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Effect of Thermodiffusion on Non-premixed Flame in MILD Regime Using a Modified Reacting Solver

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ABSTRACT

Numerical simulations for moderate and intense low oxygen dilution (MILD) combustion with essential solvers and detailed mechanisms involve more complications and computational time. Various advanced combustion modeling techniques have recently been developed to study MILD combustion characteristics. However, every combustion model has specific issues predicting the temperature and emissions of the MILD combustion flames. The diffusive nature of the MILD flame is considered, and individual Lewis numbers are investigated on a non-premixed flame. The current study analyzes the methane/hydrogen flame propagation with different Lewis number combinations in a hot co-flow environment. Individual Lewis numbers for methane and hydrogen are investigated from stochiometric to ultra-rich mixtures in non-premixed flames. Several numerical simulations are performed in the OpenFOAM9 environment using a modified EDC model with tuned turbulence and combustion model constants. The numerical simulation results with hydrogen and methane Lewis numbers of 0.4 and 0.9, respectively, show promising agreement with the experimental findings of Dally[1], *et al.* Various combustion parameters are studied with different CH_4 and H_2 Lewis number combinations. In addition, the unity Lewis number case is simulated and compared to the situations that are taken into consideration.

Keywords: OpenFOAM; MILD combustion; Non-premixed; Lewis number; Modified EDC model

NOMENCLATURE

m	: Mixture mass
v	: Velocity
Y_i	: i^{th} species mass fraction
w_i	: i^{th} species reaction rate
τ	: Stress tensor
T	: Temperature
$\bar{\bar{I}}$	: Identity tensor
N	: Number of species
F_h	: Enthalpy flux
α_i	: Thermal diffusivity of i^{th} species
S_{chem}	: Chemical source term
μ_t	: Turbulent dynamic viscosity
ε	: Turbulent kinetic energy
σ_k&σ_ε	: κ and ε turbulent Prandtl numbers, respectively
ρ	: Density of the mixture
p	: Pressure
V_i	: i^{th} species diffusion velocity
h	: Specific total enthalpy of the mixture
μ	: Dynamic viscosity
h_i	: i^{th} species-specific total enthalpy
λ	: Mixture thermal conductivity
C_p	: Local specific heat
Le_i	: Lewis number of i^{th}species
w_i	: Mass reaction rate
κ	: Turbulent kinetic energy
G_K	: Mean velocity gradient generated turbulent kinetic energy
S_K&S_ε	: κ and ε equations source terms
$C_{1\varepsilon}$&$C_{2\varepsilon}$	: Turbulent model constants

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1. INTRODUCTION

Mild combustion is characterized by an invisible flame and a unified temperature distribution. The temperature of the reactants before the primary reaction zone is perfectly suitable for igniting the fuel. The temperature rise is low inside the furnace[2]. The lower peak temperature and constant furnace temperature lessen the generation of undesirable pollutants to the environment (mostly NOx, CO, etc.) and irreversible heat loss. This will increase combustor efficiency as well[3]. When compared to conventional combustion, the MILD combustion is substantially less noisy and more stable. The researchers usually prefer non-enclosed flames, such as bi-dimensional and axisymmetric flame shapes, to study MILD combustion as measurement and diagnosis become more accessible, simplifying the complexity of numerical simulations[4]. The basic concepts and understanding of the MILD combustion are well studied on a combustor configuration with a jet-carrying fuel surrounded by preheated and diluted oxidizer[1,5]. This type of burner is usually called a Jet in the hot co-flow burner (JHC). The generation of vitiated gas in the co-flow offers a

great advantage by eliminating the need for the combustion products' recirculation. This provides an opportunity for reasonable control over the local composition, which is a positive outcome. Dally[1], *et al*. conducted an experiment in a JHC burner by employing three different oxygen levels (3 %, 6 %, and 9 %) in the co-flow. They achieved MILD combustion with a lower increment of flame temperature up to 100 K. Khalil and Gupta[6] achieved colorless distribution combustion in a swirl burner of thermal intensity 3.25 kW, employing methane, propane, and hydrogen-enriched methane as fuel in which the preheated gas (N_2+ CO_2 +O_2) temperature varied from 300-750 K. They attained an ultra-low NOx emission of 1 ppm from the varieties of fuel considered in the experiment. Khalil and Gupta[6] outlined the conditions to achieve CDC, *i.e*., for the oxygen content of 9.5 % and a peak temperature of 1800 K.

