Numerical analysis of lifted hydrogen flame

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Abstract. A numerical analysis of a turbulent lifted H_2/N_2 flame is presented. As combustion mechanisms, a large spectrum is considered including single-step and two-step, as well as detailed mechanisms. As combustion models, various models are considered that treat turbulence-chemistry interaction in different ways, including the Eddy Dissipation Concept and the Laminar Flamelet Method. For turbulence modelling Reynolds Averaged Numerical Simulation and Large Eddy Simulation approaches are used. Results are compared with measurements.

1 Introduction

Power generation by thermal machinery, including the gas turbine [1] and steam turbine [2] plants, largely depends on the conversion of the chemically bound energy by the combustion process. Parallel to the efforts for exploiting new energy sources, as well as recovery techniques [3], combustion continues to play an important role in power generation, also through the renewable energies, considering the significance of biomass in the latter.

Combustion of hydrogen and hydrogen-blend fuels plays an especially important role in clean and efficient energy supply, climate protection and resource efficiency. On the one hand, hydrogen represents an attractive alternative to storing excess energy in power generation from wind power or photovoltaics. On the other hand, instead of combustion [4,5] the gasification of biomass and coal is a good possibility for an efficient and clean power generation. The gasification product, the synthesis gas contains, in addition to carbon monoxide and small amounts of methane, significant amounts of hydrogen. In addition, there is a rapidly growing interest in hydrogen production using nuclear power plants, using the nuclear power for electrolysis, thermochemical cycles or hybrid approaches. From an environmental point of view, the subsequent combustion of hydrogen is most welcome because it produces no carbon dioxide when burned.

Use of hydrogen or hydrogen blend gases as fuel in combustion systems represents a great challenge. Hydrogen is extremely reactive and, compared to other gases, has very different material properties, so that even relatively small proportions of hydrogen can greatly alter the combustion properties of the gas mixture. Therefore, the combustion of fuel gas mixtures with hydrogen fractions requires new combustion chamber concepts. To this purpose development of accurate prediction procedures are required. This is the main motivation for the present contribution.

In power generation by gas turbines, the state-of-theart technology for the land-based gas turbine combustors is the so-called "lean premixed combustion", due to its high potential for achieving very low nitrogen oxide emissions. A principal problem in premixed combustion systems is the so-called "flashback" [6]. This means an undesirable flame propagation upstream, towards the inner parts of the burner, which cause serious damage [6]. A classical cause of flashback is an imbalance between the local flow velocity and flame speed, in the favor of the latter, which may be caused by a change/disturbance in the operation of the burner. This aspect makes the use of hydrogen fuel in premixed combustion to become an especially great challenge, since the high reactivity of hydrogen considerably increases the flame speed and flashback propensity [6].

The counterpart of flashback is the so-called "blowoff", i.e. loss of the flame, which is also an undesirable scenario, which can happen when the flow velocity is higher than the flame speed. The precursor of blow-off is the flame lift-off which starts as the flame root leaves the rim. If the jet velocity is further increased, the flame moves downstream to a position where it stabilizes, thus, a lifted flame results. Lift-off height is the distance between the lifted flame base and the jet exit. When the jet velocity reaches the blow-off velocity, the reaction cannot be sustained and the flame is extinguished. Both stability limits (flashback & blow-off) are important for operation of combustion systems and have safety implication for handling fuels, in our case, hydrogen.

For a lifted flame, a turbulent mixing region exists which is very similar to that for the unignited jet, where an accurate prediction of the subsequent ignition is crucial for the prediction of lift-off height and the blowoff behavior of the flame. The prediction of the lifted flame is, thus, highly demanding. The scope of the

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present investigation is the prediction of the lifted flame by various modelling strategies.

Besides experimental studies [7,8], computational investigations [8,9] were performed for lifted hydrogen flames. In the previous modelling work, either the 2nd generation Eddy Dissipation Concept (EDC) in combination with Reynolds Averaged Numerical Simulation (RANS) [8] or a subgrid joint probability density method in combination with Large Eddy Simulation [9] was used as the modelling strategy. In the present investigation, different combustion modelling approaches will be assessed within RANS and LES formulations for turbulence.

