article presents a model to describe the effects of non-equilibrium plasma discharges on gas temperature and species concentration, in the set of equations governing the combustion phenomena. Based on the results reported in the literature, the model is constructed by analysing the channels through which the electric energy is deposited. The two main channels by which the electrons produced during the discharge impact the flow are considered: (1) the excitation and the subsequent relaxation of electronic states of nitrogen molecules which leads to an ultrafast increase of gas temperature and species dissociation within the discharge characteristic time; and (2) the excitation and relaxation of vibrational states of nitrogen molecules which causes a much slower gas heating. The model is fully coupled with multi-dimensional flow balance equations with detailed transport coefficients and detailed combustion chemical kinetic mechanisms. This high level of NRP discharge modelling allows computing high Reynolds flows by means of Direct Numerical Simulations and, therefore, a better understanding of plasma-assisted ignition phenomena in practical configurations. A sequence of discharge pulses in air and methane–air mixture in quiescent and turbulent flow configurations are studied with this model. The results show the minor impact of the vibrational energy on mixture ignition and how the increase of the turbulence spreads this vibrational energy and intermediate combustion species around the discharge zone, minimizing the cumulative effect of multiple pulses. In contrast, the production of O atoms during the discharge has a strong impact on the ignition delays and ignition energies (number of discharge pulses). The results also underscore the impact of the initial turbulent flow Reynolds number and the spatial distribution of turbulent eddies, relative to the discharge channel, on the number of pulses needed to ignite the mixture.

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1. Introduction

New combustion technologies to reduce pollutants emissions rely on premixed or partially premixed lean combustion regimes (e.g. MILD combustion, Homogeneous Charged Compression Ignition, Exhaust Gas Recirculation). However, due to low gas temperatures, the application of these new technologies to industrial systems is limited by the difficulty to control ignition and flame stabilization over a wide range of operational conditions. Non-equilibrium plasmas produce highly reactive radicals, mostly O radicals in very short characteristic time scales, even at low mixture temperatures, and enhance combustion processes. The introduction of non-equilibrium plasmas in new technologies is

therefore a promising solution to reduce ignition delays and extend the flame stability domain. For instance, the beneficial effects of using non-equilibrium plasmas on premixed swirled burners, representative of aeronautical combustors, were recently observed in Barbosa et al. [1]. Several laboratory scale experimental studies [2–7], have shown that, among non-equilibrium plasmas, those produced by Nanosecond Repetitively Pulsed (NRP) discharges are an energy-efficient way to initiate and control combustion processes particularly when conventional ignition systems (spark ignition) are rather ineffective or too energy costly [7–9]. Mixture ignition and flame stabilization inside a supersonic combustion chamber is particularly difficult at high Mach numbers. Experimental results presented in [10,11] showed that the injection of non-equilibrium plasmas, produced with relatively small electric power, was very effective for flame stabilization under supersonic flow conditions, even at low static reactants temperature. More recent experimental studies have also shown the energy-efficiency of this kind of non-equilibrium plasmas produced by NRP

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discharges, on enhancing combustion processes [2,12,13]. The electric discharge energy is spent on ionization, excitation and dissociation of molecules, rather than just on a gas temperature increase [14–18]. Indeed, experiments and simulations in air at reduced electric fields $E/N > 100$ Td ($1 \text{ Td} = 10^{-17} \text{ V cm}^2$) have shown that, during NRP discharges, N_2 and O_2 molecules are excited to vibrational and electronic states [16,19–23], usually not in thermal equilibrium with the translational mode. The relaxation of these excited molecules by collisional quenching reactions with molecules can result in an ultrafast (time scales of nanoseconds) increase of radicals and gas temperature inside the discharge channel. In typical conditions, up to 50% of molecular oxygen can be dissociated in the inter-electrode region [18,22]. Hydroxyl radical is also formed along with hydrogen atoms when NRP discharges are applied to hydrocarbon–air mixtures, as discussed in [23,24]. Such high concentration of radicals has a positive effect on both ignition phenomena and flame stabilization [2,5,6,25–30].

The modelling of ignition by conventional spark (thermal plasmas) has been largely investigated in [31–33]. In these works, 2-D numerical simulations in quiescent flow conditions with detailed chemistry, including ionization processes, were used to study the early development of the flame kernel and the fluid motion induced by spark discharges. 3-D DNS with simplified chemistry have been then performed to study the impact of different turbulence intensities on spark ignition in inhomogeneous mixtures [34]. However, few studies [28,35] have been pursued on the multi-dimensional modelling of ignition by NRP discharges. The phenomena occurring in NRP discharge-assisted combustion are still poorly understood, especially the gas dynamics and the thermochemical coupling between the discharge and the reactive flow. Some numerical simulations have recently been conducted to study the impact of NRP discharges on the flame and mixture ignition. Coupled plasma and combustion kinetic mechanisms have been used for that purpose. As an example, [28] simulated the plasma-assisted stabilization of a laminar premixed methane/air flame. Numerical investigations of H_2 /air mixture ignition by NRP discharges in quiescent conditions were performed in [23,35].

