URN (Paper): urn:nbn:de:gbv:ilm1-2011iwk-029:7

56TH INTERNATIONAL SCIENTIFIC COLLOQUIUM
Ilmenau University of Technology, 12 – 16 September 2011
URN: urn:nbn:gbv:ilm1-2011iwk:5

CFD INVESTIGATION OF THE INJECTION AND COMBUSTION PROCESS IN A DIESEL ENGINE

Prof. Dr. W. Waidmann

University of Applied Sciences Aalen, Department of Mechanical Engineering, Aalen, Germany

ABSTRACT

This paper describes the simulation of in-cylinder diesel injection and combustion. The calculations were carried out on the basis of a Deutz 2014 heavy duty diesel engine. A discrete phase model has been used for spray simulation. A primary break-up model and two secondary spray break-up mechanisms, the Kelvin-Helmholtz theory and Rayleigh-Taylor instabilities have been investigated. Droplet evaporation, droplet collision and the influence of droplet shape on drag has been accounted for. To verify the spray simulation, droplet diameters and velocity distributions have been compared with experimental data from a Phase Doppler Anemometry (PDA) measurement in a model chamber. The combustion is calculated with available models in Fluent, the Eddy-Dissipation Model (EDM), where the turbulent mixing is the time limiting process, the Eddy-Dissipation Concept model (EDC) and the Flamelet Model which both take account for kinetic effects.

1. INTRODUCTION

The Common-Rail Diesel injection results in spray atomization with very small mean droplet diameters. This guarantees effective evaporation of the fuel and enhanced mixing of the reactants. Multi-dimensional simulation of these processes is still an issue. The spray models currently available in the literature will not work without adjustment of constants and fitting parameters based on detailed measurements. However simulation of combustion and pollutant chemistry is not possible without correctly predicting the spray. The combustion is calculated with widely applied models available for turbulent non premixed combustion. Typical engine working conditions near full load were taken to validate the calculations. The thermal loss due to the heat transfere through the cylinder head and the cylinder wall and the pressure loss through the piston rings were taken into account. The computational domain extends from the fresh air inlet duct, which operate as a vortex generator, the inlet valves to the moving piston.

2. VALIDATION CONDITIONS

The numerical investigations were carried out on the basis of a Deutz 2014 heavy duty common rail diesel engine (2100 rpm, 232 PS, rail pressure 1600 bar, compression pressure 140 bar). The flow through the inlet duct, the inlet valves and the cylinder is pre-calculated to have realistic initial flow conditions for the cause of the injection and combustion process, Figure 1. The calculation starts at minus 5 degree ahead the top dead center (T.D.C). In fact of incomplete mass exchange during the charge changing 6.8 percent of exhaust gas was assumed to remain in the fresh air. Exhaust gas recirculation was not taken into account. The pressure loss due to the piston rings was assumed to be 1.5 bar (crevice model). A cylinder pressure indicator system delivers the pressure versus the crank angle to verify the simulations. Droplet diameters and velocity distributions of the spray have been measured by Phase Doppler Anemometry (PDA) in a model chamber [1].

Figure 1: View of the inlet duct with two inlet valves and the piston bowl (Deutz).

3. NUMERICAL MODELS

The numerical calculations were carried out with the Fluent 13 CFD code. The chosen multiphase model is the Discrete Particle Model, applying the stochastic tracking of individual droplets or droplet parcels

(Lagrangian approach). All droplets are injected with the same initial diameter ('blob'-method). In general, this diameter is identical to the nozzle orifice diameter or somewhat decreased due to cavitational effects. Temperature dependencies of the air and fuel material properties have been taken into account. The Standard k-e, the Realizable k-e and the SST turbulence model have been applied in combination with the Eddy Break-up, the Eddy Dissipation Concept and the Flamelet model. For the latter the gasoil chemkin mechanism was applied. Table 1 gives some injection and model constants.