Several computational methodologies are implemented in the literature to study MILD combustion reaction physics. The JHC burners are extensively used to study the MILD combustion characteristics using Reynolds-averaged Navier-Stokes (RANS) models[7-10]. Christo and Dally[8-9] performed numerical simulations with various combustion models like the eddy dissipation concept (EDC) model, flamelet model, and transported probability density function (PDF) models with detailed chemistry to validate the experimental results of JHC burner[10].

Sarras[11], *et al.* also used the same combustion models with DRM 19 chemical mechanism to validate the experimental results of the Delft (DJHC*)* burner[5]. The numerical findings with the EDC model are better than that of flamelet and PDF models. However, the EDC model took more computational time than flamelet and PDF models, and a slight deviation between computational results using the EDC model and experimental results is observed. Compared the EDC model's capabilities to other combustion models in the literature[8,10]. These studies illustrated that the EDC model assumes fast-rate chemistry, which is invalid for the MILD combustion scenario as it is distributive and leads to a slower reaction rate of the unburnt mixture[13]. In MILD flames, the numerical results could not be better with the fast-rate chemistry assumption. However, the detailed mechanism with EDC model predictions has a lower deviation from the MILD combustion experimental results when compared with other combustion models. Furthermore, the combustion model constants' dependency on flame characteristics is reported in the literature[7,8,14] and suggested appropriate combustion constants in the basic EDC model for the MILD combustion.

Kulkarni & Polifke[15] performed large eddy simulations (LES) to understand the MILD flames in the DJHC burner, and the anticipated lift-off heights are shown to be in good promise with the experimental findings. Nevertheless, temperature findings are overpredicted with various Reynolds numbers. The predictions of temperatures are significantly improved when a progress variable is added to the LES by Ihme and See[16]. Darbyshire[17], *et al.* developed a joint PDF model to study the stratified V-flame in the MILD regime and observed slight improvements from that of the single PDF model for the temperature findings.

Klimenko[18], *et al*. and Kim[10], *et al*. used the Conditional Momentum Closure (CMC) model to solve the transport equations for the case of MILD combustion. It is observed that the flow characteristics are predicted accurately, and the NO and CO predictions do not agree with the experimental results. Labahn[19], *et al*. have implemented the conditional source-term estimation (CSE) model to study the DJHC flame by averaging the source term in the combustion equation. The temperature predictions with CSE are accurate near the burner but need to be in better agreement (more than 15 %) in the downstream direction. From the literature, computational time-wise, all the PDF-based models require less than the other combustion models. Nevertheless, PDF-based models are observed to be less accurate for temperature predictions, which affects the other combustion characteristics of the flame and results in a deviation from the emissions predictions.

Characterizing the transport processes emerging within the gaseous mixtures, particularly in premixed combustion, majorly depends on the Lewis number (*Le*)[20-22]. These studies showed that unequal heat, flame stretch, and species diffusion (*Le*) significantly impact the overall combustion phenomena. In the present study, *Le* is equivalently regarded as the thermal-to-mass diffusivity ratio of the individual species. The unity Lewis number (*Le*=1) assumption is employed in significant combustion models. From the literature, it is found that Lewis number-based studies are carried out in premixed flames by calculating the mixture of Lewis numbers by various available theories. The Lewis number gives the physical sense of the fuel and thermal diffusivity in the co-flow/oxidizer in the burner. In case of the non-premixed MILD combustion, the reactants travel together before the reaction occurs, similar to the premixed case. Therefore, *Le* has a crucial role in the reaction physics of either non-premixed or premixed cases of MILD combustion. Lots of research works are conducted on premixed flames. The present study reports a *Le*-based computational analysis for the first time for the non-premixed flames.

The current study considers the EDC model with the individual Lewis numbers of the fuel (methane and hydrogen) jet for non-premixed flame in the MILD regime. The work is carried out using a modified reacting solver in the OpenFOAM 9 environment. Various Lewis numbers are considered for analyzingthe methane-hydrogen fuel jets in the MILD regime. The range of Lewis numbers from 0.9 to 1.14 and from 0.4 to 0.7 are considered for the methane and hydrogen fuels in the steps of 0.06 based on the literature. In addition to the variation in *Le*, tuned combustion and turbulence constants are implemented according to the literature. Furthermore, the EDC model with unity Lewis number is simulated and compared with the various Lewis number combinations.

2. MATHEMATICAL MODELING

Finite volume modeling is used in the open-source C++ library code known as OpenFOAM, which can solve complex problems with reasonable accuracy compared to other commercial software. The reactingFoam is a reacting solver that solves combustion problems with a detailed chemical mechanism in OpenFOAM and is built with an

EDC combustion model. In the present work, the steady state Favre-averaged turbulence modeling is incorporated with a typical two-equation k-ε model and a standard wall function is imposed along the wall boundaries. The flow chart of the reacting solver in the OpenFOAM is shown in Fig. 1.

