Final Project Report of the DFG-Transferbereich 42:

A Method for the Prognosis of Turbulent Combustion

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Abstract. This final project report summarizes the objectives, realization, and the results of the DFG-Transferbereich 42. The report describes the flames considered, flame simulations, and results of flame simulations. A summary of project publication records, the transfer of project results and planned future activities will be also given.

1. Introduction

The extension of Reynolds-averaged Navier-Stokes (RANS) equations by probability density function (PDF) methods [1-3] has significant advantages for turbulent reacting flow simulations because there is no need to involve approximations of uncertain generality to close chemical reaction rates. Compared to the use of PDF methods in conjunction with large eddy simulation (LES) methods (which means filter density function (FDF) methods [4]), another advantage of PDF methods is given by their applicability to technical problems. Due to the exact treatment of chemical reactions, the performance of PDF methods is essentially determined by the modeling of the transport of scalars (e.g., species mass fractions and temperature). Such scalar transport models involve two ingredients: a scalar mixing frequency model that determines the characteristic time scale of mixing, and a scalar mixing model that describes the change of the PDF of a scalar [1-3].

Most previous applications of PDF methods were related to simulations of non-premixed turbulent combustion. The reason for that is given by the fact that in this case the length and time scales of scalar fields are usually larger than the length and time scales of turbulent motions. Correspondingly, the scalar mixing frequency can be assumed to be controlled by the frequency of large-scale turbulent motions. The performance of scalar mixing models for non-premixed turbulent combustion is relatively well investigated [5-12]. Merci et al. [13-16] and Xu and Pope [17] studied various scalar mixing models in turbulent natural gas diffusion flames.

Applications of PDF methods to premixed turbulent combustion are more complicated than calculations of non-premixed turbulent combustion because scalar mixing may well take place on scales which are much smaller than all scales of turbulent motions [18-22]. Correspondingly, there exist only a few applications of PDF methods to premixed flames. To overcome problems of earlier approaches, Mura et al. [21] recently suggested a PDF model where the outer parts of the flame structure (reactant side and product side) are described by a standard scalar mixing model, whereas the inner part (the inner reaction zone) is described by a flamelet model. However, this approach is complicated and related to several questions (e.g. regarding the matching of both combustion regimes). More recently, Lindstedt and Vaos [22] and Cha and Trouillet [23-24] developed models that relate the scalar mixing time scale of reacting scalars to the characteristic time scale of turbulent motions and the scalar mixing time scale of nonreacting scalars, respectively. However, the generality of assumptions used to involve the effects of chemical reactions in this way appears to be unclear [22]. Apart from that, the fact that scalar mixing may well take place on scales which are much smaller than all the scales of turbulent motions does not support the view that the scalar mixing frequency is controlled in general by the characteristic time scale of turbulent motions.

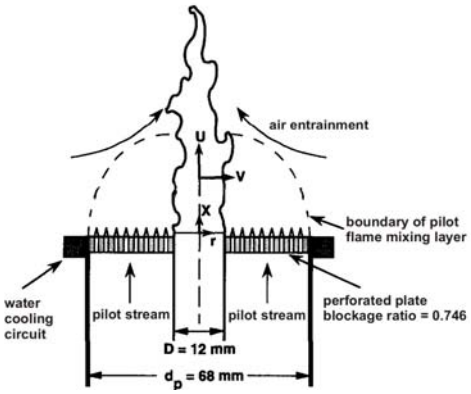

Fig. 1. The bunsen burner design [27].

Flame	F1	F2	F3
Equivalence ratio	1.0	1.0	1.0
Reynolds number	52500	40300	24200
U_0 [m/s]	65	50	30
k_0 [m²/s²]	3.8	10.8	12.7

Table 1. Global operating characteristics of the F1-F3 flames [27]. The Reynolds number Re is calculated on the basis of nozzle diameter D = 12 mm and bulk velocity U_0. k_0 is the centerline turbulent kinetic energy at the nozzle exit.

