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International Journal of Hydrogen Energy 30 (2005) 1113–1126
International Journal of HYDROGEN ENERGY
www.elsevier.com/locate/ijhydene

The effect of thermal radiation and radiation models on hydrogen–hydrocarbon combustion modelling

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Received 26 July 2004; received in revised form 1 September 2004
Available online 11 November 2004

Abstract

This paper presents numerical simulation results from the modelling of a turbulent non-premixed hydrogen (H_2) and hydrogen–hydrocarbon flame with and without radiation models. CFD studies using Fluent code were carried out for three cases; without radiation model, with the P-1 radiation model and with the discrete transfer radiation model. The model results from these three cases are compared with each other and with the experimental results. The effects of fuel composition from pure natural gas to hydrogen (100% CH_4, 70% H2 + 30% CH_4, and 100% H_2) were also investigated. The predictions are validated and compared against the experimental results obtained in this study and results from the literature. Turbulent diffusion flames are investigated numerically using a finite volume method for the solution of the conservation equations and reaction equations governing the problem. The standard k–ε model was used for the modelling of the turbulence phenomena in the combustor. The chemical combustion reactions are described by seven species and three steps. A NO_x post-processor has been used for predicting NO_x emissions from the combustor. Using the both radiation models caused over all lower temperature levels for all fuel compositions compared with the results obtained using no radiation model. The results with the radiation models are in better agreement with the measurements compared with the results without radiation model. The use of a radiation model predicts lower over all temperature, thus lower NO_x emissions.

Keywords: Combustion modelling; Hydrogen and hydrocarbon combustion; Radiation models; NO_x formation

1. Introduction

Thermal radiation heat transfer involving gases can be an important mode of heat transfer in high-temperature combustors and furnaces, even under non-soot conditions. In hydrocarbon fuel combustion, the familiar products of combustion H_2O, CO_2, CO are particularly important owing to their comparatively high absorptivities and emissivities in the near infrared region. The computation fluid dynamic (CFD) modelling of combustors burning hydrogen or hydrogen–hydrocarbon composite fuels is a great interest to researchers and designers because of the complexity of combustion process and flow field in such devices. Ignoring thermal radiation heat transfer may cause significant errors in the overall predictions. Thermal radiation affects the structure and combustion characteristics of hydrocarbon and composite fuels, as well as the NO formation due to the sensitivity of thermal NO kinetics to temperature. The non-accurate prediction of combustion phonemena in the modelling of hydrogen and hydrogen–hydrocarbon fuels causes non-accurate NO predictions. For example, higher temperature predictions will cause higher NO predictions due to the thermal NO mechanism. Therefore, the use of a radiation model for an accurate combustion simulation is essential.

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0360-3199/$30.00
doi:10.1016/j.ijhydene.2004.10.009

Nomenclature

A_k	Arrhenius pre-exponential factor	b	oxygen reaction order
E_a	activation energy, J/kmole	k_1, k_2	forward rate constants
p	pressure, Pa	k_{-1}, k_{-2}	reverse rate constants
ρ	density, kg/m^3	M_{NO}	molecular weight of NO
ϕ	mixture ratio defined as air–fuel ratio	$\nu'_{i',k}$	the molar stoichiometric coefficient for species i'
T	temperature, K	$\nu_{j',k}$	the exponent on the concentration of reactant j'
Y_k	mass fraction of the species, k	$M_{i'}$	molecular weight of species i', kg/kmol
$R_{i',k}$	the reaction rate	β_k	temperature exponent
ε	the rate of dissipation of turbulent kinetic energy	$C_{j'}$	the molar concentration of each reactant species j'
k	rate constant, turbulent kinetic energy		
f	correction factor for prompt-NO_x model		
R	universal gas constant		

Diffusion flames have been widely applied in industrial process systems, such as burners and furnaces. Both numerical and experimental investigations of turbulent diffusion (non-premixed) flames have been the subject of extensive research during recent years for several gas fuels and liquid fuels, because they are very important for the understanding of the complex interactions between the turbulent flow and chemical reactions. Good model simulations can be used in construction of furnaces or gas turbines as well as for the prediction of pollutants such as nitrogen oxides and carbon monoxide emissions.

Some detailed numerical studies on thermal radiation and radiation models may be found in literature [1–9] for hydrocarbon fuel combustions, but the numerical studies on thermal radiation and radiation models are very limited for hydrogen combustion, and not found for hydrogen–hydrocarbon combustion.

The main aim of this work is to investigate the effect of thermal radiation and radiation models on the modelling of hydrogen and hydrogen–hydrocarbon composite fuel combustion. In this paper, a detailed numerical experiment is carried out for two radiation models; the Discrete Transfer Radiation Model (DTRM) and the six-flux or P-1 model, and ignoring radiation models. Experimental measurements of radial temperature and NO distributions were previously performed at the combustor exit for three different fuel compositions (100% CH_4, 70%H_2 + 30% CH_4, and 100% H_2) [10].

2. CFD Modelling of the combustor

Simulation of the combustor was performed by the use of a CFD package Fluent [11] which was integrated with a NO_x post-processor. The boundary conditions were defined in terms of temperature and constant for inlets and walls. The gas law was used to calculate the fluid density. The other physical constants of fluid were taken from the literature. Inlet velocities were calculated from the known mass flow rates ($Q_{fuel} = 4.467 \times 10^{-4}$ kg/s, $Q_{air} = 0.015536$ kg/s for 100% H_2, $Q_{air} = 0.01320$ kg/s for 70% H_2 + 30% CH_4, $Q_{air} = 0.007768$ kg/s for 100% CH_4) according to mixture ratio ($\phi = 1.0$). For radiation calculations, absorption coefficients used in the radiation model are taken 0.6 for pure methane, 0.50 for composite fuel and 0.45 m^{-1} for pure hydrogen combustion, while scattering coefficients used are taken 0.01 m^{-1} for all cases. At the combustor walls, the heat transfer coefficient is taken 15 W/m^2 K and free stream temperature is taken 300 K for all cases.

2.1. The model combustor

The combustor modelling has been performed for three different fuel composition (100% H_2, 70% H_2 + 30% CH_4, 100% CH_4) cases. The stoichiometric mixture ratio (ϕ=1.0) was used for all cases. The standard k–ε model [12] was employed for the modelling of the turbulent flow in the combustors. The physical domain of combustors is given Fig. 1. The physical values used in combustor modelling are selected as: length of combustor $L = 2$ m, radius of combustor $R_c = 0.3$ m, radius of fuel inlet $R_f = 0.005$ m, radius of air inlet $R_a = 0.15$ m, $Q_{fuel} = 4.467 \times 10^{-4}$ kg/s, $T_{fuel} = 300$ K, $T_{air} = 300$ K.

2.2. The combustion model

Reaction rate in turbulent flow is calculated from the Arrhenius kinetic rate expression and the eddy break-up model which are given as

The Arrhenius reaction rate expression:

$$R_{i',k} = -\nu'_{i',k} M_{i'} T^{\beta_k} A_k \prod_{j'} C_{j'}^{\nu_{j',k}} \exp\left(-\frac{E_k}{RT}\right). \quad (1)$$