NUMERICAL INVESTIGATION OF TURBULENCE-EVAPORATING SPRAY INTERACTION IN A SWIRLING COMBUSTOR FLOW

M. R. Maneshkarimi*, A. Sadiki°

*Institute of Mechanics, Dept. of Mechanics, Darmstadt University of Technology, Germany
°Institute of Energy and Power Plant Technology, Dept. of Mechanical Engineering,
Darmstadt University of Technology, Germany

ABSTRACT

Employing an Euler-Lagrangian method in conjunction with advanced models for turbulence, evaporation and modulation, a numerical study of the effects of two key parameters on the evolution of sprays in a single gas turbine combustor is reported in this work. The effects of internal parameters such as turbulence intensity on the turbulent droplet dispersion, vaporization and mixing for non-reacting case are pointed out and linked to the turbulent spray combustion. Secondly the effects of external parameters such as swirl intensity on turbulent spray combustion in combination with modulation effects are analysed. 1) Based on *RANS*, the results confirm that the *EARSM* model is appropriate to represent the flow field quantities in two-phase flows for a large range of swirl intensity. 2) Under reacting conditions, it is shown how the evaporation characteristics, mixing rate and combustion process are strongly influenced by swirl intensity. 3) In particular, the turbulence modulation modifies the evaporation rate, which in turn influences the mixing and the species concentration distribution. It is demonstrated that this effect can not be neglected for low swirl intensities ($Sw.Nu.<1$).

INTRODUCTION

Dealing with spray combustion in particular internal combustion systems such as automotive engines, gas turbine combustors, an accurately controled preparation of air-fuel vapor mixing process is of great importance for efficient combustion and reduction of pollutants. In such devices the fuel is often supplied as a liquid with varying physical and chemical properties to form a combustible mixture of fuel vapor and air. This process is determined by the turbulent dispersion, the evaporation of fuel droplets and the related interaction phenomena within the turbulent carrier phase. In particular the effects of the so-called turbulence modulation, i.e. the modification of the continuous phase turbulence characteristics by droplets or by interface transport and the modification of interface transport by turbulence are confirmed by various experimental investigations [1-7]. From these studies, it is also well-known that the swirl intensity can strongly influence the turbulent mixing processes and therefore the spray combustion (see [8] and therein cited references). An accurate capture of the turbulence characteristics, in particular of the turbulent kinetic energy is therefore decisive for an accurate prediction of the spray combustion characteristics. Although in many recent works some numerical calculations have been performed in which the effects of the turbulence on droplet vaporization have been pointed out, they deal mostly with mono-dispersed sprays using numerical codes in which the standard *k-e* model was coupled to quasi-equilibrium evaporation models without a fully consideration of turbulence modulation processes[3, 9-11]. Thereby no reliable prediction of the turbulence effect could be expected. This is also the case in *LES*, where only the standard dissipative expression for two-way coupling is really available in the existing formulation of subgrid scale turbulent kinetic equation (e.g. [12]).

In this paper, interest is therefore focussed on the effects of these various phenomena on dilute sprays, and in particular on how the coupling effects of turbulence and swirl variations can influence droplet dispersion, evaporation and combustion. Numerical investigations based on *RANS* are carried out to highlight these in a single gas turbine combusor similar to that investigated by Wittig et al. [2], where we vary swirl intensities in the simulation. First the effects of turbulence properties on droplet dispersion, vaporization and mixing of a non-reacting spray are numerically predicted and compared with available experimental data. In the second case of reacting spray, focus is on conjugate effects of the turbulence, turbulence modulation and swirl intensity on the spray combustion.

GOVERNING EQUATIONS AND MODELLING

Gas phase (non-reacting), Droplet description and Two-way Coupling

To account for the instantaneous flow properties encountered by the droplets, involving each droplet history starting from the injection into the flow, an Euler-Langrangian approach is adopted.