Conditions	Parameters / Comments
Fuel	$C_{16}H_{29}$ gasoil, surrogate for diesel, 158 mm^3 inj. volume
Initial droplet injection diameter	0.167 mm, nozzle orifice
Injection velocity	max. 430 m/s, variabel
Aerodynamic drag	Including droplet deforming
Primary break-up	Solid cone injection
Secondary break-up	Kelvin Helmholtz and Rayleigh Taylor (KH-RT)
KH-RT constants	B0=0.61, B1=18,C3=2.5, c=30
Time stepping	39,4 μsec, CA = 0.5 degree
Injection time	2150 μsec
Particle streams	500 parcels

Table 1: Parameters for injection calculation[2]

3.1. Primary spray break-up

Since the spray has a conical shape near the orifice the Solid Cone Injection has been applied. The spray angle which is an unknown parameter must be given as a basic input value for the model. In the present investigation the angle is retained from the shadowgraphs available from a model chamber [1] with 50 bar backpressure. The influence of the higher in-cylinder pressure of about 140 bar was taken into account. [2]. The break up length where the primary break-up ends and the secondary break-up starts is given by an empirical equation in the literature [3].

3.2. Secondary spray break-up

The secondary break-up model is the backbone of spray simulation. The models usually applied, calculate liquid break-up by using some form of stability analysis [4]. Break-up occurs if droplets exceed a certain stability criterion, and the characteristics of the resulting droplets depend on the wavelength of the instability that caused the break-up. In the present study, Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) models are used. The KH model (also called Wave-Model) considers the stripping process of droplets due to the growth of Kelvin-Helmholtz instabilities on the droplet surface resulting from the relative velocity between the gas and the liquid phase. The RT model accounts for sudden catastrophic break-ups due to the deceleration of the droplets. The resulting droplets are larger than those of the KH model. Physical details of the different models and proposed activation conditions are described in [5]. A combination of these two models, the so-called KH-RT model, can match the measured droplet size distribution best. In the vicinity of the nozzle, until a certain path length (the so-called break-up length), it is expected that droplets undergo only the KH break-up, whereas further downstream both mechanisms are operative.

3.3. Evaporation

Although real Diesel fuel consists of a blend of hundreds of components, it is usually treated as a single component solution, $C_{16}H_{29}$ in the present case. In fact, this is an over-simplification but there is no better option. Vaporization has been assumed to take place as soon as the droplet temperature exceeds the boiling temperature. It was calculated from the vapor pressure, which is described as a piecewise linear function of temperature. Heat- and mass transfer were calculated in the usual way from a Nusselt correlation [6] with the actual droplet diameter. A constant diffusion coefficient of 3.79 E-6 m^2/s and a latent heat of 180 kJ/kg were applied.

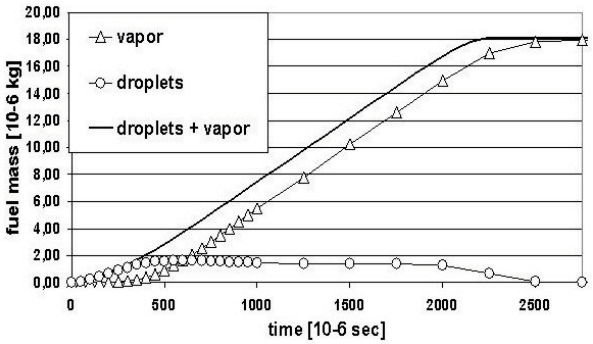

Figure 2: Calculated droplet and vapor mass during the injector time (2150 μsec).

Figure 2 illustrates the droplet and vapor mass fraction during the injection time. In the beginning, the droplet and the total mass are nearly the same while the amount of vapor mass fraction is negligible. Evaporation starts at about t = 400 μsec injection time. Subsequently, the vapor mass fraction increases nearly linearly with time until the end of evaporation at t = 2500 μsec the complete fuel is evaporated. The slope of the vapor mass fraction is almost parallel to the totally injected mass. This means the mass of droplets in the chamber remains nearly constant during this time period, and the fuel evaporation rate is proportional to the injected mass flow rate. This tendency can also be observed in the experiment, where it was found that during this time period the droplet distribution and the droplet diameter

histograms are more or less time independent [1]. Note that the chamber conditions have been 50 bar and 710 K. For the engine conditions the evaporation process is faster due to the higher temperature near the top dead center.