The numerical studies presented in the literature are limited to 1-D and 2-D simulations in quiescent flow conditions. The problem complexity increases in practical configurations as the ignition phenomena are also controlled by the flow and mixing field characteristics in and around the discharge channel. Furthermore, in NRP discharges, mixture ignition occurs due to the cumulative effect of successive pulses and not due to a single pulse energy addition, as in conventional spark ignition. The radicals formed by each pulse will enhance chain-branching reactions, increasing the local concentration of intermediate combustion species and, therefore, the mixture reactivity pulse after pulse. After a given number of pulses, the mixture ignites and a self-sustained flame kernel is developed. In turbulent flows, the high-temperature and highly-reactive kernel formed by each pulse may be stretched and convected away from the discharge zone before the next pulse, yielding a non-uniform distribution of temperature and concentration of radicals inside the discharge zone at the beginning of the following pulse. Depending on the characteristic time and length scales of turbulence and on the pulse repetition frequency, the cumulative effect of repetitively pulsed discharges may be minimized and, therefore, the number of pulses needed to ignite the mixture, as well as the ignition delay, may significantly increase.

Direct Numerical Simulations (DNS) is a powerful research tool to understand these turbulence/plasma-assisted ignition interactions. However, the computational cost of fully coupled non-equilibrium plasma and combustion detailed chemistry and high Reynolds flow simulations is prohibitive. In addition, the uncertainties associated to the coupling of these chemical models are still high.

The aim of the present paper is to provide a general phenomenological model for NRP discharges-assisted ignition, capable of taking into account the effects of non-equilibrium plasmas on the gas temperature and species concentration in the set of multicomponent reactive flow balance equations [36] governing the combustion phenomena. The model described next, is a high level modelling of non-equilibrium plasmas that avoids including detailed non-equilibrium plasma kinetics and, therefore, reduces the computational costs of high Reynolds flows DNS computations. Yet, it captures the main channels and their characteristic time scales through which the electric energy of the discharge is deposited into the flow. Nevertheless, detailed chemical kinetic model for hydrocarbons–air mixtures is considered, as well as multi-species transport model to capture the transient characteristics of NRP discharges-assisted ignition.

In the following sections the set of conservative equations of reactive systems in thermal equilibrium is briefly described. These conservative equations are then modified according to the proposed phenomenological NRP discharge model. The general model closure is presented and an analytical closure is proposed. Finally, numerical results of NRP discharges-assisted ignition are analysed for lean methane–air mixtures in quiescent and turbulent flow conditions.

2. Governing equations for plasma-assisted combustion

2.1. Reactive flow equations without plasma

The conservation equations for multicomponent reacting systems, where N_{sp} species are in thermal equilibrium, can be written as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0 \quad (1)$$

$$\frac{\partial(\rho u_j)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} \quad (2)$$

$$\frac{\partial(\rho e)}{\partial t} + \frac{\partial(\rho u_i e)}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial(\sigma_{ij} u_i)}{\partial x_j} \quad (3)$$

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho u_i Y_k)}{\partial x_i} = -\frac{\partial(\rho V_{k,i} Y_k)}{\partial x_i} + W_k \dot{\omega}_k^c \quad (4)$$

where ρ is the density, u_i the velocity component in x_i spatial direction, p the pressure and τ_{ij} the viscous tensor. In Eq. (3), e refers to the gas total energy per unit mass defined as the sum of kinetic, thermal and chemical energies as follows:

$$e = \frac{1}{2} u_i u_i + \sum_{k=1}^{N_{sp}} (e_{sk} + \Delta h_{f,k}^0) Y_k \quad (5)$$

where e_{sk} and $\Delta h_{f,k}^0$ are the sensible energy and enthalpy of formation of the k th species, respectively. Y_k and W_k are the mass fraction and molar mass of the k th species, respectively. In Eq. (4) the diffusion velocity of the k th species, $V_{k,i}$, is computed assuming complex mixture average transport phenomena as in [37]. $\dot{\omega}_k^c$, the molar production rate of the k th species due to combustion reactions, reads:

$$\dot{\omega}_k^c = \sum_{i=1}^I (v_{ki}'' - v_{ki}') Q_i \quad (6)$$

$$\text{with } Q_i = K_{fi} \prod_{j=1}^{N_{sp}} [X_j]^{v_{ji}'} - K_{ri} \prod_{j=1}^{N_{sp}} [X_j]^{v_{ji}''}$$

where Q_i is the rate of progress of the i th reaction, $[X_j]$ is the molar concentration of the j th species and K_{fi} and K_{ri} are the rate

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