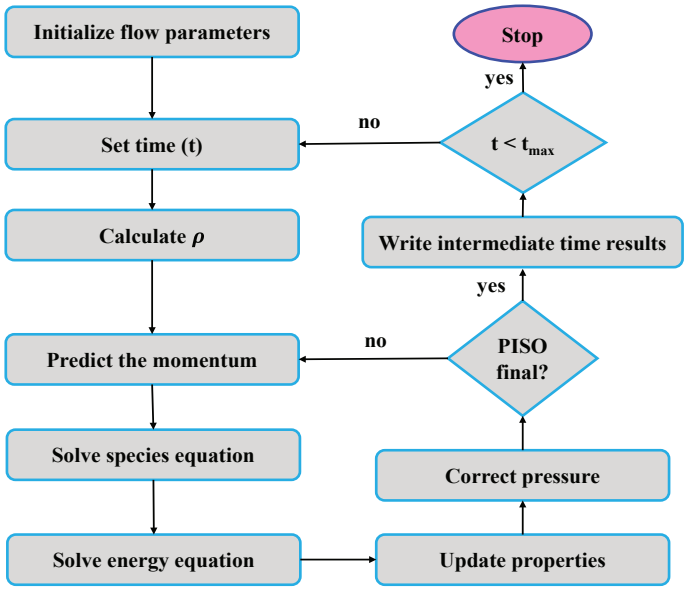

Figure 1. Algorithm for steady state reacting foam solver.

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2.1 Governing Equations

In the current study, the discrete ordinate (DO) radiation model and modified EDC combustion models are used to execute Favre-averaged-based simulations. The required conservation equations (mass, momentum, species, and energy) under steady-state conditions expressed in Eqn. (1-6) are as follows:

$$\nabla.\left(\rho v\right)=0 \tag{1}$$

$$\nabla.\left(\rho vv\right)=-\nabla p+\nabla.\left(\overline{\overline{\tau}}\right) \tag{2}$$

$$\overline{\overline{\tau}}=-\frac{2}{3}\mu\left(\nabla.v\right)\overline{\overline{I}}+\mu\left[\nabla v+\left(\nabla v\right)^{T}\right] \tag{3}$$

$$F_h=mh-\frac{\lambda}{c_p}\frac{\partial h}{\partial s}-\frac{\lambda}{c_p}\sum_{i=1}^{N}\left(\frac{1}{Le_i}-1\right)h_i\frac{\partial Y_i}{\partial s} \tag{4}$$

$$\nabla.\left(\rho v_j h\right)=\frac{\partial}{\partial x_j}\left(\Gamma_h\frac{\partial h}{\partial x_j}\right)+\nabla.\left(\alpha_i * F_h\right)\nabla\left(F_h\right)+S_{chem} \tag{5}$$

$$\nabla.\left(\rho Y_i v\right)=\left(\nabla.\left(\alpha_{eff}\,/\,Le_i\right)\nabla Y_i\right)+w_i \tag{6}$$

The present study incorporated individual Lewis numbers of fuel jet species (methane and hydrogen) into the energy and species transport equations. Accordingly, the conservation equations are modified in the OpenFOAM environment. The EDC model with modified conservation Eqns. (5 and 6) is named the modified EDC model in the present study. The below equations show the equations for the standard κ- ε model.

$$\frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{v}_i\tilde{k}\right)=\frac{\partial}{\partial x_i}\left[\left(\mu+\frac{\mu_t}{\delta_k}\right)\frac{\partial\tilde{k}}{\partial x_i}\right]+G_k-\tilde{\rho}\tilde{k}+S_k \tag{7}$$

$$\frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{v}_i\tilde{\varepsilon}\right)=\frac{\partial}{\partial x_i}\left[\left(\mu+\frac{\mu_t}{\delta_\varepsilon}\right)\frac{\partial\tilde{\varepsilon}}{\partial x_i}\right]+C_{1\varepsilon}\frac{\tilde{\varepsilon}}{\tilde{k}}\left(G_k\right)-C_{2\varepsilon}\bar{\rho}\frac{\tilde{\varepsilon}^2}{\tilde{k}}+S_\varepsilon \tag{8}$$

