# **NOZZLE – TO – SPRAY MODELLING**

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## **ABSTRACT**

In order to take into account the internal nozzle flow and its influence on the primary break-up of issuing spray, the current research project aims at a two-stage strategy for the nozzle flow and the spray formation simulations. The nozzle flow calculation is performed at first on a fine mesh necessary for the resolution of cavitating flow in the nozzle orifice. The flow properties are sampled at the exit of the nozzle orifice. This data is then transferred via a coupling file into the subsequent spray formation simulation. The spray calculation is performed using the discrete droplet model, based on Eulerian – Lagrangian approach, with the mesh resolution suitable for practical in-cylinder flow analyses. The data sampled from the nozzle flow simulation is used as the input values for newly developed primary break-up models in order to refine the spray break-up predictions and render the results less dependent on empirical constants. Adopting this two-stage strategy, it has been possible to provide the engineers with a feasible simulation tool ensuring moderate computational costs.

## **INTRODUCTION**

The automotive industry is facing the introduction of increasingly stringent emission regulations. The nozzle flow simulations as well as the spray formation simulations are commonly used to optimise the injector and the combustion chamber designs and thus, to refine the spray and combustion processes and lower raw engine emissions. The influence of the injector internal design on the spray initial formation has been investigated and confirmed both experimentally and numerically. Although there have been several attempts at simultaneous simulations of the nozzle flow and the spray formations, these are usually not feasible for practical engineering applications. The main obstacle to doing this is the difference in the length scale of the injector internal flow and that of the spray formation in engine cylinder or engine intake port. The computational efforts of such simulations are thus significant.

To provide the engineers with a feasible simulation tool, the current research project aims at a two-stage strategy for the nozzle flow and the spray formation simulations, see Fig. 1. The nozzle flow calculation is performed on a fine mesh necessary for the resolution of cavitating flows in the nozzle orifice. The flow properties are sampled at the exit of the nozzle orifice. This data is then transferred via a coupling file into the subsequent spray formation simulation. The spray calculation is performed using the common discrete droplet model (DDM), based on Eulerian – Lagrangian approach, with mesh resolution appropriate to practical in-cylinder flow analyses. The data sampled from the nozzle flow simulations is used as input values for newly developed primary break-up models to refine the spray break-up predictions and render the results less dependent on empirical constants.



**Figure 1:** A two-stage strategy for the nozzle-to-spray simulations

### **NOZZLE FLOW SIMULATIONS**

The incompressible cavitating flow is computed in the nozzle orifice and its nearest up-stream region. The results of the nozzle flow simulation are then sampled in proximity of the nozzle orifice exit and transferred to the subsequent spray formation simulation.

#### **Cavitation Model**

The implemented cavitation model basically follows that published in Ref. [6]. Writing the the transport equation for the void fraction,  $\alpha$ , in the following form,

$$
\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \, \vec{w}) = S_{\alpha}.\tag{1}
$$

the void-fraction source term can be formulated as,

$$
S_{\alpha} = \begin{cases} C_{prod} \frac{\sqrt{k}}{\sigma} \rho_L \left( \frac{2}{3} \frac{\Delta p}{\rho_L} \right)^{\frac{1}{2}} \left( 1 - \frac{\rho_V}{\rho} \alpha \right); \ \Delta p \ge 0, \\ C_{dest} \frac{\sqrt{k}}{\sigma} \rho_L \left( \frac{2}{3} \frac{|\Delta p|}{\rho_L} \right)^{\frac{1}{2}} \frac{\rho_L}{\rho} \alpha \end{cases}; \ \Delta p < 0. \tag{2}
$$

The indices L and V refer to liquid and vapour, respectively.  $\rho$  is the mixture density.  $C_{prod}$  and  $C_{dest}$  are the model coefficients for bubble production and destruction rates, respectively. They serve to allow for the differences in bubble growth and collapse behaviour and presumably other effects neglected in the present model.