4. SPRAY PATTERN

Figure 3 shows a snap-shot of the spray pattern of a typical multi orifice diesel injector. The picture is taken 1000 μsec after the injection is started and the jets penetrate into quiet air with a backpressure of 10 bar.

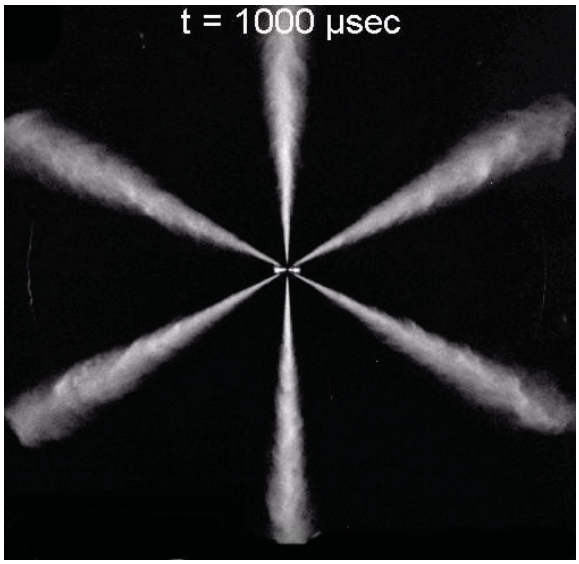

Figure 3: Spray pattern of a 6 orifice common rail injector (Bosch). Note: for the present paper an 7 hole injector is used.

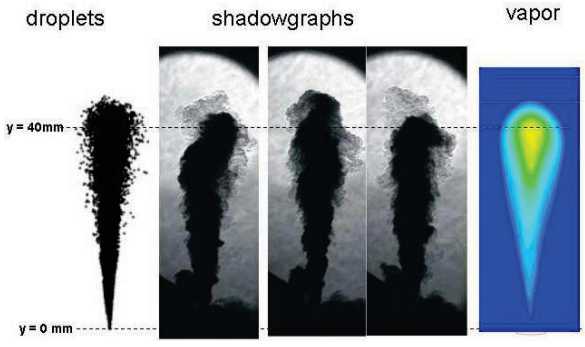

Figure 4: Nanolight shadowgraphs of one single spray and the corresponding calculated droplet (left) and vapor (right) distribution. (chamber backpressure = 50 bar, 710 K)

Figure 4 shows a more detailed shadowgraph of one single spray for the same injection time. The chamber conditions are 50 bar and 710 K. The three shadowgraphs in the middle of figure 4 should give an impression of the intermittent character of the fuel spray. The exposure time is a few nanoseconds. The shadowgraphs have been taken at different test runs at the same time and instant of injection, and show a strongly irregular spray pattern especially at the head region. The overall fuel penetration length is nearly identical in all three pictures, but the head region sometimes consists of droplets (dark colour), sometimes of vapor (brighter cords). The conical spray boundary also shows fluctuations with small outbursts of droplets or vapor.

Compared to the experiments, there are much less irregular coves visible at the simulated jet, but penetration length and overall shape of the spray are well reproduced. Note that the cone angle for the primary break-up model has been taken as a time-average from the experiments.

The calculated droplet distribution shows a dense core region near the orifice. Droplets at the jet boundaries are more exposed to the surrounding air and experience stronger deceleration than the droplets located in the central jet region. Hence, about 20 mm away from the nozzle, radial spray expansion starts. Vapor mass fraction is almost steadily distributed in the spray region, only close to the head region a maximum vapor mass fraction of about 0.3 occurs. The overall shape of the vapor distribution is nearly identical to the droplet distribution. In the real engine vapor will be transported by the swirl in the piston bowl.

