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Mixing and Evaporation Analysis of **a** High-Pressure SCR System using **a** Hybrid LES-RANS Approach

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Abstract

A hybrid Large Eddy Simulation (LES) – Reynolds-Averaged Navier-Stokes (RANS) method (HLR) has been applied to simulate an engine related selective catalytic reduction (SCR) system. Typical

SCR systems utilize low pressure urea injection together with a mixer for vapor field homogenization. Simultaneously, it is also desirable to reduce spray-wall interaction to avoid urea crystallization. The present study considers an SCR system where a high pressure (150 bar) urea spray is injected towards hot exhaust gases in exhaust pipe. The system has been shown to work well in a previous experimental study but detailed characterization of the system is missing. The novelty of the present study rises from: 1) the creation of phase diagrams with single droplet simulations that predict the optimum operation regions for the SCR system, 2) validation of the HLR method in a high Reynolds number (*Re* = 49,900) compressible pipe flow, 3) the use of HLR simulations in an engine SCR system for the first time, and 4) the detailed characterization of the present SCR system. As a result of the study, new non-dimensional timescale ratios are proposed to link the droplet size and liquid injection velocity to the exhaust pipe dimensions in future SCR systems.

Keywords: Selective Catalytic Reduction (SCR), NO_x reduction, Computational Fluid Dynamics, hybrid LES-RANS, urea mixing, SCR spray design

1. Introduction

- Selective Catalytic Reduction (SCR) systems are used to lower NO_x emissions from diesel engines. Typically urea-water solution (UWS) is injected to hot exhaust gases before the catalyst which is 30 located some distance downstream from the SCR injector in the exhaust pipe. The mixing and evaporating UWS decomposes into ammonia, which is the reducing agent needed to transform NO_x to N₂ at the catalyst. Usually, a low injection pressure (~ 10 bar) UWS is injected either directly into the exhaust pipe [1,2] or to a mixer or high-swirl generating mixing device [3,4]. In the present study, 35 the former type of SCR system is analyzed. The used injector operates at a high injection pressure (150 bar) in order to improve the spray mixing and evaporation. Engine tests with the present system have been successful yielding high NO_x conversion rates (up to 95%) [5]. However, the detailed link between high injection pressure and UWS mixing is not available. The SCR system used by Kaario et al. [5] is shown schematically in Fig. 1. The present study is related to SCR systems in heavy-duty 40 engines [5,6] but has also relevance to SCR systems in marine and power plant engines [7]. In order to obtain a deeper understanding on the UWS spray dynamics and operation, Computational Fluid Dynamics (CFD) simulations are performed utilizing a hybrid model combining Large Eddy Simulation (LES) and Reynolds-Averaged Navier-Stokes (RANS) turbulence modeling [8]. An example of a computational setup of such high injection pressure SCR concept is shown in Fig. 2.
- 45 The UWS spray injection takes typically place in a confined volume, such as the engine exhaust pipe. The combination of high Reynolds number wall bounded flow necessitates special treatment of the near wall region. In RANS modeling, good accuracy may be obtained by using wall functions to bridge the gap between the wall and the first computational cell. However, for high Reynolds number flows, the requirements for a wall resolved LES becomes prohibitive. It is estimated that the grid size

50 requirement to resolve the viscous sublayer scales as ~ Re^{1.8} for LES. This is close to the scaling Re^{2.25} required by Direct Numerical Simulation (DNS) [9]. Thus, the cost for wall resolved LES becomes high in practical applications. A solution to this problem, and used also in the present study, is to apply a hybrid LES-RANS (HLR) approach [9-11] where the near wall region is modelled in the RANS framework while other areas of the computational domain are solved with the LES approach.
55 In this way, the boundary layer can be described in an accurate way with a feasible amount of computational cells while other parts of the computational domain are treated with the LES method to capture the chaotically swirling turbulent flow field.



60 Figure 1. A schematic representation of the present SCR system used by Kaario et al. [5].

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In the following, some previous experimental studies on SCR systems are reviewed. According to the literature, the UWS is typically injected with low injection pressure into hot gases with or without an additional mixing device [1-4]. Of particular interest are the droplet sizes as they significantly affect the spray formation and evaporation processes [12]. Postrioti et al. [2] measured UWS spray droplet

sizes in a hot environment using 5 bar injection pressure and a 3-hole spray-disk –type nozzle where each hole was 200 μ m in diameter. They reported average droplet sizes between 60 - 100 μ m depending on the position they were measuring. Oh and Lee [3] analyzed experimentally an optimal mixer location in the exhaust pipe and reported an average Sauter mean diameter (SMD) of 65 μm using a 3-hole nozzle with 4 – 6 bar injection pressure. They did not report the nozzle hole size. Hua et al. [13] did not calculate the average SMD from their experimental data but showed that more than 50% of the droplets were below 10 μm and the maximum drop size they measured was 45 μm . Similar to [3], they used a 3-hole nozzle with 190 μm hole diameter with injection pressure of 10 bar. Santangelo [14] used a rather high injection pressure (60 - 80 bar) for pure water with a swirl nozzle and reported average SMD between 55 - 60 μm .



Figure 2. The computational setup of the present SCR injection system. High-pressure urea-water solution (UWS) spray is injected towards the hot (T = 523 K) and turbulent gas flow in an engine exhaust pipe from a single hole nozzle.

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Next, a review of RANS based SCR system simulations is given. RANS simulations have the advantage of requiring low computational cost but, as a trade-off, the results give a time averaged view of the situation. Cho et al. [4] optimized an SCR system equipped with different types of mixers using both experiments and simulations. They used a 4-hole nozzle with 140 μm hole size and low injection pressure. Cho et al. [4] focused especially on the uniformity of the ammonia distribution before the catalyst and found an optimal position for an 6-blade mixer yielding an uniformity index of 88 % before the catalyst (see Section 6.2 about uniformity index). Ström et al. [15] analyzed different droplet motion related forces in a low-pressure SCR system using a hollow cone injector.

90 They injected the UWS from a pipe wall which lead to a relatively strong spray wall interaction. The

evaporation model used by Ström et al [15] had a separate treatment for urea and water. For part of their simulations, monodisperse sprays were used in order to separate certain effects from one another. Improved turbulence modeling was recommended to better capture the droplet and flow dynamics. Birkhold et al. [16] developed an evaporation model for UWS and used the model to predict UWS spray evaporation in a low injection pressure RANS case. They predicted that not all the UWS will be decomposed (hydrolyzed) before the catalyst which requires some additional capacity from the catalyst. Bhattacharjee et al. [17] developed modeling capabilities, especially SCR chemistry, and analyzed ammonia concentration at the catalyst inlet. They concluded that detailed chemistry was not needed upstream the catalyst to model properly the decomposition of UWS.
Recently Varna et al. [18] studied experimentally and numerically a low injection pressure cross-flow SCR system. A six-hole disk-type injector with 210 μm hole size was used together with pure water as UWS substitute. Varna et al. [18] reported droplet sizes below 150 μm whereas the distribution peaks varied between 20 – 50 μm depending on the applied conditions.

The presented literature review showed that only a little computational research has been done on high pressure SCR systems. In particular, the link between various droplet sizes, their mixing and evaporation, is not fully understood in present-day SCR systems. In fact, a thorough characterization of high pressure UWS evaporation and mixing process is missing at the moment. Typical modern SCR systems incorporate various types of mixers to enhance vapor homogeneity. However, additional pressure losses due to the mixer are not favorable in the exhaust channel. In addition, it is desirable to reduce and remove spray-wall interaction to avoid urea crystallization. In light of these aspects, the present study considers a high-pressure UWS injection without an additional mixer. The UWS sprays are characterized as a function of droplet size. In a sense, we are applying a 'worst case evaporation scenario' for the UWS sprays by using monodisperse sprays: there is no droplet size distribution with smaller droplets that would have fast mixing and evaporation. This computational 115 setup is designed in order to point out possible problematic operating conditions for the SCR system without uncertainties due to additional submodels.

