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# Numerical and Experimental Investigation of High-Pressure Stoichiometric Hydrogen–Oxygen Combustion in a Steam Atmosphere

*The present work deals with the numerical and experimental investigation of a novel combustion system for the generation of superheated steam. This combustion system is based on the stoichiometric combustion of pure oxygen and hydrogen in an atmosphere of high-pressure, low-temperature steam (“Oxy-H<sub>2</sub> in steam” combustion). For successful steam superheating, it is important that only small quantities of unreacted hydrogen and oxygen remain in the steam. A two-stage design is therefore envisaged, in which the first stage serves mainly the purpose of combustion of hydrogen and oxygen, whereas the second stage is used to provide sufficient time for mixing and for chemistry to reach chemical equilibrium. The total amount of steam is split between these two stages. In the first stage, only a small fraction is added as a diluent to limit the combustion temperature. The bulk of the steam is added in a second stage. The detailed investigation of the first stage, i.e., the burner, is the main focus of the present work. Based on computational fluid dynamics, the combustion process and the conditions in the reaction zone are simulated numerically. Emphasis is given on an analysis of the flame structure and the mixing of the reactants with the dilution steam. For validation, measurement data for the OH\* chemiluminescence (OH\*-CL) are collected in high-pressure experiments at 10 bar in an optically accessible combustion chamber. The comparison to experimental data shows that the numerical simulation can reproduce key aspects of the combustion accurately. [DOI: 10.1115/1.4072525]*

**Keywords:** oxygen–hydrogen combustion, numerical simulation, high-pressure experiment

## 1 Introduction

**1.1 Technical Background.** Renewable energies play a major role in today’s electricity generation. Their increasing use goes hand in hand with a rising demand for energy storages. Such storages are necessary to balance the volatility of renewable energies. Various approaches for the storage of energy exist, such as batteries, pumped hydroelectric energy storages, or chemical energy carriers. Among the latter, hydrogen and oxygen obtained from the electrolysis of

water are of high technical relevance since they can be used in various ways. For example, hydrogen and oxygen can be burnt directly in order to produce heat for heat engines. Compared to conventional combustion technologies, the combustion of pure oxygen and hydrogen offers the distinctive advantage that, in addition to avoiding carbon dioxide, pollutants such as nitrogen oxides and carbon monoxide are not emitted. For this reason, a novel combustion system for the stoichiometric combustion of hydrogen and oxygen under high pressure with high levels of steam dilution is investigated in this work. This Oxy-H<sub>2</sub> in steam combustion system has been developed recently by Siemens Energy [1] for the production of superheated steam in steam cycle applications (termed “steam boosting”). The design validation presented in Ref. [1] shows that the main design objectives, i.e., safe combustion at high

<sup>1</sup>Turbo Expo: Turbomachinery Technical Conference & Exposition (GT2026), June 15–19, 2026, GT2026.

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Manuscript received May 4, 2026; final manuscript received May 6, 2026; published online September 4, 2026. Editor: Jerzy T. Sawicki.

pressure, sufficient component lifetime, and low content of unreacted hydrogen and oxygen, are achievable. The key to this technology is a two-stage combustion process where one part of the steam is added first in a combustion stage, where it mainly serves as a diluent to limit the combustion temperature. This is necessary to ensure the required component lifetime. However, the amount of dilution steam is limited in this first stage in order to permit sufficiently high temperatures for flame stabilization [1]. The bulk of the steam is added in a second stage which provides sufficient residence time for mixing and reactions. The objective of this second stage is to achieve low levels of unreacted hydrogen and oxygen.

**1.2 Previous Work.** As outlined in Ref. [1], the use of “Oxy-H<sub>2</sub>” combustion for steam generation or steam boosting is, as such, not new (see Ref. [2] for an overview). Oxy-H<sub>2</sub> steam generators for providing peak power in power plants are presented in Refs. [3–8]. These steam generators are based on burners which are derived from rocket combustor technology. Liquid water is injected in these devices directly into the hot exhaust stream at the exit of the burner in order to generate rapidly large amounts of steam. This approach leads to significant amounts of unreacted hydrogen and oxygen [3,5–8] that have to be removed from the steam for safety reasons [6]. A similar method for steam superheating is pursued in Refs. [9] and [10] where steam is supplied to the hot gases of an Oxy-H<sub>2</sub> combustion system. The system presented in Refs. [9] and [10] is intended for the use in gas turbines. Fundamental combustion characteristics of this system are investigated in Ref. [9], where the effect of various diluents such as steam, but also argon and nitrogen, is studied for a single injector element. This investigation is extended in Ref. [10] to a technically relevant configuration which involves a 36 deg sector element of a combustion chamber for a gas turbine. Finally, in Ref. [11], a burner system for the generation of superheated steam is investigated where jets of oxygen and hydrogen are injected into a swirled stream of steam. This investigation is conducted at atmospheric pressure. The objective of this work is to obtain a fundamental understanding of the system with emphasis on combustion efficiency. Depending on the strength of the swirl, jet- or swirl-stabilized flames are observed in this burner. A high combustion efficiency of more than 95% is reported for temperatures above 1100 K. All of these earlier approaches to steam generation or steam superheating aim to achieve the desired steam state in a single step: Flame stabilization, mixing, and the reduction of unreacted hydrogen and oxygen are foreseen in a single process step within a restricted space of the combustor. The process investigated in this work is based on two steps as discussed in Ref. [1]. The two steps are spatially separated, and each serves a designated purpose for generating and conditioning steam. To our knowledge, this two-step process constitutes a novel aspect and distinguishes it from previous works.

**1.3 Objectives of This Work.** The two-step process for steam superheating given in Ref. [1] consists of a first stage where part of the steam is heated by the hydrogen–oxygen combustion and a second stage where the hot steam is conditioned in terms of temperature and contents of residual hydrogen and oxygen by adding steam with lower temperature. A simplified reactor model of this process is shown in Fig. 1 in terms of plug flow reactors and mixers. This concept is developed on the basis of reactor models that assume idealized conditions in terms of mixing and reactions and is validated through tests that mainly investigate the final amount of hydrogen and oxygen in the steam [1]. However, a detailed analysis of the processes within the device is not yet available. In particular, for the first stage where the combustion in a steam atmosphere takes place, no information is available regarding flame structure and mixing processes. The present work aims to close this gap through numerical and experimental investigations. Computational fluid dynamics is used here to obtain computational data on the combustion stage. These numerical results are supplemented by experimental data which are used for a validation of the numerical

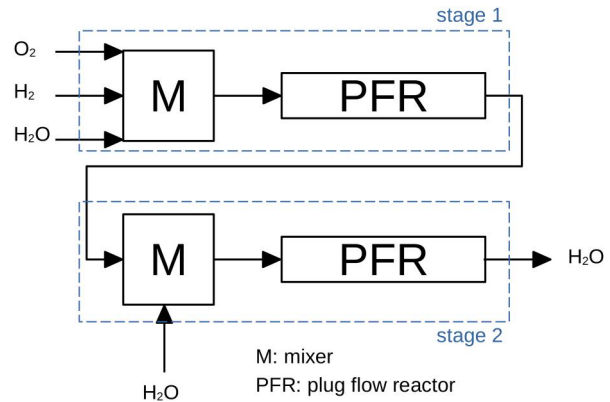


**Fig. 1 Simplified reactor model of the two-stage process for steam superheating**

modeling approach. Details on the experiment and the numerical simulation are provided in Secs. 2 and 3, respectively. The results of these investigations are presented in Sec. 4.