2.2 Computational Domain and Boundary Conditions

In the current study, Dally[1], *et al*. experimental conditions with 9 % oxygen in the co-flow (HM3) are considered for validating the solver with an individual Lewis number. A hot co-flow with a diameter of 82.8 mm surrounds a primary jet of fuel with a diameter of 4.5 mm, and it is placed inside the air duct. The fuel in the central jet combination of Natural Gas (NG) and hydrogen, is blended together in equal volume fractions. The hot co-flow with 9 % oxygen is considered for validating the solver. The co-flow operates with a secondary burner and enters the main fuel jet at non-uniform conditions. However, the actual co-flow conditions are not measured in the experiments. Hence, uniform boundary conditions are considered for the co-flow based on the literature. The inlet uniform velocity & temperature of 69 m/s & 302 K is given for the main jet and 3.2 m/s & 1300 K for the co-flow and the tunnel flow at 3.2 m/s & 302 K. The domain of a 170 mm cylindrical wedge and 500 mm along the axis is considered for the computational study. Figure 2 shows the computational domain with the boundaries. In co-flow, CO_2, H_2O, and N_2 are given as uniform mass fractions of 0.055, 0.065, and 0.79, respectively. The considered burner is operating at atmospheric pressure. Table 1 summarizes the overall inlet boundary conditions.

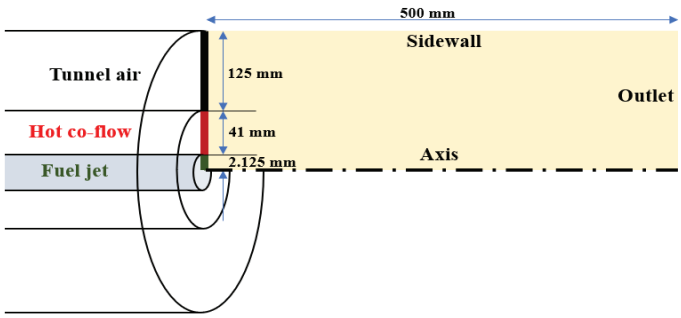


Figure 2. Computational domain is taken into account in this study.

The considered burner is operated under constant operating conditions, and there is no deviation in the distribution of the local variables with respect to the time observed. Hence, the numerical simulations are performed under steady-state conditions in the literature[1]. In the current study also, several 2D-computational simulations in steady state are performed with a detailed chemical mechanism (GRI Mech 3.0) in a modified EDC model and individual fuel Lewis numbers for the fuel jet. This study used the turbulence constant (($C_{\varepsilon 1}$)) of

Table 1. Boundary conditions at the inlets.

	Velocity (m/s)	Temp. (K)	CH_4 (%)	H_2 (%)	O_2 (%)	CO_2 (%)	H_2O (%)	N_2 (%)
Fuel inlet	69	302	50	50	-	-	-	-
Co-flow inlet	3.2	1300	-	-	9	5.5	6.5	79
Tunnel air inlet	3.2	302	-	-	21	-	-	79

1.6 instead of 1.44 for the considered turbulence model k-ε with standard wall functions[8]. In the EDC model, time scale and volume fraction constants are changed from 0.0893 and 1 to 0.4083 and 2.1377, respectively, as Kuang[13], *et al*. suggested for the MILD combustion case. The range of Lewis numbers for methane and hydrogen are collected from the literature; these are 0.9 to 1.14 and 0.4 to 0.7, respectively. The *Le* is varied in the steps of 0.06.

2.3 Grid Independence Test

The 2D domain (Fig. 2) is discretized into fine hexahedral volume elements. Since both the solution and the cost of calculation are significantly influenced by the number of cells and node connections in the computation domain. Mesh size is decisive in getting accurate predictions from the simulations. Hence, simulations are used to find reliable solutions with three different discretized domains of M1, M2, and M3 having 182355, 222444, and 250943 nodes, respectively, with a minimum grid size of 0.02125 mm and maximum grid size of 0.421 mm (Table 2).

Table 2. Grids considered for the grid independence test

Grid	No. of nodes	Deviation (%)
M1	182355	-
M2	222444	6
M3	250943	0.923

From the several simulations using three different discretized domains, the grid-independent analysis is conducted based on the temperature variation in a radial direction at 30 mm from the fuel jet. It is observed that the simulations with M2 and M3 grids showed similar predictions with a deviation of less than 1 %, as shown in Fig 3. Hence, M2 mesh having 222444 nodes is considered for further analysis in this study.

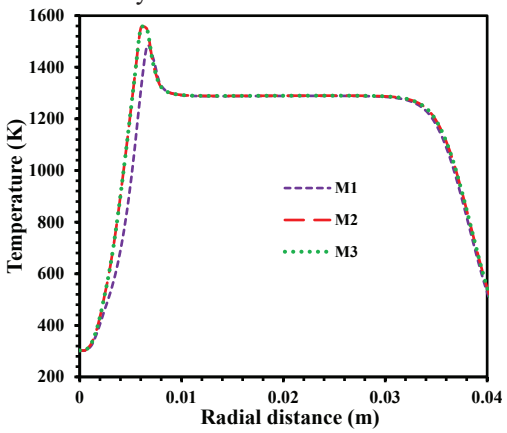


Figure 3. Radial distribution of the temperature for grid independence at 30 mm from the fuel jet.