5. DROPLET DIAMETER AND DROPLET VELOCITY DISTRIBUTION HISTOGRAMS

Figure 5 and 6 show a comparison of the calculated and measured droplet diameter and droplet velocity distribution at a position at height = 40 mm (45 mm) and radial = 2 mm. The simulated and measured diameter and velocity spectra agree very well. The parameters of the break-up models have been adapted with experimental PDA data (Phase Doppler Anemometer) in a 50 bar, 710 K model chamber [1]. Note that the pressure near the upper dead center in the real engine is about 140 bar. Only the cone angle is adapted to this higher chamber pressure. The droplet diameter and droplet velocity distribution will change with increasing in-cylinder pressure. However the comparison shows an excellent agreement for the droplet velocity and a good agreement for the droplet diameter distribution. When the break-up parameters are changed to achieve a better agreement for the droplet diameter the velocity distribution deteriorates. A balance between the quality of both histograms is necessary. In figure 5 the agreement of the velocity distribution is carried to extremes and the overall difference is very low. This good result can be observed on several positions in the spray for injector distances larger than 40 mm. Below this value the spray is to dense to apply the LDV method and there are no data available. Because of the transient behaviour of spray only between 800 and 2150 μsec

the droplet values are constant. In the beginning of the penetration the droplet diameters and velocities are not constant with time at a fixed position. This affects the evaporation and combustion calculation in the beginning of the process.

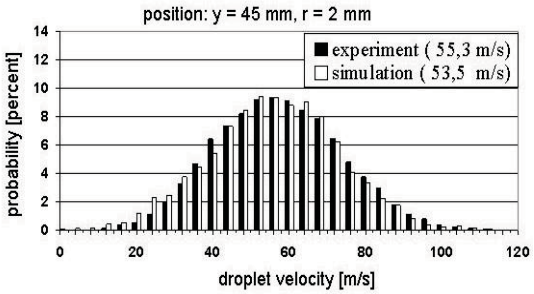

Figure 5: Droplet velocity histogram, ( ) mean values.

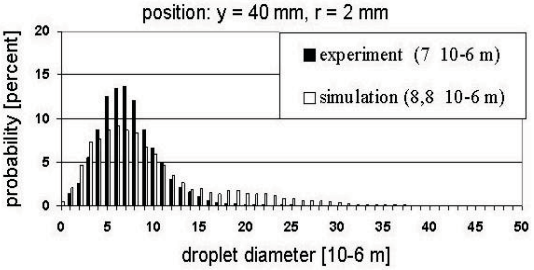

Figure 6: Droplet diameter histogram, ( ) mean values

6. COMBUSTION

6.1. Combustion Models

To simulate non premixed combustion, several models are available in the fluent code. These models are able to calculate species transport, diffusion and the reaction mechanism. The Eddy Dissipation Model (EDM), the Eddy Dissipation Concept Model (EDC) and the Flamelet Model [7]. These models are predestinated to simulate the turbulent combustion. The models can not stand alone but need to be combinated with an adequate turbulence model due to the dominant influence of turbulent mixing in such flames.The EDM uses a global one step equation assuming complete conversion of the gasoil into CO_2 and H_2O. The reaction rate is determined assuming that turbulent mixing is the rate-limiting process. The EDC model is based on a detailled description of turbulent eddies. In the EDC the total cell space is subdivided into a reaction space, which is represented by the Kolmogorov dissipation volume (smallest eddies) and the surrounding space. The homogeneous reactions take place in the fine structure. All rections in the surrounding fluid are neglected. Fluent allows reaction kinetic schemes in the chemkin format with 50 species. The Flamelet Model reduces the multidimensional combustion process to a one dimensional case. The turbulent flame is devided into a thin laminar one dimensional diffusion flames including complex reactions. The influence of the turbulence exists in the distension and folding of the flamelets.

