Simulation of Primary Break-up of Diesel Jets by a Hybrid Method Combining VOF-Calculations and the Classical DDM Rate Approach with a 3D CFD Code

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Abstract
A novel hybrid primary break-up model, which is based on coupling of direct numerical simulation (DNS), energy conservation method and linear stability analysis has been implemented into a 3D CFD code and has been tested under conditions typical for Diesel fuel injection in IC engines. Droplet spectra have been pre-calculated for the relevant range of injection and have been stored in a database. From this database actual values in the 3D code are gained during injection time using a quadrilinear interpolation technique to save computational effort. The results are compared with various experiments for non-evaporating and evaporating sprays with promising results.

Introduction
The liquid jet atomization process represents an important but not yet fully understood phenomenon within diesel engine CFD simulations. Since this process defines the spray initial conditions, it also affects spray penetration, mixture formation and thus as well the following combustion analysis. Especially penetration dynamics close to the nozzle has been difficult to predict with present standard models, since these are based on injection of big blobs of liquid instead of starting with the smaller droplets produced by primary break-up of the coherent liquid leaving the nozzle. To get a better understanding of the initial fuel disintegration processes a new primary break-up model was developed by UNIBO /1/. For testing under engine conditions this model has been implemented into the FIRE 8 CFD code. The aim of this work is to obtain an improved initialization of the spray, i.e., droplet size distribution and starting velocities within the framework of the standard discrete droplet method (DDM).

Previous work
Primary break-up is the first stage of fuel jet disintegration close to the injection nozzle. The various modelling approaches assume aerodynamic instability, liquid phase turbulence, cavitation inside the nozzle or velocity profile relaxation as decisive disintegration mechanisms /2-4/. Based on this, surface wave formation, wave crest or ligament detachment and also ligament decay are modelled. The most comprehensive of these models /4/ combines the various mechanisms mentioned above; however, it relates the primary break-up to spatially averaged nozzle flow properties. Recently a more detailed coupling to nozzle flow has been presented in /5/ by calculating the primary break-up from locally resolved flow properties in the nozzle orifice. All of these authors use the well-established rate approaches and describe primary break-up processes based on the blob injection method or the erosion of a liquid core. More sophisticated approaches are Fourier analysis of the surface evolution /6/, turbulent mixing /7/ as well as models based on large eddy simulation (LES), e.g. the volume-of-fluids (VOF) methods, which have already been applied to liquid jet break-up simulation /8/. However, although the DNS methods are most accurate, they are also very time consuming. Therefore at the present stage of computational resources, simulations of the overall injection cycle by DNS does not seem to be practical yet. In order to overcome this shortcoming, the work presented here attempts to combine a partial use of the VOF method with the faster rate approach method: the aim is to set up a model which is usable for an engineering scope of applications. In contrast to the work of Murdoch et al. /9/, who use VOF pre-calculations to define additional injection of parcels and simulate the liquid phase distribution as predicted by the VOF method, here the VOF approach is fully integrated into the DDM method providing the initial conditions for the spray parcels in each time step.

Model description

The idea behind this hybrid model is to directly simulate the ligament formation process and then to model further droplets detachments. The liquid jet surface is reconstructed by means of Stephane Zaleski's Surfer V3.1.2 2D-VOF code (see /10/). The 2D simplification is valid as long as disturbances are small compared with jet diameter. The simulations are performed on a comparatively coarse computational grid of 10 µm square cells, allowing reasonable calculation times. The domain covers a length of 2 mm after the injector and only the half jet is simulated (see Fig. 1.1). Effects of nozzle flow turbulence and cavitation are accounted for by introducing a surface velocity fluctuation of 20 percent of the injection velocity at the boundary. The adoption of such a grid size has proved to be accurate to compute directly ligament formation accounting for the physical processes driving surface wave growth. Since the atomization is mainly a three-dimensional process, an energy balance is introduced to detect liquid crests, which reach critical conditions for ligament detachments. This condition is based on a Weber number criterion We > We*. The Weber number, decisive for wave crest detachment, is calculated using the radial liquid velocity as well as a characteristic length scale taken from within the order of magnitude of the grid size.

