Comparison of Different Combustion Models with Respect to the Simulation of Combustion Induced Vortex Breakdown

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1 Introduction

This work elucidates the numerical results of uRANS simulations of a premixed flame system for three different combustion models and compares the outcomes with experimental findings from literature. The investigated configuration exhibits an extraordinary transformation of the flame when a critical equivalence ratio is reached - the system shifts into an unstable condition. This phenomenon is known as *Combustion Induced Vortex Breakdown* (CIVB) and is associated with an unintended upstream propagation of the flame nearby the axis of rotation through the mixing pipe towards the swirler ([1]).
This type of flashback is characterised by an intense interaction between the flow and the flame. Hence, the precise prediction of the local and time dependent distribution of heat release is necessary for the simulation of CIVB. The combustion model has to capture this challenging task which is even more sophisticated due to the restriction of the inherent processes to only a small volume around the axis of rotation.
The combustion models that are assessed and compared to each other with respect to the appropriate simulation of the CIVB phenomenon are slightly modified versions of the approaches of Schmidt [2], Lindstedt-Vaos [3] and Hoffmann [4].
The combustion model originally introduced by Schmidt [2] is based on the closure for the turbulent flame speed. The approaches of Lindstedt-Vaos and of Hoffmann are based on considerations for the flame surface density which in turn is determined by an algebraic formulation ([3]) or rather on a formulation for an additional transport equation ([4]).

2 Theory

All three combustion models are based on an irreversible, infinitely fast one-step chemical reaction mechanism for methane-air. This procedure reduces the determination of the mean, statistically distributed reaction state to the solution of only one progress variable. This favre averaged progress variable $\tilde{c}$ can

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be expressed as

$$\tilde{c} = \frac{T - T_u}{T_b - T_u} \tag{1}$$

for the atmospheric conditions of the configuration under consideration. Thereby, T_u stands for the unburnt temperature and T_b for the temperature of the burnt mixture.
The interaction between the combustion and the flow is captured by the effect of modified density distribution which is in turn directly related to the temperature field due to the ideal gas assumption. The effect of heat release on the flow field can therefore be described by means of the progress variable. For this reason, the applied combustion models solve a convective-diffusive differential equation for the mean favre averaged progress variable

$$\frac{\partial}{\partial t}\left(\overline{\rho}\tilde{c}\right) + \frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{u}_i\tilde{c}\right) = -\frac{\partial}{\partial x_i}\left(\widetilde{\overline{\rho}u_i''c''}\right) + \overline{S_c} \tag{2}$$

with the turbulent transport term $\widetilde{\overline{\rho}u_i''c''}$ modelled as gradient diffusion term. The utilised combustion models can be distinguished by the individually determined source term $\overline{S_c}$.

1. The combustion model of Schmidt [2]:

The source term $\overline{S_c}$ of eq. (2) is given by an algebraic equation which is determined by the turbulent time scale $\tilde{k}/\tilde{\epsilon}$, the laminar unstretched flame speed s_l^0, the turbulent Damköhler number Da_t and by the reaction state in the form of $\tilde{c} \cdot (1 - \tilde{c})$.

$$\overline{S_c} = 4.96 \cdot C_R \cdot \frac{\tilde{\epsilon}}{\tilde{k}} \cdot \left(\frac{s_l^0}{\sqrt{\frac{2}{3}\tilde{k}}} + Da_t^{*\,-\frac{1}{4}} \right)^2 \cdot 4 \cdot \tilde{c} \cdot (1 - \tilde{c}) \cdot \rho_u \tag{3}$$

with $Da_t^* = 1 + Da_t^{-2}$, ρ_u as the density of the unburnt mixture, $C_R = 0.25$ as a model constant, $\tilde{k}$ and $\tilde{\epsilon}$ as the favre averaged turbulent kinetic energy and the dissipation rate of turbulent kinetic energy, respectively.

2. The combustion model of Lindstedt-Vaos [3]:

The closure for the source term $\overline{S_c}$ of eq. (2) is based on the density of the fresh gases ρ_u, the unstretched flame speed s_l^0 and the flame surface density Σ.

$$\overline{S_c} = \rho_u \cdot s_l^0 \cdot \Sigma \tag{4}$$

The flame surface density Σ is determined by an algebraic formulation derived from fractal considerations leading to the following equation for the source term ([5]).

$$\overline{S_c} = C_R \cdot \rho_u \frac{s_l^0}{\nu^{1/4}} \cdot \frac{\tilde{\epsilon}^{3/4}}{\tilde{k}} \cdot \tilde{c} \cdot (1 - \tilde{c}) \tag{5}$$

ν stands for the kinematic viscosity of the unburnt mixture and $C_R = 3.15$ again for a model constant.

3. The combustion model of Hoffmann [4]:

The source term $\overline{S_c}$ of eq. (2) is given analogously to eq. (4). But, in contrast to the formulation of the approach of [3], the flame surface density is specified by means of solving the convective-diffusive differential equation (6) instead of using an algebraic formulation. Thus, the local and time dependent

strain and curvature effects of the flame surface and also the propagation of the flame within the flow field is taken into account.

