Validation of Combustion Models for Lifted Hydrogen Flame

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Abstract. Within a Reynolds Averaged Numerical Simulation (RANS) approach for turbulence modelling, a computational investigation of a turbulent lifted H_2/N_2 flame is presented. Various turbulent combustion models are considered including the Eddy Dissipation Model (EDM), the Eddy Dissipation Concept (EDC), and the composition Probability Density Function transport model (PDF) in combination with different detailed and global reaction mechanisms. Turbulence is modelled using the Standard k-ε model, which has proven to offer a good accuracy, based on a preceding validation study for an isothermal H_2/N_2 jet. Results are compared with the published measurements for a lifted H_2/N_2 flame, and the relative performance of the turbulent combustion models are assessed. It is observed that the prediction quality can vary largely depending on the reaction mechanism and the turbulent combustion model. The best and quite satisfactory agreement with experiments is provided by two detailed reaction mechanisms applied with a PDF model.

1 Introduction

Power generation by gas and steam turbines [1] depend largely on the combustion process. Parallel to the efforts for exploiting new energy sources [2] as well as recovery techniques [3], combustion will continue to play an important role in power generation. This is true also for renewables, as biomass [4] plays an important role.

Combustion of hydrogen and hydrogen containing fuels occupies an important role in clean and efficient energy supply, environment protection and resource efficiency. Hydrogen offers an attractive alternative for storing excess energy in power generation from photovoltaics and wind energy. Furthermore, instead of combustion [5] the gasification of waste, biomass and coal [6] offers good possibilities for efficient and clean power generation. The so-called synthesis gas (syngas), which results as the product of gasification, contains, in addition to carbon monoxide and small fractions of methane, rather significant amounts of hydrogen. Additionally, there is a growing interest in nuclear energy based hydrogen production, i.e., using the nuclear power for electrolysis, thermochemical cycles or hybrid approaches to produce hydrogen [7]. From the environmental perspective, its subsequent combustion is most welcome since it produces no carbon dioxide.

Utilization of hydrogen or hydrogen blend fuels in combustion systems represents a great challenge. Hydrogen is extremely reactive and, compared to other gases, has different material properties, so that it can alter the combustion properties of the gas mixture even in small proportions. In premixed combustion, a potential problem is increased flashback propensity [8]. The counterpart of flashback is blow-off [9]. The forerunner of blow-off is the lift-off, as the flame root leaves the rim. Following the lift-off, with a further increase of the jet speed, a stabilized flame at a distance from the rim, i.e. a lifted flame can be obtained [10].

Computational analysis of turbulent lifted flames is a very challenging task, due to the modelling of turbulence and its interaction with chemistry [11]. For turbulence modelling, although the Large Eddy Simulation (LES) approach [12-14] is being increasingly used in practical applications, its adequate use in industrial development processes is still very challenging and the RANS approach [15] is still frequently preferred to this purpose. Given this, the present work is focused on the RANS methodology, and in the following review, RANS based approaches will be considered only.

Prediction of lifted turbulent jet flames is a demanding task. A partially premixed state is reached at the flame base, which leads to complex stabilization mechanisms [16]. In configurations, where the fuel jet is issuing into a hot coflow, like the presently investigated one, autoignition emerges as a further possible mechanism of stabilization. Thus, the applied turbulent combustion model should sufficiently accommodate for the mentioned effects.

As the turbulent combustion model, Cabra et al. [17] applied a composition Probability Density Function transport model [18] (PDF) in predicting a lifted methane flame. For lifted hydrogen flames, the MIL (Modèle Intermittent Lagrangien) [19], the unsteady flamelet / progress variable [20], and the Conditional Moment Closure (CMC) [21] models were applied [22]. Several researchers used PDF as well as Eddy Dissipation Concept (EDC) [23] approaches.

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As outlined above, different and quite sophisticated models have already been used to predict turbulent, lifted hydrogen flames.