The critical value for the ligament Weber number We* was assumed as 10, according to literature and further model tuning (for more details see /1/). When a crest is defined as critical, it is detached as a ligament. Its area is erased from the computational domain and all the related dynamic properties are transferred to the ligament break-up model (see Figure 1.2) which is introduced because of the grid size adopted which cannot resolve droplet formation. The pinched-off area is not a droplet itself, but can be considered as part of a vortex ring with a relevant amount of circulation Γ around the annular surface. This is responsible for instability in circumferential direction and thus for further break-up into ligaments (see Fig. 1.3). A dispersion relation linking disturbance wave-number k with the wave growth rate ω is introduced on annular surfaces, in order to determine the critical wavelength k_{max} of the most unstable perturbations.

$$\omega^2 = \left[\frac{\sigma}{\rho_l d_r^{\,3}}\left(1-k^2 d_r^{\,2}\right)+\left(\frac{\Gamma}{2\pi d_r^{\,2}}\right)^2\right](kd_r)\frac{I_1(kd_r)}{I_0(kd_r)} \quad \Rightarrow \quad \lambda_{critic} = \frac{2\pi}{k_{max}} \quad \Rightarrow \quad D = B\cdot\lambda$$

This dispersion relation is based on Ponstein's original theory /11/: by the results of this linear stability analysis the value of the wave length λ with maximum growth rate is then linked to the detached drops diameter assuming a proportional relation.

The number and the diameter of the parcels atomized by each annular ligament are stored during VOF simulation, until the liquid phase is completely eroded by subsequent detachments. Simulation is continued until a steady state is reached. During computational time the various droplet spectra are sampled according to mass or number weighting of the atomized parcels (see Figure 1.4). From this procedure mean detachment rates and detachment angles are finally achieved.

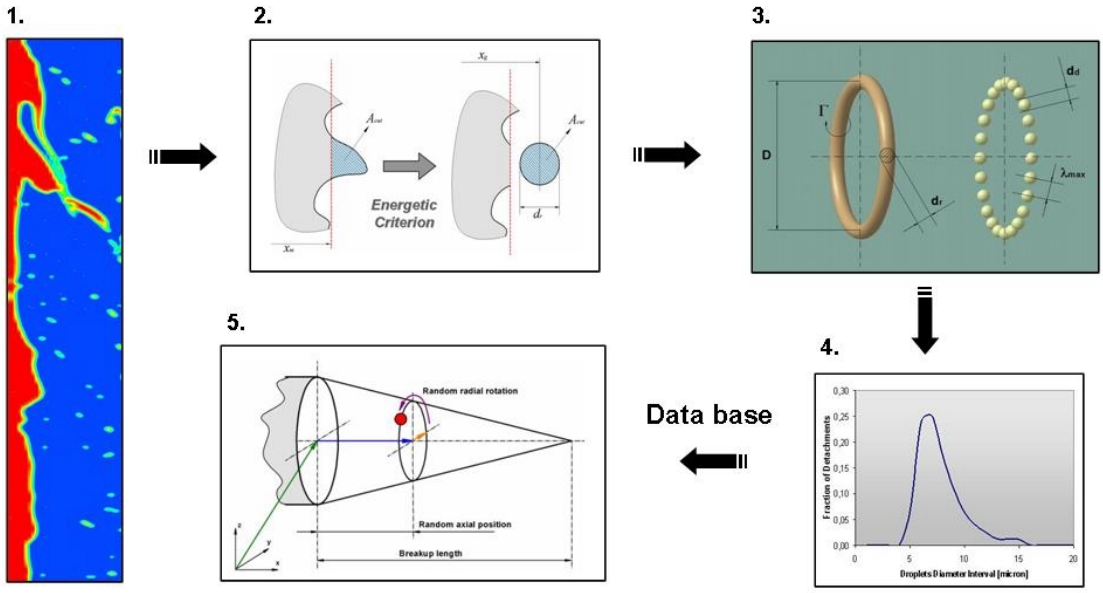

Figure 1: Work flow of the primary breakup VOF-based model linked to the classical DDM rate approach

Implementation into a 3D CFD code

The new primary break-up model has been implemented into the FIRE 8 CFD code. The basic ideas applied in the coupling procedure are to use a precalculated database and to release the parcels containing the product droplets of the primary break-up process along the surface of a coherent liquid core structure.

