

Monte-Carlo-PDF-Simulation and Raman/Rayleigh-Measurement of a Turbulent Premixed Flame

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Abstract

The simulation of turbulent flames is still a very challenging problem due to the strong coupling of chemical kinetics, turbulent transport and flow. Improvement of the existing underlying mathematical models is guided by a validation based on experimental results. This paper reports calculations and measurements of an axisymmetric 2-dimensional premixed flame. Measurements of the flame are performed using Raman/Rayleigh-laser-spectroscopy. The calculations are based on the solution of the transport equation for the joint probability density function of velocity and scalars. It is shown that the quality of the results depends crucially on the quality of the underlying mixing models.

Experimental Approach and Apparatus

Figure 1 shows the burner configuration. The premixed gas exiting through the inner tube is composed of 131 m³/h air and 14 m³/h natural gas and is surrounded by a coflow of air. The turbulence is generated by a grid in the inner tube and the flame is stabilized by the outer pilot. Non-intrusive, one-dimensional single-pulse in-situ measurements of temperature and majority species concentration are frequently obtained from combined spontaneous Raman and Rayleigh scattering techniques. In the experiment reported here a tunable, highly polarized KrF excimer laser (248.398 nm) was used as light source for assessing temperature and N₂, CH₄ and H₂O concentrations [1]. The laser beam was focussed into the flame with a $f=500$ mm spherical lens. The focal diameter of the laser profile in the observation volume was approximately 0.5 mm. Typical laser power densities were between 1,4 and 1,8x10⁹ W/cm², well below the limit for optical air break-through. The laser energy was measured with a pyroelectrical detector. As illustrated in figure 2 two large spherical quartz lenses were used to image the Raman and Rayleigh scattered light from the detection volume (0.5 x 0.5 x 0.5 mm³) onto the entrance slit of a spectrometer. The Rayleigh signal was attenuated by two orders of magnitude using a narrowband dielectric mirror to enable the simultaneous measurement of Raman and Rayleigh signal. The detection setup had a resulting magnification of 0.5 and guaranteed a maximum of light input. The spectrally resolved scattered light was imaged onto an intensified CCD camera covering a spectral range of 77 nm which resulted in a spectral resolution of 0.1 nm/pixel. Raman and Rayleigh intensities are evaluated according to [2]. The temperature dependence of the Raman cross section [2] was accounted for by determining the temperature in the first step using constant Rayleigh cross sections for burned (170x10⁻²⁸ cm²) and unburned gases (172x10⁻²⁸ cm²) [4, 5]. Temperatures are inferred according to the perfect gas law. Concentrations and temperature measurements are calibrated using a set of calibration measurements in pure gas flows and laminar McKenna flames [3].

Mathematical Modelling and Solution

Mathematical modelling of the flame is performed by solving the PDF-transport equation. The fundamentals of this method have been described by Pope [6]. In this work the transport equation is solved by a Monte-Carlo-particle-mesh-method as proposed by Pope [6]. In the Monte-Carlo-method the PDF