According to Ref. [3], the turbulent vortices can have an important influence on the inception of cavitation. The difference of the pressure in cavitation bubbles and that in the surrounding liquid,  $\Delta p$ , is thus computed as,

$$
\Delta p = p_{vap} + \frac{0.39 \,\rho k}{2} - p_{\infty},\tag{3}
$$

where  $p_{vap}$  is the saturated vapour pressure,  $p_{\infty}$  is the pressure in surrounding liquid, and  $k$  is the turbulence kinetic energy. The second term on RHS stands for the pressure increase due to the turbulence pressure fluctuations, see Ref. [6],

#### **Nozzle Flow Sampling**

The nozzle flow sampling serves to extract the values necessary for the subsequent spray simulation from the converged nozzle flow solution. A sampling surface of arbitrary geometry can be used to cut the nozzle orifice in the proximity of its exit, see Fig. 2. The sampling surface is further divided into a number of sectors.



Figure 2: Sampling of the nozzle flow properties using a sampling surface

The flow properties are sampled and the mean values evaluated along each of these sectors, which enables us to resolve spatially the jet break-up process with possible asymmetries in initial spray formation. The sampled data is stored in so-called coupling file and used as input values for the primary break-up model used in the subsequent spray formation simulation.

### **BREAK-UP MODELS**

Three versions of the primary break-up model have been developed to predict the primary break-up of sprays typical of portand direct-injection gasoline engines as well as those in diesel engines. Both the round jet and the sheet break-up can be predicted for the gasoline sprays.

### **Jet Break-Up Resolution**

The initially continuous liquid jet exiting the nozzle orifice is discretised into a number of slices, see Fig. 3. Correspondingly to the sampling surface geometry, each slice is further divided into a number of sectors in order to allow for the spatial distribution of the flow properties over the nozzle orifice area and its influence on the spray break-up. The sector initial conditions are defined by the nozzle flow properties sampled at the orifice exit. The behaviour of each of these sectors is analysed separately as they move downstream of the injector and thus, the sectors may differ in their properties and, finally, in the time of break-up and its consequences. Once break-up is predicted, the sector is transformed into a parcel of secondary droplets. These droplets may undergo further break-up, calculated using common secondary break-up models.



**Figure 3:** A simplified view of the primary break-up of a low-speed round jet

To incorporate the above described jet structure (slices and sectors) into the Lagrangian discrete spray model, each of the sectors is approximated by a primary blob, i.e. a parcel of droplets with diameter equal to that of the nozzle orifice.

The parameters sampled for each sector include orifice geometry, mass flow rate, velocity, vapour mass fraction, fuel temperature, and turbulence properties. The initial turbulence length and time scales are evaluated as,

$$
L_t(0) = C_\mu \frac{k^{3/2}}{\varepsilon}; \quad \tau_t(0) = C_\mu \frac{k}{\varepsilon}, \tag{4}
$$

where the parameter  $C_{\mu} = 0.09$ , k is the turbulence kinetic energy, and  $\varepsilon$  is its dissipation rate.

#### **Break-Up Model for Gasoline Sprays**

The break-up model for sprays typical of gasoline port- and direct-injection engines is able to predict both the break-up of solid-cone and hollow-cone sprays. The initial disturbances on the surface of an appearing jet are assumed to be further amplified by the aerodynamic interactions with surrounding gas, which may finally lead to to the detachment of wave crests in the form of droplets. The evolution of the jet surface disturbances is predicted by the linear instability analysis, assuming the existence of an initial axisymmetric disturbance on the jet surface,  $\eta_0$ , which further evolves in time as,  $\eta = \eta_0 \exp{(\omega t)}$ . The dispersion equation, which relates the wave growth rate,  $\omega$ , to the wave number was derived for round jets in Ref. [4]. The dispersion relation appropriate for liquid sheets can be found in Ref. [5]. These relations can be solved numerically yielding the range of wavelengths of growing waves and their growth rates.