The parameters entering the model are injection velocity and back pressure as well as orifice diameter and disturbance level. The database contains size distributions for all the relevant injection conditions. These conditions cover a velocity range from 100 to 500 m/s, back pressures up to 50 bars and a range for orifice diameters typical for diesel injectors nowadays, as well as the disturbance level related to nozzle flow turbulence. From the database the actual conditions during injection are extracted by means of a quadrilinear interpolation technique for each time step of the injection period covering the four-dimensional parameter space. After detection of the appropriate distribution a stochastic droplet diameter is extracted. The detachment angle can also be taken from the database, but, since there is some uncertainty introduced via the heuristic detachment criterion, it is also possible to prescribe a fixed one. Anyway the modification of detachment angles led mainly to a slight change of spray shape, without a sensible alteration on final penetration. This indicates that air entrainment is more decisive for the final spray cone angle as the initial detachment angle calculated from the primary break-up model. Droplet spectra and angle values are finally used in the spray calculation to set the initial parcel properties during the injection period. Since many parcels, e.g., 40 per time step are released, the underlying overall distributions are represented sufficiently. Further the applied method uses a quasi-steady approach with respect to temporal evolution assuming that the break-up process adjusts itself very rapidly to changing detachment conditions.

Instead of using the standard method of injecting large blobs of liquid in the nozzle orifice cross section, the parcels introduced per time step are distributed along a liquid core structure. The length of the jet core is chosen according to a mass balance applied to the injected flow with average detachment rates calculated from the VOF simulations. The coherent liquid jet is approximated by a conical shape from which the parcels are released at randomly chosen positions on the core surface. This also reflects the stochastic nature of the detachment process and together with the large number of parcels over some time steps yields a sufficient representation of the initial droplet sizes and detachment angles distributions. Fig. 1 shows the workflow of the overall procedure.

Results

Results for different test cases and for varied injection conditions are shown and compared with experimental data on spray shape as well as liquid and vapour penetrations. The first simulations were performed to test the model in cold injection environment /12/. The nozzle used was of single-hole type, with a hole diameter of 200 µm operated at rail pressures between 30 and 120 MPa. Gas density was kept at 20 kg/m^3, which is representative of the density in an HSDI diesel engine at the time of injection, and the temperature to 293 K. In Figure 2a a comparison between experimental and calculated spray shapes is shown at 2 ms after SOI yielding overall good agreement between experiments and