The turbulent fluid phase is described following an Eulerian approach. The stationary, general form of the transport equation in *RANS*-modelling context emerges as an elliptic differential equation:

$$\frac{\partial\left(r\,\overline{u}\,f\right)}{\partial x}+\frac{\partial\left(r\,\overline{v}\,f\right)}{\partial y}+\frac{\partial\left(r\,\overline{w}\,f\right)}{\partial z}-\frac{\partial}{\partial x}\left(\Gamma\frac{\partial f}{\partial x}\right)-\frac{\partial}{\partial y}\left(\Gamma\frac{\partial f}{\partial y}\right)-\frac{\partial}{\partial z}\left(\Gamma\frac{\partial f}{\partial z}\right)=S_f+\overline{S}_{f,p}+\overline{S}_{f,p,v} \qquad (1)$$

in which f may represent the mean value of mass, energy, turbulent kinetic energy, turbulent dissipation rate, and chemical species mass fraction (O_2, CO_2, vapor fuel), respectively. G represents an effective diffusion coefficient and S_f the well-known turbulence source term in monophase flow cases. The latter has been already documented in the literature (e.g. [14, 15]).

To better capture streamline curvature effects and swirled flows phenomena we apply besides the *k-e* model for comparison the algebraic Reynolds stress models by Launder, Reece & Rodi [14] and by Gatski & Speziale [15] modified for two phase flow description by including source terms for phase exchange, $\overline{S}_{f,p}$, and phase transition processes, $\overline{S}_{f,p,v}$. For simplicity, the heat flux vector in the energy equation has been postulated by means of a gradient ansatz. The latter additional source terms in Eq. (1) characterize the direct interaction of mass, momentum, energy and turbulent quantities between the two phases and account for the two-way coupling between the fluid turbulence and the droplet heat transfer. Details about these terms can be found in [13]. With regard to the two-way coupling contribution in the turbulent kinetic energy equation only models accounting separately for the induced turbulence attenuation or augmentation by the presence of particles are available, as reviewed by Crowe [9] who used the energy balance to attempt a first consistent description. To better account for the modification of the continuous phase turbulence characteristics by the dispersed phase or by interphase transport in internal combustion engines, and because all the phenomena involved are thermodynamical processes, we use in this work besides the standard expression for the two-way coupling a model compatible with the second law of thermodynamics. The particle/droplet source term for the turbulent kinetic energy is given in this model [13] by:

$$S_{k,p}=b\left(\overline{u_{pi}S_{u_i,p}}-\overline{u_i}\;\overline{S_{u_i,p}}\right)+\left(\overline{u_iS_{u_i,p}}-\overline{u_i}\;\overline{S_{u_i,p}}\right) \quad \text{where} \quad b=a'+\frac{(1-a')\left(\overline{u_{pi}S_{u_i,p}}-\overline{u_{pi}}\;\overline{S_{u_i,p}}\right)}{\left(\overline{u_{pi}S_{u_i,p}}-\overline{u_i}\;\overline{S_{u_i,p}}\right)} \qquad (2)$$

The second term in Eq. (2a) represents the usual dissipative standard contribution, while the first term accounts for the production of the turbulent kinetic energy. So, this thermodynamically consistent model captures well both the enhancement and the diminution of the turbulence of the gas phase due to the presence of both big and small droplets in polydispersed sprays. The parameter α' in Eq. (2b) depends on the particle properties. The relevance of this model has already been pointed out in [19].

To compute the properties of droplets moving in turbulent flow a Lagrangian approach is employed. The trajectories of individual particles are obtained from motion equations, where all external effects except drag, buoyancy and gravity forces are neglected [1, 6, 12, 13, 19]. For evaporating droplets, two additional equations which give the rate of change of droplet diameter and temperature with respect to time are also needed (e.g. [10, 11]).

Evaporation, Combustion and Dispersion models

To account for the 3D-evaporation of droplets, equilibrium [10] and non-equilibrium models [11] are considered. For the equilibrium model usually used, the molar mass fraction is related to the saturation pressure through the Clausius-Clapeyron equation [1-4, 6, 10]. In the case of non-equilibrium evaporation model [11], the non-equilibriun molar mass fraction is additionally related to the blowing Peclet number. According to [11], corresponding modifications are then performed in the Lagrangian equation describing the transient temperature.

For the combusting spray case, chemical source terms in the equations for O_2, CO_2 and vapor fuel must be provided. Although many efforts have been done in the last decade in combustion modeling, we chose for the complex swirled, reacting two-phase flow the Eddy dissipation model [2, 16, 17] to calculate the mean source terms.