2 Modelling

For the computational investigations, the generalpurpose finite volume method based open source CFD code OpenFOAM [10] is used, where a pressurecorrection scheme (PIMPLE which is a combination of PISO and SIMPLE schemes) was applied for treating the velocity-pressure coupling. A reacting mixture of ideal gases is considered along with a Newtonian behavior and negligible buoyancy effects. Radiative heat transfer [11] is neglected as gas radiation is obviously weaker compared to radiation encountered in flames containing liquid droplets or solid particles such as pulverized coal flames [4,5].

Flow turbulence is described either within a RANS [12] or an LES [13] framework. For RANS the SST model [14] is used as the turbulence model, which has been successfully used, so far, in a wide range of applications [15-19]. For LES, the Smagorinsky model [13,20-22] is employed as the subgrid-scale model, assuming a constant value of 0.1 for the subgrid-scale model constant C_S [13].

For scalars, a gradient-diffusion approximation is used, along with the assumption of constant turbulent Schmidt numbers of value 0.7.

A general, reversible chemical reaction involving N species can be expressed as [23]

$$\sum_{i=I}^{N} v'_{i} M_{i} \longleftrightarrow^{k_{f}, k_{b}} \sum_{i=I}^{N} v''_{i} M_{i}$$
(1)

where M_i , v_i denote the species, the stoichiometric coefficients, whereas k_f and k_b stay for the rate coefficients of the forward and backward reaction, respectively.

According to the law of mass action of chemical kinetics, the molar conversion rate of a species i $(R_{C,i})$ is expressed as [23]

$$R_{C,i} = \left(v''_{i} - v'_{i} \right) \left(k_{f} \prod_{j=1}^{N} C_{j}^{n'_{j}} - k_{b} \prod_{j=1}^{N} C_{j}^{n''_{j}} \right) \quad (2a)$$

where C_i denote the species concentrations. The exponents n_i are equal to v_i for elementary reactions. For

global reactions n_i are empirically determined and may be different from $\nu_i. \label{eq:rescaled}$

After Arrhenius [23], the rate coefficient $k_{\rm f}$ is expressed by

$$k_f = A T^m \exp\left(-E_a / R_u T\right) \tag{2b}$$

In (2b), T is the thermodynamic temperature, E_a is the activation energy, R_u is the universal gas constant, A is the so-called pre-exponential factor, m is the so-called temperature exponent. For irreversible reactions, k_b is zero, for reversible reactions, given k_f , k_b can be obtained with the help of the equilibrium constant K_C ($K_C = k_f / k_b$) [23].

The source terms of species transport equations depend on expressions as given by Eq. (2). Obviously, in a turbulent flow, where averaged/filtered equations are solved, such highly non-linear source terms lead to severe closure problems. Thus, models are needed to consider turbulence-chemistry interaction.

2.1 Turbulence-chemistry interaction (turbulence model)

Following models are considered:

2.1.1 Chemical kinetics controlled flame (C)

It is assumed that turbulent mixing is infinitely fast compared to the chemical reaction rate, so that the resultant averaged/filtered conversion rate is determined purely by chemical kinetics. Expressions such as Eq. (2) are used as they are, plugging in the averaged/filtered quantities, neglecting the fluctuations.

2.1.2 Turbulent mixing controlled flame (T)

It is assumed that the chemical kinetics is infinitely fast compared to the turbulent mixing rate, so that the resultant averaged/filtered conversion rate is determined purely by small-scale turbulent mixing. A model based on this assumption is the so-called Eddy Dissipation Concept [24]. Here the averaged/filtered molar conversion rate ($R_{T,i}$) is calculated from

$$R_{T,i} = v_i \ \alpha \ \rho \frac{\varepsilon}{k} \min\left(\frac{Y_R}{v_R^{'} M_R} \right), \beta \frac{\sum_{P} Y_P}{\sum_{j}^{N} v_j^{''} M_j} \right) (3)$$

where, ρ , k, ε denote the time-averaged mixture density, turbulence kinetic energy and its dissipation rate, respectively. The terms Y_i and M_i stay for the averaged/filtered mass fraction and molar mass of the species i. The subscripts R and P denote the each if the reacting species, and the sum of the product species, respectively. The coefficients α and β are the empirical model constants. The standard model constants [24] are used. Since an improved version of this model was proposed later (see below), the abbreviation "EDC" will be reserved to denote the improved version of the Eddy Dissipation Concept, which will be presented below. The present version will be denoted by the abbreviation "T".