Many real turbulent flames involve a variety of mixing regimes (non-premixed, partially-premixed, and premixed turbulent combustion) [25-26]. To take advantage of the benefits of PDF methods to treat chemical reactions exactly, one needs methods which are applicable to all these mixing regimes. In continuation of activities related to the improvement of PDF methods within the frame of the SFB 255 (TPA2), the main objective of the Transferbereich 42 was the development of PDF methods that can be applied to both non-premixed and premixed turbulent combustion. An important aspect of this development is given by the fact that these developments were performed such that industrial users can make use of these solutions via a close collaboration with Fluent Inc. (via the implementation of new models in the commercial fluid dynamics software code FLUENT). The original idea was that the project will be realized by Dr. S. Heinz at the Technical University of Munich. However, Dr. S. Heinz received in 2004 a professor position at the University of Wyoming, USA. Thus, the project was realized by Prof. S. Heinz and the graduate student M. Stoellinger at the University of Wyoming.

The report is organized in the following way. The flames considered, flame simulations, and the results of PDF flame simulations are described in sections 2, 3, and 4, respectively. Section 5 deals with a summary of project results, and section 6 describes the transfer of project results.

2. The flames considered

The turbulent premixed F1, F2, and F3 flames studied experimentally by Chen et al. [27] were considered to investigate the performance of the PDF modeling approach. The three highly stretched stoichiometric methane–air flames featuring a range of Reynolds and Damköhler numbers. Chen et al. [27] found that all three flames are located in the distributed reaction zones regime [25]. In particular, the F1 flame is located at the borderline to the well stirred reactor regime, and the F3 flame is located at the borderline to the flamelet regime. This wide range of combustion conditions is often found in spark ignition engines [28] which present one of the most important applications involving premixed turbulent combustion. Due to the simple configuration, the broad range of combustion conditions, and the high quality experimental database [27], the three flames considered are well appropriate to investigate the performance of PDF methods for premixed combustion [21-22, 29-31].

The three flames are generated with the same burner which is illustrated in Fig. 1. Table 1 presents the different mean nozzle exit velocities, corresponding Reynolds numbers, and centerline turbulent kinetic energy values. The burner consists of a nozzle with diameter D = 12 mm for the main stream which is surrounded by a large pilot stream to stabilize the turbulent main jet flame. The laminar pilot stream is generated by an array (1165 holes of diameter 1 mm) of small jets issued through a cooled perforated plate. Both streams have a stoichiometric

methane-air mixture (equivalence ratio $\Phi = 1$). The burner is surrounded by air at rest. The outer air is entrained into the three flames at axial positions 3-5 D, changing the flame brush to non-perfectly premixed. The experimental database includes radial profiles of the mean velocity, the turbulent kinetic energy, mean and variance of the temperature and the mean mass fractions of the major species CH_4, O_2, CO_2, H_2O and minor species CO, H_2, OH. The error for the mean velocity is estimated to be less than 1%, and the error for the mean temperature is expected to be less than 10%. The error in the measurements of the major species is between 8% to 15%, and the error regarding the minor species is within 20% to 25%.

The flames introduced above have been studied numerically using different combustion models. Prasad and Gore [29] solved RANS equations where the averaged reaction rate was closed with a flame surface density model. This model is valid under flamelet conditions. Therefore, only the F3 flame has been investigated. Herrmann [30] investigated all three flames using a modified level set approach that accounts for effects of the instantaneous flame structure and the entrainment of cold ambient air. The latter model is strictly valid only under flamelet conditions. Pitsch and De Lageneste [31] formulated the level set concept for LES of premixed flames and performed a F3 flame simulation. They reported issues regarding the strong influence of boundary conditions in their LES simulation. Concerns include the significant heat losses to the burner surface, which are estimated to reach up to 20% regarding the pilot flame.