The radiation contribution in the energy equation is evaluated by solving differential equations for the radiant fluxes following the Four-Flux method [18] in which the black body emissive power is assumed. The equations system of gas-phase, Eq. (1), is closed by the equation of state which determines the distribution of density for ideal gas.

To obtain the velocity fluctuations of gas occurred in the motion equation of droplets at droplet locations, a dispersion model following the Markov-Sequenz-ansatz (see in [13]) is used. This model is based on the calculation of Lagrangian and Eulerian correlations and exhibits a high ability in calculating the gas fluctuations.

CONFIGURATION AND NUMERICAL PROCEDURE

A single gas turbine combustor similar to that investigated in [2] is used. It consists of a single cylindrical combustor with diameter of 0.1 m and length of 0.4 m where a swirled air stream enters the chamber after flowing through two tubes and the liquid fuel (dodecane) is injected into the combustion chamber as shown in Fig. 1. According to experimental data, details of operating conditions of gas and droplet at the combustor inlet are summarized in Fig. 1. The computational domain is represented by 128 × 64 cells in axial and radial directions, respectively. Due to the

symmetry assumption, half the domain is presented in computed results. Non-reacting and reacting cases are investigated.

Under steady state conditions, two-dimensional partial differential equations of all dependent variables of gas phase? are solved using the finite volume based SPRINT code. The space discretization is based on a hybrid method and the velocity-pressure coupling is accomplished by a SIMPLE algorithm. The Lagrangian equations for droplets are discretized using first order scheme and solved explicitly. The source terms for the gas phase are computed in each cell with the contributions of all the relevant droplets [6].

Numerically, the interaction between the continuous and the dispersed phases is taken into account by means of several couplings between two modules involved. Following a steady method, after several iterations of gas phase alone, the gas variables are kept frozen and all the droplets representing the entire spray are injected in the computational domain. The computed droplets source terms are inserted in the calculations of gas phase and kept frozen till the next coupling takes place in which the old particle sources are replaced by newly calculated sources. High levels of under-relaxation technique were used in order to obtain successful convergence [1, 2, 6].

The droplet injection is based on a stochastic approach by considering the droplet mass flux and the droplet size distributions obtained from experimental measurements at the inlet far off the nozzle exit [2].

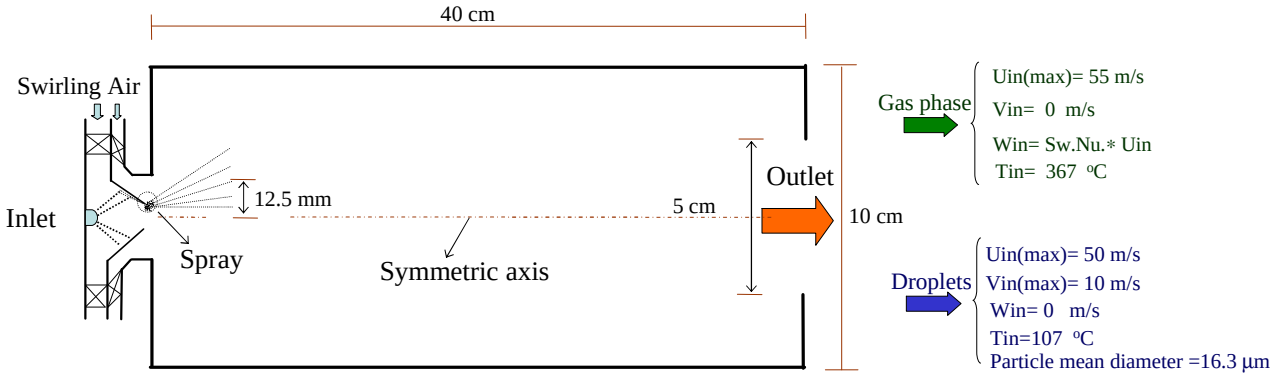

Fig. 1: Cylindrical Combustion Chamber

RESULTS DISCUSSIONS AND CONCLUSION

First Case: Non-reacting swirled Spray

The computed cross-sectional profiles of gas axial velocity component along the chamber using different turbulence models are shown in Fig. 2 and compared with available experimental data. It turns out that in the vicinity of inlet port all turbulence models deliver good agreement with experimental data without any considerable deviation from each other. In contrast, the second section where the experimental data are still available reveals a high performance of *EARSM* [15] in capturing well the velocity field in a turbulent swirling flow. Based on this result, further investigations in this paper have been carried out by using this model.