## 2 Experiment

**2.1 High-Pressure Test Rig HBK-S.** High-pressure experiments are performed here at 10 bar pressure in the high-pressure test rig “HBK-S” of the DLR Institute of Combustion Technology in Stuttgart. To perform these experiments, the burner is mounted on a test carrier which includes all required instrumentation and supply lines for different media. The test carrier is placed inside a high-pressure housing where optical access is provided through windows on each side. For the present investigation, hydrogen and oxygen are supplied from pressurized bottles. Steam is produced by a rented steam boiler system capable of pressures up to 17 bar in conjunction with an electric heater to superheat the steam to temperatures between 250 and 350 °C.

**2.2 Burner.** The burner used here is provided by Siemens Energy. A description of the burners in general terms is given in Ref. [1]. A more detailed schematic overview on the burner is shown in Fig. 2 (not to scale). There are a total of six nozzle pairs arranged along an annular channel for dilution steam. In each of those nozzle pairs, the outer nozzle supplies hydrogen and the inner one oxygen. The nozzles for hydrogen and oxygen are slightly inclined toward each other as indicated in Fig. 2 in order to enhance mixing of the oxygen and hydrogen. In addition, the mixing takes place at some distance from the nozzles, so that the resulting flame stabilizes away from the burner walls. In this way, the wall heat loads are reduced. The jets of a pair of nozzles draw also steam from the annular gap, which reduces the combustion temperature.

**2.3 Combustion Chamber.** The burner is located in the center of a combustion chamber with quadratic cross section. The combustion chamber is considerably longer than the lateral dimension. In order to provide well defined outflow conditions, a contraction is placed at the end of the combustion chamber. The combustion chamber provides optical access on all four sides through quartz glass window stacks which are convectively cooled by an air flow. Glass plates which face the flame on the inside are replaced regularly during the experiments. Due to cooling, the wall temperature inside of the combustion chamber varies in a range of 600 to 1100 K. Convective heat losses to the coolants are recorded in this work whereas radiative heat losses are difficult to quantify.

**2.4 Combustion Diagnostics.** To capture the location of the reaction zone, OH\* chemiluminescence (OH\*-CL) images are recorded in this work. OH\* denotes the OH radical in its electronically excited state. It is formed through chemical excitation

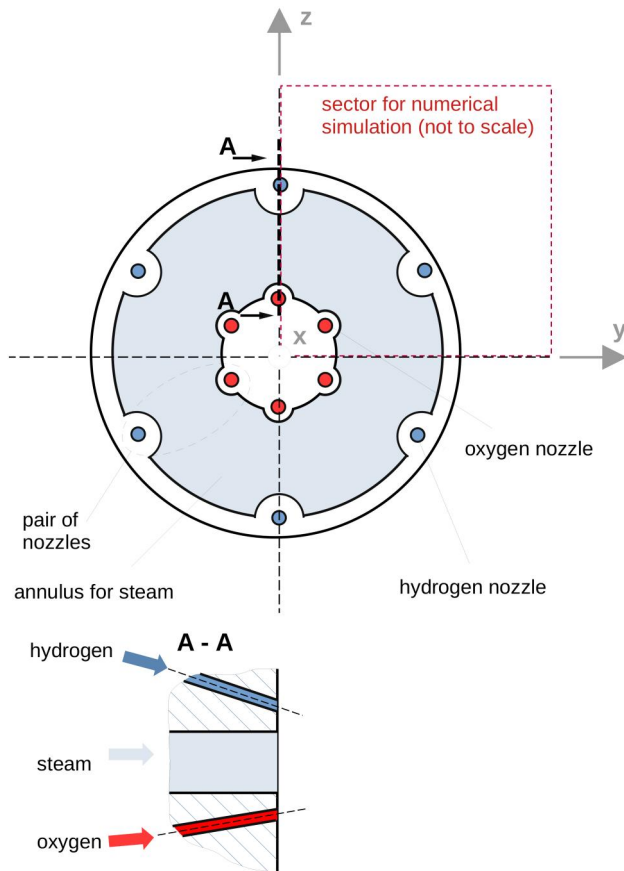


Fig. 2 Schematic sketch of burner (not to scale)

at temperatures below 2500 K [12]. At higher temperatures (such as in the present combustion system) thermal excitation becomes increasingly dominant [12]. OH\*-CL is recorded here through the use of a CMOS camera (the gate time is about 40  $\mu$ s; quartz glass objectives and interference filters ( $312 \pm 15$  nm) are used) which is placed perpendicular to the reaction zone. It records line-of-sight integrated images of OH\*-CL. After subtracting the background and correcting the sensitivity of each image, these images are averaged in order to obtain averaged information on the reaction zone.

### 3 Numerical Simulation

**3.1 Numerical Method and Modeling Approach.** To compute the turbulent reactive flow in this combustor, the in-house code THETACOM [13] of the DLR Institute of Combustion Technology is used. In THETACOM, the steady-state Favre-averaged balance equations for momentum, energy, and mass are solved numerically together with the steady-state transport equations for each species and turbulence model equations. The flow is assumed to be incompressible; therefore, the pressure-based semi-implicit method for pressure-linked equations algorithm [14] is used to compute the pressure and velocity fields. The numerical scheme is of second-order accuracy in space.

Turbulence is modeled with different turbulence models, namely, the  $k$ - $\omega$  shear-stress transport (SST) model [15],  $k$ - $\omega$  model in its 2006 version (KOM-2006) [16], and the low-Reynolds number  $k$ - $\epsilon$  model (LR-KE) given in Ref. [17]. Among those models, the SST model is a well-established two-equation model that blends dynamically between a  $k$ - $\omega$  and a  $k$ - $\epsilon$  model approach. However, the SST model is known to overestimate the decay rate of axial velocity in incompressible round jets [18,19]. As a consequence, the mixing rate of reactants is usually also overestimated which affects the position of the reaction zone in computations. For free round jets, this rapid decay of axial velocity can be countered by applying a

correction for the “round-jet/plane-jet anomaly” [16,20] which improves the computational results for free jet flames (see, e.g., Refs. [21] and [22]). As discussed in Refs. [21] and [22] for the  $k$ - $\epsilon$  model, an ad hoc method is to increase the model constant  $C_{\epsilon 1}$  to higher values, e.g.,  $C_{\epsilon 1} = 1.6$  [20]. For the SST model, such an adjustment of model constants is not available to the authors’ knowledge. For this reason, the use of the low-Reynolds number model  $k$ - $\epsilon$  in one variant denoted as LR-KE-JC is considered where  $C_{\epsilon 1}$  equals 1.6 in order to study the effect. The default variant LR-KE (i.e.,  $C_{\epsilon 1} = 1.5$  [17]), which is also considered here, serves as a reference in order to quantify the changes in the solution caused by the adjustment of  $C_{\epsilon 1}$ . Due to this, the KOM-2006 model is used as a more accurate model approach since it includes a correction for the round-jet/plane-jet anomaly in the model formulation. This correction is based on a nondimensional vortex-stretching parameter [16], i.e., an invariant, that is defined in terms of the strain-rate tensor and rotation tensor. Its definition ensures that the vortex-stretching parameter is zero for two-dimensional flows and positive for axisymmetric flows. This property is used in the KOM-2006 model in order to reduce in axisymmetric flows the model constant for the dissipation term in the transport equation of the specific dissipation rate. As outlined in Ref. [16], this behavior of the model mimics the processes in axisymmetric flows, where vortex stretching leads to an increased rate of dissipation compared to two-dimensional flows.