6.2. Ignition delay

An important parameter in combustion calculations is the ignition delay time. The ignition delay is a combination of a physical and a chemical part. In the physical part the droplets must undergo a break-up into small droplets which can evaporize. The chemical part starts now when the vapour is breaking down into carbon and hydrocarbon products. Together with the oxygen radicals they built a ignitable mixture. Some available kinetic schemes include starting rections to calculate the ignition delay time. Unfortunately all available and tested ignition delay models failed in this investigation. The combustion is therefore started by patching the temperature and some radicals at a certain time step. The value is taken from the literature for diesel oil surrogate and the surrounding conditions when the injection is started (p = 140 bar, T = 900 K). The ignition delay time is 470 µsec. Note that the injection was started minus 5 degree before the top dead center and the ignition therefore starts at about 1 degree crank angle.

6.3. In-cylinder pressure

To verify the combustion calculations the in-cylinder pressure is compared with experimental dat taken while the expansion cycle. The injection starts at minus 5 degree before the top dead center. Figure 7 shows a typical pressure course obtained by an EDC calculation in combination with the Standard k-e model. The figure shows a typical calculated pressure trace with a higher pressure maximum at the beginning of the combustion. For higher crank angels the deviation is small and indicates a good agreement. This tendency can be observed in nearly all calculations except the EBM calculations where the pressure overshooting is much higher followed by a strong decrease under the measured values. So the EBM is not the first choice for such cases of calculation.

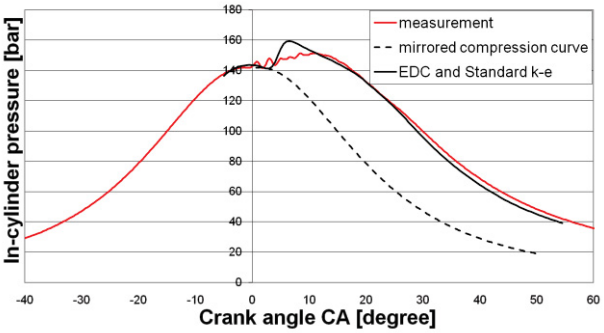

Figure 7 : Comparison of the measured and calculated pressure.

When the ignition delay time is changed the pressure curves will change too. So the correct ignition delay time is a very important parameter which must be carefully fixed. The overshooting of the pressure can be caused by many factors. The fuel could be reacting to fast and the corresponding heat release and pressure increase therefore exceed the measured value. The modelled spray break-up at the beginning of injection could be too fast or the one component diesel surrogate gasoil is too basic. Effects like the supercritical evaporation could also become an influence under the in-cylinder conditions near the top dead center.

6.4. Comparison of Combustion Models

The best results are achieved with the Flamelet and the Eddy Dissipation Concept Models in combination with the Standard k-e and the Realizable k-e model. The SST model is also a good choice but the differences in the pressure trace is very small. The EBM model leads to an overprediction of the cylinder pressure and a strong decrease for higher crank angles. The change in the shape of the flame during the calculation is comparable to the EDC approach, so the model gives a fast overview of the flame propagation. A detailed description of the different models and their pros and cons including the NO_x and the soot formation are given in [8 and 9]. The NOx calculation can be done in a postprocessing mode, with the flow field, temperature and hydrocarbon combustion species concentrations fixed. Prediction of NO_x or NO in this mode is justified on the grounds that the NO concentrations are very low and have negligible impact to the hydrocarbon combustion prediction [6]. The thermal NO delivers the highest amount in the calculations so that the prompt NO_x could normally neglected.

6.5. Piston bowl

Figure 8 shows the piston after a test run near the maximum power. The seven spays are visible at the piston crown bowl. The droplets of the spray reaches the surface and leave one´s mark. As a result of the swirl component the soot prints drift somewhat in the flow direction. Figure 8 includes the calculated droplet distribution. The penetration is high enough to reach the piston wall even at this time step and form the dark soot zones. So it is a typical example how to get a virtual insight into such complex physical phenomena. At the end of injection at about t = 2150 µsec, no new droplets were injected and the last droplets are evaporating, figure 9. In this piston expansion phase the droplets are transported at the wall over the edge to the upper side of the piston bowl before they finally disappear.