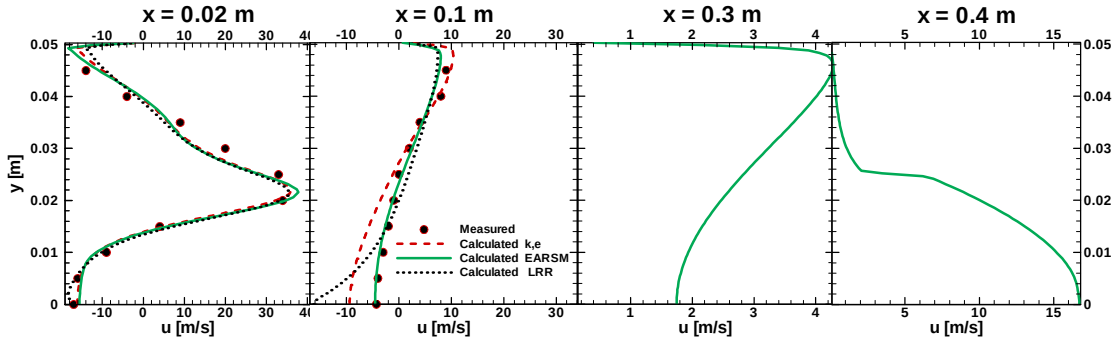

Fig. 2: Cross-sectional profiles of gas axial velocity component along the chamber (non-reacting case)

In Fig. 3 the calculated radial distribution of the droplet mass flux is shown at different axial positions using equilibrium and non-equilibrium evaporation models. Generally, the concentration of droplets decreases while moving away from the nozzle due to the evaporation. A comparison between equilibrium and non-equilibrium evaporation models does not reveal a prediction difference as long as big particles are involved (x=5mm). As expected, with decreasing droplet diameter the non-equilibrium effects become predominant (x=20; 40mm) and lead to an enhancement of droplet evaporation rate in accordance to [6]. This is also confirmed in Fig.4 which shows the droplet concentration zones inside the chamber obtained by using equilibrium and non-equilibrium models in comparison with experimental visualization.

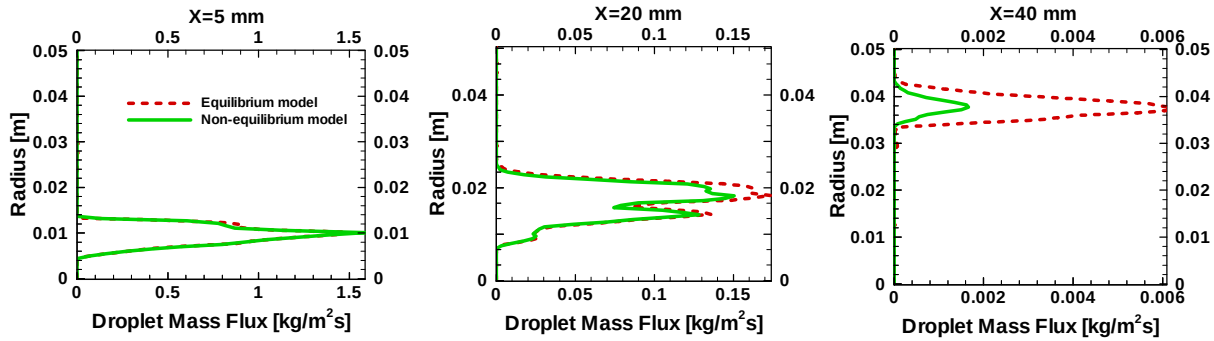

Fig. 3: Droplet mass flux along the chamber: Comparison between results with equilibrium and non equilibrium evaporation models