In practice, the optimal operation of an SCR system could be related to dimensioning of the exhaust pipe as a function of the UWS injection velocity and the characteristic droplet diameter of the spray. In other words, the injector type and injection pressure have significant impact on the UWS spray and

thereby on the SCR system operation. The present study is linked to the mentioned topics by using dimensional arguments to find optimal SCR system operation conditions as a function of UWS injection velocity and droplet size. In order to reach this goal, the following objectives are formulated. The objectives of the present study are to: 1) create phase diagrams with single droplet simulations in uniform ambient flow in order to find optimum droplet sizes and injection velocities for the UWS
injection, 2) validate the used HLR approach in high Reynolds number conditions for the present SCR pipe flow, 3) quantify UWS spray mixing and evaporation using HLR together with Lagrangian particle tracking (LPT), and 4) characterize the UWS injection with non-dimensional timescale ratios

in order to help dimensioning of future SCR systems. In order to reach these objectives, the HLR modeling is used which is capable of capturing the transient and turbulent flow field that is present in
the high Reynolds number pipe flow as well as in the high velocity UWS spray.

2. Governing Equations and Numerical Algorithms

2.1 Fluid Motion

The governing equations for the gaseous phase describe the conservation of mass, momentum, energy, and species mass fractions, and they are written as:

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$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = \mathbf{0}$$
 (1)

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial}{\partial x_j} \left(p \delta_{ij} - \tau_{ij} \right) + M_d + M_g$$
(2)

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_j h}{\partial x_j} = -\frac{\partial}{\partial x_j} (\tau_{ij} \ u_j) + \frac{\partial}{\partial x_j} (\lambda \frac{\partial T}{\partial x_j}) + M_h$$
(3)

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_j Y_k}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D_k \frac{\partial Y_k}{\partial x_j} \right) + M_Y \tag{4}$$

where M_d is the momentum source term exerted from the droplets to the gas phase, M_g is the 140 momentum source term for the gas phase to keep the average flow velocity constant, M_h is the energy source term to keep the average gas temperature constant, and M_Y is the vapor mass source term from the droplets. The M_g and M_h are source terms that are added to compensate for the friction and wall heat transfer losses, respectively. The viscous stress tensor is defined as

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \mu \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij}$$
(5)

The Navier-Stokes (NS) Eqs. (1), (2), and (5) are of the form NS = NS(ρ, u_i,...) = 0 describing the conservation of mass, momentum, and energy. In LES, Eqs. (1) - (5) are spatially filtered resulting in additional subgrid-scale terms from the non-linear part of the equations and they can be written in the form NS(ρ̃, ũ_i,...) = τ_{sgs}. The subgrid-scale terms, which need modeling, account for the interaction between the resolved and the unresolved scales. Additionally, according to the Boussinesq
hypothesis, viscosity can be written as μ = μ_g + μ_{t/sgs}, where μ is the total viscosity and μ_{t/sgs} is the turbulent viscosity in RANS or the subgrid-scale viscosity in LES calculated from

$$\mu_{tlsgs} = (1 - \lambda) C_{\mu} \rho \, k^2 / \varepsilon + \lambda \, C_{LES} \rho \, \Delta \sqrt{k} \tag{6}$$

In Eq. (6), Δ is the filter width calculated from the cell volume V_{cell} as $\Delta = V_{cell}^{1/3}$ and $C_{LES} = 0.05$. Lambda (λ) is calculated according to

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$$\lambda = 0.5 + \frac{1}{\pi} \operatorname{atan}\left(10\left(\frac{1}{\Delta/l} - 1\right)\right)$$
 (7)

The length scale *l* is obtained from $l = min(\kappa y, C_l k^{3/2} / \varepsilon)$ where $\kappa = 0.419$ is the Von Kármán constant and *y* is the normal distance from a wall. C_l is a large number in the present study which effectively forces RANS to be used only in a few near wall cells (see Section 5). In the Eq. (7), when $\Delta/l > 1, \lambda \rightarrow 0$ implying a RANS solution. Then the turbulent viscosity from the Eq. (6) reads $\mu_t =$ $C_{\mu} \rho k^2 / \varepsilon$. On the other hand, when $\Delta/l < 1$, then $\lambda \rightarrow 1$ meaning LES solution for the μ_{sgs} . In this case the subgrid-scale viscosity reads $\mu_{sgs} = C_{LES} \rho \Delta \sqrt{k}$. The Eq. (7) for λ implies smooth but fast transition from the RANS solution ($\lambda \rightarrow 0$) to the LES solution ($\lambda \rightarrow 1$).

In the present study, transport equations for both k and ε are solved in the whole computational domain. The equation for k is given as

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$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_j k}{\partial x_j} = P - \rho \varepsilon + \frac{\partial}{\partial x_j} \left(\left(\mu_g + \frac{\mu_{t/sgs}}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right)$$
(8)

Eq. (8) is formally the same for both RANS and LES models. Only the total viscosity μ changes according to the RANS/LES region. *P* is the production term calculated as

$$P = \tau_{ij} \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$
(9)

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Instead of forcing ε algebraically, a transport equation is solved as described by Schiestel and Dejoan [19], and Chaouat and Schiestel [20]

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial \rho u_j \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\left(\mu_g + \frac{\mu_{t} I_{sgs}}{\sigma_2} \right) \frac{\partial \varepsilon}{\partial x_j} \right) + \rho \frac{\varepsilon}{k} \left(C_1 P - C_2 \varepsilon \right) - F \rho \frac{C_{LES} \Delta}{2\sigma_k \sqrt{k}} \left(\frac{\partial k}{\partial x_j} \right) \left(\frac{\partial \varepsilon}{\partial x_j} \right)$$
(10)

where F = 0 for RANS and F=1 for LES. The calculation of F is based on the λ calculation in the Eq. (7). When $\lambda < 0.5$ then F=0, otherwise F=1. The parameters σ_2 , C_1 , and C_2 are calculated according to $\sigma_2 = (1 - F)\sigma_e + F\sigma_k$, $C_1 = (1 - F)C_{\varepsilon_1} + F\frac{3}{2}$, and $C_2 = (1 - F)C_{\varepsilon_2} + F\frac{3}{2}$. This means that when going from RANS to LES solution, only the coefficients C_{ε_1} : 1.44 \rightarrow

1.5, $C_{\varepsilon 2}$: **1.92** \rightarrow **1.5**, σ_e : **1.22** $\rightarrow \sigma_k$: **1.0** are changed, and an additional source term is added (last term on the right-hand side of the Eq. (10)). The calculation of ε in the whole domain enables smooth estimation of its value in the RANS/LES interphase. Importantly, however, the HLR model operating in the LES region is essentially a one equation k-l model since the subgrid-scale viscosity is calculated from $\mu_{sas} = C_{LES}\rho \Delta \sqrt{k}$ without contribution from ε .

In conjunction with the HLR approach, standard wall functions are used in the wall adjacent cell. The standard wall functions for velocity are

$$u^{+} = \begin{cases} \frac{1}{\kappa} \log(E \ y^{+}), & y^{+} > y_{m}^{+} \\ y^{+}, & y^{+} \le y_{m}^{+} \end{cases}$$
(11)

where E = 9 is an empirical constant and $y^+ = \rho u_\tau y/\mu$ is the non-dimensional wall distance, where $u_\tau = \sqrt{\tau_w/\rho}$ is the friction velocity and τ_w is the wall shear stress. The switch point y_m^+ between the linear (laminar) and logarithmic (turbulent) profile is defined at the intersection of the linear and the logarithmic curves. A second order accurate flux limited scheme is used for the spatial discretization and for the time integration a second order accurate three time level method is used. Simulations have been carried out with the Star-CD 4.22 code.