For turbulent combustion modeling, a finite-rate-chemistry approach is employed where a transport equation is solved for each species together with the balance equations for energy. Closure for the chemical source term is provided either by the “laminar chemistry” (LCH) approach or an assumed probability density function (APDF) method. In the former, the LCH approach, the reaction rates are obtained by applying the Favre-averaged mass fractions and Favre-averaged temperature to the constitutive equations of the chemical source term. In the latter, the APDF model, the expectation of the chemical source term is computed on the basis of a multivariate probability density function (PDF) in temperature and composition [23]. A clipped Gaussian PDF is used for temperature [23] and a Girimaji PDF for composition [24]. This model approach requires the solution of two additional transport equations for temperature variance and the trace of the covariance matrix of the species [23].

To describe chemical kinetics for hydrogen and oxygen combustion, the reaction mechanism in Ref. [25] is employed. This mechanism is combined with a reaction scheme for OH\* formation [26]. The combination of these two reaction mechanisms results in a total of nine species and 28 reactions.

The thermochemical equations, which consist of the balance equation of energy and the transport equations of all species, are solved simultaneously in THETACOM using an implicit scheme. To overcome the stiffness of this system of equations, the chemical source term is linearized by utilizing an analytic Jacobian matrix as outlined in Ref. [27] for both the LCH approach and the APDF model. Since an incompressible flow is assumed in this work, the thermodynamic pressure is taken to be constant over time and in space. The energy equation reduces, thus, to a balance equation for the specific enthalpy. The equation of state is given here by the ideal gas law. Thus, enthalpy is a function of temperature only. Its temperature dependence is given by the polynomial expressions in Ref. [28].

An important aspect in hydrogen combustion is the inclusion of differential diffusion. To this end, the diffusive fluxes of each species are modeled on the basis of a simplified Fickian approach as outlined in Ref. [29]. Each species has an individual diffusion coefficient which is computed on the basis of the molecular transport data. To ensure mass conservation for the diffusive fluxes, a correction term is added as described in Ref. [30].

Regarding turbulent scalar fluxes, closure is given in terms of a gradient diffusion hypothesis where turbulent Schmidt and Prandtl numbers are set to 0.7. In order to account for wall heat losses, the side windows are set to a temperature of 1100 K, and the walls of the

base plate and outflow contraction to 600 K. For the water-cooled window frames, a temperature of 500 K is assumed.

**3.2 Investigation of Mixing.** To investigate mixing of hydrogen, oxygen, and dilution steam, two variables are required. In this respect, this combustion system differs from conventional combustion systems where a third stream is usually absent and where only oxidizer and fuel participate in the mixing process. In this case, only one variable (i.e., mixture fraction) is sufficient to describe the mixing of the two media. Here, two tracers denoted by  $\tilde{\beta}_{O_2}$  and  $\tilde{\beta}_{H_2O}$  are introduced, and the following transport equation is solved for each of them:

$$\nabla \cdot (\rho \tilde{u} \tilde{\beta}_\alpha) = \nabla \cdot \left( \left( \frac{\mu}{Sc} + \frac{\mu_T}{Sc_T} \right) \nabla \tilde{\beta}_\alpha \right) \quad (1)$$

In this equation,  $\rho$  is the density,  $\mu$  is the dynamic viscosity,  $\mu_T$  the turbulent viscosity,  $Sc = 0.7$  the Schmidt number, and  $Sc_T = 0.7$  the turbulent Schmidt number. The operators  $\bar{\cdot}$  and  $\tilde{\cdot}$  denote Reynolds- and Favre-averages, respectively. Although this equation neglects differential diffusion, the tracers computed in this way still provide a good approximation to the spatial distribution of the media, since the turbulent viscosity is usually much larger than the molecular. The inflow boundary conditions for the tracers are specified such that  $\tilde{\beta}_{O_2}$  and  $\tilde{\beta}_{H_2O}$  are one at the inflow boundaries for oxygen and steam, respectively, and zero for any other inflow. At walls, zero gradient boundary conditions are employed. These boundary conditions ensure together with the elliptic character of Eq. (1) that the value of each tracer equals the mass fraction of either oxidizer or diluent. Furthermore, the tracer value of hydrogen  $\tilde{\beta}_{H_2}$  can be retrieved by

$$\tilde{\beta}_{H_2} = 1 - \tilde{\beta}_{O_2} - \tilde{\beta}_{H_2O}$$

**3.3 Computational Runs.** As outlined in Sec. 3.1, different models are employed for turbulence and combustion modeling. To study the effect of each of these models, the runs given in Table 1 are considered. Runs 1 to 4 investigate the effect of turbulence modeling on the solution. Since no stable solution is obtained for all of these turbulence models when the APDF model is used, these investigations are conducted on the basis of the LCH approach where a solution is always found. The effect of considering turbulence chemistry interaction modeling in terms of the APDF model is investigated in runs 4 and 5. This investigation is performed for the  $k-\omega$  (2006) model only.

**3.4 Computational Domain.** In order to reduce the computational cost, only one fourth of the burner and combustion chamber is modeled in the simulations. The computational domain contains one and a half nozzles. The sector of the burner and the combustion chamber (not to scale) is shown in Fig. 2. The domain is discretized with an unstructured mesh of about  $78.6 \times 10^6$  cells which is created using the software CENTAUR of CentaurSoft. The mesh consists of tetrahedrons and pyramids in the interior of the domain and prism layers at the walls. The height of the prism layers is adjusted in order to meet the required wall resolution for the turbulence model, i.e.,  $y^+$  is well below one for all computations. THETACOM solves the equations on a median dual grid that is built at each node of this

mesh. This dual grid has a total of  $16.6 \times 10^6$  control volumes. The finest mesh is in the region of flame stabilization with mesh sizes of about  $50 \mu m$ . To ensure that this grid resolution is sufficient, run 4 (given in Table 1) is repeated on a finer mesh with half the mesh width in the critical region where the flame stabilizes (the refined mesh has  $31.2 \times 10^6$  control volumes). No major changes are observed in the solution of the fine mesh (the results are not shown here to keep this work concise). For this reason, the mesh with  $16.6 \times 10^6$  control volumes is used for all computations.