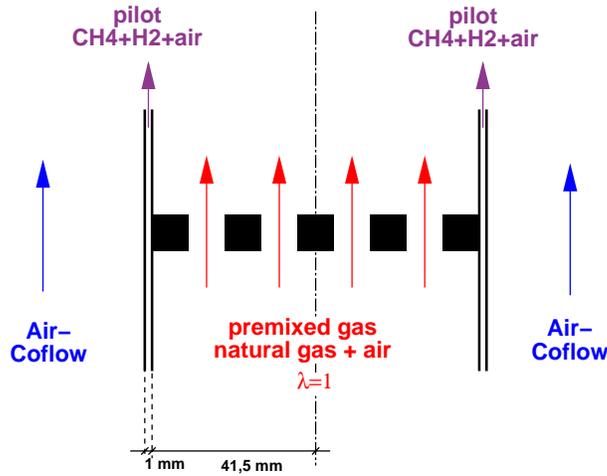


Figure 1: Burner configuration

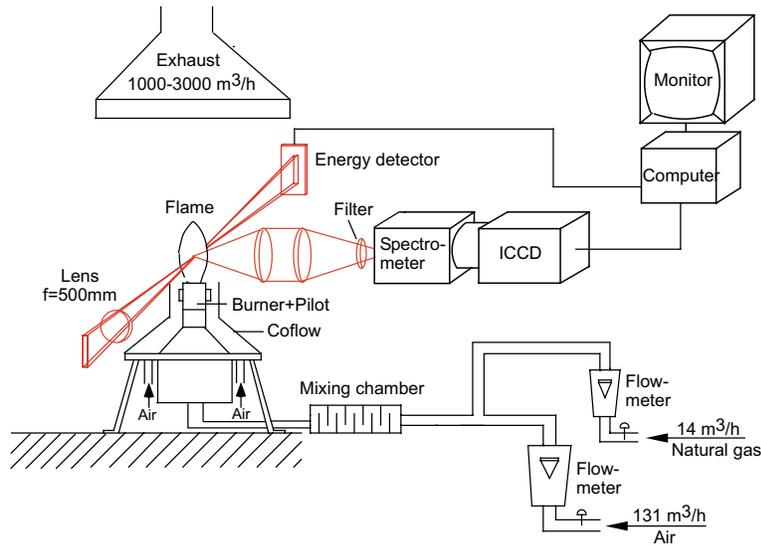


Figure 2: Experimental setup

is discretized into a large number of particles for which the particle trajectories are calculated. The mean and the higher moments of the PDF can be calculated by averaging over the particles. An important advantage of the PDF-method over the solution of the averaged Navier-Stokes-equation is that the chemical source term appears in closed form. In order to keep the dimension of the equation system treatable the chemistry is reduced by an ILDM-method [7]. The unclosed terms in the PDF-equation describing viscose dissipation and pressure fluctuations are modelled using a simplified Langevin-model [8]. The scalar micro mixing is modelled by several different models, namely the deterministic model of Dopazo (Interexchange with the mean model, IEM) [9] and some variants of Curl's model [10][11]. The IEM models the fact that molecular diffusion relaxes the composition of stochastic particles to their mean value. Curl's model describes the mixing process by a random mixing of stochastic particles. The mixing probability is chosen to reproduce the variance of the composition correctly. According to this probability the particles are chosen and mixed pairwise to mean composition of both particles. This model has been proposed first by Curl [10]. Janicka [11] proposed an improved variant of Curl's model (so called modified Curl's model). In this model the degree of mixing of the particles is an equally-distributed random variable. In order to allow an easy calculation of the mean pressure field, dissipation rate ϵ and turbulent time scale, which are difficult to calculate by solving the PDF transport equation, a simultaneous finite-volume calculation of the flow field with a presumed density field [12] is performed. After this step a Monte-Carlo-solution of the reacting flow is calculated. With the new density field a new finite-volume calculation is performed. The procedure is repeated until a statistically stationary solution of the flow field is obtained.