190 2.2 Droplet Motion

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In Lagrangian particle tracking (LPT), the motion of individual droplets is tracked through the computational domain. It is assumed that the force acting on a droplet is due to aerodynamic drag. The droplet equation of motion (assuming spherical droplets) reads [12]:

$$\frac{1}{6}\rho_p \pi d^3 \frac{du_p}{dt} = \frac{1}{2} (u_g - u_p) |u_g - u_p| \rho_g C_d \frac{\pi d^2}{4}$$
(12)

195 The expression for the drag coefficient C_d is given as

$$C_{d} = \begin{cases} \frac{24}{Re_{p}} \left(1 + \frac{1}{6} Re_{p}^{2/3} \right) & Re_{p} < 1000 \\ 0.424 & Re_{p} \ge 1000 \end{cases}$$
(13)

where Re_p is the droplet Reynolds number based on the droplet slip velocity. The present study uses the Discrete Droplet Method (DDM) [21] where parcel position is updated from

$$\frac{dx_p}{dt} = u_p \tag{14}$$

200 The droplet velocity change can be calculated from the re-cast form of the Eq. (12) as

$$\frac{du_p}{dt} = \frac{c_d}{\tau_p} \frac{Re_p}{24} \left(u_g - u_p \right) \tag{15}$$

and the droplet momentum timescale can be calculated from

$$\tau_p = \frac{\rho_d d^2}{18\mu_g} \tag{16}$$

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The parcels are advanced in time using a semi-implicit time integration method by taking five subiterations within each time step. The momentum source term M_d in Eq. (2) is evaluated for each cell separately by looping over all the parcels within the cell. The following relation for the source term is assumed [12]:

$$M = \frac{1}{2}\rho_g C_d A |u_g - u_p| (u_g - u_p)$$
(17)

where A is the projected droplet area. The total number of parcels in this study is **534,000**.

210 2.3 Droplet Evaporation

The mass transfer from the droplets due to evaporation is modeled according to Bird et al. [22]. The rate of change of the droplet mass is given as

$$\frac{dm_d}{dt} = -A_d K_g p_g ln\left(\frac{p_g - p_{\nu,\infty}}{p_g - p_{\nu,d}}\right) \tag{18}$$

where A_d is the droplet surface area, K_g is the mass transfer number, p_g is the gas pressure, $p_{\nu_{l}\infty}$ is 215 the vapor pressure in the droplet surroundings, and $p_{\nu_{l}d}$ is the vapor pressure at the droplet surface. The mass transfer coefficient K_g is modeled according to Ranz and Marshall [23] and it is given as

$$K_g = \frac{Sh D_m}{R_m T_m d} \tag{19}$$

where *Sh* is the Sherwood number, D_m the vapor-gas mixture diffusivity, R_m the mixture gas constant, T_m the mixture temperature, and *d* the droplet diameter. The heat transfer at the droplet surface is derived from the droplet energy balance and the Ranz-Marshall correlations for *Sh* and Nusselt (*Nu*) number [23] are applied in the equations for mass and heat transfer. The droplet evaporation time can be expressed as $dm_d/dt = -m_d/\tau_e$ where the evaporation time is

$$\tau_e = \frac{\rho_d \, d^2}{6 \, D_m \, Sh \, \rho_g \, ln[(p_g - p_{\nu,\infty})/(p_g - p_{\nu,d})]} \tag{20}$$

2.4 Properties of the Urea-water solution

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The liquid urea-water solution's (UWS) physical properties are modeled according to [5,24]. Accordingly, the liquid properties are modeled as a single component that represents the UWS properties. The UWS is composed of 32.5 % urea and 67.5 % of water. In brief, the UWS has 9 % higher density and approximately 25% higher viscosity than pure water at 320 K. UWS has also 10% smaller surface tension, 33% smaller latent heat, and approximately 14% smaller heat capacity than water. Due to lack of experimental data, it is assumed that UWS has similar vapor pressure as water. More details can be found from Kaario et al. [5].

2.5 Modeling assumptions

In the following, a brief list of the modeling assumptions used in the present study is given.

• A hybrid LES-RANS (HLR) method is used where the near wall region is solved in the RANS 235 framework and LES is used elsewhere.

• Lagrangian particle tracking (LPT) is utilized for the droplets (sometimes called the Discrete Droplet Method (DDM)).

• The modeling of droplet breakup is disregarded since droplet breakup only occurs at Weber numbers above $We = \rho_g |u_g - u_p|^2 d/\sigma_l > 12$. For the largest drop size (40 μm), the maximum Weber number in the simulation is We < 12.

• It is assumed that there is no interaction between the droplets. This is based on the fact that the dense spray region is relatively short, in this case roughly ~30 mm [25], compared to the maximum spray penetration (~7 %). However, another important reason to omit the modeling of droplet interaction is to simplify the spray event in order to be able to separate various effects from each other.

• No explicit subgrid-scale modeling for the droplet dispersion is used. High-resolution LES implies that the subgrid-scale velocity fluctuations are relatively weak and have therefore only a minor influence on the droplet motion. Similar approach has been utilized previously in [26-28].

- For possible effects between the droplets and the pipe wall, a model by Bai and Gosman [29] 250 is used. The model takes into account several phenomena that can happen when droplets interact with a hot surface. According to the model, and depending on the flow, wall, and droplet conditions, a droplet can either attach, rebound, slide, or breakup when hitting a wall. The possibility for the formation of a liquid film is not taken into account since in the present system there is no significant wall-droplet interaction.
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• The urea-water solution (UWS) properties are described by a single component model.

3. Computational Setup and SCR Geometry

The purpose of the following section is to provide details for proper background flow of the UWS sprays. The geometry of the present SCR system has been obtained from experiments [5]. Table 1 describes some important parameters for the UWS spray cases. The gas mass flow rate \dot{m}_g as well as the average gas temperature *T* in the pipe were measured in [5]. The characteristic flow timescale of the present system is calculated as $\tau_{char} = L/U_{bulk} = 63 \text{ ms}$. Also the injection pressure P_{inj} and the injection duration τ_{inj} are taken from the same study. The average gas density ρ_g is calculated from the ideal gas law. The average gas velocity U_{bulk} is calculated from the experimental gas mass flow rate \dot{m}_g , pipe diameter *D*, and the average gas density ρ_g . The injection velocity U_{inj} is calculated from the Bernoulli equation assuming $C_v=0.90$ and $\rho_l=1074 \text{ kg/m}^3$. The mass flow rate used for the liquid injection assumes $C_D=0.80$. A top hat profile is assumed for the liquid injection.

Table 1. Details of the UWS spray cases.

1 4010 11			
L	Pipe length	[mm]	1200
D	Pipe diameter	[mm]	110
\dot{m}_g	Gas mass flow rate in the pipe	[kg/h]	420
U_{bulk}	Average pipe flow velocity	[m/s]	19
τ_{char}	Characteristic flow timescale	[ms]	63
Т	Average gas temperature in the pipe	[K]	523
p	Pressure in the pipe	[bar]	1
$ ho_g$	Average gas density	$[kg/m^3]$	0.66
P _{inj}	Injection pressure	[bar]	150
U _{inj}	Injection velocity	[m/s]	150
d_n	Nozzle hole diameter	[mm]	0.23
	Number of nozzle holes	[-]	1
τ_{inj}	Injection duration	[ms]	4
m _{inj}	Mass injected	[mg]	23.8

The present mesh consists essentially of two parts: 1) the background pipe flow mesh, and 2) the 270 spray mesh with local cell refinement area. In the used HLR approach, RANS is used only in the near wall cells (2 - 3 wall adjacent cells). The non-dimensional height of the first cell is $y^+=38$. The 2^{nd} and the 3rd cell heights are $y^+=95$ and $y^+=130$, respectively. After this there are 14 layers of 0.5 mm cells spanning the non-dimensional distance between $y^+=150-300$. The bulk of the pipe mesh consists of 1.7 mm cells. Details of the background pipe flow mesh are shown in Fig. 3 and in Table 2. 275 In the spray mesh, the UWS nozzle is located in the middle of the pipe at z = 0 mm, where z is the axial pipe coordinate running between -L/2 < z < L/2. The most dense part of the spray mesh consists of 200 µm cells up to 200 mm from the nozzle. After this, a 400 µm region extends up to 400 mm from the nozzle. Surrounding the 200 and 400 μm resolutions is a cylindrical volume consisting of 0.85 mm cells between -10 mm < z < 450 mm. The diameter of the 0.85 mm cell cylindrical volume is 30 mm. Further details on the spray mesh are shown in Fig. 3 B) and in Table 2. 280 The simulations are run for 100 flow through times T_0 ($T_0 = L/U_{bulk} = 63$ ms). Courant (*Co*) number was kept below $Co = u \Delta t / \Delta x < 1$ at all times (during UWS injection, $u = U_{inj}$, whereas at other times $u = u_a$).

