Short Communication

Computational Fluid Dynamics Modeling of Hydrogen-Oxygen Flame

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Abstract

A non-premixed hydrogen-oxygen flame is modeled, incorporating the reactions of intermediate radical species, by the use of a computational fluid dynamic modeling technique. The computed and experimentally measured mass fractions are shown to agree well overall.

Keywords: Hydrogen flame; computational fluid dynamic; turbulent combustion modeling; non-premixed

1. Introduction

A transformational technology for alternate ironmaking is under development at the University of Utah. This novel technology is based on the direct gaseous reduction of iron oxide concentrates in a flash reduction process, with the ultimate objective of significantly increasing energy saving and reducing environmental emissions compared with the conventional blast furnace (BF) ironmaking route. The flash ironmaking process uses gaseous reducing agents, such as natural gas or hydrogen. These gases will go through partial oxidation to generate a hot reducing gas mixture. Experiments have been conducted in a drop-tube reactor and laboratory flash reactor [1, 2, 3, 4]. A large pilot-scale flash reactor has been constructed and is being installed [5].

The data generated in this type of experimental apparatus can best be presented and analyzed by the use of a computational fluid dynamic (CFD) model. Such a model will also provide a very useful tool for burner and powder injector design and the design and optimization of an industrial flash reactor. The model should be capable of describing the various processes occurring in this novel flash ironmaking process.

Hydrogen is the best fuel/reductant in the flash ironmaking process. Even when hydrocarbons are used, the oxidation of hydrogen in the flame plays an important role, and thus it has been studied by computational fluid dynamics (CFD) simulation using ANSYS Fluent [3]. Computed results of the simulation of benchmark experiments reported in the literature for a non-premixed hydrogen jet flame are thus presented here for CFD model validation.

2. Model Formulation

The CFD simulation of a turbulent hydrogen jet flame involves the numerical solution of a set of transport equations, which describe fluid flow, heat and mass transfer, and reaction kinetics. These equations are summarized below.

2.1 Fluid Flow and Heat Transfer Equations

The generic transport equation, in steady state, can be written in the following form:

$$\nabla \cdot \rho_g \vec{u} \phi - \nabla \cdot \Gamma_\phi \nabla \phi = S^\phi \quad (1)$$

Where ϕ represents the generic dependent variable, Γ_ϕ is the effective transport coefficient, and S^ϕ is the source term. Other symbols are defined in the Nomenclature section.

The following Favre averaging, a density-weighted average used for compressible flows, was used in the turbulence modeling:

$$\bar{\phi} = \frac{1}{\bar{\rho}} \int_t^{t+t_0} \rho(t) \phi(t) dt \quad (2)$$

where $\bar{\phi}$ is the Favre-averaged dependent variable, and t_0 is a long enough time to obtain a smooth-averaged value.

Table 1 presents the governing equations [6]. The standard k - ε turbulence model [7] was used, and radiation was described using the discrete ordinate (DO) model [6].

