Correlating Results from Numerical Simulation to SLIPI-based Measurements for a non-combusting Diesel Spray

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Abstract
The validation of numerical methods for the study of highly atomizing transient sprays (e.g. Diesel sprays) is a nontrivial task. One important issue concerns the fact that such sprays are optically dense making the measurement particularly difficult, especially when high accuracy is required (which is the case for model validation purposes). It has recently been demonstrated that SLIPI-based techniques are able to provide either two or three-dimensional quantitative results of the extinction coefficient even in challenging situations. More specifically, the extinction coefficient of a non-combusting Diesel sprays injected at 1100 bar in a chamber pressurized at 18.6 bar could be extracted in two-dimensions at late time (2000 \textmu s) after injection start. In this article, these experimental results are correlated with numerical data. The numerical calculations are based on Large-Eddy Simulation (LES) combined with Lagrangian Particle Tracking (LPT). The simulation includes secondary droplet break-up models, gas-liquid two-way coupling and an evaporation model. The main purpose of the work presented here is, then, to numerically deduce the extinction coefficient field which can be directly compared to the one obtained experimentally. The extinction coefficient is related to the droplet number density times the extinction cross-section which is calculated, for each droplet size, based on the Lorenz-Mie theory. We show in this article, that by extracting the extinction coefficient from numerical simulation, comparisons between simulated and SLIPI-based experimental results are becoming possible even in optically dense sprays. Thus, the presented approach is a step towards providing strong evidence of similar or different structures between the experimental and simulated description of atomizing spray systems.

NOMENCLATURE

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<tr>
<td>$d$ droplet diameter (m)</td>
<td>Re Reynolds number</td>
<td>$\alpha$ liquid phase volume fraction (–)</td>
<td>FDM Finite Difference Method</td>
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<tr>
<td>$f$ statistical number of droplets per unit volume (1/m\textsuperscript{3})</td>
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<td>$\mu$ dynamic viscosity (kg/(m·s))</td>
<td>LES Large Eddy Simulation</td>
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<td>$F$ force (N)</td>
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<td>$\mu_e$ extinction coefficient (1/m)</td>
<td>LPT Lagrangian Particle Tracking</td>
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<td>$m$ mass (kg)</td>
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<td>$\rho$ density (kg/m\textsuperscript{3})</td>
<td>SGS Sub Grid Scale</td>
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<td>$N$ number density (1/m\textsuperscript{3})</td>
<td></td>
<td>$\sigma$ surface tension (N/m)</td>
<td>SLIPI Structured Laser Illumination Planar Imaging</td>
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<td>$p$ pressure (N/m\textsuperscript{2})</td>
<td></td>
<td>$\sigma_e$ extinction cross-section (m\textsuperscript{2})</td>
<td>SMD Sauter Mean Diameter</td>
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<td>$Q$ heat flux (J/(m\textsuperscript{2}·s))</td>
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<td>WENO Weighted Essentially Non Oscillatory</td>
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<td>$R$ specific gas constant (J/(kg·K))</td>
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<tr>
<td>$T$ temperature (K)</td>
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<tr>
<td>$t$ time (s)</td>
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<tr>
<td>$u$ velocity (m/s)</td>
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<td>$V$ Volume (m\textsuperscript{3})</td>
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<tr>
<td>$Z$ mixture fraction (–)</td>
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<tr>
<td>$x, y, z$ spatial coordinates</td>
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Introduction
Numerous experimental and numerical techniques have been developed to study the structure of liquid sprays. The benefit of performing numerical simulations is the possibility of obtaining detailed quantitative information regarding the droplet size distribution, number density and velocity, which are not always accessible experimentally. In addition, a validated model would provide the underlying physics dominating the spray development and be a useful tool to accurately predict spray formation and structure at various initial conditions. Such predictions, could considerably help for the further development and optimization of liquid fuel driven combustion devices. It is then of importance to extract accurate experimental data, as well as to develop adequate procedures for the validation of modern numerical models. In this work the atomization for a non combusting Diesel spray is simulated by performing a Large-Eddy Simulation (LES) combined with Lagrangian Particle Tracking (LPT) method. It takes into account the secondary breakups, transport and evaporation phenomena occurring in the spray region.