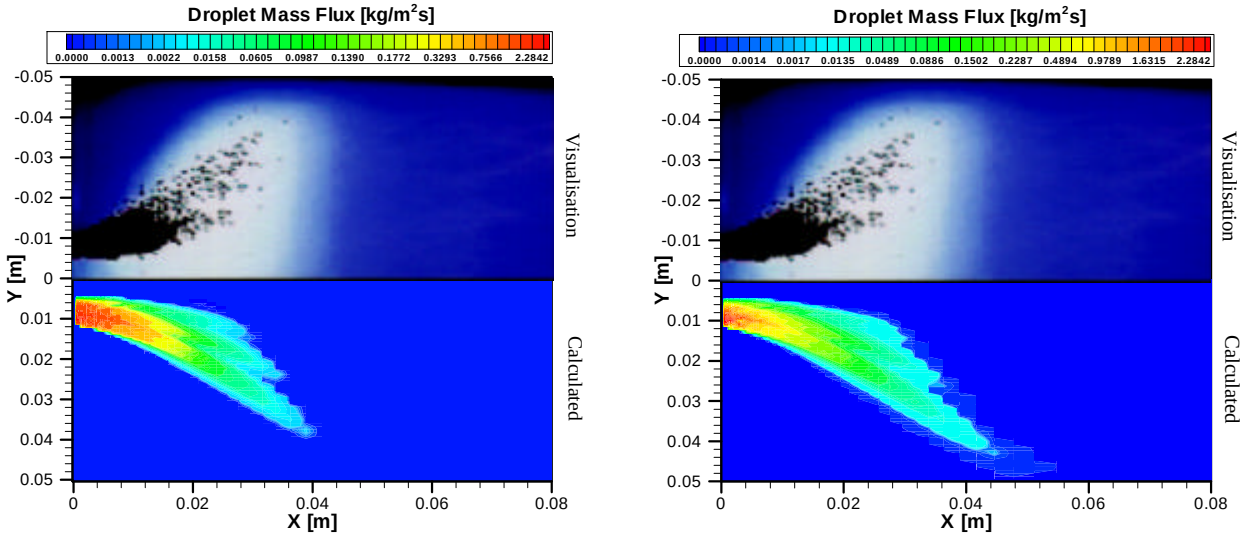

Fig. 4: Droplets concentration zones using non-equilibrium (left) and equilibrium (right) evaporation models

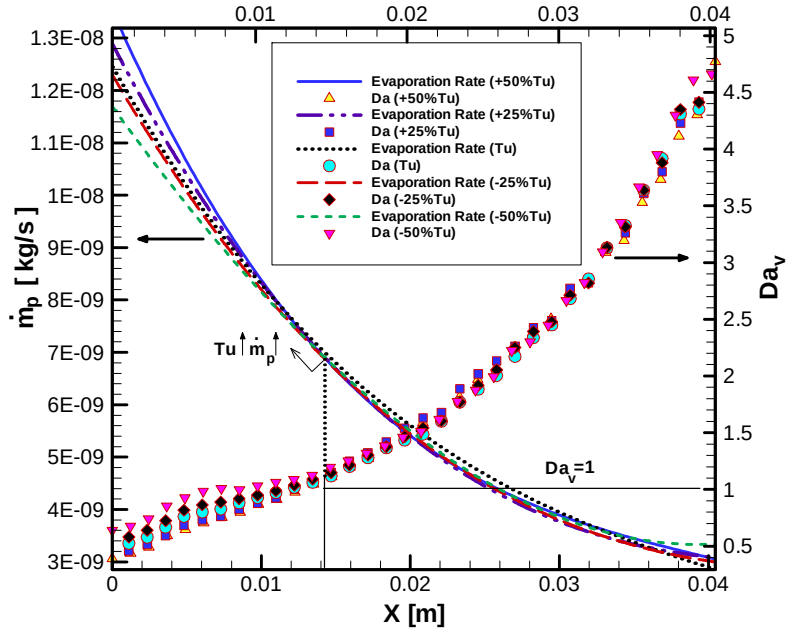

Fig. 5: Influence of the turbulent kinetic intensity on the evaporation rate of droplets and the evaporation Damkhoeler number (Da_v) along the spray core

