Numerical modeling of gas-liquid flows in a swirl nozzle

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A doctoral dissertation completed for the degree of Doctor of Science (Technology) to be defended, with the permission of the Aalto University School of Engineering, at a public examination held through remote connection (https://aalto.zoom.us/j/68406037485) on 16th of June 2021 at 12:00.

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The present dissertation belongs to the research area of fluid dynamics. In particular, scale-resolving computational fluid dynamics (CFD) methods are utilized to investigate liquid injection and atomization processes in industrial context. The two-phase flows are solved using the volume-of-fluid (VOF) method utilizing a sharp interface capturing framework. The work is motivated by high-viscosity, biomass-based renewable fuel injection where the atomization process and the size of the liquid droplets may relate to the overall quality of the combustion process. In this work, liquid injection from a large-scale asymmetric pressure-swirl atomizer is studied in different conditions. In contrast, previous research has mainly concentrated on small-scale nozzles with symmetric designs. Detailed simulations of both the inner-nozzle flow characteristics and the onset of liquid sheet breakup are carried out. Publications I and II investigate the low-Reynolds-number regime ($420 \leq \text{Re} \leq 5300$) in detail. Full understanding of the atomizer flow characteristics and key spray parameters has been so far lacking for the studied parameter range. In addition, comparison with experimental measurements is carried out in Publication II. In Publication III, bubbly flow in the atomizer is studied with relevance to injection scenarios where significant volume of gas is present inside the nozzle. Thus far, such conditions have remained relatively unexplored by detailed simulations in the context of swirl nozzles. The novelty of the present work relates to the application of highly resolved numerical simulations to study a large-scale swirl atomizer in conditions relevant for industrial applications. The main outcomes of the dissertation are as follows: (1) Detailed description of the inner-nozzle flow characteristics is provided. (2) Near-nozzle liquid sheet characteristics are analyzed and the existence of different spray patterns at different Reynolds numbers is demonstrated. (3) The effects of bubbly flow on the atomizer performance and liquid film characteristics are assessed. In addition, practically relevant nozzle key parameters, such as the spray opening angle, discharge coefficient, and film velocity, are reported. Also, the applicability of the used computational approach in the present application field is demonstrated via sensitivity tests, numerical benchmarks and experimental validation.

Keywords fluid dynamics, two-phase flow, liquid injection, atomization, swirl nozzle
The work for this dissertation was carried out in the Energy Conversion Group at Aalto University, Department of Mechanical Engineering during the period 2017-2021. The thesis would not have been possible without the help from many people, for which I am very grateful.

First, I would like to thank my supervisor Prof. Ville Vuorinen for giving me the opportunity to work in his group. I have really enjoyed my time in the group and learned immensely both on professional and personal levels. I am also grateful for my thesis advisor Prof. Mika Järvinen for his valuable comments and always positive attitude. The thesis was pre-examined by Prof. Francesco Picano and Prof. Henrik Ström, whom I sincerely thank for their positive evaluation and comments. In addition, I would like to show my deepest appreciation to Prof. Ström for acting as the opponent in the public defense.

In addition to help from individuals, this work was made possible by support from organizations and funding bodies. I wish to thank ANDRITZ Oy. for providing the general setting of the research and for continued support and feedback during the project. In addition, Aalto University Engineering Graduate School, Doctoral Education Network in Energy Technology (DENET), and Kauhajoen Kulttuurisäätiö are highly appreciated for financial support. Furthermore, I would like to acknowledge CSC – Finnish IT Center for Science Ltd. for enabling the research by providing the computational resources.

Research is teamwork and many issues faced during this work have been solved in productive discussions with past and present co-workers. Also, one should not forget the importance of co-workers in lighting up the lunch discussions and bringing well-deserved breaks to the workdays. Thank you Ossi, Karri, Heikki, Mahdi, Petteri, Bulut, Alpo, Mahmoud, Jeeva and Daulet, to name a few. Besides colleagues, I would like to acknowledge my fellow physics students Antti, Armi, Tuomas, Jaakko, Susanna, Jere, Klaara, Sampo and Samuli. In addition to heaps of unforgettable memories, you have given me plenty of examples on how to successfully pursue a PhD.
Finally, I wish to thank my parents, Riitta and Pekka, and my brother Antti with his family for always supporting me on my journey. Most of all, I am grateful to my wife Kristiina and son Eeli for showing me what is truly important in life.

Espoo, May 7, 2021,

Erkki Laurila
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This thesis consists of an overview and of the following publications which are referred to in the text by their Roman numerals.