The quantities of importance for the validation of the model presented here are the final droplet size distribution, droplet number density and velocity in two or, if possible, three dimensions. A number of experiments have been conducted in the past to analyse the global structure of atomizing sprays, e.g. [1, 2, 3, 4]. Often the geometrical characteristics such as the spray penetration distance or the spray opening angle are the only parameters compared between experimental and simulated results [5]. There have also been some attempts [6] where secondary droplet breakup models have been correlated with experiments for a single droplet suspended in air. In parallel to this work, the numerical simulation of the breakup of a liquid jet has been validated for the case of the Rayleigh regime [7] which is not optically dense and therefore easy to analyse experimentally. However, in atomizing sprays the optical density is usually quite high and the detected optical signal is strongly affected by multiple light scattering [8] blurring the recorded images and making quantitative measurements non-reliable or impossible to perform without any filtering/suppression strategy. As a result to this lack of visibility and direct observation, the physical mechanisms acting during the jet atomization are still not well known and fully understood.

In this paper a novel approach is presented where experimental results from a non-combusting Diesel spray are compared with results from numerical simulation, based on the extinction coefficient. The extinction coefficient is a quantity containing information related to both the droplet size and number density. It can be experimentally extracted after the suppression of effects induced by multiple light scattering and light extinction. This has been recently performed in two-dimension using a recent technique called Dual-SLIPI [9] (note that it can also be done in three-dimension using SLIPI-Scan [10] or Tomo-SLITI [11]). From the simulation point of view the extinction coefficient can be easily calculated from the resultant droplet size and number density given by the LPT method. The main advantage of this approach is that not only global and qualitative parameters of the spray, but a complete field of a variable, i.e. the extinction coefficient, can be accurately compared. This gives the possibility to judge the numerical modelling of the complete spray structure. Starting from this validation approach, the numerical model can, then, be used to extract further detailed information about the spray, such as the droplet diameter distributions, liquid volume fractions, droplet number densities etc.

Governing Equations and Numerical Methods
In this work, a LES of the spray is performed. The continuous gas phase is described in Eulerian and the dispersed liquid phase in Lagrangian framework. This approach assumes the droplets to be small with relatively large inter-droplet distance and not interacting with each other, i.e. no collision or history/wake effects. The droplets are assumed to be spherical so they can be tracked individually and the subsequent breakup and evaporation processes can be modelled. As the LPT is a point-particle approach it assumes that the volume occupied by the liquid in each computational cell is small compared to the volume occupied by the gas [12]. All the above assumptions might be violated in a region very close to the injection nozzle. In the current simulations the liquid occupies in average less than 5% of the volume of a cell in a region beginning 15 nozzle diameters downstream. However, as this paper focuses on the spray development at many nozzle diameters downstream, the used methods are appropriate to describe the dilute spray. While the drawback of the LPT method is that the above assumptions need to be taken, the description of the liquid phase in Lagrangian framework is computationally much more efficient than for example interface tracking methods such as Volumes of Fluid.

Continuous Phase
The continuous gaseous phase is described in the Eulerian framework by the continuity, momentum, energy and mixture fraction transport equation for Newtonian fluids with constant diffusivities, given in Eqs. 1 - 4. Low Mach number flow is assumed, which means that the density is a function of the temperature only. Thereby, acoustic effects are neglected. Due to the assumption of dilute spray, the continuous phase volume fraction $\theta$ is assumed to be unity.
\[
\begin{align*}
\frac{\partial p}{\partial t} + \frac{\partial pu_j}{\partial x_j} &= \dot{m}_S \\
\frac{\partial pu_i}{\partial t} + \frac{\partial pu_iu_j}{\partial x_j} &= -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \mu \frac{\partial u_i}{\partial x_j} + \dot{F}_{s,i} \\
\frac{\partial pT}{\partial t} + \frac{\partial pu_jT}{\partial x_j} &= \frac{\partial}{\partial x_j} \rho \alpha_v \frac{\partial T}{\partial x_j} + \dot{Q}_s \\
\frac{\partial pZ}{\partial t} + \frac{\partial pu_iZ}{\partial x_j} &= \frac{\partial}{\partial x_j} \rho \tilde{D}_i \frac{\partial Z}{\partial x_j} + \dot{\tilde{Z}}_s
\end{align*}
\]