## 4 Results

**4.1 Nondimensional Representation.** In the following, all results are presented in nondimensional form. Spatial  $x$ -,  $y$ -, and  $z$ -coordinates are normalized with the outer diameter  $D$  of the annulus for steam shown in Fig. 2. Likewise, for mass fractions (except for water), a reference value is used to compute the nondimensional mass fraction (nondimensional quantities are denoted by  $\star$ )

$$\tilde{Y}_\alpha^\star = \frac{\tilde{Y}_\alpha}{\tilde{Y}_{\alpha,ref}} \quad (2)$$

For heat release  $q$ , temperature  $T$ , and water mass fraction, the dimensionless variables are defined as

$$\tilde{T}^\star = \frac{\tilde{T} - \tilde{T}_{min}}{\tilde{T}_{max} - \tilde{T}_{min}} \quad (3)$$

$$q^\star = \frac{q - q_{min}}{q_{max} - q_{min}} \quad (4)$$

$$\tilde{Y}_{H_2O}^\star = \frac{\tilde{Y}_{H_2O} - \tilde{\beta}_{H_2O}}{\tilde{Y}_{H_2O,ref}} \quad (5)$$

min and max denote the minimum and maximum values in the computational domain, respectively. The definition of  $\tilde{T}^\star$  and  $q^\star$  ensures that these quantities vary between zero and one.  $\tilde{Y}_{H_2O}^\star$  is defined by subtracting the mass fraction of dilution steam  $\tilde{\beta}_{H_2O}$ . Hence, only the water formed by chemical reactions is considered in this variable. For the dimensionless mass fractions presented in this work, following reference values  $\tilde{Y}_{\alpha,ref}$  are used in Eqs. (2) and (5):

$$\tilde{Y}_{OH^\star,ref} = \tilde{Y}_{OH^\star,max} \quad (6)$$

$$\tilde{Y}_{H_2,ref} = \frac{\dot{m}_{H_2,in}}{\dot{m}_{H_2,in} + \dot{m}_{O_2,in} + \dot{m}_{H_2O,in}} \quad (7)$$

$$\tilde{Y}_{O_2,ref} = \frac{\dot{m}_{O_2,in}}{\dot{m}_{H_2,in} + \dot{m}_{O_2,in} + \dot{m}_{H_2O,in}} \quad (8)$$

$$\tilde{Y}_{H_2O,ref} = \tilde{Y}_{H_2,ref} + \tilde{Y}_{O_2,ref} \quad (9)$$

where  $\dot{m}_{\alpha,in}$  denotes the mass flow of the species  $\alpha$  that enters the burner system. To investigate OH\*-CL, the nondimensional OH\* concentration  $C_{OH^\star}^\star$  is defined here as

$$\tilde{C}_{OH^\star}^\star = \frac{\tilde{C}_{OH^\star}}{\tilde{C}_{OH^\star,ref}} \quad (10)$$

where the reference value is set to  $\tilde{C}_{OH^\star,ref} = \tilde{C}_{OH^\star,max}$ .

For all computational runs, the same reference values are used. Maxima and minima of variables (which are required to compute some of the reference values and some nondimensional variables) are taken across all computations. In this way, all nondimensional variables can be compared directly between the different computations.

**Table 1 Overview on computational runs**

| Run | Turbulence model | Combustion model |
|-----|------------------|------------------|
| 1   | SST              | LCH              |
| 2   | LR-KE            | LCH              |
| 3   | LR-KE-JC         | LCH              |
| 4   | KOM-2006         | LCH              |
| 5   | KOM-2006         | APDF             |

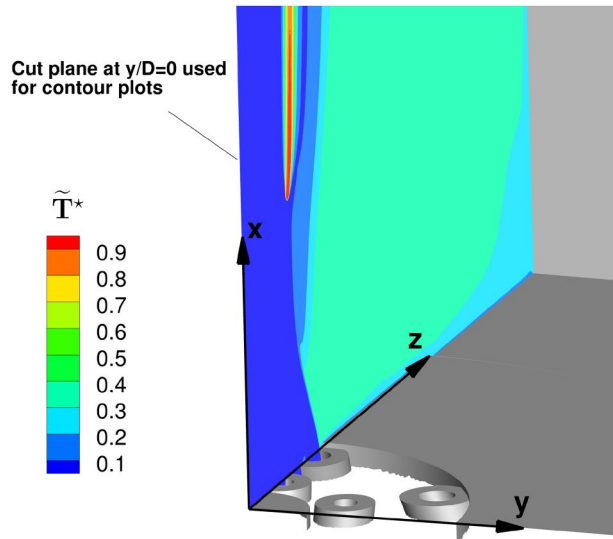


**Fig. 3** View showing cut plane for contour and streamline plots and global coordinate system

**4.2 Evaluation of Simulation Data.** In order to compare field data of different simulations, a cut plane is used for contour and streamline plots, which is shown in Fig. 3 together with the global coordinate system. The global coordinate system is located in the center of the combustion chamber as indicated in Fig. 2. The location  $x/D = 0$  coincides with the exit plane of the burner. The cut plane in Fig. 3 is placed along the cut “A–A” given in Fig. 2, i.e., the  $x$ – $z$  plane at  $y/D = 0$ . It intersects a pair of nozzles.

An exception is the evaluation of the line-of-sight integrated  $\text{OH}^*$ -CL. The line-of-sight integration is performed in direction of the  $z$ -axis. For this reason, the results of this integration are shown in an  $x$ – $y$  plane.

In addition to these two-dimensional plots, diagrams of different properties are plotted along the  $x$ -axis. For this one-dimensional representation of results, averages are computed at different  $y$ – $z$  planes in the combustor.

**4.3 Reaction Zone Position.** In order to provide a first impression on the location of the reaction zone, the isosurface of nondimensional  $\text{OH}^*$  mass fraction is shown in Fig. 4. Isosurfaces of the hydrogen and oxygen mass fraction highlight the location of the jets that issue from the nozzles. It is clear from the  $\text{OH}^*$  distribution, that lifted discrete reaction zones are formed between each pair of hydrogen and oxygen nozzles. As the contour plot on the slice given in Fig. 4 indicates, the reaction zones have a thin curved shape in all computational runs. It appears, however, in Fig. 4 that the models LR-KE-JC and KOM-2006 which utilize a correction for the round-jet/plane-jet anomaly lead to a distinctively higher lift-off height in runs 3 to 5 than the SST and LR-KE model in runs 1 and 2. In order to correlate these computational data to  $\text{OH}^*$ -CL recorded in the experiment, the  $\text{OH}^*$  concentration is computed for each computational run and summed up in  $z$ -direction (cf. coordinate system in Figs. 3 and 4) to obtain a line-of-sight integrated image. The concentration is used here based on the intuitive argument that  $\text{OH}^*$ -CL should be correlated with the number of  $\text{OH}^*$  molecules per volume. The evaluation of  $\text{OH}^*$  concentration is shown in Fig. 5 together with experimental data of  $\text{OH}^*$ -CL. A distinctive asymmetry is observed in  $\text{OH}^*$ -CL in the experiment which might be due to the presence of liquid water that accumulates at the bottom side of the combustion chamber. In agreement to the data of the numerical simulation in Fig. 4, separate reaction zones are observed in the experiment which are located between a pair of hydrogen and oxygen nozzles. In the experiment, only three separate zones of  $\text{OH}^*$ -CL are visible because the line-of-sight detected  $\text{OH}^*$ -CL signal from two nozzle pairs (oxygen and hydrogen) overlaps in