$$\frac{\partial}{\partial t}\left(\overline{\rho}\tilde{\sigma}\right)+\frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{u}_i\tilde{\sigma}\right)=-\frac{\partial}{\partial x_i}\left(\widetilde{\overline{\rho}u_i''\sigma''}\right)+\overline{S_\sigma} \tag{6}$$

with $\sigma=\Sigma/\rho$ as the mass weighted flame surface density and the source term $\overline{S_\sigma}$ given by

$$\overline{S_\sigma}=\left\langle\frac{\partial u_i''}{\partial x_i}-n_in_j\frac{\partial u_i''}{\partial x_j}\right\rangle_s\cdot\overline{\rho}\tilde{\sigma}+\left(\frac{\partial\tilde{u}_i}{\partial x_i}-\langle n_in_j\rangle_s\frac{\partial\tilde{u}_i}{\partial x_j}\right)\cdot\overline{\rho}\tilde{\sigma}-\frac{\partial\left(\langle n_is_l\rangle_s\cdot\overline{\rho}\tilde{\sigma}\right)}{\partial x_i}+\left\langle s_l\left(\frac{\partial n_i}{\partial x_i}\right)\right\rangle_s\cdot\overline{\rho}\tilde{\sigma}. \tag{7}$$

The strained flame speed s_l which is determined by the strain field expressed by the turbulent Karlovitz number Ka_t and the Markstein number Ma of laminar strained premixed flames was applied. Additionally, the efficiency parameter I_{eff} was introduced according to [6] to account for the effective turbulent strain on flamelet behaviour.

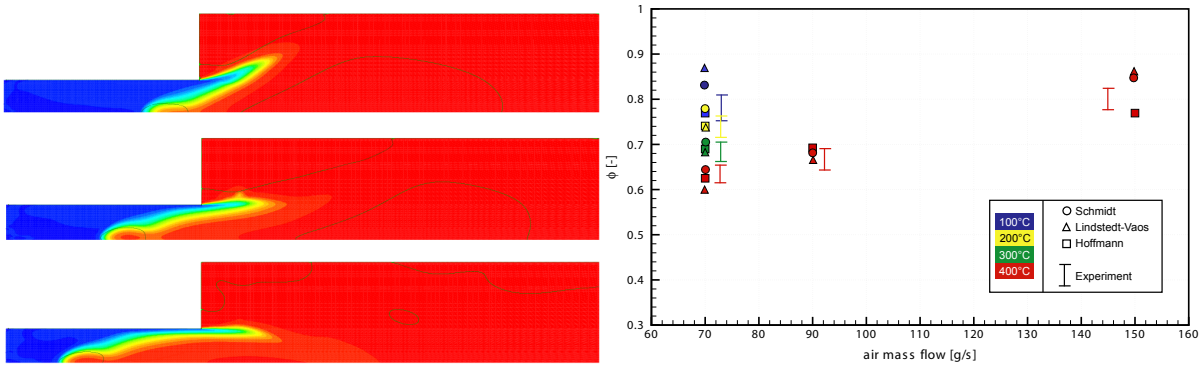
$$\frac{s_l}{s_l^0}=1-I_{eff}\cdot Ma\cdot Ka_t \tag{8}$$

3 Numerical Features

The simulations were performed using the uRANS method for the momentum equations with a Reynolds-Stress turbulence model as approach for the closure of the turbulence. The simulated domain consists of a combustion chamber (cc) and a mixing pipe (mp) both rotational of diameter $D_{cc}=0.225\ m$, $D_{mp}=0.075\ m$ and length $L_{cc}=0.50\ m$, $L_{mp}=0.22\ m$, respectively. The walls were treated as smooth and the no-slip condition was applied. The zero-gradient approach was utilised for the static pressure at the domain outlet. Profiles for the mean and the rms-fluctuating velocity correlations and for the dissipation rate of kinetic energy were set for the inlet at the upstream end of the mixing pipe. The values for the boundary conditions were adopted from the experiments of [1] and from preliminary simulations of [7], respectively.
The combustion models of [2] and [3] were implemented as additional C-code using the commercial FLUENT solver ([8], [5]). The approach of [4] was integrated as fortran user code into the commercial ANSYS CFX solver. The second order discretisation scheme for space and time was applied for all simulations. The mesh of the domain was similar to each other guaranteeing grid independency with a local resolution of about one millimetre around the axis of rotation.

4 Results

Each of the applied combustion models perform the simulation of the CIVB phenomenon in an excellently accordance with the conducted experiments regarding all important parameters. One of these features is the formation and maintenance of the characteristically small recirculation bubble in front of the flame. Also, all models predict the process of flashback nearby the rotational axis and the propagation speed of the flame to be of the very same magnitude as detected in the experiments. Figure 1 (a) shows three snap-shots of the upward propagating flame during the simulated flashback illustrating the aforementioned attributes of CIVB (cf. [8]).
The simulations were performed for different operation conditions that are expressed by the different preheat temperature and air mass flux varying from $T_u=100\ ^\circ C$ to $T_u=400\ ^\circ C$ and from $\dot{m}_{air}=70\ g/s$ to $\dot{m}_{air}=150\ g/s$, respectively. The critical equivalence ratios of the numerical results for all these operation conditions are summarised and compared with the experiments in figure 1 (b). The listed critical equivalence ratio expresses the limit at which the flame shifts into the unstable condition and the flashback is initiated. For this purpose, starting from a stable flame configuration, the equivalence ratio was increased in consecutive steps till the process of CIVB occurred.



(a) Reaction progress variable $\tilde{c}$ during simulated flashback; illustration of three snap-shots

(b) Flashback limits: Comparison between simulations and experiment

Figure 1: Simulated flashback (a) and comparison of critical equivalence ratios with the experiment (b)

All applied combustion models predict the limit to CIVB in good accordance with the experimental observations (cf. figure 1 (b)). However, for the simulations using the combustion models of [2] and [3], the model constants had to be modified and were adjusted to an experimental determined flashback limit ($T_u = 400\ °C,\ \ \dot{m}_{air} = 70\ g/s$). On the contrary, the model of the extended approach of [4] was able to predict the critical flashback limits without adjustment of any parameter.

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