Table 1. Transport Equations for a Hydrogen Flame

Overall continuity:	$\frac{\partial}{\partial x_i} (\bar{\rho}_g \bar{u}_i) = 0 \quad (3)$
Momentum:	$\begin{aligned} \frac{\partial}{\partial x_j} (\bar{\rho}_g \bar{u}_i \bar{u}_j) = & -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu_g \left(\frac{\partial \bar{u}_j}{\partial x_i} + \frac{\partial \bar{u}_i}{\partial x_j} - \frac{2}{3} \delta_{ij} \frac{\partial \bar{u}_k}{\partial x_k} \right) \right] + \\ & \frac{\partial}{\partial x_j} (-\bar{\rho}_g \overline{u'_i u'_j}) + \bar{\rho}_g \bar{g}_i \end{aligned} \quad (4)$
Turbulent kinetic energy:	$\frac{\partial}{\partial x_j} (\bar{\rho}_g \bar{u}_j k) = \frac{\partial}{\partial x_j} \left[\left(\mu_g + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + \bar{\rho}_g \varepsilon - Y_M + S_k \quad (5)$
Turbulent dissipation rate:	$\begin{aligned} \frac{\partial}{\partial x_j} (\bar{\rho}_g \bar{u}_j \varepsilon) = & \frac{\partial}{\partial x_j} \left[\left(\mu_g + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} G_k \\ & - C_{2\varepsilon} \bar{\rho}_g \frac{\varepsilon^2}{k} + S_\varepsilon \end{aligned} \quad (6)$
Energy:	$\frac{\partial}{\partial x_i} (\bar{\rho}_g \bar{u}_i h_g) = \frac{\partial}{\partial x_i} \left[k_g \frac{\partial T_g}{\partial x_i} \right] + Q_{rg}^h + S_g^h \quad (7)$
Species:	$\frac{\partial}{\partial x_i} (\bar{\rho}_g \bar{u}_i \bar{Y}_k) = \frac{\partial}{\partial x_i} \left[\left(\bar{\rho}_g D_{k-mix} + \frac{\mu_t}{Sc_t} \right) \frac{\partial \bar{Y}_k}{\partial x_i} \right] + S_k \quad (8)$
Reynolds stresses:	(9)

$$-\bar{\rho}_g \overline{u'_i u'_j} = \mu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left(\bar{\rho}_g k + \mu_t \frac{\partial \bar{u}_k}{\partial x_k} \right)$$

Equation (7) is the governing equation for the transport of heat in the gas phase under steady state. The term on the left-hand side represents heat transfer by convection (bulk flow). The first term on the right-hand side (RHS) represents heat transfer by conduction and eddy motion. The second term on the RHS denotes the net radiative heat transfer to the gas phase. The last term on the RHS represents a source term due to gas-phase chemical reactions.

2.2 Turbulent Combustion Modeling

In typical combustion processes where the mixing of the fuel and oxidant takes place outside the gas injector, it is customary to assume that the intrinsic gas-phase reaction rate is very fast and thus the reaction rate is controlled only by the turbulent mixing of the reactants. The combustion rate can therefore be calculated using the Eddy-Dissipation Model (EDM) [8].

The partial combustion of hydrogen with oxygen is not a typical combustion process. In fact, it has not received much attention due to its lack of industrial application. In our early modeling effort, the partial combustion of hydrogen with oxygen was modeled by the EDM technique. The maximum flame temperatures were significantly over-predicted. In such a chemical system, the heat evolution in H_2/O_2 flames may be dominated by the reactions of intermediate species such as H and OH radicals and consequently the simple mixed-and-burnt approach does not provide sufficient details. A more realistic approach considering the reaction rate of these intermediate species was thus required.

In this work, a reaction mechanism for H_2/O_2 mixtures composed of seven elementary reactions to represent the combustion process was thus adopted together with the Eddy Dissipation Concept approach [9]. In this approach, chemical reaction kinetics are calculated in small constant-pressure cells, the dimensions of which are defined by the small scales of turbulence.

The gas-phase reaction mechanism shown in Table 2, proposed by Eklund and coworkers [10], was used in this work. It consists of seven chemical reactions involving six species: H_2 , O_2 , H_2O , OH, H, and O. The chemical reactions are represented in the following general form:

for which the reaction rate was defined by

$$R_j = k_{f,j} C_A^a C_B^b - k_{r,j} C_C^c C_D^d \quad j = 1, 2, \dots, J. \quad (11)$$

The forward and reverse rate constants were computed from

$$k_{f,j} = A_j T^{\beta_j} \exp\left(-\frac{E_j}{RT}\right), \quad (12)$$

$$k_{r,j} = k_{f,j} / K_{c,j}. \quad (13)$$

The equilibrium constants $K_{c,j}$ were calculated internally within Fluent using its built-in thermodynamic data.