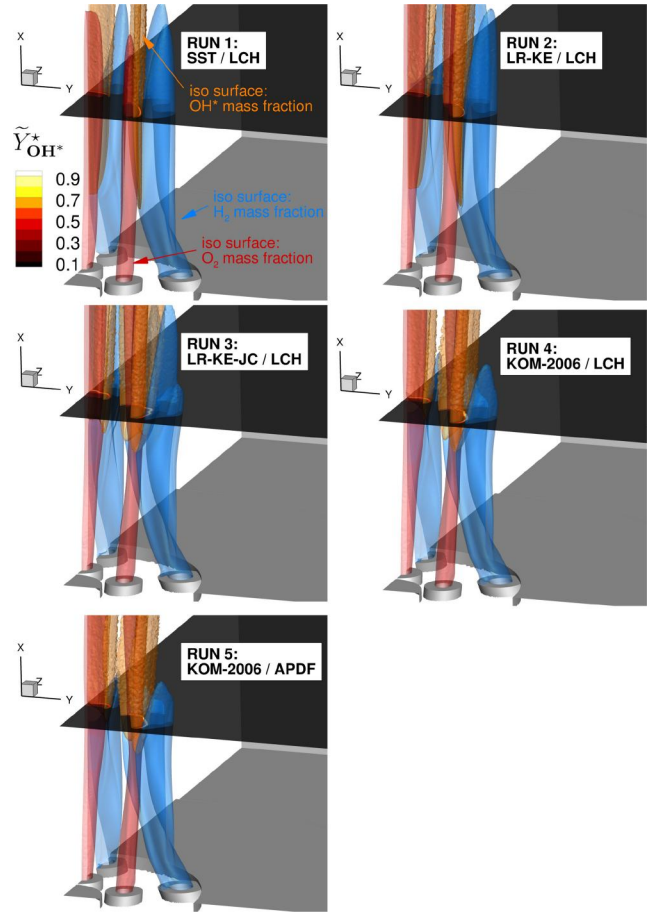


**Fig. 4** Isosurfaces of hydrogen, oxygen, and  $\text{OH}^*$  mass fraction for different turbulence and combustion models

each zone. A comparison of these experimental data to numerical results confirms that the models LR-KE-JC and KOM-2006 increase indeed the lift-off height to a degree that the lift-off height matches experimental data. Here, lift-off height is defined in terms of the lower edge of the zone where  $\text{OH}^*$ -CL is detected. It equals approximately  $0.55D$ . Models without a correction for the round-jet/plane-jet anomaly yield a lift-off height that is significantly smaller than in the experiment. In contrast, the use of the APDF has no drastic effect on flame position. It merely increases the concentration of  $\text{OH}^*$  in the computation. A distinctive difference between all computations and the experiment is the shape of the reaction zone. In the simulation, a thin area of maximum intensity is observed. This is essentially an artifact of the three-dimensional shape of the reaction zone which is thin and curved as observed in Fig. 4. By contrast, the experiment gives the impression of a broad reaction zone. This is due to the highly unsteady flow in the experiments where rapid flame fluctuations are observed in the streamwise direction over a distance of about  $2D$ . Such processes cannot be modeled adequately with the present steady simulation approach which explains this difference in shape.

Figure 5 shows large differences in the absolute value of  $\text{OH}^*$  between runs 1 to 4 that utilize the same combustion model. To quantify the exact causes for these differences is difficult, since various effects such as differences in the local strain rate, different shapes of the reaction zone in each run, and differences in the local dilution by steam overlap simultaneously in the computation. However, a closer inspection of the dimensionless  $\text{OH}^*$  concentration given in Fig. 6 reveals that  $\text{OH}^*$  concentration seems to correlate with the dilution by steam. To quantify this dilution, the tracer  $\beta_{\text{H}_2\text{O}}$  is plotted in Fig. 6. It is found for run 1 with the lowest  $\text{OH}^*$  concentration that  $\text{OH}^*$  is mainly formed in regions with  $\beta_{\text{H}_2\text{O}}$

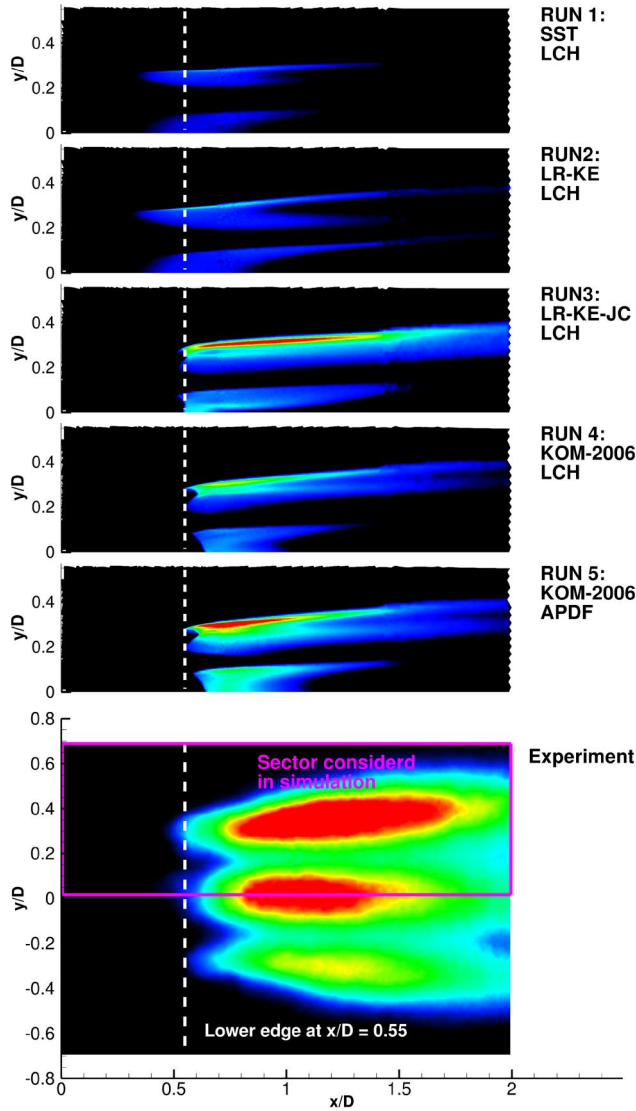


**Fig. 5 Comparison of computed and measured OH\* distribution for different turbulence and combustion models. The data are line-of-sight integrated in z direction and plotted in an x-y plane.**

above 0.21. In contrast, for run 3 with the highest OH\* concentration among runs 1 to 4, OH\* is formed in an area with a lower amount of steam ( $\tilde{\beta}_{\text{H}_2\text{O}}$  equals about 0.13). For runs 2 and 4, the situation is less clear. It seems, however, that OH\* is formed in these runs in areas which have less steam compared to run 1. Consequently, OH\* concentration is higher for runs 2 and 4 than in run 1.