However, to the authors' opinion, there is still need for further investigation. The purpose of the present paper is to present a "coherent" validation study, for a cascade of different turbulent combustion modelling strategies in a wide range. This coherent validation study based on the consistent/comparable strategies in all further aspects of the mathematical modelling, numerical methods and gridding is believed to be of additional value to the research community, as it will provide a basis for a direct comparison of a wide range of turbulent combustion models, unmasked by the other effects, for the present problem.

2 Problem definition

The "main" considered test case is the atmospheric, lifted flame of a turbulent H_2/N_2 jet in vitiated coflow, which was experimentally investigated by Cabra et al. [24]. This comprises a free jet of H_2/N_2 mixture (with H_2 volume fraction of 25.37%) in a co-flow of exhaust gases stemming from lean hydrogen combustion (with oxygen volume fraction of 14.74%).

In comparing the predictions with the experimental results, mainly, the lift-off heights of the flames for different values of the coflow temperatures are monitored. For this purpose, the experimental data of Wu et al. [25] is considered which was obtained on an experimental setup, which was equivalent to that of Cabra et al [24].

For selecting the turbulence model to be used, a study has been carried out, where turbulence models are validated in an isolated manner from the combustion model, on an isothermal, non-reacting test case, which, however, resembles the setup of the main, combusting test case, in so far that the gas composition (containing H_2), and, thus, density, is variable.

As test case for this purpose, the measurements of Sautet and Stepowski [26] are considered. The test rig was an open, atmospheric one at ambient conditions. In the experiments, non-reacting turbulent jets of H_2/N_2 mixtures discharging into a coflow air stream were investigated.

3 Models

The general-purpose, finite volume based CFD code ANSYS Fluent 18.0 [27] is used in the computational analysis of the problem.

3.1 Outline

A two-dimensional, axisymmetric formulation is used. The medium is considered to be an ideal gas mixture with Newtonian behavior. Buoyancy effects are neglected, which is reasonable due to the prevailing rather high Froude numbers [28]. The radiative heat transfer [29] is also neglected and the reacting system is assumed to be adiabatic. An accurate modelling of the molecular material properties is attempted. For all species, the specific heat capacities are represented by a pair of (low and high temperature ranges) fourth order polynomials of temperature [30]. The viscosities, thermal conductivities, as well as the multi-component diffusion coefficients are calculated according to the kinetic theory [9].

The flow turbulence is described within a RANS framework [15], as already mentioned above. Among the two-equation turbulence models the specific dissipation rate (omega, ω) based models have gained popularity [15,31]. However, since the present problem is of completely free-shear type, among the two-equation models, the dissipation rate (epsilon, ε) based models are considered only, in particular, the Standard k-ε [27,32], the RNG k-ε [27,33], and the Realizable k-ε models [27,33,34]. For scalar turbulent fluxes, the gradient-diffusion approximation is used assuming constant turbulent Schmidt numbers. For the latter, 0.85 is used for the energy equation, whereas 0.7 is assumed for the further scalars.

The velocity-pressure coupling is treated by the SIMPLEC scheme [27]. For the discretization of the convective terms, the QUICK scheme [27] is used, which is considered to possess formal accuracy of third order. As no under-relaxation is applied to pressure, the under-relaxation factors range between 0.4-0.7 and 0.8-1.0 for the velocities and the scalar quantities, respectively.

For convergence, the threshold value for the normalized residual has been set to 10^{-8} for the energy equation and to 10^{-5} for the remaining equations.

3.2 Combustion models

As single-step global mechanisms, those of Kudriakov et al. [36] (KU) and Marinov et al. [37] (M) are considered (comprising the main species, H_2, O_2, H_2O), where the former and latter consider an irreversible and a reversible reaction, respectively.