The PDF method was first applied to F3 and F2 flame simulations by Mura et al. [21]. The authors showed that the IEM mixing model combined with the standard model for the scalar mixing frequency ($\omega_\alpha = C_\alpha / (2\tau)$, where τ is the dissipation time scale of turbulence and $C_\alpha = 2$) is inapplicable to the two premixed flames close to the flamelet regime. The standard model corresponds to the idea that the scalar mixing frequency is controlled by the inertial range turbulent motions. This assumption is valid for distributed combustion, but in the flamelet regime the mixing process is controlled by the laminar flame length scale. Mura et al. [21] suggested a PDF model where the outer parts of the flame structure (reactants side and products side) are described by a standard mixing model and the inner part (inner reaction zone) by a flamelet model. This approach, however, is complicated, and it is related to several questions regarding the matching of both combustion regimes. More recently, Lindstedt and Vaos [22] applied a transported PDF model to the F1, F2, and F3 flames. The authors demonstrated the applicability of the transported PDF model to premixed combustion in the flamelet regime under the condition that the modeling of the scalar mixing frequency is modified. The molecular mixing term was closed by using the modified coalesence-dispersion (CD) mixing model [6, 32]. The scalar mixing frequency model applied relates the scalar mixing time scale of reacting scalars to the characteristic scalar mixing time scale of nonreacting scalars. However, the generality of assumptions used to involve the effects of chemical reactions in this way appears to be unclear [22].

3. PDF flames simulations

A hybrid PDF-RANS approach was used to simulate the turbulent premixed flames described above. The realizable k−ε turbulence model [33] was used to calculate the mean velocity field and turbulence characteristics. A scalar PDF transport equation was solved via Monte Carlo simulation, where the scalar mixing frequency was calculated by using a generalized frequency model [34-35]. In particular, the scalar mixing frequency was calculated for the fuel (CH_4) mass fraction because combustion takes place only if fuel is available. The chemical reaction rates are provided by a skeletal chemical mechanism called DRM22 [36] consisting of 23 species (H_2, H, O, O_2, OH, H_2O, HO_2, H_2O_2, CH_2, $CH_2(S)$, CH_3, CH_4, CO, CO_2, HCO, CH_2O, CH_3O, C_2H_2, C_2H_3, C_2H_4, C_2H_5, C_2H_6, N_2) and 104 elemental reactions. The applicability of the DRM22 mechanism

Domain	2-d axisymmetric, 6.5 D x 20 D in radial by axial direction, discretized by 70 x 220 = 15,400 non-equidistant grid cells
Turbulence model	Realizable k-ε with $C_{\varepsilon 1} = 1.44$, $C_{\varepsilon 2} = 1.79$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.2$, $Sc_t = 0.6$
Mixing model	IEM model combined with the VC frequency model
Chemistry model	DRM 22 integrated with the ISAT method
Wall treatment	Low Reynolds number model [39]
Solver	Steady, segregated with implicit formulation
Discretization schemes	Presto for pressure, PISO for pressure-velocity coupling, Second-order upwind for velocities, k, and ε
Monte Carlo statistics	80 particles per cell, averaging over the last 100 iterations
ISAT parameters	ODE error tolerance = 10^{-8}, ISAT error tolerance $\varepsilon_{tol} = 5\ 10^{-4}$
Hardware	four 2.8 GHz Opteron processors each equipped with 4GB of SDRAM
Simulation time	About 15 hours (approximately 30 000 iteration steps)

Table 2. Summary of PDF flame simulation details.

was demonstrated by comparisons to results obtained with the full GRI-2.11 mechanism [37]. The composition change due to chemical reactions was handled by the in situ adaptive tabulation (ISAT) method developed by Pope [38]. Details of the numerical methods are listed in Table 2.

The model equations were solved by using the FLUENT code [39]. The RANS equations for the mean mass, momentum and energy were solved in conjunction with the equations for the turbulent kinetic energy k and dissipation rate ε of turbulent kinetic energy. The equations were discretized with a finite volume method and solved on a 2-d axisymmetric domain. The modeled scalar PDF equation was solved by the Monte Carlo method. The Monte Carlo equations were solved by a mid-point rule in order to achieve second order accuracy in time. Details of the simulation data are given in Table 2, and further details may be found elsewhere [34-35].

The jet inlet profiles for the axial velocity and turbulent kinetic energy have been taken from the experimental database of Chen et al. [27]. The profile for the turbulence dissipation rate has been calculated from the profile of the turbulent kinetic energy and measurements of the lateral length scale λ according to $\varepsilon = (2k/3)^{1/2} / \lambda$ [27].

The pilot composition was calculated from the chemical equilibrium of a stoichiometric methane-air mixture with 20% heat loss. The convergence rate of PDF simulations can be drastically increased if they start from realistic initial conditions. Thus, the simulations have been performed in two steps to reduce the computational time. First, a laminar flame model was used to generate realistic initial conditions for the PDF simulations. The PDF simulations were then initialized by results from the laminar flame model.