For the background pipe flow, standard RANS wall functions are used in the wall adjacent cells.
Therefore, the y⁺ value of the 1st cell needs to be close to y⁺~ 30 - 40 for accuracy reasons implying a rather large first cell. Then, the sensitivity of the RANS/LES domain border was tested with several different computational grids. It was found out that it is beneficial to set the domain border to some distance away from the 1st cell. In the present case, y⁺~130 was chosen based on extensive testing and according to the findings of e.g. Temmerman et al. [9]. This provides a smooth development for the turbulence quantities in the RANS region compared to starting the LES region closer to the 1st RANS cell. On the other hand, taking the domain border too far, decreases the eddy-resolving capability of the HLR method. The spray mesh resolution was based on previous experiences from LES spray simulations [28,30,31] where it has been shown that cell size somewhat below the nozzle

hole size is sufficiently small. In [30], it was observed that 5% of the total turbulent kinetic energy was modeled implying that 95% was resolved. According to literature [32,33], at least 80% of the turbulent kinetic energy should be resolved for good quality LES. Hence, the resolution used herein is considered feasible for the subsequent UWS spray analysis.

Table 2. The mesh variants used in the pipe flow validation and in the spray simulations.

	Case	Re	ρ	Tave [K]	<i>D</i> [mm]	Length	Cells
1	Superpipe	56,700	const.	const.	129	5D	2.2 × 10 ⁶
2	Compressible pipe flow	49,900	varying	523	110	10.9D	3.1 × 10 ⁶
3	Spray	49,900	varying	523	110	10.9 <i>D</i>	9.4 × 10 ⁶

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Figure 3. A) The HLR methodology pipe flow mesh topology used in the present study. B) The mesh refinement area in the spray mesh.

305 4. Single Droplet in Uniform Ambient Flow

In order to gain insight to the UWS spray injection before 3D simulations, single droplet simulations in uniform ambient flow have been performed. Here, Eqs. (13) - (16), and (18) - (19) are integrated for an evaporating single droplet assuming constant gas velocity. In the performed simulations, it is assumed that droplet temperature is constant $T_d = 323$ K, droplet density is constant $\rho_l = 1074$ kg/m³, and the surrounding vapor pressure is $p_{v,\infty} = 0$. Droplet vapor pressure is constant $p_{v,d} = 11700$ Pa

and gas temperature is set to T = 523 K. The chosen T_d value is based on HLR/LPT results where only a small variation was observed in the droplet temperature. The chosen vapor pressure value $p_{v,\infty} = \mathbf{0}$ is considered to be reasonable implying that 'no vapor' is assumed in the far field.

The problem in an SCR system is to find the optimal value of injection velocity U_{inj} and droplet size 315 *d* for the UWS spray. Here, the aim is to find optimal conditions defined as: 1) droplet stays between -L/2 < z < L/2 and 2) droplet evaporates completely within the characteristic flow timescale $\tau_{char} = L/U_{bulk} = 63 \text{ ms}$ of the present system. Consequently, it is not beneficial if the droplet meets the ends of the pipe or does not evaporate completely within τ_{char} .

Fig. 4 A) characterizes the injection process as a function of the gas phase velocity and droplet size. Since the gas phase velocities vary both spatially and temporally, all combinations of U_g in the present 320 system are investigated. Three different situations are distinguished: I) droplets experience gas phase velocity that equals the bulk velocity ($U_{bulk} = -19$ m/s), II) droplets experience gas phase velocity that is zero, and III) the gas phase velocity equals the injection velocity. In the case I), there is a maximum upstream penetration (when droplet velocity goes to zero) after which the droplet switches 325 its direction and starts to follow the bulk gas flow. It can be observed that the 40 μm droplet size has a too long downstream penetration whereas the 10 μm droplet evaporates quickly. In the case II), the droplet upstream position first increases, but after some time, the droplet velocity goes to zero because of drag force acting on the droplet. This leads to the droplet staying in a constant position. If the droplet diameter is large enough, as is the case with the 40 μm droplet size, the evaporation rate is too slow to take place within the $\tau_{char} = 63 \text{ ms}$. Finally, in the case III), the upstream penetration 330 is fast and the droplet will soon meet the upstream end of the pipe.

Figs. 4 B) – D) show phase diagrams as a function of the initial droplet diameter and velocity. The optimal area vs conditions I – III (defined above) is shown with red color. In case there is a too long downstream penetration, the area is colored dark blue. If the droplet evaporates too slowly, the area

has a light blue color. In case the droplet has a too high upstream penetration, the area is colored light green. It is observed that most influential factors to the droplet evaporation and penetration are the droplet diameter and the assumed gas phase velocity. In contrast, the effect of the initial droplet velocity is significantly lower compared to droplet diameter and gas velocity. Furthermore, the analysis reveals that to stay in the optimal area, droplets should preferably be small with high slip velocity.



Figure 4. Phase diagrams for single droplet in uniform ambient flow. A) Characterization of the droplet position and evaporation as a function of gas velocity U_g and droplet size d. B) Phase diagram of droplet position when $U_g = U_{bulk}$, C) when $U_g = \mathbf{0} m/s$, and D) when $U_g = U_{Inj}$.

Fig. 5 A) shows a phase diagram comparing the droplet momentum timescale τ_p (Eq. (16)) to the evaporation timescale τ_e (Eq. (20)). It is seen that for all slip velocities and droplet sizes, τ_p is always small compared to τ_e indicating that droplets will adjust to velocity changes much faster than it takes them to evaporate. When the slip velocity is close to zero, the evaporation process is rather long. When the slip velocity or the droplet size is increased, inertial effects (i.e. τ_p) are increasing. Fig. 5 B) compares the evaporation timescale τ_e to the characteristic flow timescale $\tau_{char} = L/U_{bulk} =$ **63** *ms*. The dashed white line shows where τ_e is equal to τ_{char} . Below this line, $\tau_e > \tau_{char}$ implying too long evaporation time for the present system. It is seen that high slip velocity is beneficial for fast evaporation. Part of the operating area of the present work is in the area where the evaporation is slow and, thus, long evaporation times may be expected for low slip velocity conditions. In particular, when $\tau_e > \tau_{char}$ too long evaporation time may be expected. This leads to $1/2 U_{inj} \tau_p < 1/2 L \rightarrow \tau_p < \tau_F$, where $\tau_F = L/U_{inj} = 8 \times 10^{-3}$, and 2) droplet evaporation should take place before the lower end of the pipe leading to $\tau_{char} < \tau_{char}$.



Figure 5. Phase diagrams for single droplet in uniform ambient flow. A) Droplet timescale τ_p compared to the evaporation timescale τ_e as a function of the slip velocity and droplet size. B) Evaporation timescale τ_e compared to the characteristic simulation time $\tau_{char} = 63$ ms. Below the dashed white line $\tau_e/\tau_{char} > 1$.

Table 3 shows the droplet momentum timescale as well as the minimum and maximum evaporation timescales calculated with 150 m/s or zero slip velocity, respectively. Also shown is a worst case scenario where $max(\tau_e)$ (calculated with zero slip velocity) is divided by the flow timescale τ_{char} to indicate what droplet sizes may produce too slow evaporation in the present system $(max(\tau_e)/\tau_{char} > 1)$. It is seen that the constraint 1) is always fulfilled $(\tau_p < \tau_F)$ whereas constraint 2) only for $d < 30 \ \mu m$.