As detailed reaction mechanisms, four mechanisms are considered, each of which comprising a large number of elementary reactions (approx. 20 without counting the reverse reactions) between eight species, names, H_2, O_2, H_2O, H, O, OH, HO_2, H_2O_2. The considered detailed mechanisms are the Gri-Mech 3.0 [38] (GRI), the mechanisms of Li et al. [39] (LI), Conaire et al. [40] (CON) and Keromnes et al. [41] (KER).

For purely mixing controlled combustion, the time-averaged consumption rate is calculated, in Eddy Dissipation Model (EDM), from the dissipation rate of turbulence eddies [42]. The chemical kinetics effects (K) are taken in an ad-hoc manner into account, calculating the rate from an Arrhenius expression neglecting fluctuations [9], comparing the two rates and taking the smaller one [27].

As an improved version of the eddy dissipation idea is the Eddy Dissipation Concept (EDC), where the time-averaged conversion rate is calculated by taking the mixing and kinetics effects in a combined manner into

account, in a more sophisticated way, treating the small turbulent scales to behave as well stirred reactors [27,43].

In the composition PDF transport (PDF) model, for obtaining the averaged values thermochemical variables a single-point, joint probability density function is obtained from its transport equation, which is derived from the governing equations under the application of some closure models [18,27].

4 Results

4.1 Isothermal turbulent flow

The solution domain is two-dimensional axisymmetric, having rectangular shape in plane of the axial (x) and radial (r) coordinates.

The domain is starting at the exit plane of the jets, extending 22d in the axial direction. Its radial extension is 11d. The inlet boundaries representing the central and coaxial jet are placed on the left boundary of the domain (x=0), whereas the right boundary (x=22d) is defined to be pressure boundary with a prescribed constant pressure and zero gradient conditions for the remaining variables. The lower (r=0) boundary is a symmetry axis, whereas the upper one (r=11d) is also defined to be a symmetry surface.

On the left boundary (x=0), the part that surrounds the annular jet is defined to be a pressure boundary, again, (ambient pressure) that allows an inflow, i.e. the suction of ambient air by the ejector effect. At inlet, the measured values are prescribed as the inlet boundary conditions. Boundary conditions of turbulence quantities are derived from assumed turbulence intensities and length scales.

Computational grids are generated as structured, rectangular grids, with axial and radial concentration of the nodes near the jet inlet. For determining the adequate grid resolution, a grid independence study is performed. In the grid independence study, the Standard k-ε model is used as the turbulence model.

Table 1 displays the variation of the potential core length (L) with grid fineness, where N is the total number of nodes. One can see that sufficient grid independence is achieved for $N \geq 5{,}000$. In the further calculations for the validation of turbulence models, the finest grid is used, which had 16,200 nodes.

The predicted variations of the half value radius (δ) at the axial position of x/d=20 are compared with the experimental values in Table 2.

One can see that the predictions delivered by the Standard k-ε model agree rather well with the experiments, better than the Realizable and RNG versions, for the present, variable density H_2/N_2/Air jet (Table 2). Thus, the Standard k-ε model is selected.

Table 1. Potential core length as function of total number of grid nodes.

N	1375	2450	2925	3250	4590	6405	16200
L/d	2.08	2.64	2.79	3.06	3.50	3.51	3.51

Table 2. Variation of half-value radius (δ) along jet axis.

	δ/d	% Error
Experiment	1.36	-
Standard k-ε	1.45	6.6 %
Realizable k-ε	1.55	13.9 %
RNG k-ε	1.62	19.1 %