4. PDF simulation results

Radial profiles of the normalized mean axial velocity U/U_0 at different axial positions are presented in Fig. 2 for the F3, F2, and F1 flames. The mean velocity is normalized by the bulk velocity U_0 = 30, 50, 65 m/s for the F3, F2, and F1 flames, respectively. The overall agreement between simulation results and measurements is excellent. The thermal expansion within the turbulent jet can be recognized by the increase of the axial velocity at radial positions $r/D > 0.5$ along the axis for all three flames. As a result of this expansion, the shear layer (which is roughly located at the position of the maximum gradient of the mean axial velocity) is pushed outward in radial direction. The latter fact can also be observed on the right-hand side of Fig. 2 where

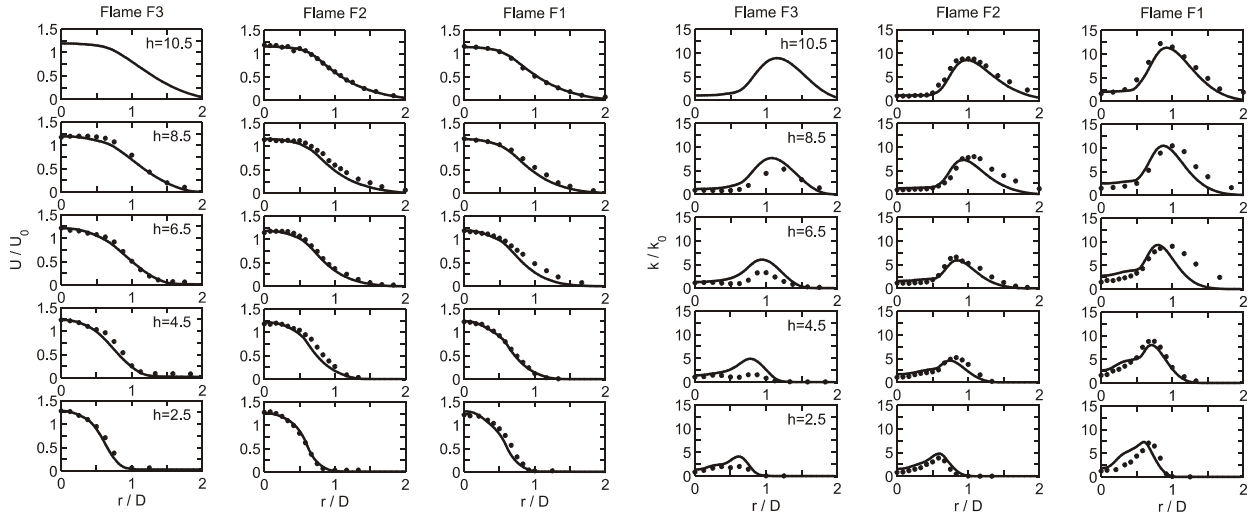

Fig. 2. Radial profiles of the normalized mean axial velocity U/U_0 (left-hand side) and turbulent kinetic energy k/k_0 (right-hand side) for the F3, F2, and F1 flames (h is the axial position normalized on the nozzle diameter D). Dots refer to experimental results [27], and lines denote simulation results.

radial profiles of the normalized turbulent kinetic energy k/k_0 are shown (k_0 = 12.7, 10.8, 3.8 m^2/s^2 for the F3, F2, and F1 flames, respectively). The peaks of the turbulent kinetic energy are shifted outward for increasing axial positions. The results for the higher Reynolds number F2 and F1 flames agree very well with the measurements whereas an overprediction of the turbulent kinetic energy can be seen for the F3 flame, especially close to the burner head. Similar overpredictions have been reported by Lindstedt and Vaos [22]. The F3 flame was also studied by Pitsch and de Lageneste [31] using LES and a level set approach. Their results of the turbulent kinetic energy show better agreement at h = 2.5 but a similar disagreement at h = 6.5. Since the flame F3 has the lowest axial velocity and the highest temperature, low Reynolds number effects which are not accounted for in the k−ε model applied could be the reason for the overprediction of the turbulent kinetic energy.