2.1.3 Turbulence & chemistry controlled flame (TC)

A rather simple method for considering of both effects is the following combination of the previously mentioned two methods, where the resulting averaged/filtered conversion rate is obtained from

$$R_i = \min(R_{C,i}, R_{T,i}) \tag{4}$$

2.1.3.1 Eddy Dissipation Concept (EDC)

The initial Eddy Dissipation Concept [24] assumes an infinitely fast chemistry. An improved version of the Eddy Dissipation Concept was proposed, later, again by Magnussen [25] where, chemistry and turbulence effects are considered in a combined manner (in a more sophisticated form compared to the "TC" approach expressed by Eq. (4)) Here, the averaged/filtered source/sink term of the species transport equation for a species i (S_i), is modelled as

$$S_{i} = \rho \frac{\gamma^{*} \psi}{1 - \gamma^{*} \Psi} \frac{1}{\tau^{*}} (Y_{i} - Y_{i}^{*})$$
(5)

where γ^* and τ^* denote the mass fraction occupied by the fine structures and the corresponding time scale, ψ representing the reacting fraction of the fine structures (constant estimated by stoichiometry). The terms Y_i and Y^*_i represent the averaged/filtered and fine structure values of the species mass fractions. Assuming adiabatic, isobaric perfectly stirred reactors for the fine structures, the fine structure mass fractions are obtained from

$$\frac{dY_i^*}{dt} = R_i(p, T, Y_i^*) + \frac{1}{\tau^*} \Big(Y_i^0 - Y_i^*) \Big)$$
(6)

where Y_i^0 denotes the surrounding value of the mass fraction and R_i is the reaction rate obtained from chemical kinetics (Eq. (2)). The two key parameters γ^* and τ^* are modelled based on turbulence quantities.

2.1.3.2 Laminar Flamelet Model (LFM)

The Laminar Flamelet Method is an elegant way of combining turbulence and chemistry effects [26]. In the present study, a flamelet model based on the mixture fraction (Z) and the reaction progress variable (C) is adopted, which was originally proposed by Pierce and Moin [27]. Within this concept, all thermo-chemical variables (ϕ) are expressed functions of Z and C as

$$\phi = \phi(Z, C) \tag{7}$$

Such functional relationships are obtained by performing 1D laminar flame calculations, once for all, and made available in tabulated form (flamelet libraries) for the subsequent CFD analysis.

Assuming Z and C are independent, with the help of presumed probability density functions (PDFs), the average values of the thermo-chemical variables are obtained. In the present work, a single-delta PDF is assumed for C, where a beta PDF is used for Z.

The model requires the solution of modelled transport equations for three quantities, i.e. for Z, its variance and the reaction progress variable [28].

The elegance of the approach lies therein that the number of equations to be solved does not increase with the complexity of the underlying reaction mechanism, since species transport equations are not solved during the CFD calculation, but extracted out of the libraries, which were prepared by detailed chemistry calculations in a preceding step.

Thus, LFM is very convenient to use with a detailed reaction mechanism, and, it is normally used, as such. In the present work, the flamelet libraries are constructed using the FlameMaster code [29].

2.2 Reaction mechanisms

The combustion reactions consist of elementary reactions between a large number of species, which are expressed by the so-called "detailed mechanisms" [23]. However, except for LFM, the computational overhead increases with the number of species considered in the mechanism. Thus, simplified mechanisms comprising a small number of mechanisms are required for practical purposes. These are, however, less universal compared to the detailed mechanisms and necessitate a careful evaluation and validation for the specific purpose. The following global and detailed mechanisms are considered in the present study:

2.2.1 Single-step global mechanisms

Here, the mechanism of Varma et al. [30] (VCB) and Marinov et al. [31] (MWP) are considered. Note that the reaction of MWP is a reversible one, whereas the reaction of VCB is an irreversible reaction.

2.2.2 Two-step global mechanisms

Here, the mechanism of Hsu and Jemcov [32] (HJ) is considered. Both reactions are formulated as reversible reactions.

2.2.3 Detailed reaction mechanisms

A detailed mechanism that is considered is the one suggested by Conaire et al. [33] (CCSPW).

A further detailed mechanism considered is the full GRI Mech 3.0 [34]. Referring to the definitions above (Eq. (2)), the single-step and two-step global reaction mechanisms [30-32] are summarized in Table 1.

Table 1. Global mechanisms (units: cm³, mol, s, kcal, K).