3. RESULTS AND DISCUSSION

Several numerical simulations are conducted in the present study employing an OpenFOAM 9 modified reacting solver. The combinations of the Lewis numbers are artificially implemented to see the dependency of the *Le* on the flame characteristics.

The radial distributions of various combustion characteristics are analysed at an axial location of 30 mm. The findings of the current numerical modeling of combustion and flow parameters are compared with the experimental measurements of Dally *et al*.[1] experimental result. Figure 4(a) compares the radial temperature distribution at a 30 mm axial location between the experimental results[1] and presents numerical simulations with different Lewis number combinations. The peak temperature is observed around 9 mm from the axis. The simulation results of *Le*_0.4_0.9 (hydrogen *Le*=0.4 and methane *Le*=0.9) are a close match to the actual findings. However, the variation in peak temperature is observed as 40 K, which is less than 2 %. In other Lewis number cases, the peak has shifted the axis outwards, and the peak temperatures are under-predicted.

Figure 4(b) compares radial distributions of CO mass fractions at an axial location of 30 mm. The CO mass fraction variation trend in *Le*_0.4_0.9 is observed to be the same as the experimental results. However, a slight deviation is observed in peak CO prediction. Because of the assumed uniform inlet co-flow boundary conditions, the radial variation of temperature (Fig 4(a) and CO mass fraction (Fig 4(b)) predictions in the co-flow region does not exhibit close promise with the actual findings. The OH mass fraction distribution shows close agreement with the actual results for *Le*_0.4_0.9 case, as shown in Fig. 4(c). The OH peak locations for other Lewis numbers are slightly shifted towards the outer radial locations, similar to the case of temperature (Fig 4(a)).

Figure 4 (d) and (e) shows the comparison of obtained NO and H_2O mass fractions with experimental results. In both cases, computational results with the *Le*_0.4_0.9 are in very close agreement with the experiential findings. Nevertheless, a slight deviation in the peak values is observed, where the deviation error is within 3%.

Based on the literature, in the case of rich flames, the Lewis numbers are less than unity. In MILD flames the local oxygen availability is less. Hence, the predictions with Lower *Le* cases (*Le* = 0.4 and 0.9 for hydrogen and methane) are in close agreement with the experimental findings of Dally *et al*.[1]. However, the present study is not a premixed flame to decide the adequate Lewis number for the fuel and oxidizer mixture.

Figure 5 depicts the temperature variation in the domain for various combinations of the fuel Lewis numbers. In the case of *Le*_0.4_0.9, the flame is distributive as the Lewis numbers