Table 3. Characteristic momentum and evaporation times for several droplet sizes. $Max(\tau_e)$ is calculated with zero slip velocity and $min(\tau_e)$ with 150 m/s slip velocity from Eq. (20). τ_{char} = $L/U_{bulk} = 63 ms$ and $\tau_F = L/U_{inj} = 8 ms$. Dashed red line indicates successful droplet size 375 according to the constraint 1) and solid red box successful droplet size according to the constraint 2).

Droplet size	$ au_p$ [s]	$\max(\tau_e)$ [s]	<i>min(τ_e)</i> [s]	$max(\tau_e)/\tau_{char}$	τ_p/τ_F
10 µm	3.3 × 10 ⁻⁴	1.1 × 10 ⁻²	2.8 × 10 ⁻³	0.18	0.041
20 µm	1.3 × 10 ⁻³	4.4 × 10 ⁻²	1.1 × 10 ⁻²	0.70	0.16
30 µm	2.9 × 10 ⁻³	9.9 × 10 ⁻²	2.5 × 10 ⁻²	1.57	0.37
40 µm	5.2 × 10 ⁻³	1.8 × 10 ⁻¹	4.5 × 10 ⁻²	2.86	0.65

5. HLR Model Validation

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In order to validate the present high Reynolds number compressible pipe flow case, experimental data from a high-Re number pipe flow facility, so called 'Superpipe' wind tunnel data from the Princeton University [34,35] (Princeton/DARPA-ONR Superpipe facility), is used for the validation. The present HLR approach is first validated in incompressible isothermal conditions using mesh #1 (Table 2). Then, compressible pipe flow validation is carried out using mesh #2. After this, four UWS spray injection cases are calculated to analyze the effect of droplet size on spray mixing and evaporation using mesh #3. 385

5.1 Incompressible isothermal pipe flow

In the Superpipe facility, pipe flow has been measured over a large range of Reynolds numbers between 5 × 10³ and 38 × 10⁶. The pipe diameter is D = 129.36 mm. The present validation simulation is carried out for Re = UD/v = 56,700. The corresponding friction Reynolds number is $Re_{\tau} = u_{\tau}D/\nu = 2700$, where u_{τ} is the friction velocity. The experiments and the simulations have 390 been conducted in room temperature (298.97 K). The flow is pressure driven in order to keep the average flow velocity constant, and the flow field is recycled in order to yield a realistic turbulent flow profile. A momentum source term has been added to keep the average velocity constant (a constant volumetric source term). The simulation is run until 100 flow through times ($T_0 = 100$). Then the result is spatially and temporally averaged for each y^+ value. The result is shown in Fig. 6 A). It 395 is seen that the averaged non-dimensional velocity profile is in reasonable agreement with the experimental Superpipe data. Comparing the results to those in Temmerman et al. [9], where Re_{τ} = **2000** was used in a channel flow, the results of the present study are very similar or even better. Standard wall functions (Eqs. (11)) are also plotted in the same figure for reference and they are seen 400 to closely match the experimental data.



Figure 6. A) Experimental Superpipe data (Re = 56,700) compared to the HLR simulation. Also shown is the HLR result from the compressible pipe flow case (Re = 49,900) and the analytical wall functions. B) Top: Axial velocity from compressible pipe flow (Re = 49,900) at $y^+ = 130$. B) Bottom: Cross-section from the middle of the compressible pipe flow showing the temperature field.

5.2 Compressible pipe flow

Practical SCR systems operate in high temperature conditions implying the presence of strong temperature and density gradients. Thereby, a compressible pipe flow case with temperature and 410 density variations is validated next following the satisfactory agreement with the Superpipe data. The details of the case are given in Table 2. The pipe wall has been set to a constant temperature of 450 K. Similarly as before, the flow is pressure driven and the flow field is recycled with cyclic boundary conditions at the pipe ends. In addition, to compensate for the heat loss through the walls, a heat source term has been added to keep the average temperature constant (a constant volumetric heat source term). In a similar fashion as in the above Superpipe case, the case is run up to $T_0 = 100$ after 415 which the result is spatially and temporally averaged for each y^+ . The result is shown in Fig. 6 A). Very good agreement is seen between the Superpipe data and the compressible pipe flow case. Fig. 6 B) shows the axial velocity distribution from $y^+=130$ and the temperature field from the middle of the pipe at $T_0 = 100$. These observations imply that the setup offers a feasible background lies.

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6. UWS Spray Results

In the following, monodisperse UWS sprays using 10, 20, 30, or 40 μm droplets are analyzed. The droplet sizes were selected according to the single droplet simulations in uniform ambient flow (Section 4). Because the exact details of the UWS sprays are not known, monodisperse sprays are used to quantify the spray mixing and evaporation as a function of the droplet diameter. This approach enables us to quantify the mixing and evaporation processes specifically related to droplet diameter.

6.1 Spray Evolution

Since the UWS spray is injected towards the main flow, a strong turbulent shear layer is formed between the spray-accelerated gas jet and the main pipe flow. This is shown in Fig. 7 A) where the 430 strongly accelerated gas jet is shown at 4 ms (end of injection). Fig. 7 B) shows the averaged axial velocities from the spray centerline. Small droplets lose their momentum faster than bigger droplets, and hence small droplets produce higher gas phase velocity. This is clearly visible at t = 4 ms. At t = 10 ms, the spray centerline velocity has decreased significantly and has mostly switched direction.



Figure 7. A) Axial velocity distribution from the middle of the UWS spray at t = 4 ms (end of injection).
B) Averaged axial gas velocity from the spray centerline at t = 4 ms and t = 10 ms. Negative values imply flow direction to the main pipe flow direction.

Fig. 8 shows the UWS sprays at t = 4 ms. Clear differences are seen between the different droplet sizes. 40 μ m spray evolves with distinct formation of an outer 'shell' together with a region with only a small amount of droplets (void). This structure is formed due to the shearing of droplets from the tip area of the spray. The 10 μ m droplets evolve in a more homogenous manner and droplets are seen to follow the local flow field. The following of the local flow field leads to regions accompanied by many droplets (preferential concentrations) and to void regions without droplets [36]. Considering

the droplet Stokes (*St*) number $St = \tau_p / \tau_f^{100 \ mm}$, where $\tau_f^{100 \ mm} = D_{jet}^{100 \ mm} / U_{jet}^{100 \ mm}$, the *St* numbers for the 40, 30, 20, and 10 μm droplets are 32, 20, 10, and 3, respectively. Thereby, the biggest droplets will respond slowly to the flow field changes compared to the smallest droplets

according to Eq. (16). However, droplets will be influenced by the strong evaporation rates that efficiently reduce their St number.

450 Fig. 8 shows that the sprays exhibit a relatively narrow and sharp tip area. This is in line with experimental observations from low gas density sprays [37]. In the present case, the shape is also related to the dispersion of the droplets. Since the sprays are injected towards the main flow, the droplets dispersed in the tip area leave the spray-accelerated gas field and thus face higher gas resistance. This effectively decelerates the axial movement of the dispersed droplets. Hence, in the 455 spray tip area, a narrow tip is formed due to the strong deceleration of the dispersed droplets. In addition, the bulk pipe flow accelerates the dispersed droplets to follow the opposite flow direction.



Figure 8. UWS sprays and vapor concentration at t = 4 ms.

460 Scatter plot of droplet axial velocity vs droplet axial position is shown in Fig. 9. It is seen that many of the droplets have high velocity (~150 m/s) and are located below 100 mm from the nozzle at 4 ms. On the one hand, the 40 μm spray has a lot of droplets that have already switched their velocity

direction and are located between 50 mm < z < 150 mm. These are the outer 'shell' droplets seen also in the Fig. 8. On the other hand, for the 10 μm spray, all the way between the nozzle and the spray tip, there are droplets which have switched their velocity direction ($U_z < 0$.) At 10 ms, it is seen that the 40 μm spray has penetrated longer and has generally higher droplet velocities compared to the 10 μm spray. Most of the droplets have switched their velocity direction at 10 ms.