\(\dot{m}_S, \dot{F}_{s,i}, \dot{Q}_s \) and \(\dot{\tilde{Z}}_s\) are source terms for mass, momentum, energy and mixture fraction, which account for the coupling from the liquid to the gaseous phase. The system of equations is closed by the equation of state for incompressible, non-isothermal flows, \(p_0 = \rho RT\), where \(p_0\) is the constant reference pressure.

The governing equations are discretized by the FDM. The convective terms are approximated by an up to fifth-order Weighted Essentially Non Oscillatory (WENO) scheme, which was developed by [13]. The pressure terms and the diffusive terms are approximated by a forth-order scheme and the time derivatives are approximated by an implicit second-order upwind scheme. For grid points close to the boundary of the domain, lower order approximations are used. The resulting system of equations is solved applying the Semi-Implicit Method for Pressure Linked Equations (SIMPLE) algorithm, according to [14] and [15].

When the momentum equation (Eq. 2) is solved several numerical errors are introduced, out of which the spatial truncation error is the largest. This error has a form of a numerical stress and is depending on the cell size. In this work no explicit turbulence model is used, but the truncation error is assumed to be of the same magnitude as the residual stresses. As both, the residual and the numerical stresses depend on the cell size (if the numerical grid is used as spatial filter), this assumption is true for small cells. The filtering and residual stress modelling is done implicitly by the numerical schemes. This approach has been applied successfully in previous works, e.g. [16, 17, 18].

**Dispersed Phase**

The droplet distribution function is given by Eq. 5.

\[
f(x, \tilde{u}, d, T, y, \tilde{y}) \, dx \, d\tilde{u} \, dd \, dT \, dy \, d\tilde{y}
\]

This function gives the number of droplets that are currently at a position between \(x\) and \(x + dx\), of a speed between \(\tilde{u}\) and \(\tilde{u} + d\tilde{u}\), of a diameter between \(d\) and \(d + dd\), of a temperature between \(T\) and \(T + dT\) and of distortion parameters between \(y\) and \(y + dy\) and the distortion rates \(\tilde{y}\) and \(\tilde{y} + d\tilde{y}\). The liquid phase is described by the stochastic parcel method, which is a discrete representation of the continuous droplet distribution function. The total number of droplets is gathered in parcels which each represent the corresponding number of droplets, \(f\). Each parcel is considered as a particle and tracked individually in the Lagrangian particle tracking framework.

Only aerodynamic forces are taken into account for the momentum exchange between gaseous and liquid phases. The acceleration of a spherical, isolated, rigid droplet is according to Newton’s second law of motion,

\[
\frac{du_d}{dt} = -\frac{3\rho_g C_d |u_{rel}| u_{rel}}{4\rho_d d_d^2}
\]

where \(C_d\) is the drag coefficient of the droplet. \(C_d\) is depending on the droplet Reynolds number and follows the standard drag curve for a smooth sphere which can be found in standard textbooks, [19]. There are other forces acting on the droplet such as the virtual mass force, the Faxen force, the Basset history term, gravitational forces, the Magnus force and the Saffman forces. These are neglected in the current work, as well as in most other similar spray simulations, which is justified in [20] for similar spray conditions.

To account for secondary droplet breakup, in this work the approach of [21] is followed: The two breakup regimes that are considered to be dominating are modelled, namely bag breakup and stripping breakup. The Wave Breakup model according to [22] is applied as long as the droplets contain more than 95% of the initially injected mass. The model describes both, the stripping breakup and the bag breakup regime. If the droplet has less than 95% of the injected mass the Taylor Analogy Breakup model according to [23] is applied. The model describes the bag breakup regime and uses the analogy between a distorted droplet and a spring-mass system.

