



The effects of multicomponent fuel droplet evaporation on the kinetics of strained opposed-flow diffusion flames

Chenguang Wang^a, Anthony M. Dean^{a,*}, Huayang Zhu^{b,c}, Robert J. Kee^b

^a Chemical and Biological Engineering, Colorado School of Mines, Golden, CO 80401, USA

^b Mechanical Engineering, Colorado School of Mines, Golden, CO 80401, USA

^c College of Petroleum Engineering, Xi'an Shiyou University, Shaanxi 710065, PR China

ARTICLE INFO

Article history:

Received 23 July 2012

Received in revised form 9 October 2012

Accepted 13 October 2012

Available online 14 November 2012

Keywords:

Multicomponent fuel droplets

Fuel pyrolysis

Opposed-flow nonpremixed flame

Modeling

ABSTRACT

With the increasing use of alternative fuels, it becomes important to understand the impacts of their different chemical and physical properties on combustion processes. The objective of this paper is to explore the impact of the vaporization of a multicomponent liquid fuel on the combustion kinetics using an opposed-flow diffusion flame model. The model fuel consisted of a *n*-heptane, *n*-dodecane, and *n*-hexadecane mixture, selected to represent a Fischer–Tropsch fuel. A computational model is developed to describe the multicomponent vaporization process. Gas-phase chemical kinetics is modeled using a reduced mechanism containing 196 species. Results compare pre-vaporized fuel streams with those containing monodispersed initial droplet sizes of 20, 25 and 30 μm . The separation distance between the fuel and air inlets is either 5 and 10 mm. In all cases the fuel is carried in nitrogen, the pressure is 10 atm, and the fuel and air inlet velocities are 1 m s^{-1} . The fuel loading is set to achieve an overall equivalence ratio of unity. Results show that the finite evaporation rate significantly impacts the chemical kinetics. In particular, if the combination of separation length, stream velocity, and fuel volatility is such that fuel droplets penetrate into the higher temperature region near the flame-front, the rapid increase in evaporation rate significantly enhances the local vapor phase fuel mole fraction. The high temperature increases reaction rates, leading to higher peak temperatures as well as increased pyrolysis in the pre-flame region. For example, the peak temperature predicted for 30 μm droplets is 330 K higher than that for the pre-vaporized case. This increase occurs in spite of an initial decrease in temperature as a consequence of fuel vaporization. A similar effect is observed for the pre-flame pyrolysis products; ethylene, acetylene, and butadiene all increase by about a factor of two for the 30 μm droplet case. The implications of these findings regarding the use of alternative fuels is discussed.

© 2012 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

1. Introduction

The objective of this paper is to analyze the impact of the vaporization of a multicomponent fuel on the kinetics of non-premixed strained flames. Such flames occur in diesel engines and turbines, where the vaporization process is most closely connected to the combustion event. Analysis of these flames is especially important with the advent of alternative fuels that might have significantly different chemical and physical properties than conventional ones. Such fuels (e.g., biomass-derived Fischer–Tropsch fuels) might have substantially different hydrocarbon compositions, such as a higher concentration of branched alkanes and different boiling point curves than petroleum-derived diesel fuels [1]. A convenient framework in which one can examine this coupling of physical and

chemical properties of the fuel is an opposed-flow diffusion flame (Fig. 1). This provides the advantage of a well-defined flow field that can be modeled as a one-dimensional boundary value problem. As a result, this device is often used for combined experimental/modeling efforts, such as the analysis of pre-vaporized fuels [2,3]. Different models have been developed to predict the behavior of fuel evaporation [4–6]. In this work such efforts are extended by explicitly coupling the description of the evaporation of a multicomponent model fuel with the subsequent gas-phase kinetics of its components. To our knowledge, this is the first instance of such an analysis in an opposed flow diffusion flame. Of course, such coupling is frequently accomplished in CFD codes such as KIVA or Fluent to describe the combustion kinetics in engines and turbines [7,8]. In this work the goal is to develop a more explicit understanding of the impact of differential vaporization on the detailed kinetics in a diffusion flame environment. With a simpler physical configuration to model, it is possible to work with a more complex kinetic mechanism.

* Corresponding author. Tel.: +1 303 273 3643; Fax: +1 303 273 3730.

E-mail address: amdean@mines.edu (A.M. Dean).

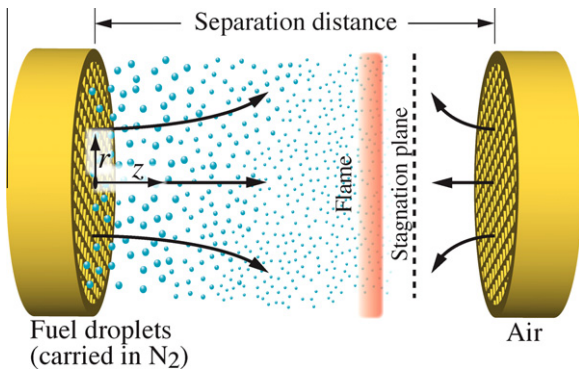


Fig. 1. Illustration of the opposed-flow nonpremixed-flame configuration.

