Vaporization and gas-phase combustion of electrosprayed heptane in a small chamber

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ABSTRACT

A model is formulated of the vaporization and gas-phase combustion of a dilute spray of electrically charged droplets of heptane with a coflow of preheated air in a mesoscale combustion chamber. The model includes an Eulerian/Lagrangian treatment of the gas and the droplets, an equilibrium vaporization submodel, and a single step mechanism for the combustion of heptane vapor. The effects of the inlet air temperature, the fuel flow rate and the overall equivalence ratio are investigated. Two combustion modes are described for globally lean systems. When rapid vaporization leads to a kernel of high fuel vapor concentration, combustion may begin before the fuel diffuses in the air coflow, in a layer of intense reaction that locally depletes the oxygen and leaves behind a region of high temperature fuel vapor surrounded by a diffusion flame. When the vaporization rate and the maximum fuel vapor concentration are decreased by increasing the size of the droplets or the inlet velocity of the air, combustion occurs in a lifted lean premixed flame after the fuel has fully vaporized and mixed with the air coflow. Ignition and extinction conditions are discussed. The degree of accuracy that can be expected from the single step reaction mechanism is also discussed.

1. Introduction

The energy density of liquid hydrocarbons is about 100 times larger than that of the currently available batteries, which makes power-generation systems based on the combustion of these fuels a promising technology in the quest for better power sources for portable equipment and other applications [1,2]. Many conventional techniques and operation principles of macroscopic combustion systems become impractical for miniaturized system, although the extent of the modifications required is smaller for devices with overall dimensions of several centimeters intended to generate powers of 10–100 W, referred to as mesoscale devices, than for smaller microdevices. Difficulties are also smaller when the liquid fuel is vaporized and burned under steady conditions in a chamber coupled to a direct energy conversion module such as a thermoelectric or thermovoltaic generator, or to a Stirling engine, than when conventional engines using classical thermodynamic cycles are miniaturized. Only mesoscale, steady combustion devices are considered here.

Reduction or disappearance of turbulent mixing, heat transfer, and flame wrinkling in small systems are important differences with their macroscopic counterparts, though Wu et al. [3] were

able to stabilize a non-premixed flame in a mesoscale combustor by means of a vortex flow that extends the concept of whirl combustion of macroscopic combustors. Increased heat losses due to the augmented surface-to-volume ratio is another effect of miniaturization, which increases the vaporization and chemical times, and may compromise combustion efficiency. A third effect of miniaturization is the reduction of the residence time, which should be larger than the vaporization and chemical times in order to achieve complete combustion and prevent the emission of pollutants such as CO and unburned hydrocarbons.

The notion of heat recuperation or excess enthalpy for miniature devices, whereby part of the thermal enthalpy of the combustion products is used to preheat the reactants, was first studied by Weinberg and coworkers [4–6] and later extended to many meso- and micro-scale combustors to achieve steady combustion under conditions of large heat losses or lean mixtures, which would otherwise result in extinction.

With exceptions [7], the liquid fuel must be atomized into small droplets that have to disperse and vaporize in the short residence time available. Flow-blurring atomizers relying on aerodynamic forces have been used by Sadasivuni and Agrawal [8] to atomize kerosene in an annular heat recuperator surrounding a cylindrical combustion chamber, where the droplets vaporize and the vapor mixes with the air before entering the chamber. Gomez and coworkers used electrosprays to atomize JP8 into electrically

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charged droplets in their mesoscale combustor [9–12]. Electrosprays have also been used in combination with flame-attaching grids in narrow tubes [13,14].

Catalytic combustion may improve combustion stability and reduce pollutant emission in the conditions of short residence times and low temperature typical of small scale combustors. Catalytic combustion in a series of catalyst-coated grids at the outlet of a chamber where fuel droplets vaporize in a coflow of preheated air has been successfully used by Gomez and coworkers [9–12]. Despite the favorable properties of catalytic combustion, gas-phase combustion may still retain some advantages in excess enthalpy mesoscale systems, stemming from their volumetric rather than superficial character, provided heat recuperation overcomes heat losses to a sufficient extent to make gas-phase combustion possible.

The purpose of this paper is to numerically study the feasibility of gas-phase combustion in a small chamber similar to those used by Deng et al. [11] in their experiments with multiplexed electrospray sources and catalytic grids. A two-way coupled model of the dispersion, vaporization and gas-phase combustion of a single electrospray from a multiplexed source in a coflow of hot air has been developed which is based on the model proposed in Ref. [15] to study the heating and vaporization of a spray of heptane droplets in a chamber. This model, which in turn builds on a model of Arumugham-Achari et al. [16], consists of a combination of an Eulerian mesoscale description of the gas and a Lagrangian description of the spray of droplets, carried out with a method of particles. The flow in the chamber is laminar (Reynolds number in the range 100–500), which makes the results free from the uncertainties of turbulence modeling. The model relies on the validation of Ref. [16] (see also references therein) against an individual electrospray source, and on the previous computations in Ref. [15], which were qualitatively compared to the experiments of Refs. [9–12] to the limited extent permitted by the available data. The previous model is extended here to account for the combustion of heptane vapor by means of a single step mechanism calibrated to reproduce the ignition delay times measured for heptane–air mixtures in conditions similar to those found at ignition in the chamber. The degree of accuracy that can be expected from this drastic simplification of the heptane–air kinetic mechanism depends on the structure of the computed solutions and is discussed in Section 3. The model of Ref. [15] is also improved by using a more realistic droplet heating and vaporization submodel.