Relating the inertia and surface-tension forces on the wave crest, the droplet detachment criterion is based on the Weber number, which is defined using the surface disturbance wavelength and its radial velocity. From the detachment criterion,

the wave amplitude necessary for the break-up,  $\eta_{bu}$ , can be derived. For the break-up time then follows,

$$
\tau_{bu} = \frac{1}{\omega} \ln \left( \frac{\eta_{bu}}{\eta_0} \right).
$$
 (5)

The amplitude of the initial disturbance on the jet surface,  $\eta_0$ , is assumed to be proportional to the turbulence length scale, sampled from the nozzle flow properties,  $L_t(0)$ , see Eq. (4).

For the gasoline sprays, it can be assumed that the parent blob disintegrates totally once the break-up time elapses and its whole volume is transformed into a parcel of secondary droplets. The size of the detached droplets is chosen randomly from a distribution function, with the Sauter mean diameter set to the wavelength of the fastest growing wave.

Due to the conical liquid sheet tightening as the sheet diverges from the cone axis, the sheet thickness at break-up time is dependent on the break-up time. This also affects the growth rates of the surface disturbances. Nonetheless, a simplified droplet detachment criterion is used according to Ref. [5], which simply equals the complex of  $\ln(\eta_{bu}/\eta_0)$  to 12, see Eq. (5).

Correspondingly to Ref. [5], it is assumed that a toroidal ligament is formed when the conical sheet breaks up, which further disintegrates into droplets. The ligament diameter,  $d_l$  is calculated from the mass balance assuming that the ligaments are formed from the tears in the sheet once per wavelength,

$$
h_{bu}\lambda_{bu} = \frac{\pi}{4}d_l^2,
$$
\t(6)

where the sheet thickness at the break-up time,  $h_{bu}$ , is calculated from the initial sheet thickness using the continuity equation. The Weber's dispersion equation for capillary pinching of a viscous cylinder is then used to predict the wavelength of the wave decisive for the ligament break-up,

$$
\lambda_l = 2\pi d_l \sqrt{\frac{1}{2} + \frac{3\mu_L}{2\sqrt{\rho_L \sigma d_l}}}.\tag{7}
$$

Finally, the Sauter mean diameter of the secondary droplets is evaluated from the assumption that one droplet is created from a ligament segment of the length equal to that of the wave decisive for the break-up,

$$
\frac{\pi}{4}d_l^2\lambda_l = \frac{\pi}{6}d_{32}^3,
$$
\n(8)

while the actual diameter of droplets in the created parcel is chosen randomly from a distribution function.

#### **Break-up Model for Diesel Sprays**

The proposed model is basically an extension of previous attempts at allowing for the influence of nozzle flow turbulence on the jet break-up, see e.g. Ref. [1].

Following the cited models, it is postulated that the turbulence fluctuations are responsible for the initial perturbations on the surface of liquid jet. These perturbations are further amplified by aerodynamic effects until they are detached and form droplets.

Hence, the turbulence length scale is assumed to be the dominant length scale of the jet atomisation. The atomisation length scale,  $L_A$ , and the wavelength of the jet surface perturbations,  $L_w$ , are thus expressed as functions of the turbulence length scale,  $L_t$ ,

$$
L_A = C_2 L_t; \quad L_w = C_3 L_t. \tag{9}
$$

The relation between the constants  $C_2$  and  $C_3$  is provided by further consideration that half a surface wave is detached as a secondary droplet,  $L_A = 0.5L_w$ .