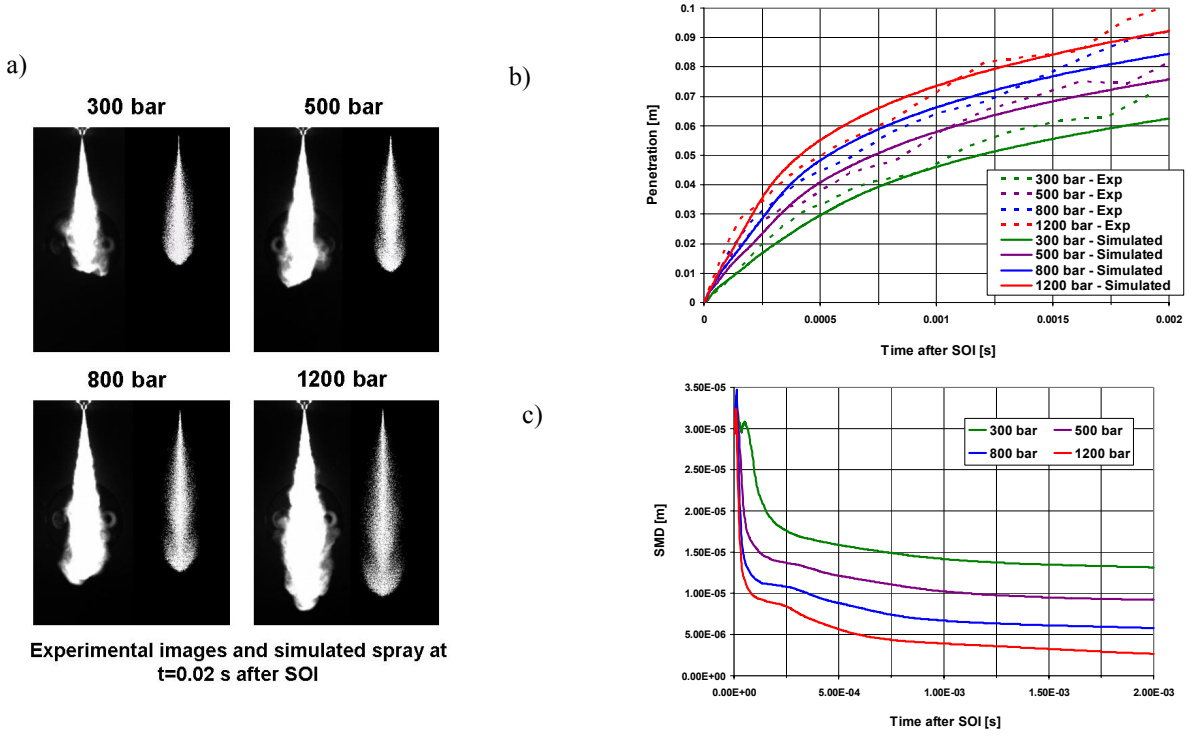

Figure 2: Comparison of measured and computed spray penetrations and SMD values for cold chamber conditions /12/ : a) spray shape, b) spray penetration, c) SMD evolution

simulations. This is confirmed by a detailed comparison between penetration curves of the leading edge of the spray: the graphs in Fig. 2b show a correct trend with pressure as well as also good quantitative agreement. The corresponding SMD results in Fig. 2c predict decreasing droplet size with increasing pressure, which is also the correct trend; however, the results at higher injection pressures seem to be somewhat underestimated. All these results were achieved with the WAVE secondary breakup model activated additionally, setting the standard parameters B_0 and B_1 as $B_0 = 0.61$ and $B_1 = 60$. The comparatively high value chosen for B_1 takes into account the already reduced initial size of droplets due to primary break-up.

Another test case was considered according to the experimental data presented by *Bensler et al.* /13/. The chamber pressure was set to 4 MPa with a constant temperature of 573 K. A valve-covered-orifice (VCO) 5-hole Diesel injector of 165 µm hole diameter was adopted and rail pressure was set to 800 bar. The presence of spray images allowed a direct comparison between simulated and experimental shapes, as shown on Figure 3a. The lack of experimental penetration and SMD diagrams prevented other comparisons, although the overall spray shape appears very similar to the experimental findings. A closer look shows differences in the spray angle in the region close to the orifice. This corresponds to the fact that detachment angles from the VOF method are somewhat too low. This also may be related to the detachment criterion applied and the related distribution of energy from instability growth to surface formation and initial kinetic energy of the droplets. With this respect further modeling work is required. Nevertheless penetration of the spray tip is predicted well (see Fig. 3a). Spray evaporation appears to be minimally affected by this low injection angle near the injector, as the scarceness of vapor close to the nozzle is evident (see Fig. 3b). Anyway vapor development and shape appears reasonable.

