Numerical simulations of flashback in lean premixed combustion systems using probability density function methods

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In this paper we present a model to predict and investigate flashback phenomenas in turbulent lean premixed combustion systems numerically. The main focus is put on flashback triggered by combustion induced vortex breakdown (CIVB) in swirling flames. The mathematical modelling of turbulent swirling flames is a difficult task due to the intense coupling between turbulent transport processes and chemical kinetics in particular for instationary processes like CIVB. The presented model consists of two parts. Chemical kinetics is taken into account with automatically reduced detailled chemical reaction mechanisms which have been generated using the recently developed REDIM method ("Reaction-Diffusion Manifold"). The turbulence-chemistry interaction is modeled by solving the transport equation for the joint probability density function of velocity and scalars (JPDF). The modell is applied to a close-to-real combustion system.

1 Introduction

Lean premixed flames are in the focus of many state of the art develoments in industrial applications. This is mainly due to the potential of lean combustion reducing emissions of NO_x signifficantly. In todays applications , e.g. gas turbines or jet engines, turbulent swirling lean premixed flames are widely applied. Nevertheless some characteristical instabilities like combustion induced flashbacks can occur in these systems which are critical with respect to a save operation. In this paper we precent a hybrid CFD/transported PDF model and check the ability of transported PDF models to predict flashback in swirling flames. The test case is close to a real application. Chemical kinetics is taken into account with automatically reduced chemical reaction mechansims. The recentlly developed REDIM model is applied here [1] which allready includes the effect of molecular transport within the state space.

While the simulation of non-reacting flows has become a standard task and can be tackeled using RANS (Reynolds-averaged Navier-Stokes) or LES (Large-Eddy Simulation) models the simulation of turbulent reacting flows is still a challenging task because of the strong non-linearity of the chemical source term which can not be modeled satifactorily by using oversimplified closure models.

Probability density function (PDF) methods show a high capability for modeling turbulent reactive flows, because of the advantage of treating convection and finite rate non-linear chemistry exactly [7]. Only the effect of molecular mixing and the fluctuating pressure gradient has to be modeled. PDF methods can be classified roughly in two different approches: those that use an a priori assumed shape of the PDF and those that solve the transport equation of the PDF to evaluate it. The second approach can be regarded as more general. Furthermore assumed shape PDF models suffer from the commonly used product ansatz of the functions which may lead to severe errors handling statistically not independent scalars (like mass fractions).

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The PDF transport equation can be derived from the Navier-Stokes equations and is a multidimensional transport equation. Due to its high dimensionality it is not feasible to solve the equation using finite-difference of finite-volume methods. For that reason Monte Carlo methods have been employed, which are widely used in computational physics to solve problems of high dimensionality, because the numerical effort increases only linearly with the number of dimensions.

Using the Monte Carlo method the PDF is represented by an ensemble of stochastic particles [7]. The transport equation for the PDF is transformed to a system of stochastic ordinary differential equations. This system is constructed in such a way that the particle properties, e.g. velocity, scalars, and turbulent frequency, represent the same PDF as in the turbulent flow. To overcome stability problems arising from the strong bias of the particle representation, the transport equation for the PDF is solved in a hybrid scheme together with an ordinary finite-volume solver for the flow field which calculates the mean pressure field.

In the presented paper the general capability of a hybrid CFD/transported PDF model to predict and investigate combustion induced vortex breakdown in close-to-real combustion systems shall be shown.

2 Numerical Model

The modelling equations which are solved in our model and the numerical issues included shall only be discused here briefly. Further details can be found in [5].

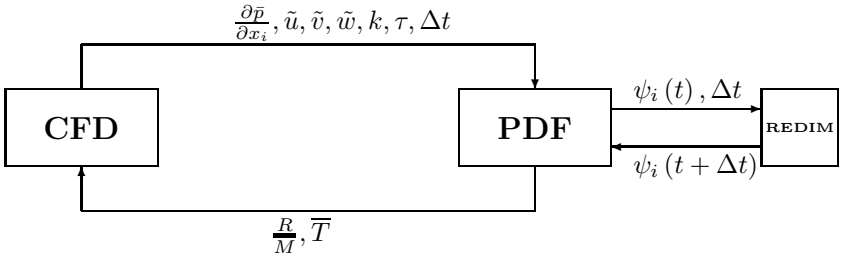


Figure 1: Scheme of the coupling of CFD and PDF

Figure 1 depicts a sketch of the whole model. As mentioned the model consists of two parts. The simualtion starts with a CFD step in which the Navier-Stokes equations for the flow field are solved by a finite-volume method. As an intermediate result the mean pressure gradient together with the mean velocities, the turbulence quantities and the time step are handed over to the PDF part. Here the joint probability density function of the scalars and the velocity is solved by a particle Monte Carlo method. The reaction progress is calculated from a lookup table based on a mechanism reduced with the REDIM method. As intermediate result of this step the mean molar mass, the composition vector and the mean temperature field are returned to the CFD part. This iteration cycle is performed until convergence is achieved for steady flames or the maximum number of time steps is reached for instationary cases.