The reaction progress variable is defined by $C = (\overline{T} - T_u) / (T_b - T_u)$. Here, $\overline{T}$ is the mean temperature, T_b = 2248 K is the adiabatic flame temperature, and T_u = 298K is the temperature of the surrounding air. Radial profiles of the mean reaction progress variable C are shown in Fig. 3 at different axial positions for the three flames. The simulation results of the F3 flame agree very well with the measurements, indicating that the new method to calculate the scalar mixing time scale is well applicable to flamelet conditions. The simulation results at an axial position h = 2.5 for the F2 and F1 flames show an overprediction of the progress variable. Lindstedt and Vaos [22] found a similar overprediction in their simulation results of the F1 flame using the same pilot inlet conditions. The reason for the observed temperature overprediction close to the burner exit in the F2 and F1 flames may be given by the complex interaction between the turbulent jet and laminar pilot stream. Such flow conditions, which are essential to the understanding of ignition and stabilization of turbulent flames, are difficult to predict within the RANS framework. A combined LES-FDF approach would represent more accurately such laminar – turbulent flame stabilization effects. However, LES results have not been reported so far for the F2 and F1 flames. The mean mass fractions of species are found to agree well with experimental data. The mean product mass fraction Y_{H_2O} is shown in Fig. 3 as an example. One observes that the calculated H_2O mass fraction agrees very well with the measurements for all three flames.

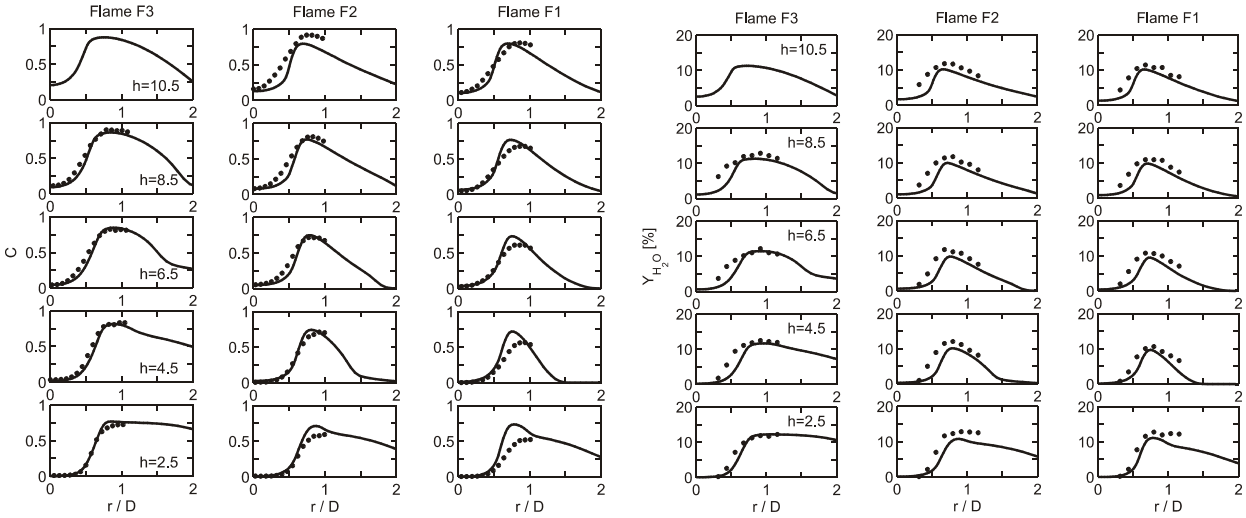

Fig. 3. Radial profiles of the mean reaction progress variable C (left-hand side) and H_2O mass fraction Y_{H_2O} in percent (right-hand side) for the F3, F2, and F1 flames (h is the axial position normalized on the nozzle diameter D). Dots refer to experimental results [27], and lines denote simulation results.