**4.4 Model Comparison.** In order to investigate the effect of the different model approaches for combustion and turbulence in detail, the nondimensional temperature field is plotted in Fig. 7 along with isolines for the tracers  $\tilde{\beta}_{\text{H}_2}$  and  $\tilde{\beta}_{\text{O}_2}$ . This plot shows the fields in the cut plane defined in Fig. 3. The contour plot of temperature reveals the same effect observed in Fig. 5 for runs 1 and 2. Both runs, which do not involve a correction for the round-jet/plane-jet anomaly, lead to a reaction zone that is located at  $x/D = 0.25$  from the burner exit plane, which is at  $x/D = 0$ . For runs 3 to 5, the reaction zone is shifted further downstream to about  $x/D = 0.55$ . In addition, the flame zone appears to be also significantly wider for runs 3 to 5. In terms of mixing, the use of models with a correction for the round-jet/plane-jet anomaly seems hardly to affect the fuel jet in the vicinity of the reaction zone. If major differences between those runs were present, the fuel distribution in terms of  $\tilde{\beta}_{\text{H}_2}$  would differ significantly. Such major differences are not observed between

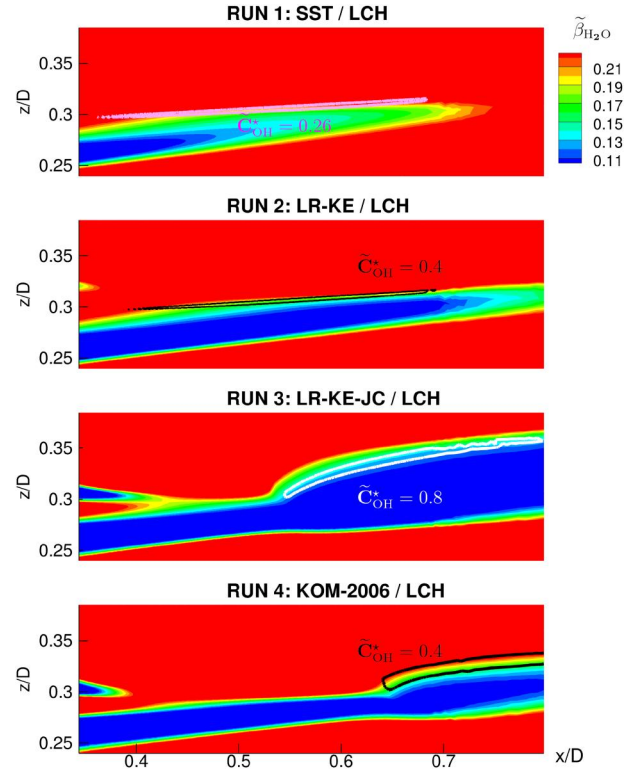


**Fig. 6 Contour plots of  $\tilde{\beta}_{\text{H}_2\text{O}}$  with isolines of  $\tilde{C}_{\text{OH}}^*$ . The data are plotted in the cut plane shown in Fig. 3.**

$x/D = 0$  and  $x/D = 0.4$ , as the isoline for  $\tilde{\beta}_{\text{H}_2}$  indicates. The location of this isoline is almost same for all runs in this region. However, differences are observed for the oxygen jets between the different runs. The use of a correction for the round-jet/plane-jet anomaly changes significantly the penetration of the oxidizer. For example, the downstream extent of the isoline of  $\tilde{\beta}_{\text{O}_2}$  moves from about  $x/D = 0.77$  for the LR-KE model to  $x/D = 1.2$  for the LR-KE-JC model. A similar increase is observed for the  $k-\omega$  based models, where the penetration depth based on the isoline of  $\tilde{\beta}_{\text{O}_2}$  increases from  $x/D = 0.58$  for the SST model to approximately  $x/D = 0.83$  for the KOM-2006 model. In addition, the models LR-KE-JC and KOM-2006 lead to a spread of oxidizer in the vicinity of the flame zone which is highlighted in Fig. 7. This spread has its origin in the wide reaction zone for these computations which leads to a region of low density that causes flow dilatation (cf. Ref. [31] for the effect of heat release on the flow field).

Differences between runs 1 to 5 are also ascertained further downstream of the flame stabilization region. In Fig. 8, streamlines and isolines for  $\tilde{\beta}_{\text{H}_2\text{O}}$  are shown in the same cut plane as in Fig. 7. The use of the models LR-KE-JC and KOM-2006 appears to extend the length of the recirculation zone in the burner by a factor of two compared to the models SST and LR-KE. Likewise, the downstream flow of reactants is affected by the choice of turbulence model. The jets of oxidizer and fuel merge in the shear layer into a single jet which moves with high momentum through the combustion chamber. To visualize the location and the spreading behavior of this jet, an isoline of  $\tilde{\beta}_{\text{H}_2\text{O}}$  is shown in Fig. 8. For the LR-KE-JC and KOM-2006 models, this jet penetrates further into the combustion chamber as the isoline of  $\tilde{\beta}_{\text{H}_2\text{O}}$  indicates.

The differences in flow and mixing shown in Fig. 8 are also noticeable in the chemical conversion of hydrogen and oxygen. This is shown in Figs. 9 and 10 where the nondimensional mass-flow averaged profiles for these quantities, i.e.,  $\bar{Y}_{\text{H}_2,\text{avg}}^*$  and  $\bar{Y}_{\text{O}_2,\text{avg}}^*$ , are plotted along the burner axis. In addition, the nondimensional average of water which is formed by chemical reactions (cf. Eq. (5)), i.e.,  $\bar{Y}_{\text{H}_2\text{O},\text{avg}}^*$ , is also given. In agreement with a shorter recirculation zone and a more rapid mixing for the models SST and LR-KE, the

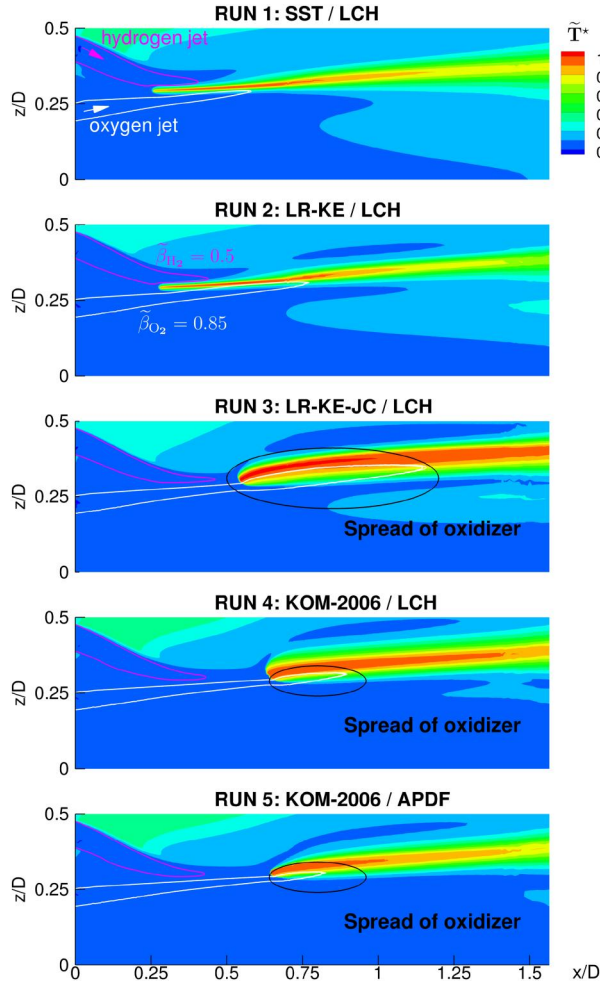


**Fig. 7** Contour plots of nondimensional temperature for different turbulence and combustion models. The data are plotted in the cut plane shown in Fig. 3.

conversion of hydrogen and oxygen to water completes at about  $x/D = 12$  as shown in Fig. 9. By comparison, the conversion continues until  $x/D = 20$  for the models LR-KE-JC and KOM-2006 which both utilize a “round-jet/plane-jet” correction. Surprisingly, the modeling of turbulence–chemistry interaction does not alter the results significantly. As shown in Fig. 10, the APDF model slightly slows down the reaction. The difference to the LCH approach appears to be almost negligible. Likewise, the differences between runs 4 and 5 are also minor in Fig. 8.