2. Formulation

Kyritsis et al. [9] and Deng et al. [11] used two-dimensional periodic arrays of identical electrospray sources to inject small, nearly monodisperse, electrically charged fuel droplets through one of the bases of a cylindrical chamber. To approximately model this system, the invariance of the array under certain discrete angle rotations is replaced here by axial symmetry. A single electrospray source of the periodic array is considered that injects droplets and a coflow of air through a circular orifice of radius r_h at one of the bases of a cylindrical chamber, and symmetry conditions (see Eq. (16) below) are applied at a distance R from an axis through the center of the orifice, as sketched in Fig. 1. The source generates Φ droplets per unit time with radius a_0, electric charge e_0, temperature T_0 and velocity v_{p_I}, and the air enters the chamber with velocity v_{g_I} and temperature $T_1 > T_0$ through the same orifice. The droplets heat up and vaporize in the chamber due to the heat transferred by conduction from the hot air, generating fuel vapor that reacts with the oxygen of the air. The combustion products leave the chamber through the opposite base, at a distance L from the injection orifice.
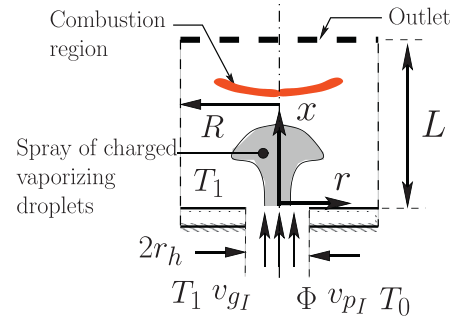

Fig. 1. Schematic of the investigated configuration with indication of relevant dimensions. The grey area represents the vaporizing spray. The heptane vapor burns in a combustion region represented by a red line in the figure. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

A dilute spray is considered. The mean distance between droplets, ℓ_d, is large compared to the radius of a droplet and small compared to the size of the chamber; i.e. $a_0 \ll \ell_d \ll L$. In these conditions, an Eulerian, mesoscale description of the gas flow [17] combined with a Lagrangian, particle-in-cell description of the droplets [18,19] can be used.

2.1. Droplets

The droplets interact mainly through the surrounding gas and through the electric field induced by the electric charges they carry. Direct interactions between droplets are rare events when $a_0 \ll \ell_d$.

The mass, momentum and energy conservation equations for droplet i are

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i, \quad m_i \frac{d\boldsymbol{v}_i}{dt} = \boldsymbol{F}_i + e_i \boldsymbol{E}_i,$$

$$\frac{dm_i}{dt} = -\dot{m}_i, \quad m_i c \frac{dT_i}{dt} = q_{g_i} - \dot{m}_i L_v, \tag{1}$$

where $\boldsymbol{x}_i(t)$ and $\boldsymbol{v}_i(t)$ are the position and velocity of the center of the droplet, $m_i = \frac{4}{3}\pi \rho_l a_i^3$ with ρ_l the density of the liquid and $a_i(t)$ the radius of the droplet, $T_i(t)$ is the temperature of the droplet, which is approximately uniform because the thermal conductivity of the liquid is large compared to the thermal conductivity of the gas, and $e_i(t)$ is the electric charge of the droplet, whose time evolution is computed as described below. In these equations $\boldsymbol{F}_i$ is the force exerted by the gas on the droplet, q_{g_i} is the heat flux reaching the droplet, and $\dot{m}_i$ is the vaporization rate. These quantities depend on the radius, velocity and temperature of the droplet, and on the local velocity, $\boldsymbol{v}_{g_i}$, temperature, T_{g_i}, and composition of the gas seen by the droplet. Finally c and L_v are the specific heat and the latent heat of vaporization of heptane, and $\boldsymbol{E}_i$ is the electric field at the position of the droplet.

As a case representative of the conditions of interest (see Section 2.3), the vaporization time of a droplet of heptane of initial radius $a_0 = 8.75$ μm injected with initial velocity $v_{p_I} = 10$ m/s and temperature $T_0 = 293$ K in quiescent air at a pressure of 3 atm and various temperatures has been computed. The model of Abramzon and Sirignano [20], the correlations of Clift et al. [21] for the drag coefficient, Nusselt and Sherwood numbers, and the 1/3 rule for the average gas properties have been used to evaluate the right-hand sides of equations (1) without electric force. The simple power laws $\mu_g/\mu_{g_0} = k_g/k_{g_0} = (T_g/T_0)^\kappa$ with $\kappa = 0.75$ are assumed for the viscosity and thermal conductivity of the gas, together with constant values of the Prandtl and Lewis numbers. The results, shown by the solid curve in Fig. 2(a), are very similar to the vaporization time for a droplet at rest with the same initial and gas