Table 2: Gas-phase reaction mechanism for H_2/O_2 combustion.

	Reaction	A_j	β_j	E_j
1	$\text{H}_2 + \text{O}_2 = \text{OH} + \text{OH}$	0.170×10^{14}	0.0	48151
2	$\text{H} + \text{O}_2 = \text{OH} + \text{O}$	0.142×10^{15}	0.0	16401
3	$\text{OH} + \text{H}_2 = \text{H}_2\text{O} + \text{H}$	0.316×10^{08}	1.8	3030
4	$\text{O} + \text{H}_2 = \text{OH} + \text{H}$	0.207×10^{15}	0.0	13750
5	$\text{OH} + \text{OH} = \text{H}_2\text{O} + \text{O}$	0.550×10^{14}	0.0	7000
6	$\text{H} + \text{OH} = \text{H}_2\text{O} + \text{M}$	0.221×10^{23}	-2.0	0
7	$\text{H} + \text{H} = \text{H}_2 + \text{M}$	0.653×10^{18}	-1.0	0

3. Results and Discussion

The experimental data from experiments reported in the literature for a non-premixed hydrogen jet flame [11, 12, 13] were simulated. Barlow [11] simultaneously measured the gas temperature, mass fractions of major species (O_2 , N_2 , H_2 , H_2O), and mass fractions of OH and NO in a turbulent non-premixed hydrogen jet flame at various axial and radial positions. These multi-scalar measurements were obtained by combining spontaneous Raman scattering, Rayleigh scattering, and laser-induced fluorescence.

In this work, the model predictions of gas temperature and mass fractions of H_2 , O_2 , H_2O , and OH were compared with Favre averaged measurements. Table 3 presents the model parameters used for the simulation. Figure 1 shows a schematic representation of the geometry of the experimental hydrogen jet flame. It also shows the computational domain used in the simulation. Due to the axial symmetry of the experimental setup, one half of the physical domain was sufficient for simulation. Along the symmetry axis and the far-field boundary in the radial direction, the gradients of all dependent variables were set equal to zero, whereas the remaining boundary conditions were specified according to the information listed in Table 3. Computationally, the mesh was a biased mesh of 17700 cells and as usual, several mesh sizes were tested to verify that a further increase in the cell number to 36550 cells did not change the computed results. In addition, an angular discretization of 3 theta divisions and 3 phi division was used for the simulation of radiation heat transfer. The burner wall was assumed to be stainless steel with an emissivity of 0.35 and the weighted sum of gray gas model was used to compute the absorption of radiation by the gas.

Table 3: Parameters for the Simulation [11].

Parameter	Value
<u>Geometry, mm</u>	
H_2 inlet radius, R_{fuel}	1.875
Visible flame length, L	675
<u>Hydrogen Jet</u>	
Inlet Velocity components, m/s	
Axial	296
Radial	0
<u>Turbulent model parameters</u>	
Intensity, %	5

Hydraulic diameter, m	0.00375
Temperature, K	295
Mass Fraction, kg/kg	1.0
<u>Air Coflow</u>	
Inlet Velocity components, m/s	
Axial	1.0
Radial	0.0
Turbulent model parameters	
Intensity, %	5
Hydraulic diameter, m	0.295
<u>Outlet</u>	
Turbulent model parameters	
Intensity, %	5
Hydraulic diameter, m	0.3

Figure 2 shows predicted and experimental radial gas temperature profiles at various axial positions. In spite of the complex interaction of turbulence, gas-phase chemistry and aerodynamics, the computer model yields a satisfactory prediction of the flame temperature.

Figures 3 – 6 show the comparison between experimental and computed mass fractions for the gas-phase species H_2 , O_2 , H_2O , and OH . Overall, the computer model show good agreement with the experimental measurements. The % RMS (the standard deviation as a percentage of the mean value) of the experimental measurements ranged from 2.5 for temperature to 7.5 for OH . The model slightly over-predicts the consumption rate of oxygen (Figure 4) and the production rate of OH radicals (Figure 6). The content of the latter is very low and more accurate prediction of such a species would be difficult.