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Figure 9. Axial droplet velocity as a function of their axial position at t = 4 ms and at t = 10 ms in 470 the 10 and 40 μ m cases. Color indicates the droplet number density from zero (dark blue) to a high value (red).

Fig. 10 shows the UWS spray evolution from a slice of cells. The first time frame is from t = 10 ms when the sprays reach the maximum upstream penetration. After this, all droplets start to follow the

gas flow towards the exit of the pipe. The sprays exhibit a relatively narrow and sharp tip area seen also at earlier time (4 ms) in the Fig. 8. A lot of internal structures (voids and preferential concentrations) are seen within the sprays which are related to their *St* numbers [36]. It is seen that roughly at ~20 ms for all cases, droplet dispersion has spread the droplets so that small part of them are already near the pipe walls. Fig. 10 also shows the strong evaporation that is closely related to droplet size. The 10 µm droplets have all evaporated at 20 ms whereas a significant amount of droplets is still present at 50 ms for the 40 µm case.



Figure 10. UWS spray evolution in the hot exhaust gases as a function of time for the various droplet sizes (10, 20, 30, and 40 μ m). The injector is located in the middle of the pipe and marked with a blue dot.

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Fig. 11 shows the spray penetration based on the 98% cumulative liquid mass. In the Fig. 11, zero position marks the location of the nozzle. Positive values indicate distance travelled towards the hot exhaust flow whereas negative values indicate that droplets have traveled past the nozzle location downstream within the exhaust flow. It is seen that the maximum upstream penetration is reached

roughly at 10 ms for all droplet sizes. The maximum penetration ranges from 38 to 44 cm for the $10 \ \mu m$ and $40 \ \mu m$ droplets, respectively. One might expect to see bigger differences in the maximum upstream penetration as a function of the droplet size. However, smaller droplets accelerate the gas phase much faster than bigger droplets as could be seen from the Fig. 7 B). Consequently, the key issue in the relatively similar maximum upstream penetration between different droplet sizes lies in the fact that although small droplets have lower momentum, they produce higher gas phase velocity and thus experience lower drag force.



Figure 11. HLR/LPT spray penetration based on 98% cumulative liquid mass.

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The additional value of the above HLR/LPT simulations compared to the single droplet simulations is in the ability to visualize the local UWS spray behavior and point out possible problematic situations, such as too long upstream or downstream spray penetrations. According to HLR/LPT, no problems were observed in the maximum upstream penetration of the droplets which is in line with the single droplet simulations (Section 4). In contrast to the single droplet simulations, according to HLR/LPT only the 40 μm droplets evaporate too slowly.

6.2 Mixing of the UWS

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Compared to the single droplet simulations, HLR/LPT allows the analysis of the UWS spray mixing. Fig. 12 shows the UWS vapor concentration field at different times from the middle of the pipe. The evaporated mass for each droplet size is different due to the large variation in the evaporation rate.

For example, the strong early evaporation can be observed in the 10 μm case compared to the 40 μm case. The vapor concentration for the 40 μm drop size shows a sharp peak and reduced mixing at initial times due to slow evaporation. In the 10 and 20 μm cases, the vapor cloud soon occupies a larger volume compared to the 40 μm case. On the other hand, the vapor cloud, although having different mass for each case, seems to move in a rather similar fashion especially at later times for all cases.

the second strategy and the second	10 ms	2000 March 1990 March 1990	10 ms
	15 ms		15 ms
and the state of the	20 ms		20 ms
and the second second	30 ms		30 ms
C. M. Contraction	40 ms		40 ms
and the second sec	50 ms		50 ms

40 µm initial droplet size

30 µm initial droplet size

10) ms		10 ms
15	5 ms		15 ms
20) ms		20 ms
30) ms		30 ms
40) ms		40 ms
50) ms	and the second sec	50 ms



10 µm initial droplet size



Figure 12. Urea-water solution vapor evolution as a function of the initial droplet size and time.

Fig. 13 displays the evaporated percentage for each droplet size. It is seen that at t = 10 ms, for example, 80% of 10 μm droplets have evaporated whereas only 27% have evaporated from the 40 μm drops. It is also seen that the evaporation rate is not linear, especially not for the biggest droplets. The slow evaporation rate seen for the last droplets (evaporated liquid amount > 99 %) for each droplet size class is mainly due to small amount of droplets interacting with wall or located in high UWS concentration region with low temperature. In addition, the 30 μm droplet size is a "critical" size above which the droplets will not be able to completely evaporate within τ_{char}. It is seen that for the 40 μm droplets about 1 % of the injected liquid mass does not evaporate before τ_{char}. Based on the evaporation history of the 40 μm droplets, it is estimated that they require approximately 400 mm longer pipe (in the downstream direction) for complete evaporation.



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Figure 13. Evaporated liquid amount for the different initial droplet sizes in the HLR/LPT cases. Red lines indicate the complete evaporation times for the different droplet sizes and the dashed red line the characteristic flow through time.

Table 4 shows the evaporation times for the HLR/LPT spray cases. According to the Eq. (20), droplet evaporation time scales as $\sim d^2$. Thereby, one would expect to observe quadrupling of the evaporation

time when doubling the droplet size. However, it is seen that the HLR/LPT spray cases are relatively far from the $\sim d^2$ evaporative scaling implying that local changes in the flow environment (temperature, vapor concentration, slip velocity, and less importantly wall effects) are significant.

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Table 4. Evaporation times for the HLR/LPT sprays. Also shown are the evaporation times calculated from the Eq. (20).

Droplet size $[\mu m]$	10	20	30	40	
HLR/LPT spray [s]	0.0194	0.0339	0.0584	0.083*	
$\tau_e (\text{Eq.}(20))^{**} [s]$	0.0053	0.0214	0.0481	0.0854	

*Estimated based on the evaporation history

** Estimated based on a constant 20 m/s slip velocity between the droplet and the gas phase

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In order to analyze the mixing of the UWS solution, Fig. 14 shows the UWS distribution at two axial locations (-L/4 and -L/2) in the pipe. It is seen that the local instantaneous vapor concentrations are strongly fluctuating. The 10 μm droplets are completely evaporated at t = -L/4 whereas the 40 μm droplets are not. Thus two separate situations can be distinguished: 1) for the 10 μm droplets the maximum vapor concentration is decreasing towards the exit of the pipe, but 2) for the 40 μm droplets, however, the maximum vapor concentration is increasing when approaching the pipe exit. Additionally, considering mixing at z = -L/4, there are large regions without any vapor whereas at downstream cross-section z = -L/2 there is hardly any region without vapor. This is mainly due to mixing of the UWS vapor traveling towards the end of the pipe.



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Figure 14. Urea-water solution (UWS) vapor evolution at z = -L/4 and at z = -L/2 (pipe exit) for the 40 and 10 µm initial drop sizes. At z = -L/4 the result is taken from $t = \tau_{char}/2$ whereas at z = -L/2 from time $t = \tau_{char}$. Also shown are the local UI.

560 For the quantification of the mixture distribution, uniformity index (UI) is calculated according to [4]

$$UI = \mathbf{1} - \frac{\sum_{i}^{N} |Y_i - \bar{Y}| A_i}{2|\bar{Y}| \sum_{i}^{N} A_i}$$
(21)

where A_i is the cell face area of cell *i* in a plane of *N* cells, and Y_i is the vapor mass fraction of cell *i*. The uniformity of the vapor distribution is somewhat non-uniform at the end of the pipe at z = -L/2showing maximum values close to $UI \cong 0.8$. Interestingly, all droplet sizes in the present study yield roughly similar maximum *UI*. For example, Cho et al. [4] reached *UI* = 0.89 with an optimized mixer setup.

Finally, Fig. 15 shows a probability density of vapor mass fraction distribution from two time instants. At $t = \tau_{char}/2$, the case with the smallest droplets has the lowest maximum vapor concentrations while the cases with the largest droplets have the highest maximum concentrations. At later time 570 $t = \tau_{char}$, the 40 μm droplets show higher maximum concentration which is related to the ongoing evaporation. Importantly, a significant amount of vapor mixing has occurred during the $\tau_{char}/2$ time reducing the maximum vapor concentrations substantially.