The utilized CFD code Sparc is an inhouse development of the Department of Fluid Machinery at Karlsruhe University [6]. It solves the full compressible Navier-Stokes equations on block structured domains. A two equation model serves as turbulence closure which solves two additional transport equations for the turbulent kinetic energy and a turbulent time scale, respectively.

In the work presented here a joint PDF of velocity and composition is employed. The basic idea of the joint probability density function is that the state of a reacting fluid flow at one point in space and time can be fully described by the velocity vector $\vec{V} = (V_1, V_2, V_3)^T$ and the composition vector $\vec{\Psi}$ containing the mass fractions of $n_S - 1$ species and the enthalpy h ($\vec{\Psi} = (\Psi_1, \Psi_2, \ldots, \Psi_{n_s-1}, h)^T$). For the joint probability density function a transport equation is derived [7]. This equation is solved due to its high dimensionality with a particle based Monte-Carlo solver which makes use of the fact that the PDF in each cell of the solution domain can be represented as a sum of delta functions. In this context

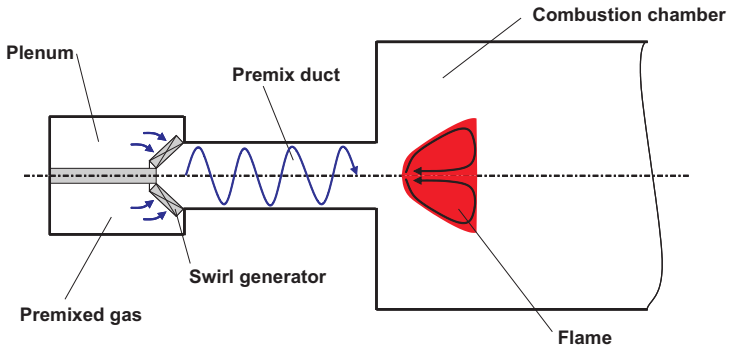


Figure 2: Sketch of the investigated combustion chamber

two unclosed terms appear. Namely the term describing the influence of pressure fluctuations p' and viscous stresses τ_{ij} upon the PDF which is modeled by the commonly used simplified Langevin Model (SLM, [7]) and the term describing molecular diffusion within the fluid which is modeled by a modified Curl model [2]. But as main advantage the chemical source term appears in closed form and needs no further modeling.

The chemical source term is calcuated from a lookup table created in a preprocessing step with the resently developed REDIM method. This method allows an accurate desripition of the reaction progress with a very narrow number of parameters. In the presented case chemical kinetics is described with only two parameters: the mixture fraction and the specific mole number of CO_2.

The coupling of the CFD and the PDF part of the model is done with the calculation of the pressure via the equation of state in the CFD part which closes the equation system.

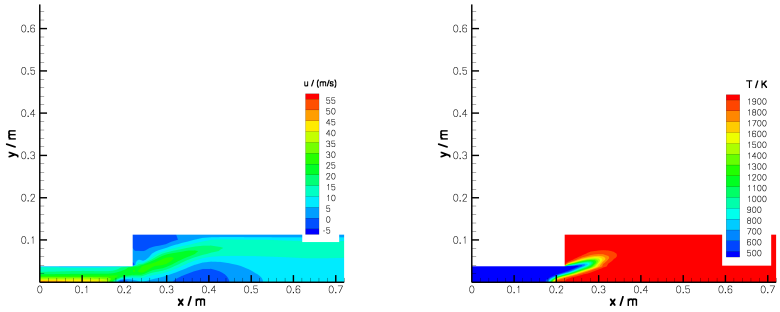
3 Results

As a test case for the model an aerodynamically stabilized confined swirling flame is used. The experimental data base is taken from [4]. Figure 2 shows a sketch of the combustion system. It consists of three parts: the plenum containing a premixed methane-air mixture, the premixing duct and the combustion chamber. Numerically only the premixing duct and the combustion chamber are modelled using a 2D axisymmetric mesh. Appropriate boundary conditions are taken from [3]. Global operation parameters are an inlet massflux of 70 g/s and a preheat temperature of 373 K.

Flashback is triggered by enriching the mixture and causes the internal recirculation zone to shift upstream into the premixing duct. Figure 3 shows the axial velocity and the temperature field before and after flashback for two different air-fuel ratios. One can observe that the flame moves upsteam into the premixing duct flowing the movement of the small recirculation bubble. The critical air-fuel ratio at which flashback occurs is 1.2 for these global operation parameters in the simulation which agrees reasonably well with the experimental finding of a critical air-fuel ratio in the rage of $\lambda = 1.25 - 1.3$ [4].

4 Summary and Outlook

In this paper a hybrid transported PDF/CFD model is presented and its ability to predict flashback caused by combustion induced vortex breakdown in swirling flames is investigated. The model predicts well the flashback limit both qualitativlly and quantitativlly at least for the operation point shown. The influence of a variaing premixing temperature and a variaing inlet mass flux is focus of current investigations and will be presented in detail at the conference.



(a) $\lambda = 1.3$ (b) $\lambda = 1.3$

(c) $\lambda = 1.2$ (d) $\lambda = 1.2$

Figure 3: Axial velocity field und temperature field before and after CIVB

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