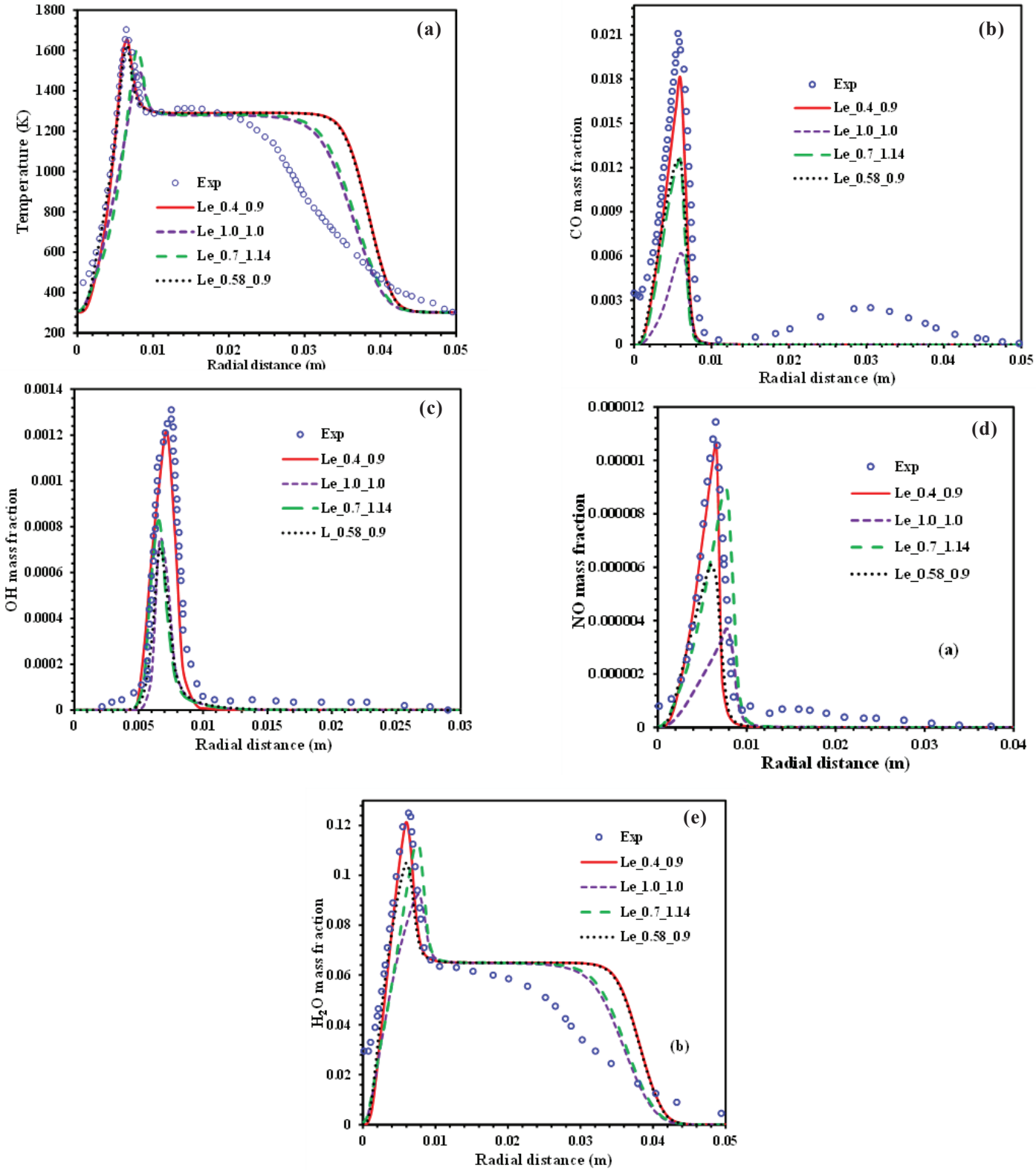


Figure 4. Comparison of experimental data and predicted radial distributions of (a) Temperature, (b) CO, (c) OH, (d) NO, and (e) H_2O mass fractions.

are lower. For the case of *Le*_0.4_0.9, as the *Le* is lower, the flame is more distributive and contacts with more oxygen, resulting in more fuel consumption. Hence higher heat release rate and peak temperatures are observed with lower *Le* case.

Figure 6(a) shows various Lewis number cases' OH mass fraction contours. The OH destruction is considered the crucial parameter for the Lift of height calculations for different Lewis numbers of the fuels. The minimum OH mass fraction of 0.001 is considered for the lift-off height calculation. Variation in the lift-off height concerning various Lewis number cases is shown in Fig. 6(a). Due to the fast-rate chemistry of the basic EDC model, the unity Lewis number scenario exhibits the lowest