A qualitatively better agreement with experiment is achieved by using a non-equilibrium model delivering the correct spray penetration length. In figure 5 the influence of the turbulent kinetic energy on the vaporization rate is shown along the axial direction. It appears that when the turbulence intensity increases, the efficiency of the mass transfer increases, approximately during the first half of the droplet lifetime. This influence decreases with decreasing droplet diameter. It also appears clearly that there exists a critical number below which the turbulence energy is able to increase the mass

transfer. For higher value of this number an inverse behavior is even observed. Focusing on the pure turbulence effect, this result confirms the experimental and numerical findings in [5, 6]. From them, a so called vaporization Damkhoeler number, $Da_v = T_t / T_v$, may be introduced. For $Da_v<1$ the evaporation rate is increased with the increase of the turbulence intensity, while in the case $Da_v>1$ an inversed phenomenon can even be observed. For the mean droplet size used in calculations, this behaviour is observed independently from evaporation models.

The influence of the swirl intensity on the mixing process is depicted in Fig. 6 in which the variations of a spatial mixing deficiency parameter (*SMD*) are shown. This parameter describes the heterogenity of the distribution of the fuel vapor in the chamber. The curves show that an enhancement in swirl intensity leads to a rapid and efficient mixing process providing a homogeneous mixture very close to the inlet port. This fact may be related to the presence of two (internal and corner) recirculation zones formed in the flow for high degrees of swirl (*Sw.Nu.*>0.6). As pointed out in [6], an increase in swirl number obviously enhances the size of the internal recirculation zones.

Second Case: Swirled Combusting Spray

In this section, some results of scalar distribution obtained under consideration of the conjugate effects of the swirl intensity, the turbulence and the combustion are presented. In Fig. 7 the effects of swirl intensity on combustion process are shown. An increase in swirl number enhances the temperature and the size of the hot zone in chamber. The hot zone appeared at the outlet area (Fig. 7a) is shifted inside the combustor which leads to a homogenization of the temperature distribution in the combustion chamber (Fig. 7b). This is due to the modification of the flow and mixing dynamics.

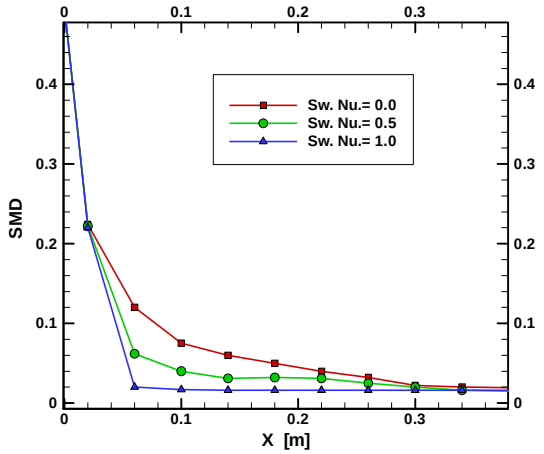

Fig. 6: Spatial Mixing Deficiency (*SMD*) along the chamber (Non-reacting case).

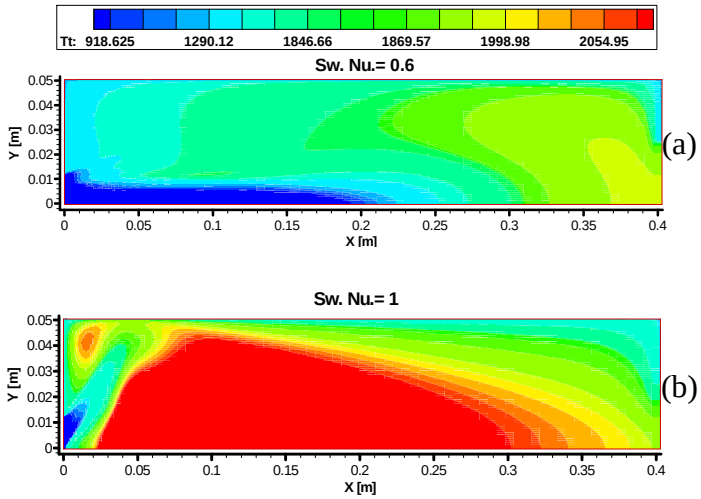

Fig.7: Effects of swirl intensity on temperature [K] distribution (reacting case).

