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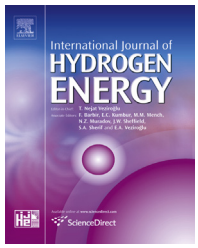

Predicting radiative characteristics of hydrogen and hydrogen/methane jet fires using FireFOAM

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ABSTRACT

A possible consequence of pressurized hydrogen release is an under-expanded jet fire. Knowledge of the flame length, radiative heat flux as well as the effects of variations in ground reflectance is important for safety assessment. The present study applies an open source CFD code FireFOAM to study the radiation characteristics of hydrogen and hydrogen/methane jet fires. For combustion, the eddy dissipation concept for multi-component fuels recently developed by the authors in the large eddy simulation (LES) framework is used. The radiative heat is computed with the finite volume discrete ordinates model in conjunction with the weighted sum of grey gas model for the absorption/emission coefficient. The pseudo-diameter approach is used in which the corresponding parameters are calculated using the formulations of Birch et al. [24] with the thermodynamic properties corrected by the Able-Noble equation of state. The predicted flame length and radiant fraction are in good agreement with the measurements of Schefer et al. [2], Studer et al. [3] and Ekoto et al. [6]. In order to account for the effects of variation in ground surface reflectance, the emissivity of hydrogen flames was modified following Ekoto et al. [6]. Four cases with different ground reflectance are computed. The predictions show that the ground surface reflectance only has minor effect on the surface emissive power of the smaller hydrogen jet fire of Ekoto et al. [6]. The radiant fractions fluctuate from 0.168 to 0.176 close to the suggested value of 0.16 by Ekoto et al. [6] based on the analysis of their measurements.

Introduction

Hydrogen is regarded as an important clean energy carrier in the future energy landscape. However, safety issues related to pressurized hydrogen release are of concern and are being incorporated in the development of hydrogen safety Codes and Standards. A related particular hazard which needs to be addressed is hydrogen jet fires. If the pressure in storage tanks or transportation systems is more than 1.9 times the ambient pressure, the release is choked with the resulting jet being under-expanded and has sonic speed at the leak/rupture point. The resulting radiative jet fire extends to several metres and even more than ten metres. Direct impingement, convective or radiative heat from such jet fires can cause human casualties and damages to the directly affected and

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surrounding equipment/facilities and in some severe cases can cascade to catastrophic consequences. There are only a handful of experimental facilities in the world wide scientific community which are able to test large scale hydrogen jet fires. Such full scale testing is extremely costly. In the mean time, it is also questionable to extrapolate the results from the limited conditions that can be tested. It is hence of considerable importance to develop and validate predictive tools which can quantify the flame and radiative characteristics of such under-expanded jet fires.

Several previous experimental studies [1–6] have focused on the radiative characteristics of under-expanded hydrogen jet fires, but relatively less computational fluid dynamics (CFD) efforts have been attempted. Brennan et al. [7] employed large eddy simulation (LES) approach to simulate hydrogen jet fires with laminar flamelet models and assumed PDF shape. They found that turbulence intensity only has limited effect on the flame length for which the predictions achieved reasonable agreement with the measurements. Houf et al. [8] also simulated hydrogen jet fires using Reynolds-averaged Navier–Stokes equations (RANS) and the eddy dissipation concept (EDC) model for combustion. Since subsonic inlet boundary conditions are specified at the pseudo-diameter, they found that the mesh size, turbulence model and turbulent intensity all influences the predictions of the flame length while similar to the findings of Brennan et al. [7], the effect of the turbulent intensity was found to be limited. The predicted flame length was also in reasonably good agreement with the measurements [2]. However, none of these numerical studies [7,8] addressed the radiative characteristics of under-expanded hydrogen jet fires.

The present study aims to validate the FireFOAM code, an LES solver based on open Source CFD toolbox OpenFOAM [9]. The development of FireFOAM [10] has been extensively supported by FM Global through internal effort as well as collaboration with worldwide institutions. FM Global also releases the developed models to the entire fire research community. The present study is part of effort to validate a recently modified EDC model for fuels with mixed components and radiative treatment for the predictions of hydrogen and hydrogen/methane jet fires. Particular attention is focused on the accurate predictions of radiative characteristics. The measurements from several published papers [2,3,6] including both hydrogen and hydrogen/methane jet fires are used for comparison as well as examination of the variation in ground reflectance.

