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Simulations of planar non-thermal plasma assisted ignition at atmospheric pressure

Tiernan A. Casey [a,*], Jie Han [b], Memdouh Belhi [b], Paul G. Arias [c], Fabrizio Bisetti [b,d], Hong G. Im [b], Jyh-Yuan Chen [a]

[a] Department of Mechanical Engineering, University of California, Berkeley, CA 94720, USA
[b] Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia
[c] Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI 48109, USA
[d] Department of Aerospace Engineering and Engineering Mechanics, University of Texas at Austin, Austin, TX 78712-1085, USA

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Abstract

The opportunity for ignition assistance by a pulsed applied voltage is investigated in a canonical one-dimensional configuration. An incipient ignition kernel, formed by localized energy deposition into a lean mixture of methane and air at atmospheric pressure, is subjected to sub-breakdown electric fields (E/N ≈ 100 Td) by a DC potential applied across the domain, resulting in non-thermal behavior of the plasma formed during the discharge. A two-fluid approach is employed to couple thermal neutrals and ions to the non-thermal electrons. A two-temperature plasma mechanism describing gas phase combustion, excitation of neutral species, and high-energy electron kinetics is employed to account for non-thermal effects. Charged species transported from the ignition zone drift rapidly through the domain, augmenting the magnitude of the electric field in the fresh gas during the pulse through a dynamic-electrode effect, which results in an increase in the energy of the electrons in the fresh mixture with increasing time. Enhanced fuel and oxidizer decomposition due to electron impact dissociation and interaction with excited neutrals generate a pool of radicals, mostly O and H, in the fresh gas ahead of the flame's preheat zone. In the configuration considered, the effect of the nanosecond pulse is to increase the mass of fuel burned at equivalent times relative to the unsupported ignition through enhanced radical generation, resulting in an increased heat release rate in the immediate aftermath of the pulse.

Keywords: Plasma assisted combustion; Electric field; Ignition

1. Introduction

Flames act as weakly ionized plasmas, generating weak self-induced electric fields due to local charge separation over small distances of length

* Corresponding author.
E-mail address: tcasey@berkeley.edu (T.A. Casey).

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comparable to the reaction zone. As such, externally applied electric fields have the potential to augment flame behavior non-intrusively. Investigations of applied electric fields have shown the ability to enhance burning velocities [1], stabilize flames near flammability limits [2], and support ignition [3]. If the strength of the electric field is high enough to produce a sufficient level of non-thermal electrons, it is understood that enhancement occurs due to fragmentation of fresh gas molecules resulting in an increased population of reactive intermediates such as O and H [4].

In the context of ignition, simulations of multiple nanosecond pulsed plasma discharges in n-heptane have been shown to decrease ignition delay time significantly [5] through the generation of non-thermal electron plasma in a breakdown process. Furthermore, it has been demonstrated experimentally that microwave frequency electric field excitation reduces the flame development time of inductive spark ignition of methane–air mixtures in a constant volume chamber [3]. The experiments in Ref. [3] suggested that enhancement arises as a result of flame wrinkling due to the perturbative effect of the applied field, indicating that both chemistry and hydrodynamics play important roles. As a practical concern to ignition strategies based on breakdown discharges, increasing the energy of the discharge itself (e.g. increasing the spark energy) can have undesirable effects in terms of device wear due to electrode ablation, which presents significant challenges for igniting lean high-pressure mixtures typical of future advanced engine technologies. As such, it is desirable to investigate means of ignition and ignition-support that occur in the sub-breakdown regime that deliver necessary performance, while avoiding excessive device wear. Furthermore, with increasing interest in using natural gas as a clean fuel alternative, the plasma-assisted ignition of methane is an important process due to the difficulty of initiating the first H abstraction from CH_4. Analysis of non-thermal electron transport properties and energy coupling to bulk mixtures in the sub-breakdown regime in premixed methane–air flames suggests a breakdown threshold of approximately 150 Td [6]. The purpose of this paper is to investigate sub-breakdown electric field assisted combustion of an established ignition kernel at higher pressure than is typically employed when simulating plasma combustion, in order to shed light on the multiple electrodynamic and chemical processes involved in increasing the overall mass of fuel burned as a result of a nanosecond pulse.

2. Configuration and modeling

The physical domain is a 1 cm region filled with premixed methane and air (79% N_2 and 21% O_2 by volume) with equivalence ratio 0.5 at 1 atm. The boundaries are open fluid outlets with imposed potentials, conceptually representing wire mesh electrodes unobstructive to fluid. This configuration is chosen such that the ignition event occurs at constant pressure. The nanosecond pulse is applied with positive 4.5 kV and negative 4.5 kV on the left and right electrodes respectively, for a total of 9 kV across the domain. Pulses are applied for up to a maximum of 35 ns. These pulse parameters are chosen to represent the typical values employed when applying nanosecond pulse discharges to ignite or enhance the ignition of reacting mixtures [7].

2.1. Models and approximations

The two-temperature methane–air plasma mechanism is built upon the GRI-Mech 3.0 methane–air mechanism [8]. Ion chemistry pathways containing thermal electrons are added following the mechanism in Ref. [9]. The rates of inelastic electron impact reactions, resulting in the decomposition of neutral molecules, ionizations, and excitations, are precomputed using a representative lean unreacted methane–air mixture and parameterized by the electron temperature in the CHEMKIN framework using Janev, Langer, Evans, and Post [10] fits. Using a representative lean mixture to pre-calculate the rates is justified by the fact that electron/neutral interactions that control the overall evolution of the system are expected to take place in the fresh gas only, where the electron temperature is sufficiently high. Collision cross-section data for these electron neutral interactions are obtained from the LXCat database [11,12]. The complete reaction list is available in Ref. [12]. Mechanism reduction is performed using ignition delay targets via the TSA algorithm [13] for lean methane–air mixtures at 300 K, 1 atm, using a variety of initial electron densities and electric fields, thus reducing the detailed mechanism from 106 species and 2141 reactions to 45 species and 514 reactions. The mechanism, including ground state and excited neutral species, e.g. $N_2(B^3)$, $N_2(C^3)$, $N_2(a')$, $O_2(a^1)$, $O(^1D)$, electron, and several ions, e.g. CH_4^+, O_2^+, O_2^-, N_2^+, HCO^+, H_3O^+, is available as Supplementary material, with validation performed against available ignition data under discharge conditions [14].

2.2. Numerics

A compressible reacting flow solver employing high-order central differencing and an explicit Runge–Kutta time integration scheme is used to advance the conservation equations governing the planar ignition problem. The outlet boundaries are implemented in the governing equations using a non-reflecting treatment based on characteristics [15]. The Poisson equation for Gauss's Law for the electric potential is solved using a geometric multigrid scheme. Electron fluxes are specified in the

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