This paper is an extension of an earlier effort [9] in which various single-component fuels, ranging from heptane to diesel fuel, were modeled with a very simplified kinetic mechanism. The vaporization model is extended to account for a multicomponent fuel, and a much more detailed kinetic mechanism is used to explore the impact of the various fuel components on the kinetics within the diffusion flame. A three-component fuel, consisting of *n*-heptane, *n*-dodecane, and *n*-hexadecane is used to create a simple surrogate for a Fischer–Tropsch fuel. This combination provides a wide range of vaporization rates to better define the impact of this parameter. A reduced version of the comprehensive *n*-alkane mechanism developed by Westbrook and co-workers [10] is used to predict the flame structure. The results of using monodispersed droplet sizes of 20, 25 and 30 μm are compared to those obtained using pre-vaporized fuel. The strain rate is varied by changing the separation distance of the inlet streams. This change has the added advantage of exploring the impact of different residence times of the fuel vapor in the hot nitrogen stream prior to entering the flame-front region.

Calculations are carried out at a pressure of 10 atm, with room temperature liquid fuel droplets evaporating into a 950 K nitrogen stream. These conditions approximate those encountered when fuel is injected into a diesel engine. The results suggest that the variation in evaporation rate of the various components can produce surprisingly large variations in flame behavior, leading to large changes in the peak flame temperature as well as to substantial differences in the amount of pre-flame chemistry. These results are most pronounced when the evaporation of the heavier components occurs near the flame-front. The increased temperature in that region leads to a much higher rate of vaporization, producing an enhancement of the local fuel vapor mole fraction that increases the reaction rate.

2. Mathematical model

As discussed in previous models, the overall approach is based upon an iterative algorithm, solving gas-phase conservation equations in an Eulerian framework and droplet tracking in a Lagrangian framework [9,11]. The coupling is accomplished by source terms in the gas-phase equations that are derived from the droplet equations. The droplet equations depend upon the local gas-phase environment.

2.1. Eulerian gas-phase conservation equations

The conservation equations for gas-phase steady-state strained laminar axisymmetric opposed-flow flames in similarity form are well known [9,12–17]. A detailed derivation of the stagnation-flow similarity equations may be found in Kee et al. [17]. After incorporating the source terms associated with droplet vaporization, the equations can be summarized as

$$\frac{d(\rho u)}{dz} + 2\rho V = S_M, \quad (1)$$

$$\rho u \frac{dV}{dz} + \rho V^2 = -A_r + \frac{d}{dz} \left(\mu \frac{dV}{dz} \right) + S_V - VS_M, \quad (2)$$

$$\rho \sum_{k=1}^K (u + V_k) Y_k c_{p,k} \frac{dT}{dz} = \frac{d}{dz} \left(\lambda \frac{dT}{dz} \right) - \sum_{k=1}^K \dot{\omega}_k W_k h_k - Q_{\text{rad}} + S_T - \sum_{k=1}^K h_k S_k, \quad (3)$$

$$\rho u \frac{dY_k}{dz} + \frac{d(\rho Y_k V_k)}{dz} = \dot{\omega}_k W_k + S_k - Y_k S_M. \quad (4)$$

The axial coordinate z is the independent variable. The dependent variables include the axial velocity u , temperature T , and species mass fractions Y_k . The scaled radial velocity $V = v/r$ is also a dependent variable, with v and r being the radial velocity and radial coordinate, respectively. The mass density ρ is evaluated using an ideal-gas equation of state. Thermodynamic parameters include the species molar weights W_k , specific heats $c_{p,k}$, and enthalpies h_k . The pressure-gradient parameter $A_r = (1/r)(dp/dr)$ is an eigenvalue that is determined during the course of the solution. Transport properties include mixture viscosity μ and thermal conductivity λ . The diffusion velocity is represented as

$$\mathbf{V}_k = \frac{1}{X_k \bar{W}} \sum_{j \neq k}^K W_j D_{kj} \nabla X_k - \frac{D_k^T}{\rho Y_k} \frac{\nabla T}{T}, \quad (5)$$

where X_k are the mole fractions, D_{kj} is the matrix of ordinary multicomponent diffusion coefficients, and D_k^T are the thermal diffusion coefficients [17]. The molar production rates of gas-phase species by chemical reaction are represented as $\dot{\omega}_k$. Radiation heat transfer between gaseous species and the environment is represented as Q_{rad} [9,18]. Thermodynamic properties and reaction rates are evaluated through CHEMKIN software interfaces [17].

As noted above, the purely gas-phase equations are extended to include source terms associated with droplet vaporization. These terms include S_M representing the net gas-phase mass addition, S_k representing the source of gas-phase species k , S_V representing the source of radial momentum, and S_T representing the source of thermal energy. The quantitative evaluation of these terms is discussed in a subsequent section.

2.2. Lagrangian droplets dynamics

The present model assumes slow-vaporization-limit behavior [6], neglecting any spatial variations within individual droplets. Thus, the droplet trajectories, mass, temperature, and composition can be represented using a system of Lagrangian ordinary differential equations as

$$\frac{dz_d}{dt} = u_d, \quad \frac{dr_d}{dt} = r_d V_d, \quad (6)$$

$$\frac{dm_d}{dt} = \dot{m}_d, \quad (7)$$

$$\frac{du_d}{dt} = \frac{F_z}{m_d}, \quad \frac{dV_d}{dt} = -V_d^2 + \frac{F_r}{m_d r_d}, \quad (8)$$

$$\frac{dT_d}{dt} = \frac{\dot{q}_d}{m_d c_{p,d}}, \quad (9)$$

$$\frac{dY_{d,k}}{dt} = \frac{\dot{m}_d}{m_d} (\epsilon_k - Y_{d,k}), \quad (10)$$

$$\frac{d\mathcal{F}}{dt} = -2\mathcal{F}V_d. \quad (11)$$

Download English Version:

<https://daneshyari.com/en/article/10264725>

Download Persian Version:

<https://daneshyari.com/article/10264725>

[Daneshyari.com](https://daneshyari.com)