The evaporation of liquid mass is taken into account by an evaporation model, which assumes that the droplet is composed of a single-component and has a spherical shape with uniform properties as described in [24].
Figure 1. Relation between the extinction cross-section and the droplet diameter. Here the incident wavelength equals $\lambda = 355$ nm. Three cases of refractive index have been selected: the first one is a non-absorbing fuel of refractive index $n = 1.40 - 0.0i$, the second one is an absorbing fuel of refractive index $n = 1.40 - 0.1i$ and the third one is a non-absorbing fuel of $n = 1.45 - 0.0i$. It is observed that over a range between 1 and 40 microns, differences between the three cases are not significant. In our case, the refractive index selected was assumed to be equal to $n = 1.40 - 0.0i$.

**Extinction Coefficient**

The extinction coefficient, $\mu_e$ can be directly derived from the results of the numerical simulation. For monodisperse particles illuminated at a single wavelength, $\mu_e$ is defined as

$$\mu_e = \frac{\sigma_e \cdot N}{V_c},$$

where $\sigma_e$ is extinction cross-section and $N$ is the droplet number density. The extinction cross-section corresponds to the effective area of interaction between the incident light and the droplets. It is equal to the sum of the absorption and scattering cross-sections. If the particles are non-absorbing at the excited wavelength, then, only scattering occurs and the extinction cross-section equals the scattering-cross section. The value of the extinction cross-section depends on the droplet diameter, the incident wavelength and the refractive index of both the droplets and of the surrounding medium. By assuming the droplets to be spherical, $\sigma_e$ is calculated from the Lorenz-Mie theory \[25\]. The relationship between the extinction cross-section and the droplet diameter is shown in Fig. 1 for three different refractive index of the droplets. By applying these data, the extinction coefficient can be deduced using the droplet distribution function as

$$\mu_e = \frac{1}{V_c} \int_{V_c} \sum_{d_i} n_p \sigma_e(d_i) \cdot f \, dV_c,$$

where $V_c$ is the size of the analysed volume and $n_p$ is the number of parcels contained in this volume. The volume $V_c$ is given as $V_c = \delta x \cdot \delta y \cdot \Delta z$, which has been chosen according to the volume measured in the experiments: $\delta x$ and $\delta y$ correspond to the resolution of the used CCD camera (here $30 \mu m$) and $\Delta z$ corresponds to the distance between the two laser sheets ($2 \text{ mm}$), see the next chapter for details.

**Characteristics of the Simulation**

The computational domain used for the simulation is a cube with an edge length of $0.1 \text{ m}$. Grid refinements are used, the finest grid which is located where the spray develops has a cell size of $1.5 \cdot 10^{-3} \text{ m}$ in all three directions. This leads to $2.2 \cdot 10^6$ grid cells. The diameter of the injection nozzle equals $d_{noz} = 105 \mu m$, corresponding to the one used in the experiment \[26\]. The liquid velocity at the injection was unknown in the experiment. However it could be estimated from the pressure difference between the rail and the vessel (which is approximately $1080 \text{ bar}$) by using the Bernoulli equation to $130 \text{ m/s}$. The diameter of the droplets at the injection, are assumed to follow a
Rosin-Rammler distribution and a Sauter Mean Diameter (SMD) of 10 μm. The injected liquid is n-decane. Due to uncertainties in the boundary conditions, a sensitivity study for different mass flow rates is performed, as shown later.

Description of the Experiment

Dual-SLIPI

Results of laser sheet imaging techniques suffer from multiple scattering issues, especially when applied to dense transient sprays. Since 2008, a laser sheet imaging based approach called SLIPI [27] has revealed efficient capabilities to "only" detect singly scattered photons (see [28] for details). The idea is to use a modulated laser sheet with a sinusoidal incident intensity pattern. While the single light scattering does keep the modulation from the incident pattern, the intensity from the multiple light scattering looses the modulated information. Thus, the intensity from single light scattering can be reconstructed from the amplitude of the modulated component of the detected scattered light. The complete SLIPI image is finally reconstructed using three single images, where the modulation is shifted vertically one third of the spatial period between each of these images.