	А	m	Ea	n' _{H2}	n' _{O2/OH}
VCB [30]:					
$\mathrm{H}_2 + {}^1\!\!/_2 \operatorname{O}_2 \longrightarrow \mathrm{H}_2\mathrm{O}$	$3.53 \cdot 10^{12}$	0	7292	1.1	1.1
MWP [31]:					
$H_2 + {}^1\!\!/_2 \operatorname{O}_2 \leftrightarrow H_2 O$	$1.80^{-10^{13}}$	0	34979	1	0.5
HJ [32]:					
$H_2 + O_2 \leftrightarrow 2 \ OH$	$2.50^{\cdot}10^{26}$	-3	23900	1	1
$\mathrm{H_{2}\!\!+\!\!2OH}{\leftrightarrow}2\ \mathrm{H_{2}O}$	8.10.1035	-5	18800	1	2

The detailed reaction mechanism of Conaire et al. [33] is presented in Table 2 (note that the concentration exponents, n_i , are not explicitly given in Table 2, as the reactions are elementary reactions)

The applied models with different combinations are summarized in Table 3 (note that for the combustion model TC, the backward reaction is disabled, if the reaction mechanism is reversible).

Table 2. Detailed mechanism [33] (units: cm³, mol, s, kcal, K).

	Reaction	А	m	E_a
H ₂ /O ₂ Chain Reactions				
1	$H + O_2 = O + OH$	$1.91 \cdot 10^{14}$	0.00	16.44
2	$O + H_2 = H + OH$	$5.08 \cdot 10^4$	2.67	6.292
3	$OH+H_2 = H + H_2O$	$2.16 \cdot 10^8$	1.51	3.43
4	$O + H_2O = OH + OH$	2.95x10 ⁶	2.02	13.40
	H ₂ /O ₂ Dissociation/Combination Reactions			
5 ^a	$H_2 + M = H + H + M$	4.57·10 ¹⁹	-1.40	105.1
6 ^a	$O + O + M = O_2 + M$	$6.17 \cdot 10^{15}$	-0.50	0.00
7 ^a	O + H + M = OH + M	$4.72 \cdot 10^{18}$	-1.00	0.00
8 ^b	$H+OH+M = H_2O+M$	$4.50^{\cdot}10^{22}$	-2.00	0.00
Formation and Consumption of HO ₂				
9°	$H + O_2 + M = HO_2 + M$	3.48 [.] 10 ¹⁶	-0.41	-1.12
	$H + O_2 = HO_2$	$1.48 \cdot 10^{12}$	0.60	0.00
10	$HO_2 + H = H_2 + O_2$	$1.66 \cdot 10^{13}$	0.00	0.82
11	$HO_2 + H = OH + OH$	$7.08 \cdot 10^{13}$	0.00	0.30
12	$HO_2 + O = OH + O_2$	$3.25 \cdot 10^{13}$	0.00	0.00
13	$HO_2 + OH = H_2O + O_2$	$2.89 \cdot 10^{13}$	0.00	-0.50
	Formation and Cons	sumption of I	H_2O_2	
14	$HO_2 + HO_2 = H_2O_2 + O_2$	4.20.1014	0.00	11.98
	$HO_2 + HO_2 = H_2O_2 + O_2$	$1.30^{\cdot}10^{11}$	0.00	-1.629
15 ^d	$H_2O_2+M=OH+OH+M$	$1.27 \cdot 10^{17}$	0.00	45.5
	$H_2O_2 = OH + OH$	$2.95 \cdot 10^{14}$	0.00	48.4
16	$H_2O_2 + H = H_2O + OH$	$2.41 \cdot 10^{13}$	0.00	3.97
17	$H_2O_2 + H = H_2 + HO_2$	$6.03 \cdot 10^{13}$	0.00	7.97
18	$H_2O_2 + O = OH + HO_2$	$9.55 \cdot 10^{6}$	2.00	3.97
19	$H_2O_2+OH=H_2O+HO_2$	$1.00^{\cdot}10^{12}$	0.00	0.00
	$H_2O_2+OH=H_2O+HO_2$	5.80 ^{-10¹⁴}	0.00	9.56
а	Efficiency factors: H ₂ O	$=12.0; H_2 = 2$	2.5	
b	b Efficiency factors: $H_2O = 12.0$; $H_2 = 0.73$			
с	Troe param.: $a=0.5$, $T^{***}=10^{-30}$, $T^{**}=10^{30}$, $T^{*}=10^{100}$			
	Efficiency factors: H ₂ O	$=14.0; H_2 = 1$	1.3	
d	Troe param.: $a=0.5$, $T^{***}=10^{-30}$, $T^{**}=10^{30}$			
	Efficiency factors: H ₂ O	$=12.0; H_2 = 2$	2.5	

Table 3. Summary of applied models.