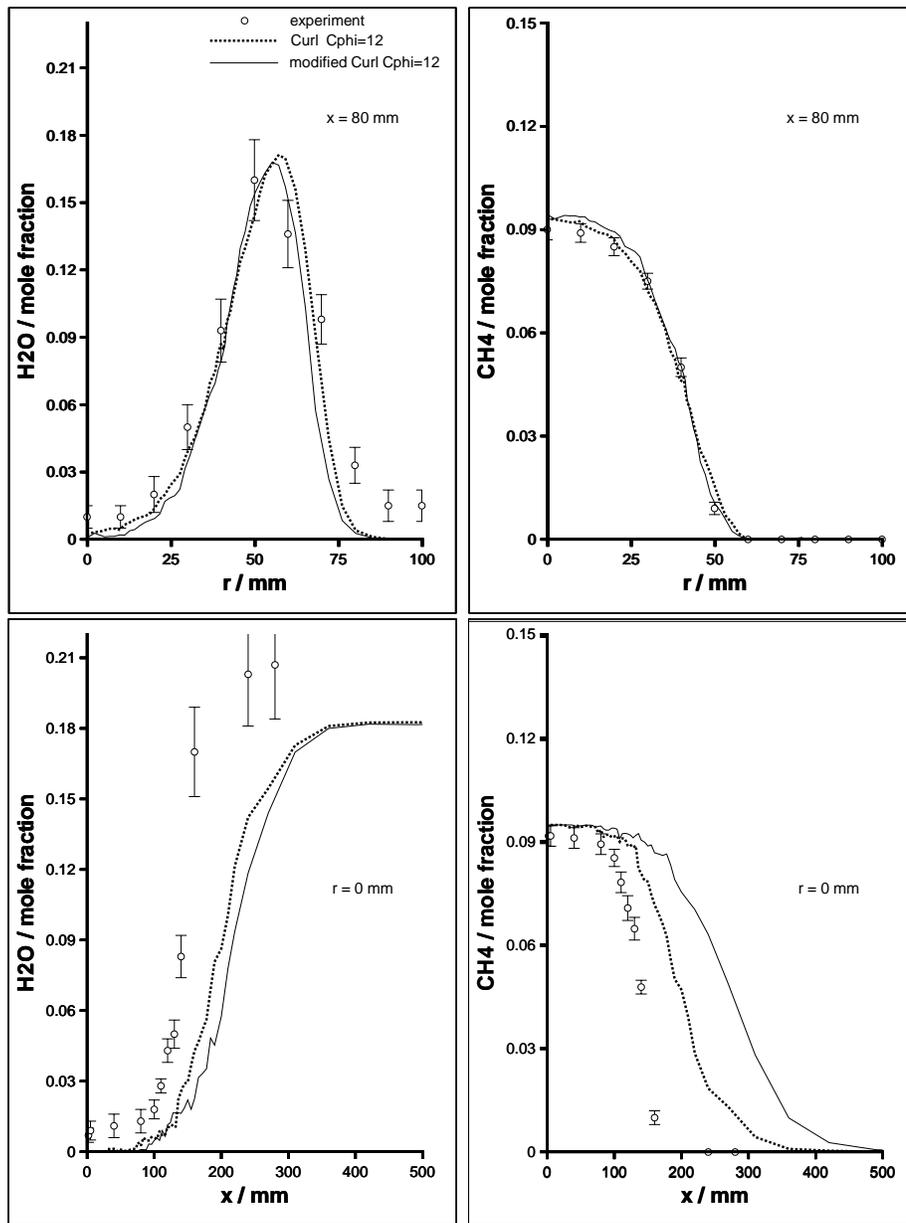


Figure 3: Radial (upper) and axial profiles of mole fraction of CH_4 and H_2O

Using the solution algorithm described above a simulation of the premixed flame has been performed. The boundary conditions for the velocity field and the field of the turbulent kinetic energy are taken from two dimensional PIV-measurements at the burner head. The $\text{C}_2\text{H}_4\text{-H}_2\text{-air-pilot}$ flame has been assumed to be a fully burned CH_4 -flame. This introduces an error into the enthalpy-balance. This error is small because the overall enthalpy of pilot is small compared to the that of the main stream. The simulation was performed using the original and modified Curl's model and the IEM. Furthermore the model constant C_Φ has been set to 2.6 (standard) and to 12 respectively. Simulations with the standard C_Φ do not reproduce a burning flame. This can be contributed to shortcomings of the simplified mixing models that over-simplify the coupling of the turbulent transport with chemical kinetics. The IEM overestimates the length of the flame strongly. Figure 3 shows the radial profiles of the measured mole fraction of CH_4 and H_2O in comparison to the calculated ones at a distance of 80 mm from the burner head. The calculated profiles have been obtained using the modified and the original Curl's model with C_Φ equal to 12. In this case the radial profiles are very close to the measured ones. In the lower part of Figure 3 the corresponding axial profiles at the axis of symmetry are shown. The profiles are relatively close to the experimental one. However, a significant difference in flame length can be seen in both, the H_2O and the CH_4 profile. This can be attributed to shortcomings in the mixing model. Within

the experimental uncertainties, peak H_2O concentrations match the mole fraction of 0.19 for complete combustion of stoichiometric CH_4 -air flames. However, averaged values were found to be significantly higher. There are two possible causes why C_Φ has to be increased: one possibility is that the strong coupling between chemical reaction and turbulence in this premixed flame is not represented by the standard C_Φ adequately. Another possibility is that determination of the boundary conditions related to turbulent time scales are difficult. (e.g. the condition for ϵ). Thus there is strong need for improving mixing models in order to allow accurate modelling of turbulent premixed flames.

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