Figure 15. Probability density of urea-water solution vapor mass fraction at time A) $t = \tau_{char}/2$ and 575 B) $t = \tau_{char}$ from the start of injection.

7. Conclusions

An SCR system has been analyzed where a high-pressure UWS spray ($P_{inj} = 150$ bar) was injected towards hot exhaust gases (T = 523 K) coming from an engine in a high Reynolds number (Re =49,900) compressible flow case. The present study uses single droplet simulations to gain insight to the SCR system operation. Phase diagrams have been created to predict optimum operation regions for the SCR system. Then, hybrid LES-RANS (HLR) simulations have been performed for the SCR system for the first time. The HLR methodology was validated against experimental data from the Princeton Superpipe facility. Four monodisperse UWS sprays were simulated with droplet sizes ranging between 10 to 40 μm selected according to the single droplet simulations. The monodisperse sprays were used to characterize the behavior of different droplet sizes in a real high-pressure SCR system. With this approach the mixing and evaporation processes can be quantified specifically related to droplet diameter.

The main findings of the present study are:

- A combination of two non-dimensional timescale ratios is proposed to link the droplet size and liquid injection velocity to the exhaust pipe dimensions in SCR systems. The proposed numbers are related to the maximum upstream penetration (τ_p/τ_F) and to the evaporation time of the droplets (τ_e/τ_{char}). The condition for the maximum upstream penetration is τ_p/τ_F < 1 and the condition for the evaporation time is τ_e/τ_{char} < 1.
 - From the viewpoint of SCR operation, the single droplet simulations in uniform ambient flow revealed optimal conditions for the UWS sprays such that the droplets do not reach the ends of the pipe and they evaporate within the pipe length. The created phase diagrams showed that the gas velocity and the droplet size are the most important properties to be considered in the UWS sprays.
 - The HLR method applied in the present high Reynolds number flow gives an accurate prediction of wall flows with a feasible number of computational cells.
 - The added value from HLR/LPT was the ability to visualize the UWS sprays and identify possible problems such as a too slow evaporation rate. The results suggest that the 30 μm droplet size is the upper limit for complete evaporation in the present 1200 mm pipe. It was estimated that approx. 400 mm longer pipe would be needed for the 40 μm droplets for complete evaporation.
 - HLR/LPT gave also additional value to the evaporation and mixing analysis of the UWS sprays. Droplet size was not a key factor in the uniformity of the vapor distribution at the pipe exit. The maximum vapor concentrations were reduced by

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30 % – 40% within $\tau_{char}/2$ downstream of the nozzle. Thereby, the uniformity of the vapor distribution could be improved by a relatively small pipe length increase.

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The present analysis has significantly improved the understanding of the SCR system operation. New non-dimensional timescale ratios ($\tau_p/\tau_F < 1$ and $\tau_e/\tau_{char} < 1$) have been obtained for the design of such a system. Suggestions for future continuation of the work includes an extension of the geometrical analysis further downstream to investigate possibilities for improved vapor uniformity. Additionally, the proposed timescale ratios point to the direction of smaller droplet size and hence towards higher injection pressures.

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Nomenclature

	DDM	Discrete droplet method
	HLR	Hybrid LES-RANS
	LES	Large eddy simulation
630	LPT	Lagrangian particle tracking
	RANS	Reynolds-Averaged Navier-Stokes
	Re	Reynolds number
	Re_{τ}	Friction Reynolds number
	SCR	Selective catalytic reduction
635	Sh	Sherwood number
	UI	Uniformity index

	UWS	Urea water solution
	We	Weber number
640	A	Projected droplet area [m ²]
010	A ,	Droplet surface area $[m^2]$
		Discharge coefficient
	C_{u}	$T_2, \sigma_2, \sigma_3, \sigma_4, \sigma_2, \sigma_3, \sigma_2$ Turbulence model coefficients
	D	Diffusivity $[m^2s^{-1}]$ or nine diameter $[m]$
645	D	Vanor-gas mixture diffusivity $[m^2s^{-1}]$
045	D_m	Dronlet diameter [m]
	а F	Parameter for LES / RANS transition in the ε -equation
	h	Enthalny $[Ik\sigma^{-1}]$
	Ka	Droplet mass transfer number [sm ⁻¹]
650	k	Turbulent kinetic energy $[m^2s^{-2}]$
000	L	Pipe length [m]
	l	Turbulent length scale [m]
	P	Production of turbulent kinetic energy
	p_{a}	Gas pressure [Pa]
655	$p_{m \infty}$	Vapor pressure in the droplet surroundings [Pa]
	\mathcal{D}_{nd}	Vapor pressure at the droplet surface [Pa]
	Pvja Rm	Mixture gas constant [Jkg $^{-1}$ K $^{-1}$]
	T	Gas temperature [K]
	T_d	Droplet temperature [K]
660	T_m	Mixture temperature [K]
	T_0	Flow through time [s]
	ť	Time from the start of simulation [s]
	U _{bulk}	Average gas velocity in the pipe [ms ⁻¹]
	U_q	Gas velocity in the single droplet simulations [ms ⁻¹]
665	U_{Ini}	Injection velocity [ms ⁻¹]
	u_a	Gas velocity [ms ⁻¹]
	u,	Velocity component [ms ⁻¹]
	u_n	Droplet velocity [ms ⁻¹]
	u^{+}	Non-dimensional velocity
670	Y_{k}	Species mass fraction
	v V	Normal distance from a wall [m]
	y^+	Non-dimensional distance from a wall
	Z	Axial pipe coordinate between $-L/2 < z < L/2$.
675	Δ	Filter width [m]
	ε	Dissipation rate of turbulent kinetic energy [m ² s ⁻³]
	λ	Parameter for LES / RANS transition in the viscosity equation
	μ_{sgs}	Turbulent subgrid-scale viscosity [kgm ⁻¹ s ⁻¹]

	μ_t	Turbulent viscosity [kgm ⁻¹ s ⁻¹]
680	ρ	Fluid density [kgm ⁻³]
	$ ho_d$	Droplet density [kgm ⁻³]
	σ_l	Liquid surface tension [Nm ⁻¹]
	$ au_{char}$	Characteristic flow through time in the pipe [s]
	$ au_e$	Evaporation time [s]
685	$ au_F$	Characteristic injection time [s]
	$ au_{ij}$	Viscous stress tensor

References

- Grout, S., Blaisot, J.-B., Pajot, K., and Osbat, G., Experimental investigation on the injection of an urea–water solution in hot air stream for the SCR application: Evaporation and spray/wall interaction, Fuel, 106, pp. 166-177, 2013. http://dx.doi.org/10.1016/j.fuel.2012.09.022
 - Postrioti, L., Brizi, G., Ungaro, C., Mosser, M., and Bianconi, F., A methodology to investigate the behavior of urea-water sprays in high temperature air flow SCR de-NOx applications, Fuel, 150, pp. 548-557, 2015. http://dx.doi.org/10.1016/j.fuel.2015.02.067
 - Oh, J., and Lee, K., Spray characteristics of a urea solution injector and optimal mixer location to improve droplet uniformity and NOx conversion efficiency for selective catalytic reduction, Fuel, 119, pp. 90-97, 2014. http://dx.doi.org/10.1016/j.fuel.2013.11.032
 - Cho, Y.S., Lee, S.W., Choi, W.C., and Yoon, Y.B., Urea-SCR system optimization with various combinations of mixer types and decomposition pipe lengths, Int. J. Automotive Technol., 15(5), pp. 723-731, 2014. doi:10.1007/s12239-014-0075-x
 - Kaario, O., Sarjovaara, T., Ranta, O., Hulkkonen, T., Keskinen, K., Larmi, M., Halonen, S., and Amberla, A., Comparing Breakup Models in a Novel High Injection Pressure SCR System using Polyhedral Meshing, SAE Technical paper series, 2014-01-2816, 2014. doi:10.4271/2014-01-2816
 - 6. Sarjovaara, T., Alantie, J., and Larmi, M., Ethanol dual-fuel combustion concept on heavy duty engine, Energy, 63, pp. 76-85, 2013. http://dx.doi.org/10.1016/j.energy.2013.10.053
 - Keskinen, K., Kaario. O., Nuutinen, M., Vuorinen, V., Künsch, Z., Liavåg, L.O., and Larmi, M., Mixture formation in a direct injection gas engine: Numerical study on nozzle type, injection pressure and injection timing effects, Energy, 94, pp. 542-556, 2016. http://dx.doi.org/10.1016/j.energy.2015.09.121