The time evolution of the turbulence properties as the blobs move downstream of the nozzle is predicted from the initial values sampled from the nozzle flow simulation, see Eq. (4), according to the correlation published in Ref. [2],

$$
L_t(t) = L_t(0) \left[ 1 + \frac{0.0828t}{\tau_t(0)} \right]^{0.457}, \quad (10)
$$

$$
\tau_t(t) = \tau_t(0) + 0.0828t.
$$
 (11)

The atomisation time scale is supposed to be a linear function of the time scale of spontaneous growth of the initial jet perturbations and the time scale of exponential growth of the perturbations due to aerodynamic effects,

$$
\tau_A = \tau_{spn} + \tau_{exp} = C_1 \tau_t + C_4 \tau_w, \qquad (12)
$$

where  $\tau_t$  is the turbulence time scale and  $\tau_w$  is derived from the Kelvin–Helmholtz instability theory of an infinite planar surface, neglecting the surface tension and viscosity effects,

$$
\tau_w = \frac{L_w}{w} \sqrt{\frac{\rho_L}{\rho_G}}.\tag{13}
$$



**Figure 4:** A simplified view of the primary break-up of a high-speed round jet

Contrary to the above-described models, for high-speed sprays the primary blobs are permitted to gradually decrease in their diameters due to the droplet shedding from their surfaces as they move downstream of the injector, see Fig. 4. The radius of a parent blob is assumed to decrease continuously with time due to the droplet shedding according to the following relation,

$$
\frac{dd_B}{dt} = C_A \frac{L_A}{\tau_A}.\tag{14}
$$

The droplets are detached from the parent blob after a time at which a sufficient mass to create a new droplet parcel has been shed. This mass is set to 5 per cent of the initial parent blob mass. The Sauter mean diameter of the detached droplets is assumed to be equal to the atomisation length scale, with the actual droplet diameter in the created parcel chosen randomly from a distribution function. The initial velocity of the detached droplets is evaluated as a superposition of the parent blob velocity and the normal component computed as,  $L_A/\tau_A$ .

The model constants that appeared in the previously introduced relations are set upon the recommendations given in the cited literature,  $C_A = 2, C_1 = 1, C_2 = 2,$  and  $C_4 = 4$ .

#### **RESULTS**

To demonstrate the capabilities of the proposed two-stage strategy, a simplified case of diesel injection using a six-hole microsac nozzle has been computed. In Fig. 5, the computational domain for the nozzle flow simulation is shown. It comprises one nozzle orifice and corresponding section of the needle seat and sac volume. The geometry corresponds to the fully opened needle. The orifice diameter and length are 0.15mm and 0.6mm, respectively. The pressure difference across the nozzle is  $80MPa$ . The sampling orifice, which consists of 8 sectors, is also shown in the detail.



**Figure 5:** Nozzle flow computational domain



The computed steady-state nozzle flow in terms of the velocity magnitude and void fraction distributions is shown in Fig. 6.

**Figure 6:** Velocity magnitude (on the left) and void fraction (on the right) distributions in the nozzle orifice axial cross-section

The spray formation has been computed assuming the constant properties during the injection interval, sampled from the steady-state nozzle flow simulation. The spray is injected into still gas in a section of cylindrical chamber. The initial gas pressure and temperature are 5MPa and 800K, respectively. The droplet secondary break-up is computed using the TAB model. The spray formation at  $0.4ms$  after the start of injection is shown in Fig. 7.



**Figure 7:** Spray formation at 0.4ms ASOI; droplets coloured according to diameters, fuel/air equivalence ratio distribution.

#### **CONCLUSIONS**

A two-stage strategy for the nozzle flow and the spray formation simulations has been developed. The nozzle flow simulation is performed at first and the flow properties at the exit of the nozzle orifice are sampled, evaluated and stored in a coupling file. In the subsequent spray formation simulation, the newly developed primary break-up models use the properties sampled from nozzle flow simulation to allow for the injector design and its influence on the spray break-up. The break-up models are capable of predictions of the primary break-up of sprays typical of port- and direct-injection gasoline engines as well as of diesel engines. Depending on injection conditions, the models account for all the process that are commonly identified as decisive for the jet break-up—nozzle flow turbulence, cavitation, and aerodynamic interactions with surrounding gas. The strategy developed has been applied to the simple case of diesel direct injection. Further verifications of the models is being done.

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