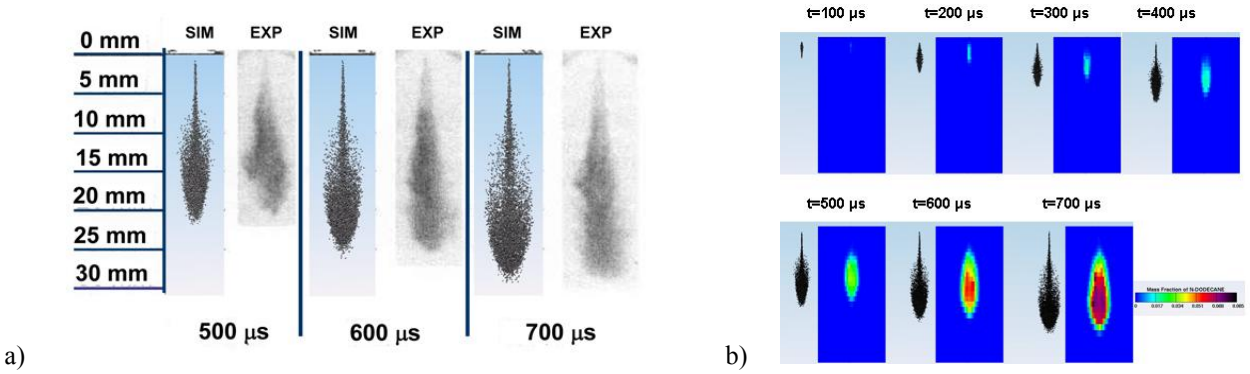

Figure 3: Comparison of measured and computed spray shape (left) and spray and vapour development after injection (right) for hot chamber conditions (experimental data taken from /13/).

Another set of validation calculations was performed using data sets supplied by CMT covering a large range of injection pressure (30-110 MPa) and backpressure conditions (6-8 MPa). Experiments were performed in a hot spray test rig, which provides a thermodynamic environment at TDC realistic for current D.I. Diesel engines. The rig is made up of a loop-scavenged two-stroke single cylinder engine, an electric motor as a motoring system and a set of thermal conditioners that control the temperature of the working fluid, coolant and engine lubricant. The injection chamber is machined in a customized cylinder head provided with wide optical accesses, so that the engine acts as a mere compression machine. The injection event is carried out by a second-generation Bosch common-rail system, with mini-sac single-hole axial nozzles, with hole diameter of 0.15 mm.

The Planar Laser Induced Exciplex Fluorescence (PLIEF) technique has been used to visualize and measure the spray geometrical characteristics and the fuel/air concentration fields in both liquid and vapor phases of D.I. Diesel sprays, using as fuel a blend of 90% hexadecane, 9% α-methyl-naphthalene and 1% TMPD to separate spectrally the fluorescence signal from the liquid and vapor phases of the spray. This mixture provides vapor phase fluorescence dominated by the excited monomer, TMPD*, while the exciplex emission, [TMPD+1-Me-Np]*, dominates the liquid phase fluorescence. To avoid oxygen TMPD quenching, the engine runs in a closed-loop circuit with pure nitrogen as intake gas.

The illuminating source used is a Nd:YAG pulsed laser working at 355 nm. A slow scan 16-bit ICCD camera with a resolution of 512x512 pixel is used for image acquisition, with an image stereoscope to take the two phases images simultaneously with just one ICCD camera. Further details on the experiments, as well as an analysis of results for the vapor phase can be found in /14/.

The results depicted in Fig. 4 show very good agreement for both liquid and vapor penetration, especially for the most relevant cases of high injection pressure and high back pressure. For low injection pressure and low back pressure a slight underprediction of vapor penetration can be detected. This may be attributed to limited applicability of the model for low injection velocities and uncertainties concerning determination of injection velocity from injected mass, which might cause too low initial velocities in the very first phase of injection. In contrast to the standard blob injection method, where spray angles have to be prescribed, the new method allows calculation of the initial spray angle. The

results gained from the model were in the range of 8 to 10 degrees for the initial liquid phase full spray cone angle. This is somewhat smaller than the experimental values of approximately 10 to 15 degrees. Thus further model improvement is necessary in this respect.