Case	Reaction mechanism	Combustion model	Turbulence model
Т	VCB [30]	Т	RANS
V-C	VCB [30]	С	RANS
V-TC	VCB [30]	TC	RANS
V-EDC	VCB [30]	EDC	RANS
M-C	MWP [31]	С	RANS
M-TC	MWP [31]	TC	RANS
M-EDC	MWP [31]	EDC	RANS
H-C	HJ [32]	С	RANS
H-TC	HJ [32]	TC	RANS
H-EDC	HJ [32]	EDC	RANS
C-C	CCSPW[33]	С	RANS
C-EDC	CCSPW[33]	EDC	RANS
LES-LFM	GRI [34]	LFM	LES

3 The test case

The considered test case is the atmospheric, vitiated coflow burner, which was investigated by Cabra et al. [8], which is depicted in Figure 1



Fig. 1. The investigated flame [8].

This consists of a central H_2/N_2 turbulent jet with a coaxial flow of hot combustion products from a lean premixed H_2/A ir flame. The central jet exit diameter is

d=4.57 mm. The coflow is stabilized on a perforated disk with 87% blockage and an outer diameter of D=210 mm. The central jet extends 70 mm above the surface of the perforated disk. The boundary conditions are summarized in Table 4 (X_{N2} =1- X_{H2} - X_{O2} - H_{H2O}).

Table 4. Inlet velocity (V), temperature (T), mole fract. (Xi).

	Central Jet	Coflow
V (m/s)	107	3.5
T (K)	305	1045
X_{H2}	0.2537	0
X _{O2}	0	0.1474
X _{H2O}	0	0.0989

4 Results

The grids are generated using a combination of rectangular/hexahedral and triangular/tetrahedral cells with a fine discretization near the central jet, and decreasing resolution towards outer parts.

Grid independence is ensured by detailed grid studies that are not discussed here in detail. For all models with RANS turbulence modelling (Table 3), a 2D-axisymmetric grid is used, utilizing the axisymmetry of the time-averaged fields. For LES turbulence model (GRI-LFM, Table 3), a 3D grid is used. The 2D $(2.2 \cdot 10^4 \text{ cells})$ and 3D $(1.1 \cdot 10^6 \text{ cells})$ are displayed in Figure 2.





Predicted fields of temperature (in K), Z, C by LES-LFM (Table 3), in a longitudinal plane through the middle of the jet flame at an instant of time are presented in Figure 3. Development of vortex structures in the edges of the jet, as well as lifting effects can be recognized.



Fig. 3. Predicted fields of temperature (in K), mixture fraction and reaction progress variable in a longitudinal plane through middle of jet flame at an instant of time by LES-LFM (Table 3).

Predicted temperature field by C-EDC (Table 3) is displayed in Figure 4. The lifting of the flame can be seen by inspecting the temperature field.



Fig. 4. Predicted temperature field (in K) by C-EDC (Tab. 3) (a) complete domain, (b) detail near central jet.

Predicted radial temperature profiles at x/d=1 (x: axial distance measured from nozzle outlet) are compared with measurements in Figure 5. M-C, M-TC, M-EDC, C-C, C-EDC and LES-LFM perform similarly and quite well.



Fig. 5. Radial temperature profiles at z/d=1 (a) 1-Step reaction mechanism, (b) 2-Step & detailed reaction mechanism.

4 Conclusions

A numerical analysis of a turbulent lifted H_2/N_2 flame is presented. As combustion mechanisms, a large spectrum is considered including single-step and two-step, as well as detailed mechanisms. As combustion models, various models are considered that treat turbulence-chemistry interaction in different ways, including the EDC and the LFM. For turbulence modelling RANS and LES approaches are used. Results are compared with measurements. The mechanism of Marinov et al. [31] is observed to perform quite well, for its being a single-step mechanism. The Hsu and Jemcov mechanism [32] shows, an inferior performance compared to the mechanisms of Varma et al. [30] and Marinov et al. [31], although it is a two-step mechanism [32], whereas the former [31,32] are single-step ones.

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