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Investigation of soot transport and radiative heat transfer in an ethylene jet diffusion flame

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Abstract

Numerical and experimental investigations highlighting the heat and mass transfer phenomena in a laminar co-flowing jet diffusion flame have been carried out. The fuel under consideration is ethylene, with ambient air as the co-flowing oxidizer. The diffusion flame is modeled using a 17-step reduced reaction mechanism with finite rate chemistry and the effects of soot on the radiative heat transfer of the flame have been demonstrated. Soot growth and oxidation processes are studied using a two-equation transport model, while the radiative heat transfer is modeled using the P1 approximation. An in-house finite volume code has been developed to solve the axi-symmetric Navier–Stokes equations in cylindrical coordinates, along with the soot mass fraction, soot number density, energy and species conservation equations. Comparison of predictions with experimental results shows reasonable agreement with regard to the flame height and temperature distribution. A parametric study is also presented, which illustrates the effects of the fuel jet Reynolds number and the flow rate of co-flow air.

Keywords: Numerical and experimental investigations; Laminar; Co-flow; Ethylene jet diffusion flame; Soot; Radiation

1. Introduction

Soot produced in a flame has both beneficial and detrimental effects. In applications like furnaces, the radiation heat transfer associated with soot particles provides a more uniformly heated environment. On the other hand, the presence of un-oxidized soot particles in any combustion exhaust is viewed as environmental pollution. Soot formation is significant, particularly in the case of unsaturated hydrocarbons with double and triple carbon–carbon bond structure (for example ethylene, acetylene and benzene). The present work investigates the effects of soot formation and oxidation on radiative heat transfer from the flame as well as on the overall combustion process, in an ethylene diffusion flame.

Several experimental and numerical studies are available on the modeling of diffusion flames [1–4]. Mitchell et al. [5] studied the laminar diffusion flame of methane in air and predicted the distributions of temperature, velocity and species concentrations. More recently, the application of detailed chemical kinetic models has become an important tool in combustion simulation [6]. Frenklach and co-workers [7] considered about 600 elementary reaction steps and 200 species, including those related to soot chemistry, during acetylene pyrolysis. Such detailed kinetic models, however, are cumbersome to handle due to the large computational times involved. A reduced reaction mechanism for methane combustion has been discussed by Peters and Kee [8]. Various semi-empirical soot models have also been developed, improved and used extensively in laminar diffusion flames [9–12]. Guo et al. [13] have investigated the influence of thermal diffusion on soot formation in an ethylene flame. Ethylene diffusion flame with co-flow air has been studied using a detailed 64-step reaction mechanism by Kennedy et al. [14]. The formation and growth of soot particles in co-annular ethane and ethylene diffusion flames have been studied by Santoro et al. [15],

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Nomenclature

a	absorption coefficient, m^{-1}
A_s	soot surface area per unit volume, m^{-1}
Ca	soot agglomeration rate constant
C_{min}	number of atoms per soot particle
C_P	specific heat, kJ/kg K
d	diameter, m
D	mass diffusivity, m^2/s
E_a	activation energy, kJ/kmol
Fr	Froude number ($u_j/g^{0.5}d_j^{0.5}$)
g	acceleration due to gravity, 9.81 m/s^2
h	specific enthalpy, kJ/kg K
k	thermal conductivity, W/m K; also, rate constant of a reaction
K	Boltzmann constant, J/K
L	length of flame, m
M	molar mass, kg/kmol
N	number density of soot
N_A	Avogadro's number, particles/kmol
p	pressure, N/m^2
Pr	Prandtl number (υ/α)
q	heat flux (W/m^2)
r	radial coordinate, m; also, reaction rate.
Re	Reynolds number ($\rho u_j d_j/\mu$)
R_u	universal gas constant
Sc	Schmidt number (υ/D)
S_m, S_n	source terms for soot mass and number density
t	time, s
T	temperature, K
u, v	axial and radial velocity components, m/s
Y	mass fraction
z	axial coordinate measured from jet exit, m

Subscripts and superscripts

i	species i
j	fuel jet inlet conditions
m, mix	corresponding to gaseous mixture
ref	reference quantities at free stream conditions
R	radiation
s	soot
(S)	solid state
T	thermophoretic
*	dimensional quantities

Greek symbols

ρ	density, kg/m^3
μ	coefficient of viscosity, N s/m^2
$\dot{\omega}$	mass based reaction rate , kg/m^3 s; mass rate of production
θ	angular coordinate
σ,τ	normal and shear stress fields, N/m^2

using laser extinction/scattering technique for particle size measurement.

Although a large number of studies have been carried out on diffusion flames and several soot models have been developed recently, there is still a strong need to develop a coupled soot model including radiative heat transfer effects, for the analysis of unsaturated hydrocarbon combustion. It is also desirable to arrive at suitable reduced kinetic mechanisms that provide accurate predictions of the overall combustion process, while being computationally very economical. Such reduced chemistry models will be useful for conducting detailed parametric studies and for highlighting the effects of important process parameters, in practical combustion problems. With these objectives in mind, an axi-symmetric diffusion flame of ethylene with co-flow air has been studied experimentally and numerically in the present work. The numerical predictions have been validated with experimental measurements at different fuel jet Reynolds numbers and mass flow rates of co-flow air.

2. Mathematical formulation

The physical configuration of an ethylene jet diffusion flame with co-flow air is shown in Fig. 1. Ethylene gas is injected vertically through a central pipe and the co-flowing air stream enters through the annular area surrounding the fuel pipe. In the numerical model of the present study, the flow is assumed to be axi-symmetric and laminar. An ideal gas mixture formulation is used to account for the variations in density and other physical/transport properties, with temperature and concentration. Second order phenomena like Soret and Dufour effects have been neglected.

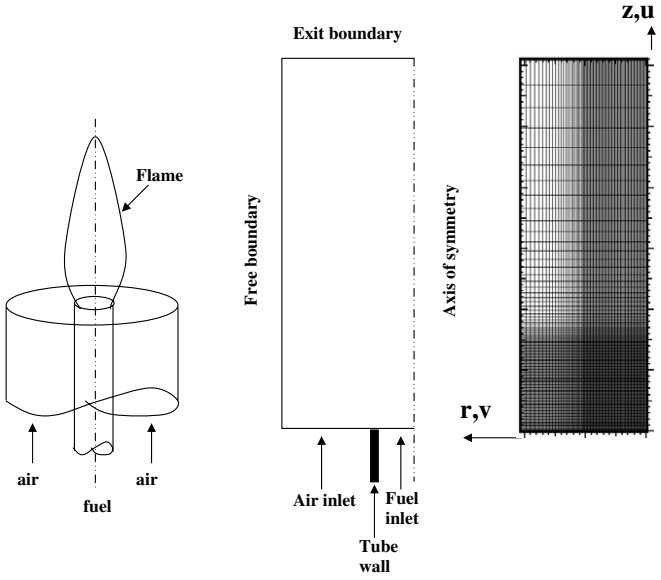

Fig. 1. Geometry of the problem along with the computational domain and grid pattern.