Fig. 4 demonstrates that the new scalar mixing frequency model predicts the position of the mean flame front in close agreement with the measurements for combustion regimes ranging from flamelet to distributed combustion. The use of the standard model and of the Lindstedt and Vaos model [22] results in a significant overestimation of the axial position of the flame tip regarding the F3 and F2 flames. The turbulent burning velocity has to balance the high axial velocity of the jet in the flame tip. Thus, predictions of the axial position of the flame tip are very sensitive to an accurate prediction of the turbulent burning velocity. In the F3 and F2 flames which are close to the flamelet regime, there are strong axial scalar gradients in the flame tip. These gradients increase the scalar mixing frequency and thereby enhance the scalar mixing and the turbulent burning velocity. The new mixing frequency model includes the effects of the strong gradients in the flame tip and allows for an accurate prediction of the flame tip position. The standard model and the Lindstedt and Vaos model [22] do not include any effects of scalar gradients on the mixing. Thus, they underestimate the turbulent burning velocity, which explains the overestimation of the flame tip position. The predictions of the three scalar mixing frequency models are almost the same regarding the mean flame front position of the F1 flame. The F1 flame is close to the distributed combustion regime, and the scalar gradients in the flame tip are not as strong as in the F3 and F2 flames. Thus, the mixing enhancement is less intense than in the F3 and F1 flames.

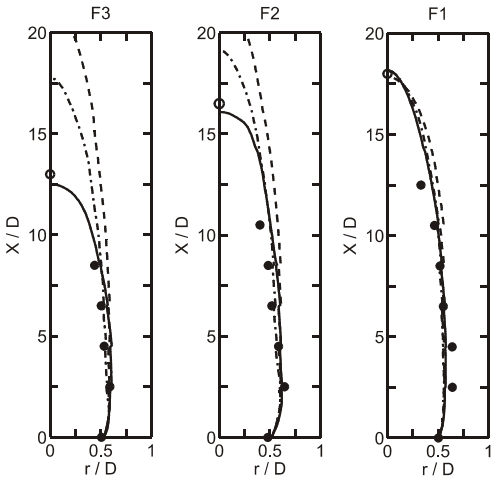

Fig. 4. The position of the mean turbulent flame front for the F3, F2, and F1 flames. Solid lines denote results obtained with the new frequency model, dashed lines denote results obtained with the standard mixing frequency model $\omega_\alpha = C_\alpha / (2\,\tau)$ combined with $C_\alpha = 6$, dashed-dotted lines denote results obtained with the Lindstedt and Vaos model [22], and dots denote experimental results [27]. The circles denote curve fit results to the measured values.

5. Summary of project results

The main objective of the project was to extend the range of applicability of PDF methods such that both non-premixed and premixed turbulent combustion problems can be addressed. The latter requires a generalization of the scalar mixing frequency used in PDF simulations: this frequency is not controlled by the frequency of turbulent motions under flamelet conditions. The results of PDF simulations reported in section 4 reveal the success of the modeling approach applied: the new scalar mixing frequency model allows accurate simulations of premixed turbulent combustion. It was proved that it is also applicable to the non-premixed Sandia flames.

The publication records of the DFG-Transferbereich 42 are summarized below. This includes three talks given by Prof. S. Heinz and M. Stoellinger at international conferences, and currently three publications (one paper is still under review). Three other publications which are related to the project results are also mentioned. One of the most important project results is given by the qualification of M. Stoellinger. He wrote successfully his Master Thesis on PDF simulations of turbulent flames. The DFG-Transferbereich 42 results will represent a significant ingredient of his Ph.D. thesis on stochastic methods for turbulent combustion.

a) Talks at International Conferences

1. Stoellinger, M. K. & Heinz, S. PDF Simulation of Premixed Bunsen Flames, 5th International Symposium on Turbulence and Shear Flow Phenomena, Munich, August 27-29, 2007.
2. Stoellinger, M. K. & Heinz, S. Mixing Modeling for Stochastic Simulations of Turbulent Premixed Flames, 6th International Congress on Industrial and Applied Mathematics (ICIAM 07), Zurich, July 16-20, 2007.
3. Heinz, S. & Stoellinger, M. K. Stochastic Mixing Models for Non-Premixed and Premixed Turbulent Combustion, 11th Internat. Conference on Numerical Combustion, Granada, April 24-26, 2006.