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695

700

705

- Ferziger, J., and Perić, M., Computational methods for fluid dynamics, Springer, 2nd edition, ISBN 3-540-59434-5, 1997.
- Temmerman, L., Hadžiabdić, M., Leschziner, M.A., and Hanjalić, K., A hybrid two-layer URANS-LES approach for large eddy simulation at high Reynolds numbers, Int. J. Heat and Fluid Flow, 26, pp. 173-190, 2005. doi:10.1016/j.ijheatfluidflow.2004.07.006

 Spalart, P.R., Detached-Eddy Simulation, Annu. Rev. Fluid Mech., 41, pp. 181-202, 2009. doi:10.1146/annurev.fluid.010908.165130

11. Hanjalić, K., and Kenjereš, S., Energy, 30, pp. 1481-1497, 2005.

- doi:10.1016/j.energy.2004.05.001
 - 12. Crowe, C.T., Schwarzkof, J.D., Sommerfeld, M., and Tsuji, Y., Multiphase Flows with Droplets and Particles, 2nd edition, CRC Press, ISBN 978-1-4398-4050-4, 2012.
 - Hua, L., Zhao, Y.-G., Hu, J., Tao, T., and Shuai, S.-J., Comparison between air-assisted and airless urea spray for diesel SCR system by PDA and CFD, SAE Technical paper series, 2012-01-1081, 2012. doi 10.4271/2012-01-1081
 - Santangelo, P.E., Characterization of high-pressure water-mist sprays: Experimental analysis of droplet size and dispersion, Exp. Thermal and Fluid Sci., 34, pp. 1353-1366, 2010. doi:10.1016/j.expthermflusci.2010.06.008
- Ström, H, Lundström, A., and Andersson, B., Choice of urea-spray models in CFD simulations of urea-SCR systems, Chemical Engineering Journal, 150, pp. 69-82, 2009. doi:10.1016/j.cej.2008.12.003
 - 16. Birkhold, F., Meingast, U., Wassermann, P., and Deutschmann, O., Modeling and simulation of the injection of urea-water-solution for automotive SCR DeNOx-systems, Applied Catalysis B: Environmental, 70, pp. 119-127, 2007.
- 735 doi:10.1016/j.apcatb.2005.12.035
 - Bhattacharjee, S., Haworth, D., and Moores, R., CFD Modeling of Processes Upstream of the Catalyst for Urea SCR NOx Reduction Systems in Heavy-Duty Diesel Applications, SAE Technical paper series, 2011-01-1322, 2011. doi 10.4271/2011-01-1322
- 18. Varna, A., Spiter, A.C., Wright, Y.M., Eggenschwiler, P.D., Boulouchos, K., Experimental and numerical assessment of impinging and mixing of urea-water sprays for nitric oxide reduction in Diesel exhaust, Applied Energy, 157, pp. 824-837, 2015. http://dx.doi.org/10.1016/j.apenergy.2015.03.015
 - Schiestel, R., and Dejoan, A., Towards a new partially integrated transport model for coarse grid and unsteady turbulent flow simulations, Theoret. Comput. Fluid Dynamics, 18, pp. 443-468, 2005. doi: 10.1007/s00162-004-0155-z

720

715

725

- 20. Chaouat, B., and Schiestel, R., Partially integrated transport modeling method for turbulence simulation with variable filters, Phys. Fluids, 25(12), 2013. http://dx.doi.org/10.1063/1.4833235
- 21. Dukowicz, J.K., A particle-fluid numerical model for liquid sprays, J. Comput. Phys., 35, pp. 229-253, 1980.
- 22. Bird, R.B., Stewart, E.W., and Lightfoot, E.N., Transport Phenomena, John Wiley & Sons, New York, 1966.
- 23. Ranz, W.E., and Marshall, W.R., Evaporation from drops parts I and II, Chem. Eng. Prog., 48(3), p. 141, 1952.
- 755 24. BASF, AdBlue Technical Leaflet, BASF, 2005.

750

760

765

770

775

- 25. Elghobashi, S., On predicting particle-laden turbulent flows, Appl. Sci. Res., 48, pp. 301–314, 1991. doi: 10.1007/BF00936835
- 26. Luo, K., Klein, M., Fan, J.-R., and Cen, K., Effects on particle dispersion by turbulent transition in a jet, Phys. Lett. A, 357, pp. 345–350, 2006. http://dx.doi.org/10.1016/j.physleta.2006.04.069
- 27. Apte, S., Gorokhovski, M., and Moin, P., LES of atomizing spray with stochastic modeling of secondary breakup, Int. J. Multiphase Flow, 29, pp. 1503–1522, 2003. http://dx.doi.org/10.1016/S0301-9322(03)00111-3
- 28. Wehrfritz, A., Vuorinen, V., Kaario, O., and Larmi, M., Large Eddy Simulation of High Velocity Fuel Sprays: Studying Mesh Resolution and Breakup Model Effects for Spray A, Atomization and Sprays, 23(5), pp. 419-442, 2013. doi: 10.1615/AtomizSpr.2013007342
 - 29. Bai, C., and Gosman, A., Development of methodology for spray impingement simulation, SAE Technical paper series, 950283, 1995. doi 10.4271/950283
 - 30. Kaario, O., Vuorinen, V., Hulkkonen, T., Keskinen, K., Nuutinen, M., Larmi, M., and Tanner, F.X., Large Eddy Simulation of High Gas Density Effects in Fuel Sprays, Atomization and Sprays, 23(4), pp. 297-325, 2013. doi: 10.1615/AtomizSpr.2013006784
 - 31. Pei, Y., Som, S., Pomraning, E., Senecal, P., Skeen, S., Manin, J., and Pickett, L., Large eddy simulation of a reacting spray flame with multiple realizations under compression ignition engine conditions, Combustion and Flame, 162(12), pp. 4442-4455, 2015. doi: 10.1016/j.combustflame.2015.08.010
 - 32. Pope, S., Turbulent flows, Cambridge University Press, Cambridge England, 2001.
 - 33. Celik, I.B., Cehreli, Z.N., and Yavuz, I., Index of resolution quality for large eddy simulations, Journal of Fluids Engineering, 127(5), pp. 949-958, 2005. doi:10.1115/1.1990201

- 780 34. Zagarola, M.V., and Smits, A.J., Scaling of the Mean Velocity Profile for Turbulent Pipe Flow, Physical Review Letters, 78(1), pp.239-242, 1997. doi:http://dx.doi.org/10.1103/PhysRevLett.78.239
 - 35. Zagarola, M.V. and Smits, A.J., Mean Flow Scaling of Turbulent Pipe Flow, Journal of Fluid Mechanics, 373, pp. 33-79, 1998. doi: http://dx.doi.org/10.1017/S0022112098002419
 - 36. Vuorinen, V., Hillamo, H., Kaario, O., Nuutinen, M., Larmi, M., and Fuchs, L., Large Eddy Simulation of droplet stokes number effects on mixture quality in fuel sprays, Atomization and Sprays, 20(5), pp. 435-451, 2010. doi: 10.1615/AtomizSpr.v20.i5.50
 - 37. Hillamo, H., Optical fuel spray measurements, Doctoral dissertation 124/2011, ISBN 978-952-60-4379-1, 2011.