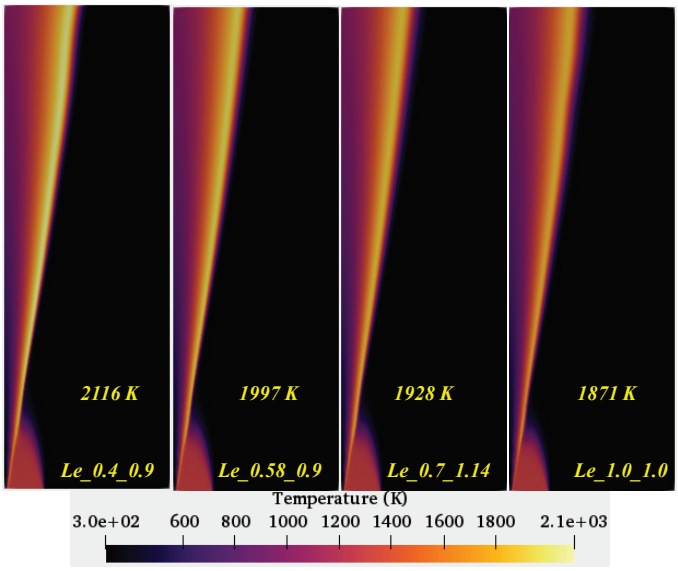
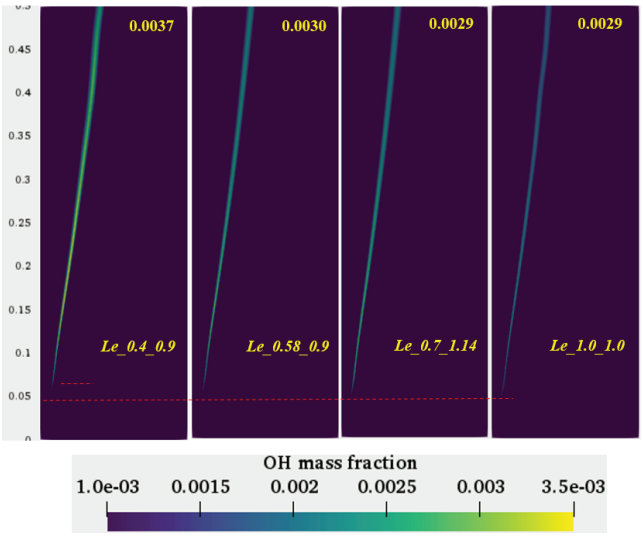
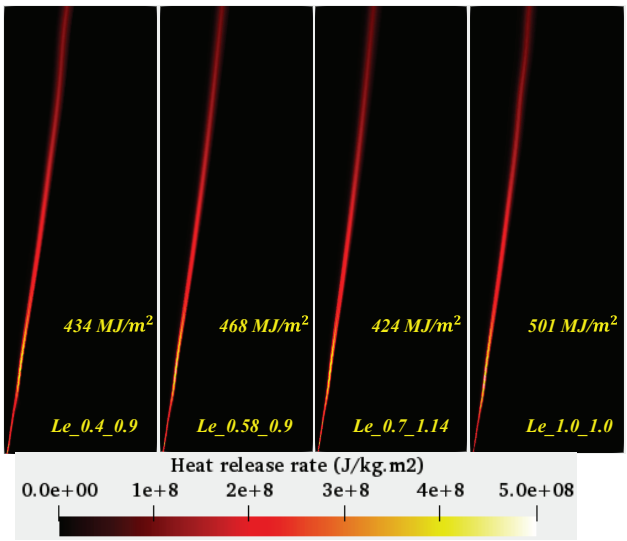


Figure 5. Temperature contours for various Lewis number cases.



(a)



(b)

Figure 6. (a) OH mass fraction; and (b) Heat release rate distribution in the computational domain for various Lewis number cases.

lift-off height. While in the case of the *Le*_0.4_0.9 highest lift-off heights are observed, all other predictions also agree with the actual findings of Dally[1], *et al*.

Figure 6(b) shows the variation of heat release rate distribution in the computational domain with peak heat release rate (HRR) values. Due to the faster reaction rate characteristics of the basic EDC model, the peak HRR was observed for the case of the unity Lewis number.

Figure 7(a) shows the peak temperature variation for the different Lewis number combinations of hydrogen and methane fuels. While changing the hydrogen Le from 0.4 to 0.46, the peak temperature variation in the domain is observed to be ~ 70K; with a further increase in Le of H_2 (0.46 to 0.52), the peak temperature variation is reduced to ~ 40K. Similarly, in the case of methane, a one-step increases in Le, the peak temperature increase is observed as ~ 5K, which is very small. Therefore, it is clearly shown that the diffusivity of hydrogen affects the solution significantly. Hence, considering the Le for hydrogen in hydrogen-involved flames fuels helps improve the computational predictions. Figure 7(b) depicts the radial distributions of temperature at the computational domain's exit for various combinations of the Le. Temperature is an indicator of fuel consumption in the industrial burner. The higher consumption of fuel is observed with the lower Le cases.The NO variation at the exit is considered to see the effect of the computational solution with various Lewis numbers, shown in Fig. 7(c). Significantly higher NO formation is observed in the case of Le_0.4_0.9, and it is due to the peak temperatures in the domain. However, the peak magnitude is in the range of 10^{-4}, which is very small. Figure 7(d) shows the radial distribution of theH_2O mass fraction at the end of the domain for the given different combinations of the Le for H_2 and CH_4. The H_2O production is higher in lower Le case. Therefore, the individual Lewis number significantly affects predicting the various combustion and flow parameters of the non-premixed flames.

3. CONCLUSIONS

The present work performed an artificial treatment of Le for the main fuel jet species (CH_4 and H_2) for a non-premixed flame. The numerical simulations are performed in OpenFOAM by modifying the built-in reacting solver with a detailed chemical mechanism using tuned turbulent and combustion model constants. The following are observed from the performed numerical simulation results.