b) Refereed Journal Papers and Proceedings

1. Stoellinger, M. K. & Heinz, S. 2007 PDF Modeling and Simulation of Turbulent Premixed Flames. (submitted).
2. Stoellinger, M. K. & Heinz, S. 2007 Mixing Modeling for Stochastic Simulations of Turbulent Premixed Flames. Proceed. Applied Math. Mechanics (submitted).
3. Stoellinger, M. K. & Heinz, S. 2007 PDF Simulation of Premixed Bunsen Flames. In: Proceedings of the 5th International Symposium on Turbulence and Shear Flow Phenomena, edited by Adams, N., Eaton, J. K. & Friedrich, R., Munich, 1131-1136.

c) Related Refereed Journal Papers

1. Heinz, S. 2007 Unified Turbulence Models for LES and RANS, FDF and PDF Simulations. Theor. Comput. Fluid Dyn. 21, 99-118.
2. Heinz, S. 2007 Some Questions Regarding the Understanding and Prediction of Turbulent Flow. Dynamics of Continuous, Discrete and Impulsive Systems (Series A), 14 (S2) 232-237.
3. Heinz, S. 2006 Turbulent Supersonic Channel Flow: Direct Numerical Simulation and Modeling. AIAA Journal 44, 3040-3050.

d) Master Thesis

1. M. Stoellinger, "Three-dimensional PDF Simulation of a Piloted Turbulent Non-Premixed Jet Flame" Master Thesis, University of Wyoming, Laramie (2005).

e) Ph.D. Thesis

1. M. Stoellinger, "Stochastic Methods for Turbulent Combustion" Ph.D. Thesis, University of Wyoming, Laramie (to be expected in 2009).

6. Transfer of project results

Dr. M. Braun (Fluent Germany, Head of the Discrete Phase Modeling Group) and Dr. G. Goldin (Fluent USA, Head of the Combustion Modeling Group) contributed significantly to the success of the Transferbereich 42. Dr. M. Braun's support enabled the realization of this project. Based on his recommendation, Fluent Inc. provided 26 free FLUENT licenses required to realize efficiently the relatively time consuming PDF computations. Dr. M. Braun helped over all the project with regard to upcoming questions (for example, the update of FLUENT licenses). In the same way, Dr. G. Goldin supported the progress of project work enormously. He was always helpful with regard to questions about the use of the FLUENT code. He helped with problem solutions (for example, subroutines for performing specific calculations) and new research results related to the application of the FLUENT PDF combustion code.

A first type of transfer of project results is provided by publications and talks that demonstrate further successful and feasible applications of the FLUENT PDF combustion code to problems of technical relevance. In addition to previous successful applications of the FLUENT PDF combustion code to non-premixed turbulent flames [40-42], the results of the DFG-Transferbereich 42 demonstrate the applicability of the FLUENT PDF combustion code to premixed turbulent flames [34-35]. Such evidence of successful applications is relevant regarding the predominant opinion that PDF codes are still too expensive computationally to be really useful for computations of practical relevance. The applications reported will encourage industrial users to make use of the PDF approach (and, in particular, the FLUENT PDF combustion code) to solve their problems considered.

A second type of transfer of project results is provided by publications and talks that demonstrate the relevance and new ideas regarding the modeling of scalar mixing frequencies. The latter problem was hardly addressed over the last 20 years: basically all the developments of PDF methods were focused on improvements of scalar mixing models (which describe the change of the PDF of a scalar), and the scalar mixing frequency was assumed to be controlled by the frequency of large-scale turbulent motions. Evidence that this approach is inappropriate to cover many mixing regimes of turbulent flames is important to stimulate more complex research focused on both the improvement of scalar mixing models and scalar mixing frequencies.

A third type of transfer of project results is given by the improvement of the flexibility of the FLUENT PDF combustion code. After the evaluation of the new approach developed for the modeling of both premixed and non-premixed turbulent flames, the new models can be made available for other users by offering corresponding subroutines. The latter allows industrial users to work with more general models in order to calculate, for example, turbulent combustion processes involving a variety of mixing regimes (as given for the so-called Delft-III flame). It also appears to be possible to offer future FLUENT versions that work with bridging models to perform continuously PDF or FDF simulations [43]. Such methods may be expected to be extremely helpful to improve the accuracy and efficiency of calculations.

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