As shown in Fig. 5, models incorporating a correction for the round-jet/plane-jet anomaly seem to show better agreement with the available OH\*-CL experimental data than models that do not apply this correction. However, applying this correction also affects the solution in other regions of the combustion chamber, such as the recirculation zone (cf. Fig. 8). To enable a definitive evaluation of the different modeling approaches, additional experimental data—particularly flow velocity measurements—are planned.

**4.5 Stabilization of Reaction Zone.** To investigate the mechanism of reaction zone stabilization, the results of run 5 are considered in detail. This run takes turbulence–chemistry interaction into account, making it the most accurate simulation in terms of modeling. Furthermore, the results of this run show a good agreement to the experimental data in terms of flame position (cf. Fig. 5). In Fig. 11, a close-up view of the results in the stabilization area of the reaction zone is shown in the cut plane defined in Fig. 3. In

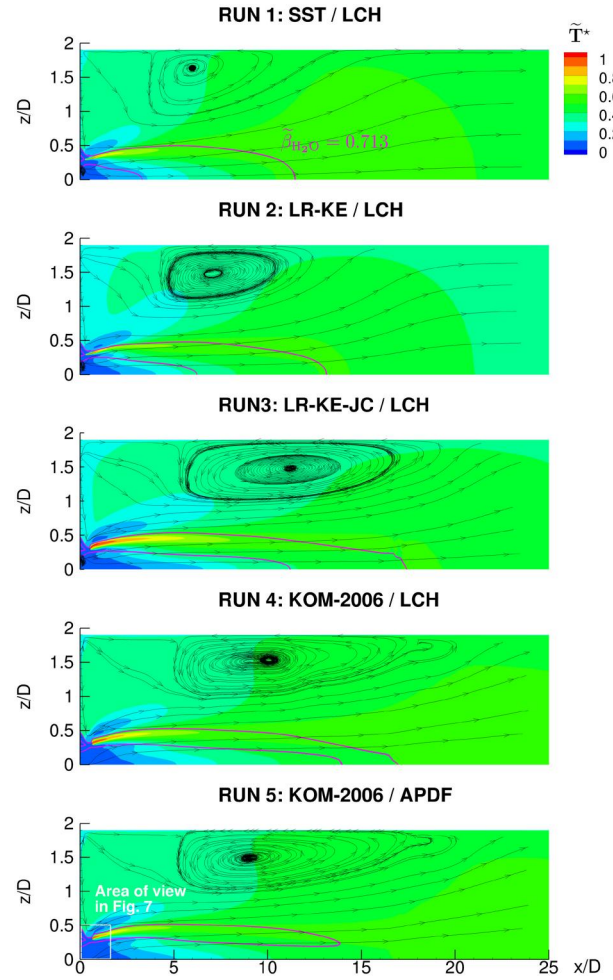


**Fig. 8** Streamlines and contour plot of nondimensional temperature for different turbulence and combustion models. The data are plotted in the cut plane shown in Fig. 3.

this figure, the normalized Takeno flame index  $G$  [32,33], which is defined according to

$$G = \frac{\nabla \tilde{Y}_{H_2} \cdot \nabla \tilde{Y}_{O_2}}{|\nabla \tilde{Y}_{H_2}| |\nabla \tilde{Y}_{O_2}|} \quad (11)$$

is shown. This index is essentially the cosine of the angle between  $\nabla \tilde{Y}_{H_2}$  and  $\nabla \tilde{Y}_{O_2}$ . If these gradients are aligned with each other, the index takes positive values. Such a situation is found in premixed combustion. If the gradients are oppositely directed, as in regions of nonpremixed combustion, the index becomes negative. Hence, the index is useful for identifying regions of premixed and nonpremixed combustion. In addition, the dimensionless temperature, the dimensionless heat release, and the dimensionless OH\* mass fraction are plotted in Fig. 11. In the contour plots of these variables, isolines for the dimensionless heat release, the dimensionless OH\* mass fraction, and the element mole fraction of hydrogen at stoichiometric conditions, i.e.,  $\tilde{\zeta}_{H_2} = 2/3$ , are also shown. The latter line separates fuel-rich and fuel-lean areas in the combustion chamber. The reaction zone appears to stabilize along this stoichiometric mixing line where the highest values of dimensionless heat release are found. This is to be expected since fuel consumption rates are highest at stoichiometric conditions. Another aspect that becomes clear from Fig. 11 is that the areas of high OH\* mass fractions do not coincide with the regions of high heat release. This is due to the fact that OH\* is mainly formed here by thermal excitation since temperatures are above the limit of 2500 K [12]. Such high temperatures are reached downstream of the maximum