In 2011, a technique called Dual-SLIPI was developed [9] to further correct issues related to laser extinction and signal attenuation. Thanks to this new technique, quantitative measurements of the extinction coefficient could be obtained in two-dimension within the spray region. In Dual-SLIPI the laser sheet is simultaneously imaged from both sides with two cameras, resulting to two first SLIPI images. Then the laser sheet is displaced by a distance Δz within the spray and two more SLIPI images are extracted. Thus, four SLIPI images, \( S_{P1,C1} \), \( S_{P1,C2} \), \( S_{P2,C1} \) and \( S_{P2,C2} \) are created. \( P_1 \) and \( P_2 \) correspond to the two positions of the laser sheets, \( C_1 \) and \( C_2 \) correspond to the two cameras. From this four images, the extinction coefficient can be directly determined as

\[
\mu_e = \ln\left( \frac{S_{P1,C1} \cdot S_{P2,C2}}{S_{P2,C1} \cdot S_{P1,C2}} \right) \cdot \frac{1}{2\Delta z},
\]

where \( \Delta z \) is the distance between the two laser sheets. By using Dual-SLIPI, the extinction coefficient can be rapidly measured in two-dimension at the center of the probed spray without the need of advanced reconstruction algorithms.

Characteristics of the Experiment

A detailed description of the experimental setup can be found in [26]. The injection nozzle diameter is \( d_{noz} = 105 \mu m \), the injected liquid is n-decane. The rail pressure is 1100 bar, the pressure in the vessel is 18.6 bar. The temperature in the vessel is ambient, ca. 20 °C. The liquid is injected during a period of 1.5 ms prior to the closing of the needle. The distance between the two laser sheets is 2 mm. The SLIPI images are taken with two intensified CCD cameras with 1280 · 1024 pixels, resulting to an image pixel resolution of 30 μm · 30 μm.

Results and Discussion

The extinction coefficient fields, experimentally measured from the Dual-SLIPI technique, are shown in Fig. 2 for, \( t = 2000, 2500 \) and \( 3000 \mu s \). Time \( t = 0 \) corresponds to the beginning of injection of the liquid spray. The shown planes are cuts through the spray including the injection nozzle, which is located at the bottom of the figures. The extinction coefficient field obtained numerically is shown for \( t = 500, 1000, 1500 \) and \( 2000 \mu s \) in Fig 3. Here, \( t = 0 \) corresponds to the beginning of injection of the liquid spray as well, and the shown planes are also cuts through the spray including the injection nozzle, which is located at the bottom of the figures.

An obvious difference when comparing the experimental to the numerical obtained extinction coefficient is the capturing of the closing of the nozzle. In the numerical simulation the nozzle closes completely at 1500 μs, thus, the extinction coefficient fields show that the spray is not attached to the nozzle anymore at 2000 μs and has moved already approximately 10 mm downstream. The experimental results however show that the spray is at 2000 μs as well as at 2500 μs and 3000 μs still attached to the nozzle, even if it is getting more dilute for later timesteps. This can be explained by the fact that the nozzle in the experiment does not close sharply at 1500 μs, but it starts closing. Thus there is still liquid injected for some time, only less as before. Therefore it has been decided to choose \( t = 1500 \mu s \) from the numerical simulation and \( t = 2000 \mu s \) from the experiment to compare with each other as those seem to reflect the most similar available state of the spray.

When comparing these two extinction coefficient fields, the experimental one shows a larger spray opening angle and a stronger droplet dispersion than the numerical one, especially in the region close to the nozzle. This can have several reasons: Large heavy droplets are known to be less sensitive to turbulent dispersion (due to a large Stokes number) than small light droplets. As the boundary conditions at the exit of the nozzle are not known
Extinction coefficient fields measured experimentally using the Dual-SLIPI technique in a non-combusting Diesel spray for $t = 2000 \mu s$, $2500 \mu s$ and $3000 \mu s$ (from left to right). It is observed from these images that the extinction coefficient reduces over time due to both evaporation and the expansion of the droplets position over time.

from the experiments, the droplet diameter distribution is assumed to be a Rosin-Rammler type and the SMD to be 10 $\mu m$. If the droplets in the experiment in fact were in average smaller, this can explain a stronger turbulent dispersion. Besides the droplet diameter distribution also other parameters as the velocity distribution are assumed, which also introduces errors. In the experiment the liquid is injected vertically and the nozzle is directed upwards. Also if gravitational forces are judged to be not dominant, they slow down the droplets in streamwise direction but don’t change the velocity in spanwise direction. Thus, the spray opening angle is increased. In numerics, gravitational forces are not taken into account. While the gas phase in the simulation is at the beginning of the injection quiescent, the gas in the experiment contains turbulent structures resulting from previous injection pulses. These structures enhance the spray dispersion and liquid-gas mixing significantly, as it was shown in [29].