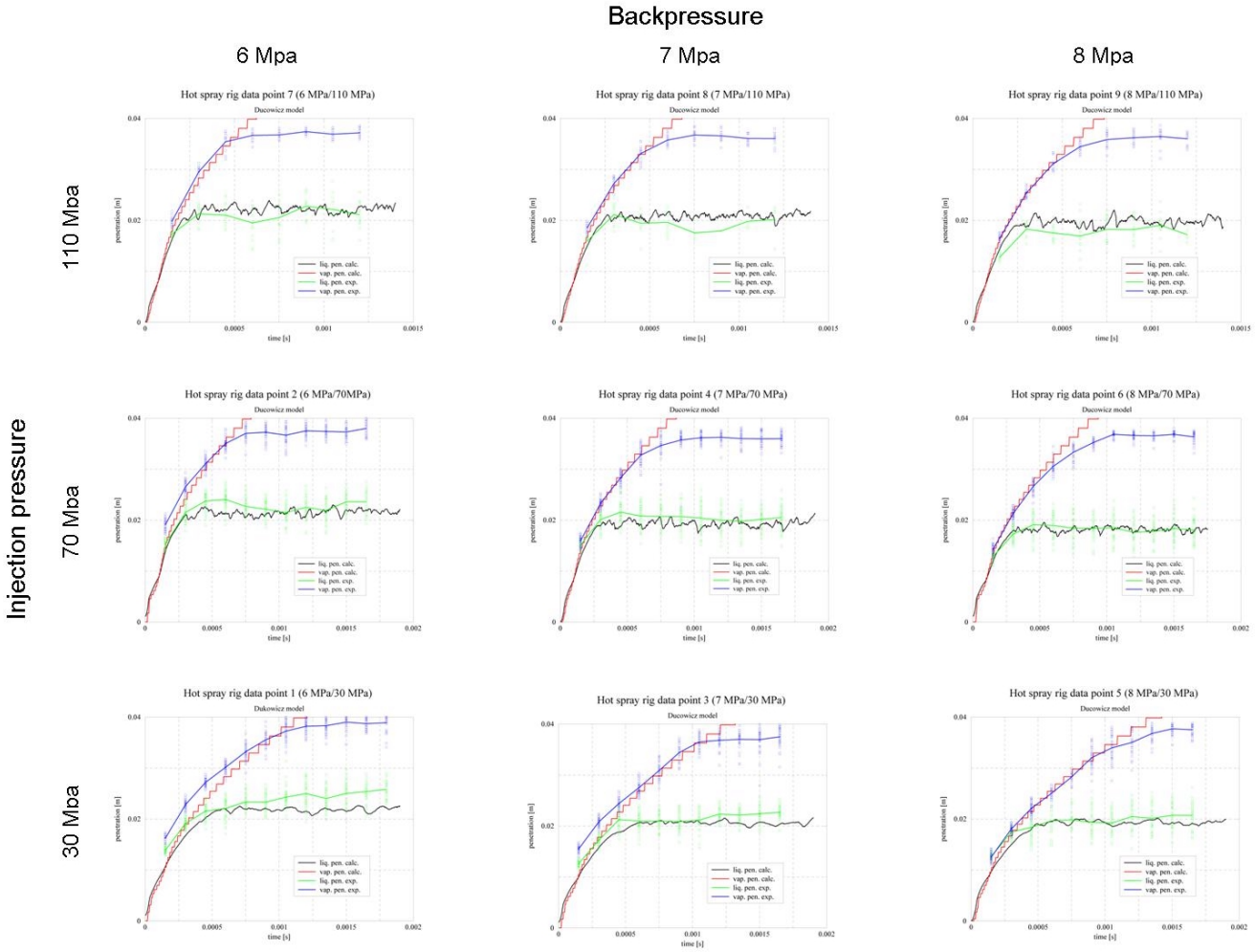

Figure 4: Comparison of measured and computed spray and vapour penetrations for CMT experimental data. Note: Observation window at height of 40 mm cuts off experimental vapor penetration curves.

Summary and conclusions

The approach presented links the accurate and properly physically based VOF method for evolution of surface instabilities together with an energetic criterion for ligament detachment as well as with the easy and fast formulation of a linear stability analysis for ligament decay into primary droplets. This allows achieving a better spray initialization within reasonable computational times. The main steps of the method are:

1. Perform the VOF method on a planar 2D geometry, until surface disturbances have been evolved sufficiently.
2. Detach annular ligaments from the jet surface crests by using energy balances and determine mass and diameter of the ligaments.
3. Calculate ligament decay from a linear stability analysis performed on annular surface.
4. Sample droplets size and detachment angle distributions along overall cone length, which is determined from a mass balance, and store results in database.
5. Apply interpolation technique within 3D-code to get actual droplet size distribution and initialize parcels according to data base values and injection rate.