Figure 8 shows the influences of swirl intensity on the concentration of oxygen and carbon dioxide along the centerline at the radial position r =10 mm computed by using two different modulation models. It can be observed that the increase of the swirl intensity enhances the speed of chemical reaction in O_2-consumption and CO_2-creation in combustion chamber. It is also clear that for low swirl intensities (*Sw.Nu.*=0.6) the oxidator is not consumpted entirely and can even be observed at the outlet.

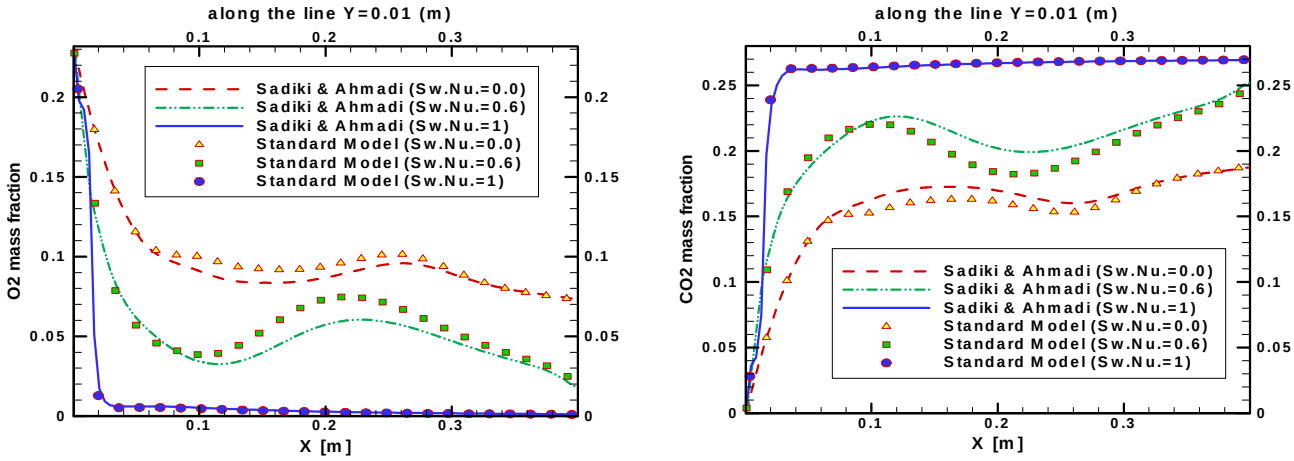

Fig.8: Effects of swirl intensity on concentration of O_2 and CO_2 along the combustion chamber using two different modulation models (standard model and model by Sadiki & Ahmadi)

Comparing the results of different modulation models, the model by Sadiki & Ahmadi [13] causes a considerable reduction in predicting the chemical reactions approximately in the middle of combustion chamber up to *Sw.Nu.*<1. It turns out that the modulation affects the concentration distribution only for low swirl numbers. In this case an accurate modulation modelling is required. Because of its reliable capability in accurately predicting the modulation effects as demonstrated in [19], the model by Sadiki & Ahmadi may be then recommendable.

NOMENCLATURE

EARSM	Explicit Algebraic Reynold's Stress Model	*Sw. Nu.*	Swirl number
LRR	Launder, Reece and Rodi (implicit) Algebraic Model	T_t	Turbulent macro time scale
		T_v	Time scale of the vaporization
k	Turbulent kinetic energy [m^2/s^2]	u_i (u,v,w)	Gas velocity components [m/s]
LES	Large Eddy Simulation	u_{pi}	Particle velocity components [m/s]
$\dot{m}_p$	Droplet evaporation rate [kg/s]	x,y,z	Position coordinates
RANS	Reynolds Averaging based Numerical Simulation	e	Turbulent dissipation rate [m^2/s^3]
		r	Gas-phase density [kg/m^3]
$S_{k,p}$	Particle source term for k-equation		
$S_{u_i,p}$	Particle source term for momentum equations	$\overline{(\cdot)}$	Average value