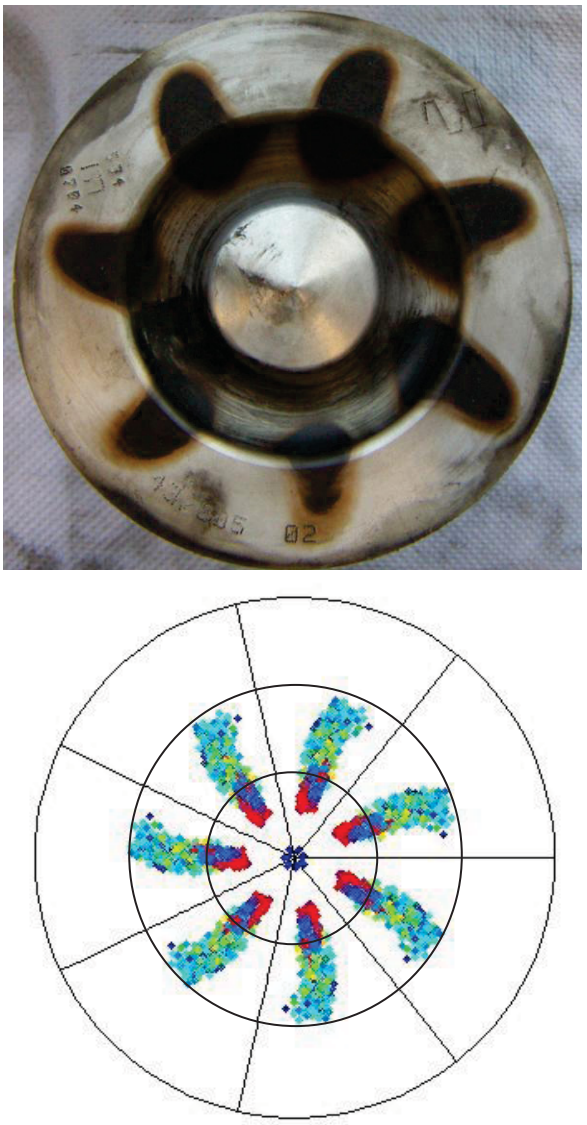

Figure 8: Piston bowl with soot trails after a test run and calculated droplets at (t = 1000 µsec).

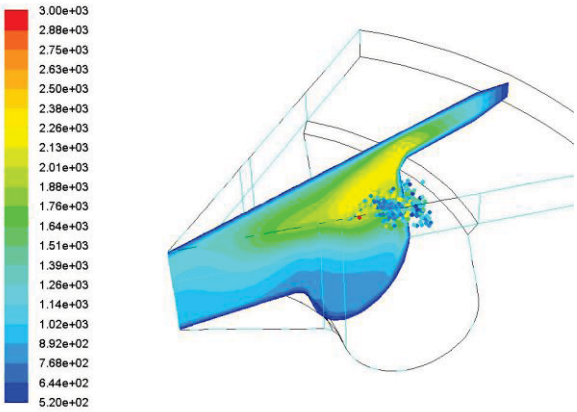

Figure 9: Droplet and temperature distribution at the end of evaporation (t = 2200 µsec).

6.6. Temperature and vapor spreading

Figure 10 shows the temperature and vapor distribution for several crank angles which describes the flame propagation. The color map for the temperature reaches from 500 K to 2600 K. The contour lines reaches to a maximal fuel mass fraction of 0.2. The ignition is started at CA = 1 (t = 473 µsec after injecton) by patching a high temperature inside a few cells near the injector. Until CA = 2 there is no temperature increase visible and the value is somewhat decreased due to the evaporation cooling. At CA = 3 the flame starts and begins to elongate into the piston bowl. The highest temperatures are at the vapor / air boundary. The spreading of the temperature (yellow = 2400 K) which shows that the flame does not fill up the whole piston bowl and there is a remaining rest of air inside the lower bowl region. Thus figure 10 shows an example where the geometry is not ideal designed or the spray angel is not correct adjusted, especially for this calculated loading condition, near full load.