- The previous combustion models (LES, EDC, PDF, CMC, and CSE) noticed the divergence in flow/temperature/species in computational predictions. In the present work simulations with lower Le case, the computational predictions of all the combustion characteristics are in close agreement with the actual findings.
- Higher flame distribution is observed in case of the lower Lewis number (Le_0.4_0.9).
- Hydrogen has a larger diffusivity and flammability range than methane fuel. Consequently, when considering H_2 mixing with fuels with lower diffusivity, the Le consideration of each species in the fuel jet yields better computational predictions

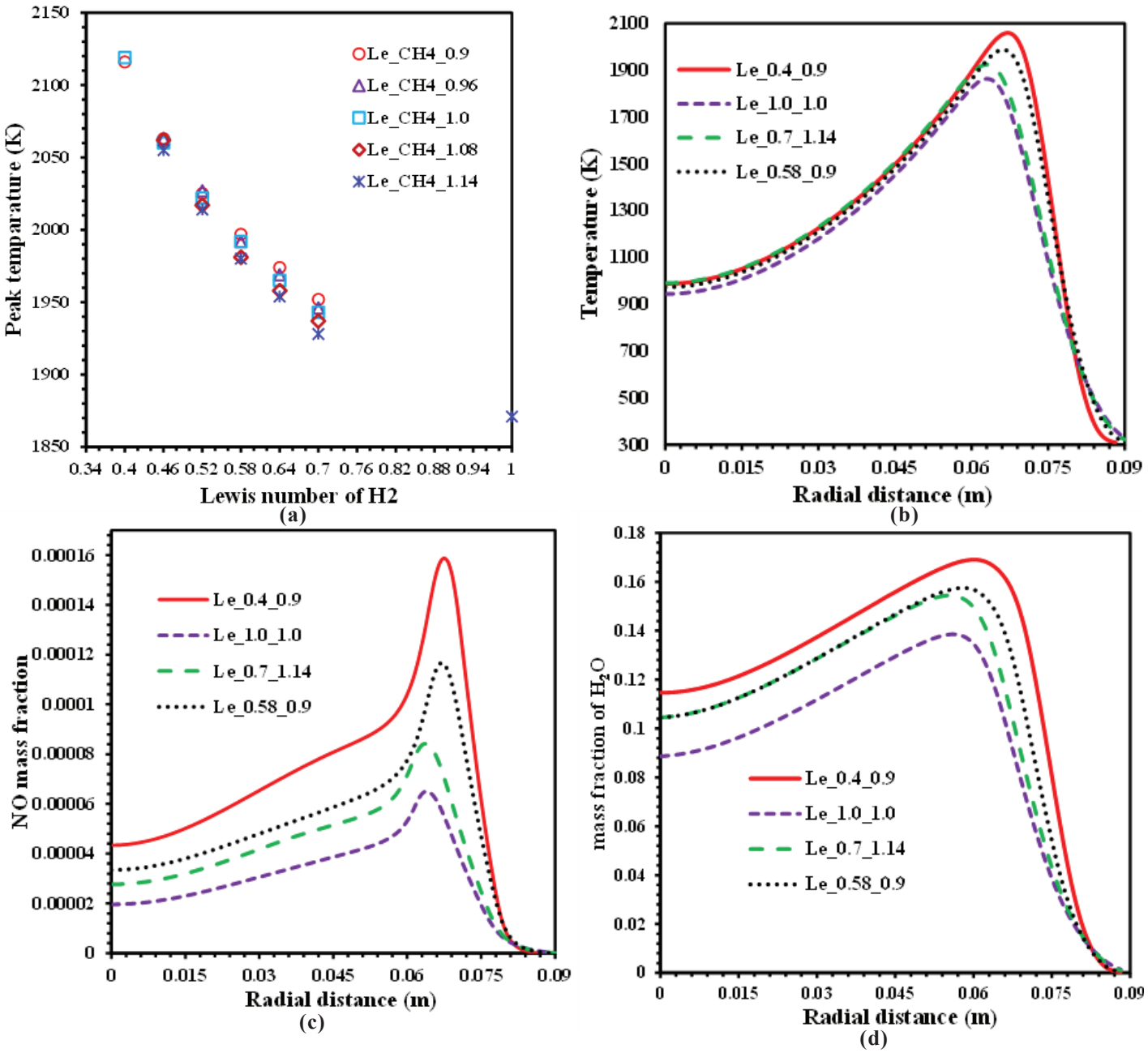


Figure 7. (a) Variation of peak temperatures in the domain. radial distribution of: (b) Temperature, (c) NO, and (d) H_2O mass fractions at the exit of the computational domain for various Lewis number combinations.

- The current work suggests that lower Lewis numbers be used to analyse non-premixed MILD combustion flames.

The main benefit of the current approach, which makes it suited for complicated MILD combustion flames, is the expansion of the solver by providing an individual Le in the accessible open-source code (OpenFOAM) for non-premixed flames without any extra modeling assumptions or complications

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