4.2 Flame

Similar to the isothermal test case, the solution domain consists of a cylinder, the bottom of which is placed at the jet exit. The axial coordinate (x) extends along the axis, in the main flow direction, with x=0 placed at the jet exit (jet inlet boundary is centered at the cylinder bottom). The domain size in the radial and axial directions are about 20d and 80d, respectively. The cylinder bottom is covered by two inlet boundaries, i.e. a central (jet), and an annular (coflow) one. Both inlets are separated by a thin, ring shaped wall boundary, representing the nozzle the lip. The top of the cylinder is defined as the outlet boundary, whereas the jacket of the cylinder is assumed to be an impermeable slip boundary. At the outlet boundary, a constant static pressure is prescribed, along with vanishing normal-gradient conditions for the remaining quantities. At the inlets, top-hat profiles are prescribed for all convective-diffusively transported variables, in accordance with the measured values. For turbulence quantities, a turbulence intensity of 4% is assumed at the both inlets. The jet diameter and the size of the individual holes in the outer disk are taken as basis in assuming the length scale for the jet, and coflow, respectively.

Computational grids are generated as structured, rectangular grids, with axial and radial concentration of the nodes near the inlets as well as in the central and mixing zones. The grid independence study is performed using the EDM+K turbulent combustion model in combination with the global reaction mechanism (KU).

Table 3 presents the variation of the predicted centerline temperature (T) at ten diameters downstream the jet inlet (x/d=10) for six different grids with changing number of total nodes (N). One can see that sufficient grid independence is achieved for the finer grids. In the further calculations, the finest grid having 16,000 cells is used.

The temperature and oxygen mole fraction fields predicted by the EDM+K model, using the global mechanism M are presented in Figure 1 for the coflow temperature (T_{CO}) of 1060 K.

The lifted flame can easily be recognized in the temperature field (Fig. 1a). In Fig. 1b, one can see that oxygen penetrates into the fuel jet along the lift-off distance, and, is, then, rapidly consumed by the combustion reactions starting at the flame root, causing a local oxygen depleted zone.

Table 3. Centerline temperature at x/d=10 as function of total number of grid nodes.

N	2436	4260	7525	9900	12480	16000
T(K)	573	456	410	392	384	384

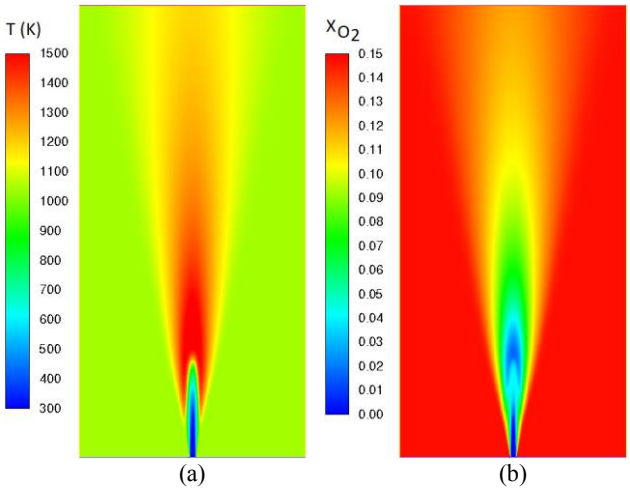

Figure 1. Predicted fields of (a) temperature and (b) oxygen mole fraction by EDM+K-M for T_{CO}=1060 K.

Inspecting the data of Wu et al. [6] one can deduce that the measured lift-off heights in their dependence to the temperature of the coflow-stream can be represented by the following relationship with a quite good accuracy

$$\frac{h}{d} = 81.37\left(\frac{T_{CO}}{1000}\right)^{-68.12} \quad (1)$$

with a coefficient of determination of 0.98.

Predicted lift-off heights by the single-step reaction mechanism (M), in combination with EDM, EDC models, i.e. by EDM+K-M, and EDC-M, as nondimensionalized by the central jet diameter, and the experimental results (EXP), as represented by the correlation expressed by Eq. (1), are presented in Table 4, for different coflow temperatures.

One can see that the calculations predict qualitatively the right trend, i.e. decreasing lift-off height with increasing temperature. However, this trend is strongly underpredicted by the calculations and the quantitative deviations from the measurements are quite large.