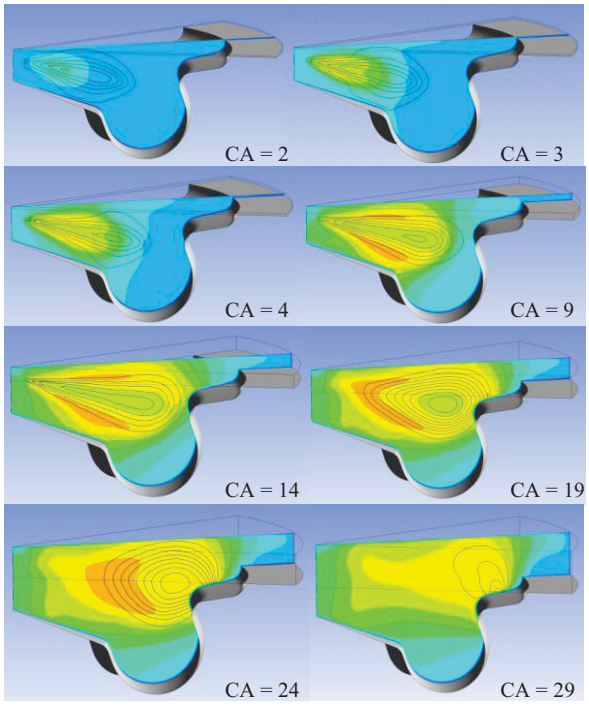

Figure 10: Temperature (filled) and vapor mass fraction (contour) for several crank angles CA.

7. CONCLUSION

The present work shows a way to simulate the in-cylinder diesel injection with combustion. The main aim was a complete simulation of all governing effects and the application of common available models. The work allows a virtual insight into the complex phenomena of the injection and combustion processes. It can be helpful for the design of a piston bowl and the optimization of the injection angel. It could also increase the knowledge of the influence of the swirl flow for the flame propagation and pollutant formation. A very sensitive phase in the transient simulation was the quality of the simulated spray. In the early phase, in the beginning of the injection, the spray cannot be correctly calculated. Because the adjustment of the spray model parameters has been carried out when the spray has been completely developed. This leads together with the sensitive ignition delay time to uncertainties in such calculations. However the simulation technique can serve as a very useful tool for engine optimizations.

acknowledgment:
many thanks to Dr. Andreas Boemer, Deutz AG and Daniel Gonsior for supplying the engine data and discussion.

8. REFERENCES

[1] Staudt M.; Pawlowski A.; Strömungs-untersuchungen mit optischer Messtechnik; Lehrstuhl für Wärme- und Stoffübertragung, Aachen University; Ergebnisbericht Deutz AG; 2004.
[2] Prof. Dr. Waidmann, Dr. Boemer, Dr. Braun; Adjustment and Verification of Model Parameters for Diesel Injection CFD Simulation; SAE-paper 06P-160,2006.
[3] Naber, J.D.; Siebers, D. L.; Effects of gas density and vaporization on penetration and dispersion of diesel sprays, SAE 960034, 1996.
[4] Patterson M. A., Reitz R.D.; Modeling the Effects of Fuel Spray Characteristics on Diesel Engine Combustion and Emission; SAE paper 980131, 1998.
[5] Reitz, R.D.; Modeling Atomization Processes in High Pressure aporization Sprays; Atomization and Spray Technology 3, 1987.
[6] W. E. Ranz, W. R. Marshall, Jr.; Evaporation from Drops, Part I.; Chem. Eng. Prog., 48(3), 1952.
[7] FLUENT User's manual, Version 13, 2011.
[8] D. Gonsior, A. Boemer, W. Waidmann; CFD Simulation des Verbrennungsprozesses in einem DEUTZ-Dieselmotor; Fluent CFD-Forum 2005, Bad Nauheim, Germany.
[9] D. Gonsior; CFD Untersuchungen zur Simulation eines dieselmotorischen Verbrennungsprozesses. Diplomarbeit, FH Aachen und Deutz AG 2005.