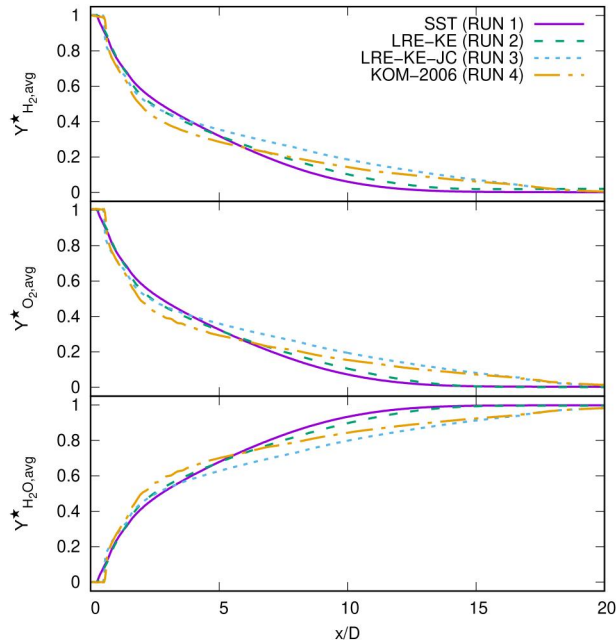


**Fig. 9 Average nondimensional mass fractions along  $x$ -axis for different turbulence models**

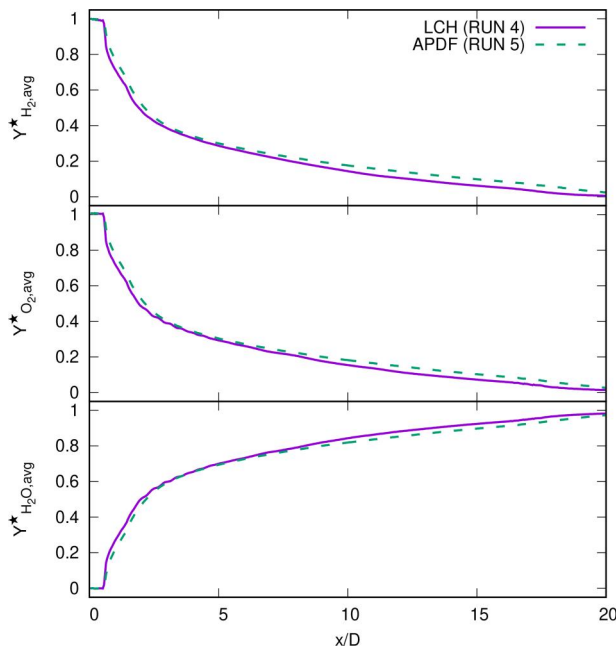


**Fig. 10 Average nondimensional mass fractions along  $x$ -axis for different combustion models**

high heat release where a region of nonpremixed combustion forms, as the negative values of the flame index indicate. The fact that  $\text{OH}^*$  is mainly thermally excited and not chemically must be taken into account when interpreting the experimental data for  $\text{OH}^*\text{-CL}$  in this burner. In the area of maximum heat release a positive flame index is present which indicates premixing of reactants. Thus, the reaction zone stabilizes along the stoichiometric mixing line on the basis of premixed combustion. The oxidizer-rich or fuel-rich gases of this reaction zone react further behind this premixed flame zone in a nonpremixed combustion regime.

The observations made here regarding the stabilization of the lifted reaction zone can be related to results of direct numerical simulation (DNS) [34] and large-eddy simulation (LES) [35] for

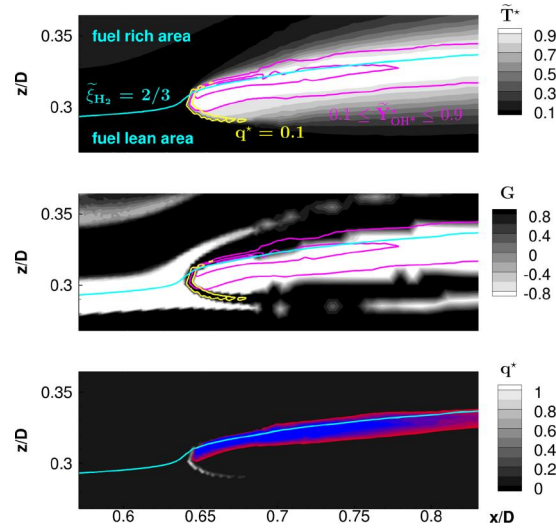


**Fig. 11 Close-up view of tip of reaction zone for run 5. The data are plotted in the cut plane shown in Fig. 3.**

lifted hydrogen–air flames. Both the DNS and LES observe flame stabilization along the stoichiometric mixing line. For DNS, the leading edge which stabilizes the flame has a triple flame-like structure, where two premixed branches, located on the fuel-rich and fuel-lean sides each, engulf a nonpremixed flame branch. Such premixed branches are observed also in LES at the point of flame stabilization. These observations sustain the results shown in Fig. 11, where two premixed branches, each in the fuel-rich and fuel-lean region, are found at the location where the reaction zone stabilizes.

## 5 Summary and Conclusions

In this work, the combustion of hydrogen and oxygen in an atmosphere of superheated steam is investigated by numerical and experimental means. High-pressure experiments are performed that provide data in terms of  $\text{OH}^*\text{-CL}$  for a qualitative validation of numerical results. In order to reproduce these experimental data, different two-equation turbulence and combustion models are used in steady simulations. It is found that the  $k\text{-}\omega$  (2006) turbulence model is capable of reproducing the experimental data in conjunction with a multivariate assumed probability density function model for turbulence–chemistry interaction. In particular, this simulation can successfully reproduce important observations from the experiment, i.e., the formation of individual reaction zones between pairs of nozzles and the lift-off height of these reaction zones. However, the shape of the flame zone is poorly modeled which is attributed to the highly unsteady behavior of the flame that is not captured by the present steady computations. Comparing different modeling approaches for turbulence and combustion, it appears that the turbulence models have a major influence on the results. In particular, the inclusion of a correction of the round-jet/plane-jet anomaly improves the agreement to the experiment in terms of reaction zone position significantly. By comparison, the effect of different combustion models on the numerical results is found to be negligible.

Based on the results of this qualitative validation, the structure of the flame zone is analyzed more closely. It is found that each individual reaction zone is stabilized by a premixed flame zone that forms in areas where stoichiometric mixing conditions prevail. Highest heat release occurs within this flame zone. Directly downstream in the wake of this premixed flame zone, a region of nonpremixed combustion forms where high temperatures are found. Due to thermal excitation,  $\text{OH}^*$  concentration reaches its maximum value in this region. Thus,  $\text{OH}^*$  concentration and  $\text{OH}^*\text{-CL}$  are not markers for the heat release zone in this burner.

## Acknowledgment

The investigations were conducted as part of the joint research project Hydroxy. The work was supported by the Bundesministerium für Wirtschaft und Klimaschutz (BMWK) as per resolution of the German Federal Parliament under Grant No. 03EE5125B. The authors would like to thank S. Peukert and T. Schiek for the installation as well as R. Schieferstein and T. Gall for the test rig operation. Furthermore, the authors gratefully acknowledge the scientific support and HPC resources provided by the German Aerospace Center (DLR). The HPC system CARA is partially funded by “Saxon State Ministry for Economic Affairs, Labour and Transport” and “Federal Ministry for Economic Affairs and Climate Action.” The HPC system CARO is partially funded by “Ministry of Science and Culture of Lower Saxony” and “Federal Ministry for Economic Affairs and Climate Action.”

## Conflict of Interest

There are no conflicts of interest.

## Funding Data

- Bundesministerium für Wirtschaft und Klimaschutz (BMWK) (Grant No. 03EE5125B; Funder ID: 10.13039/100021130).

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## Data Availability Statement

Data under embargo. Data are not available.

## Nomenclature

$C$  = concentration (mol/m<sup>3</sup>)  
 $C_{el}$  = model constant  
 $D$  = diameter (m)  
 $G$  = flame index  
 $\dot{m}$  = mass flow (kg/s)  
 $q$  = heat release (W/m<sup>3</sup>)  
 $Sc$  = Schmidt number  
 $Sc_T$  = turbulent Schmidt number  
 $T$  = temperature (K)  
 $\mathbf{u}$  = velocity vector (m/s)  
 $x$  = coordinate (m)  
 $y$  = coordinate (m)  
 $Y$  = mass fraction  
 $y^+$  = dimensionless near wall distance  
 $z$  = coordinate (m)

## Greek Symbols

$\beta$  = tracer  
 $\mu$  = dynamic viscosity (kg/(m s))  
 $\mu_T$  = turbulent viscosity (kg/(m s))  
 $\xi$  = element mole fraction  
 $\rho$  = density (kg/m<sup>3</sup>)

## Superscripts and Subscripts

avg = average value  
in = inflow  
max = maximum  
min = minimum  
ref = reference value

$\star$  = dimensionless quantity  
 $\alpha$  = index of species or tracer

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