Similarly, the calculated lift-off heights by detailed reaction mechanisms (CON, LI, KER), in combination with EDC, i.e. EDC-CON, EDC-LI and EDC-KER models are compared with experiments in Table 5. Empty boxes in the table indicate that no flame could be predicted for the corresponding temperature. One can see that the detailed mechanisms with EDC predict too small lift-off heights at high temperatures, with a very sudden and rapid increase with decreasing temperature followed by blow-off, beyond a certain value. Using the reaction

Table 4. Lift-of heights predicted by EDM+K-M, EDC-M, compared with experiments.

	h/d		
T_{CO} (K)	EXP	EDM+K-M	EDC-M
1010	41.3	7.5	20.4
1020	21.1	6.5	15.9
1030	10.9	5.2	11.4
1040	5.6	4.1	7.5
1045	4.1	3.7	6.3

Table 5. Lift-off heights predicted by EDM-CON, EDC-LI, EDC-KER, compared with experiments.

	h/d			
T_{CO} (K)	EXP	EDC-CON	EDC-LI	EDC-KER
1010	41.3	-	-	-
1020	21.1	-	24.8	21.4
1030	10.9	38.9	3.0	2.8
1040	5.6	3.8	1.0	0.8
1045	4.1	2.0	0.7	0.6

mechanism GRI with EDC, no flame could be predicted for the listed temperatures.

Calculated lift-off heights by detailed reaction mechanisms (GRI, CON, LI, KER), in combination with PDF, i.e. PDF-GRI, PDF-CON, PDF-LI and PDF-KER models are compared with experiments in Table 6. Empty boxes in the table indicate that no flame could be predicted for the corresponding temperature. With the GRI mechanism, a flame could be predicted only for the highest temperatures, however, with an extremely large lift-off height. With the mechanism CON, a flame is predicted for all temperatures, with an overprediction of the lift-off height throughout. The mechanisms LI and KER show a very good agreement with each other (except for the lowest temperature 1010 K, where PDF-KER overpredicts PDF-LI) and a quite fair agreement with the measurements. For high temperatures, PDF-LI and PDF-KER predict very close values to the experiments, and the degree of agreement is decreases as the temperature is reduced and the lift-off height increases. Still the overall agreement of PDF-LI and PDF-KER with the experiments is much better than that of the other simulation methods considered here.

5 Conclusions

A computational investigation of a turbulent lifted H_2/N_2 flame is presented, based on a RANS turbulence modelling approach, using the Standard k-ε model. Detailed reaction mechanisms of Li et al. [39] and Keromnes et al. [41] applied with PDF are observed to deliver the best predictions of the lift-off height (h) as function of the coflow temperature (T_{CO}).The mechanism of Conaire et al. [40] with PDF overpredicts h. These reaction mechanisms do not perform that well, when applied with EDC, underpredicting h for high T_{CO} with an abrupt increase of h for T_{CO} lower than a certain value, followed by a too early blow-off. The GRI Mech 3.0 [38] predicted a blow-off for all T_{CO} when applied with EDC, and a lifted flame, with an extremely

Table 6. Lift-off heights predicted by PDF-GRI, PDF-CON, PDF-LI, PDF-KER, compared with experiments.

	h/d				
T_{CO}(K)	EXP	PDF-GRI	PDF-CON	PDF-LI	PDF-KER
1010	41.3	-	79.1	54.6	65.0
1020	21.1	-	55.1	30.6	31.4
1030	10.9	-	33.9	14.0	13.9
1040	5.6	59.7	15.9	7.4	7.9
1045	4.1	50.1	11.5	5.7	5.6

overpredicted h, for T_{CO} > 1045K, when applied with PDF. The global mechanism of Marinov et al. [37] applied with EDM+K and EDC could deliver the trend of increasing h with decreasing T_{CO}, whereas the EDC version delivered quantitatively better results. The global mechanism of Kudriakov et al. [41] with EDM+K predicted attached flames for all T_{CO}.

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