Another apparent discrepancy between experiment and simulation is much higher absolut values for the extinction coefficient in the simulations. While the fields in Fig. 3 are scaled to the maximum value measured in experiments, $\mu_e = 0.45 \text{ mm}^{-1}$, the simulated field shows in fact a maximum value of $\mu_e = 52.5 \text{ mm}^{-1}$. To investigate the influence of the boundary conditions on this value, a parameter study is performed which is shown in Fig. 4. One obvious reason for the discrepancies is the mass flow rate at injection which was chosen to be $\dot{m} = 1.75 \cdot 10^{-3} \text{ kg/s}$. Thus, a simulation with identical conditions as above are run, but with a mass flow rate of $\dot{m} = 0.5 \cdot 10^{-3} \text{ kg/s}$, which leads to a maximum $\mu_e = 18.2 \text{ mm}^{-1}$. As mentioned above, the experimental fields are derived after the closing of the nozzle. As the nozzle does not close sharply it is assumed that the low absolut values for the extinction coefficients actually stem from a low mass flow exiting the nozzle after the nozzle started to close. A second parameter that has been investigated is the influence of the SMD. The three fields in Fig. 4 originate from the same mass flow rate of $\dot{m} = 0.5 \cdot 10^{-3} \text{ kg/s}$, the SMD is decreased to 5 $\mu m$, which leads to a maximum $\mu_e = 82.2 \text{ mm}^{-1}$, and increased to 15 $\mu m$, which leads to a maximum $\mu_e = 8.9 \text{ mm}^{-1}$. Thus larger droplets lead to a smaller extinction coefficient than smaller droplets, if the mass is the same.

It has to be pointed out that the extinction coefficient field is not a representation of a unique spray, it results from a certain combination of a droplet number density and related droplet diameters. Thus the same extinction coefficient field can be obtained from e.g. a spray consisting of many small droplets and of a spray consisting of less larger droplets. Nevertheless, the comparison of the experimental and numerical obtained extinction coefficient fields as shown above give a strong hint that the simulation reflects globally the spray structure that can be seen in experiments. Starting from this conclusion the strengths of numerical simulations can be used and the results can be analysed further to a level of resolution that cannot be obtained from experiments.

Summary and Conclusions

In this work a novel method has been developed to correlate results obtained from a spray experiment and from a numerical spray simulation, which is based on comparing the local extinction coefficient. The method has been applied to a Diesel type spray. The global features of the spray could be captured, while the differences
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Figure 3. Extinction coefficient fields numerically simulated for $t = 500 \mu s$, 1000 $\mu s$, 1500 $\mu s$ and 2000 $\mu s$ (from left to right).

Figure 4. Extinction coefficient fields numerically simulated for different conditions at $t = 1500 \mu s$.

mainly stem from the unclear boundary conditions used in the experiment. However, the main goal of this paper, to develop the numerical method to extract the extinction coefficient from simulations, has been reached successfully. The extinction coefficient has been shown not to be a representation of a unique spray, but a combination of droplet number and droplet diameter, but it can give a strong argument for the validation of the numerical methods. The potential of this approach for future works is shown in this paper by first correlating the experimental and numerical extinction coefficient fields. Afterwards the strengths of numerics is used to give in depth and spatially and temporally highly resolved information about the spray structure, e.g. about droplet radii, droplet diameters and velocity fields of the liquid and gaseous phase. The extinction coefficient can be used for validation purposes as it contains information of both droplet size and number density. When a liquid jet is injected, in the second wind induced or the atomization regime, under high pressure into still air, it breaks up into droplets either directly at the nozzle or some nozzle diameters downstream and to form a spray.

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