REFERENCES

1. B. Zamuner, P. Gilbank, D. Bissieres and C. Berat, Numerical Simulation of the reactive two-phase flow in a kerosene/air tubular combustor, *Aerospace Sci. and Tech.*, Vol. 6, pp.521-529, 2002.
2. G. Klose, R. Schmehl, R. Meier, G. Meier, R. Koch and S. Wittig, Evaluation of advanced two-phase flow and combustion models for predicting low emission combustors, *Proc. of ASME Turbo Expo*, May 8th-11th, Munich, Germany, 2000.
3. C. Hollmann and E. Gutheil, Flamelet-Modelling of Turbulent Spray Diffusion Flames based on Laminar Spray Flame Library, *Combust. Sci. and Tech.*, Vol. 135, pp. 175-192, 1998.
4. R. J. Sornek, R. Dobashi and T. Hirano, Effect of Turbulence on Vaporization, Mixing, and Combustion of Liquid-fuel Sprays, *Combustion and Flame* 120:479-491, 2000.
5. I. Gökalp, C. Chauveau, O. Simon and X. Chesneau, Mass transfer from Liquid fuel droplets in turbulent flow, The combustion Institute 1992.
6. A. Sadiki, M. Chrigui, M. R. Maneshkarimi and J. Janicka, CFD-Analysis of conjugate effects of turbulence and swirl intensity on spray combustion in a single gas turbinr combustor, *Proc. of ASME Turbo Expo*, june 14th-17th, Vienna, Austria, 2004.
7. S. Geiß, Z. Stojanovic, M. Chrigui, A. Sadiki, A. Dreizler and J. Janicka, Investigation of Turbulence Modification in a non-reactive Two-phase Flow, *Exp. in Fluids*, 36, pp. 344 - 354, 2004 .
8. M. A. R. Sharif and Y. K. E. Wang, Evaluation of the Performance of the three turbulence closure models in the prediction of confind swirling flows, *Computers and Fluids*, vol. 24, n1, pp. 81-100,1995.
9. T. Crowe, On models for turbulence modulation in fluid-particle flows, Int. *J. of multiphase flow*, vol. 26, pp. 719-727, 2000.
10. B. Abramzon and W.A. Sirignano, Droplet vaporization Model for Spray Combution Calculations, *Int. J. Heat Mass Transfer*, vol. 32, pp. 1605-1618, 1989.
11. R. S. Miller, K. Harstad and J. Bellan, Evaluation of equilibrium and non-equilibrium evaporation models for many-droplet gas-liquid flow simulations, *Int. Journal of Multiphase Flow* vol. 24, pp. 1025-1055, 1998.
12. V. Sankaran and S. Menon, LES of spray combustion in compressible high Reynolds number swirling flows, *Proc. of the 2nd International Symp. on Turbulence and Shear Flow Phenomena*, Stockholm, Sweden, 2001.
13. M. Chrigui, G. Ahmadi and A. Sadiki, Study on Interaction in Spray between Evaporating Droplets and Turbulence Using Second Order Turbulence RANS Models and a Lagrangian Approach, *Progress in Computational Fluid Dynamics*, Special issue, 2004.
14. W. Rodi, A new algebraic relation for calculating the Reynolds stresses, *ZAMM*, 56, pp. 219, 1976.
15. T. B. Gatski and C. G. Speziale, On explicit algebraic Reynolds stress model for complex turbulent flows, *Journal of Fluid Mechanics*, vol. 254, pp. 59-78, 1993.
16. L. I. Lilleheie, S. Byggstyl and B. F. Magnussen, Calculations of a Methane Turbulent Diffusion Flame Using Detailed Chemical Kinetics in the Eddy Dissipation Concept, Technical reports, SINTEF/Norwegian Institute of Technology, Division, 1989.
17. W. Krebs, U. Gruschka, C. Fielenbach and S. Hoffmann, CFD-analysis of reacting flow in an annular combustor, *Progress in Computational Fluid Dynamics*, vol.1, Nos 1/2/3, pp. 104-116, 2001.
18. A. D. Gosman and F. C. Lockwood, Incorporation of a flux model for radiation into a finite-difference procedure for furnace calculations, *14th Symp (int.) on Combustion*, The Combustion Institute, pp. 661-671, 1973.
19. M. Chrigui and A. Sadiki, Prediction Performance of a Thermodynamically Consistent Turbulence Modulation Model for Multiphase Flows, 3rd *Int. Sym. On Two-Phase Flow Modelling and Experimentation*, September 22th-25th, Pisa, Italy, 2004.

ACKNOWLEDGMENTS: The authors acknowledge the financial support by the *DFG* through the SFB568 (TPA4).