A better overall simulation of a hydrogen flame would require more comprehensive reaction mechanisms. Such a complex simulation requires large computing capacity and time, and thus is more difficult to incorporate into the simulation of a larger process in which hydrogen combustion is only a part. In this work, the objective was to develop an adequate simulation tool capable of representing particle-laden flows in a combustion environment. Therefore, prediction with reasonable accuracy of the gas temperature and species distributions of a non-premixed H_2/O_2 jet flame is sufficient.

NOMENCLATURE [Commonly used symbols are omitted.]

D_{k-mix}	$m^2 s^{-1}$	Diffusion coefficient of the k th species in the vapor mixture
h_g	$J kg^{-1}$	Gas specific enthalpy
k	$m^2 s^{-2}$	Turbulent kinetic energy
$k_{f,j}$	Various	Rate coefficient of the j th forward reaction
K_g	$W m^{-1} K^{-1}$	Gas thermal conductivity
$k_{r,j}$	Various	Rate coefficient of the j th backward reaction
$K_{c,j}$	Various	Concentration equilibrium constant
P	Pa	Pressure
R	$J mol^{-1} K^{-1}$	Gas constant
R_j	$mol m^{-3} s^{-1}$	Net rate of the j th reaction
S_i	$kg m^{-3} s^{-1}$	Net mass generation of the i th species by gas-phase reactions
S^ϕ	Various	Net source term of dependent variable ϕ
t	S	Time
t_o	S	Long enough time to obtain a smooth-averaged value
T	K	Temperature
T_g	K	Gas temperature
$\vec{u}$	$m s^{-1}$	Gas velocity vector
x_i	M	Coordinate length in the i th direction
Y_i	1	Favre-averaged mass fraction of the i th species
Z	m	z -coordinate length

*Greek
Symbols*

β	1	Pre-exponential factor used in Equation 12
Γ_ϕ	Various	Effective transport coefficient
δ_{ij}	1	Kronecker delta function
ϵ	$\text{m}^2 \text{s}^{-3}$	Turbulent dissipation rate
μ_g	Pa s	Gas viscosity
μ_t	Pa s	Turbulent viscosity
ρ	kg m^{-3}	Density
ρ_g	kg m^{-3}	Gas density
ϕ	1	Generic dependent variable
$\bar{\phi}$	Various	Favre-averaged generic dependent variable

Subscripts

i	i th species or i th coordinate direction
j	j th coordinate direction
g	Gas
k	k th species

Operators

∇	m^{-1}	Nabla operator in Cartesian coordinates; $\nabla = \frac{\partial}{\partial x} \delta_x + \frac{\partial}{\partial y} \delta_y + \frac{\partial}{\partial z} \delta_z$
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FIGURE CAPTIONS

Figure 1: Schematic representation of the geometry of the experimental hydrogen jet flame [11] simulated in this work.

Figure 2: Radial gas temperature profiles at various axial positions. $z/L =$ (a) $1/8$, (b) $3/8$, (c) $5/8$, and (d) 1.

Figure 3: Radial H_2 mass fraction profiles at various axial positions. $z/L =$ (a) $1/8$, (b) $3/8$, (c) $5/8$, and (d) 1.

Figure 4: Radial O_2 mass fraction at various axial positions. $z/L =$ (a) $1/8$, (b) $3/8$, (c) $5/8$, and (d) 1.

Figure 5: Radial H_2O mass fraction profiles at various axial positions. $z/L =$ (a) $1/8$, (b) $3/8$, (c) $5/8$, and (d) 1.

Figure 6: Radial OH mass fraction profiles at various axial positions. $z/L =$ (a) $1/8$, (b) $3/8$, (c) $5/8$, and (d) 1.