The new method combines the VOF simulations with the fast and approved rate approaches adopted in the DDM for subsequent secondary break-up processes. This finally results in a methodology, which is applicable in large-scale IC engine CFD calculations with promising potential for an improved prediction of spray penetration and mixture formation. The results gained up to now with this new method showed in general a good agreement with the experimental penetration curves and also with the observed spray shapes. The predicted droplet sizes and also the detachment angles partly seemed to be too small. This indicates the need for further model refinement focussing on the

formulation of detachment criteria with respect to distribution of energy from surface instability growth into surface energy and initial kinetic energy of detached ligaments. In future work the VOF database will be extended quantitatively and also qualitatively by using a 3D method. Additionally the link to nozzle flow will be refined by using locally resolved boundary conditions as well as initial disturbances related to nozzle flow.

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Nomenclature

We = Weber number
We* = ligament Weber number
ρ_l = liquid density
σ = surface tension
Γ = circulation
k = disturbance wave number
I_1 , I_0 = modified Bessel functions
D = droplets diameter
d_r = ring radius
λ = disturbance wave length
ω = maximum growth rate
B = proportionality constant

Literature

/1/ G. M. Bianchi, P. Pelloni, S. Toninel, D. Paganelli and D. Suzzi: A 2D Simulation Method for Computing Droplet Size Spectrum during the Atomization of High-Speed Liquid Jets, accepted for publication at ASME-ICE Fall Conf. 2004, Long Beach, CA, USA

/2/ C. Arcoumanis, M. Gavaises and B. French: Effect of Fuel Injection Processes on the Structure of Diesel Sprays.SAE-Paper 970799

/3/ R. Tatschl, C. v. Künsberg Sarre, A. Alajbegovic and E. Winklhofer: Diesel Spray Break-up Modelling Including Multidimensional Cavitation Nozzle Flow Effects. 16thILASS-Europe Conf., 11-13.9.2000, Darmstadt

/4/ G.M. Bianchi, P. Pelloni, F.E. Corcione, L. Alloca and F. Luppino: Modeling Atomization of High-Pressure Diesel Sprays .ASME Journal of Engineering for Gas Turbines and Power, April 2001, Vol. 123, pp 419-427

/5/ E. v. Berg, W. Edelbauer, R. Tatschl, A. Alajbegovic; M. Volmajer, B. Kegl; L. Ganippa: Validation of a CFD Model for Coupled Simulation of Nozzle Flow, Primary Fuel Jet Break-up and Spray Formation. 2003 Spring Technical Conf. of the ASME ICE Division (ICES03), May 11-14, 2003, Salzburg, Austria

/6/ Y. Yi and R. Reitz: Modelling of Primary Breakup of High-Speed Jets. Atomization and Sprays, vol. 14, No.1, 2004

/7/ G. Blokkeel, X. Silvani, F.X. Demoulin and R. Borghi: An Eulerian Model to Improve the Primary Braekup Modelling of Atomizing Jet. ILASS-Europe 2002, Zaragoza, 9-11 Sept.

/8/ E. de Villiers, A.D. Gosman and H.G. Weller: Large Eddy Simulation of Primary Diesel Spray Atomization. SAE paper 2004-01-0100. SAE World Congress, March 8-11 2004, Detroit, MI, USA

/9/ P. Murdoch et al.: A combined CFD and experimental Analysis of the spray produced by an air-assisted GDI injector. Proc. of 15th ILASS-Europe conference, Darmstadt, Germany, 11-13 September 2000

/10/ S. Zaleski: Computation of Multiphase Flow by Volume of Fluid and High-Order Front Tracking Methods. Modèlisation en Mècanique, Universitè Pierre et Marie Curie, Paris.
URL:http://www.lmm.jussieu.fr/~zaleski/drops2.html.

/11/ Ponstein, J., 1959. “Instability of Rotating Cylindrical Jets”. Appl. Scientific Research, **8** (6) , pp. 425-456.

/12/ G. König, DaimlerChrysler, Stuttgart, Germany: Private communication

/13/ H. Bensler, F. Bühren and A. Lozet: An Experimental and Numerical Study of Diesel Injection Spray Phenomena. Volkswagen AG, SAE_NA Technical Paper, 2001-01-10.

/14/ F. Payri, J.V.Pastor, J.M.Pastor and J.E.Julia: Analysis of Evaporating Diesel Sprays by Means of Laser Induced Exciplex Fluorescence. SAE-NA Paper 2003-01-68, 6th International Conference on Engines for Automobiles ICE2003, Capri, Italy