Mathematical modelling

Governing equations

Hydrogen can be treated as an ideal gas at pressure lower than 172 bar [2]. The flow is governed by spatial filtering and Favre averaging of the reactive Navier–Stokes equations in the LES framework.

$$\frac{\partial \overline{\rho}}{\partial t}+\frac{\partial \overline{\rho}\tilde{u}_j}{\partial x_j}=0 \tag{1}$$

$$\frac{\partial \overline{\rho}\tilde{u}_j}{\partial t}+\frac{\partial \overline{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\overline{\rho}(\upsilon+\upsilon_t)\left(\frac{\partial \tilde{u}_i}{\partial x_j}+\frac{\partial \tilde{u}_j}{\partial x_i}-\frac{2}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right)\right)-\frac{\partial \overline{p}_d}{\partial x_i}-g_i x_i\frac{\partial \overline{\rho}}{\partial x_i} \tag{2}$$

$$\frac{\partial \overline{\rho}\tilde{h}_s}{\partial t}+\frac{\partial \overline{\rho}\tilde{u}_j\tilde{h}_s}{\partial x_j}=\frac{D\overline{p}}{Dt}+\frac{\partial}{\partial x_j}\left[\overline{\rho}\left(D+\frac{\upsilon_t}{Pr_t}\right)\frac{\partial \tilde{h}_s}{\partial x_j}\right]+\dot{q}'''-\nabla\cdot\dot{q}_r''' \tag{3}$$

$$\frac{\partial \overline{\rho}\tilde{Y}_m}{\partial t}+\frac{\partial \overline{\rho}\tilde{u}_j\tilde{Y}_m}{\partial x_j}=\frac{\partial}{\partial x_j}\left[\overline{\rho}\left(D+\frac{\upsilon_t}{Pr_t}\right)\frac{\partial \tilde{Y}_m}{\partial x_j}\right]+\overline{\omega}_m \tag{4}$$

$$\overline{p}=\overline{p}_d+\overline{\rho}g_j x_j \tag{5}$$

where ρ, u, p, h_s and Y are the density, velocity, pressure, sensible enthalpy and mass fraction of gas mixture, respectively. υ, υ_t, D, Pr_t denote laminar dynamic viscosity, turbulent dynamic viscosity, laminar diffusion coefficient and turbulent Prantl number. $\overline{\omega}_m$ is the production/sink rate due to gas reaction. $\dot{q}'''$ is the heat release rate per unit volume from a chemical reaction. $\dot{q}_r''$ is the sum of the radiative fluxes of all gas species, mainly water (H_2O) and carbon dioxide (CO_2).

The modified EDC combustion model

The eddy dissipation concept for the computation of turbulent combustion was originally proposed by Magnussen et al. [11,12] based on energy cascading. It assumes that turbulent mixing and combustion take place in fine structures (or smaller dissipative eddies) close to the Kolmogonov scale. The original EDC formulations were successful in RANS applications but various attempts [e.g. Refs. [13,14]] to extend it to LES had been problematic since the total kinetic energy required in the computation is not available and only the sub-grid scale (SGS) kinetic energy, which is a small part of the former, is resolved. This essentially requires the EDC model in the LES framework to be formulated with the SGS kinetic energy and eddy viscosity. Fureby et al. [13,14] directly replaced the total kinetic energy and its dissipation rate using SGS kinetic energy k_{SGS} and other SGS parameters. This approach has been adopted by some commercial CFD codes like FLUENT. However, it was reported that the predicted reaction rate is strongly dependent on grid size [13]. The problem was thought to be caused by the direct replacement of the total kinetic energy with the SGS kinetic energy, which is much smaller than the total kinetic energy and varies with the grid resolution.

Chen et al. [15] followed the energy cascade concept and derived the total kinetic energy and its dissipation rate using the SGS quantities as follows:

$$k=\left(\frac{3}{2C_{D1}^2}\right)^{1/3}(\varepsilon L')^{2/3} \tag{6}$$

$$\varepsilon=\sqrt{\frac{3}{2}}C_{D1}\frac{k_{SGS}^{3/2}}{\Delta}+\frac{2}{9}C_{D2}\upsilon\frac{k_{SGS}}{\Delta^2} \tag{7}$$

where $C_{D1}=0.135$ and $C_{D2}=0.5$. υ and Δ are the molecular kinetic viscosity and the filter size. k_{SGS} is obtained together with SGS ε_{SGS} and υ_t by using the one-equation LES model of Menon et al. [16] to close the above governing equations. The

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