Author’s Contribution

Publication I: “Analysis of viscous fluid flow in a pressure-swirl atomizer using large-eddy simulation”

The author was responsible for preparing the simulation setup, carrying out the simulations and analyzing the results. In addition, the author prepared the manuscript. Support for adaptive mesh refinement in the isoAdvector code was implemented by J. Roenby. The co-authors assisted in preparing the simulation setup and aided in writing the manuscript.

Publication II: “Computational and experimental investigation of a swirl nozzle for viscous fluids”

The author was responsible for the numerical part of the study. The author carried out the simulations and the data analysis as well as prepared the manuscript. S. Koivisto, A. Kankkunen and K. Saari designed and carried out the experiments. The co-authors assisted in processing the experimental results and supported in writing the manuscript.

Publication III: “Numerical study of bubbly flow in a swirl atomizer”

The author carried out the simulations, post-processed the results and analyzed the data. In addition, the author was responsible for preparing the manuscript. The co-authors provided valuable suggestions regarding the data analysis and supported in writing the manuscript.
1. Introduction

1.1 Scope of thesis

This work belongs to the research fields of fluid dynamics and interfacial two-phase flow. Liquid injection from a large-scale swirl atomizer is resolved by numerical simulations. The present investigations focus on the inner-nozzle flow and the near-nozzle liquid film characteristics as illustrated in Figure 1.1. The results of the thesis are relevant for various high-viscosity, low-Reynolds-number liquid injection applications.

The thesis consists of this summary and the appended Publications I-III. The objective of the summary is to provide a general overview of the research topic and more information on background topics which were not extensively covered in the publications. Last, the main results of the work are summarized in the end of the thesis.

1.2 Black liquor spraying

One example of a high-viscosity liquid injection application is the spraying and combustion of black liquor in recovery boilers. This application has motivated the present studies, and therefore, a brief overview of the application area and its significance is provided here. Black liquor is a by-product of the kraft pulping process which accounts for over 90% of world’s chemical pulp production [1]. Black liquor consists of inorganic cooking chemicals and organic components dissolved in water [2, 3]. In the process, black liquor is burned in a recovery boiler to recover the cooking chemicals and to convert the organic residues into usable energy. An illustration of a recovery boiler and the main processes in its furnace section are shown in Figure 1.2.

Black liquor constitutes a significant source of renewable energy as its organic components originate from wood, a renewable raw material. On
average, the production of 1 kg of pulp produces approximately 1.5 kg of dry black liquor solids [1, 4]. Based on the world's pulp production, 195 million tons of black liquor solids are combusted in the world annually [5] which amounts to 731 TWh in terms of energy [6]. In Finland, 10% of electricity and 22% of renewable electricity was produced by black liquor combustion in 2019 [7]. Therefore, even a modest improvement in the efficiency of the energy conversion process can have a significant impact on renewable energy production.

Black liquor is introduced to the boiler by spraying it to the lower part of the furnace as shown in Figure 1.2 (b). Upon injection, the spray disintegrates into fairly large and irregular droplets with diameters of approximately 2–10 mm [4]. Likewise, the used nozzles are large in size with discharge orifice diameters of a few centimeters. Commonly used nozzle types include the splash plate, pressure-swirl and V-jet atomizers [4]. All the common injectors can be categorized as sheet-forming nozzles [3]. The nozzles first produce a liquid film which subsequently breaks up into ligaments and droplets as is later discussed in Section 1.4.2. Good control over the generated droplet size is important for efficient boiler operation. In typical combustion systems, the droplet size is minimized to maximize the surface area for quick evaporation and combustion. However, this is not the aim in recovery boilers where droplets in the millimeter range are desired. If the droplets are too small, they may be carried away by the upward convection currents. The escaped droplets, i.e. the carry-over, may deposit on and foul the heat exchanger surfaces at the upper part of the boiler [5, 8]. On the other hand, too large droplets reach the char bed with too high water content causing negative effects on the chemical conversion process [3]. Black liquor spraying has been studied experimentally in
spraying chambers [9–11], in real furnace conditions [4, 12, 13], and with numerical modeling [14–16].

The chemical, physical and combustion properties of black liquor are subject to considerable variation due to its complex chemical composition. Regarding spraying, the most important physical parameters are the viscosity, density, surface tension, solids fraction and the boiling point rise [4]. The density of high solids fraction black liquor varies in the range of 1300-1500 kg/m$^3$ [3, 4], while the surface tension has been very difficult to reliably measure [4]. The viscosity is mainly affected by the solids fraction and the temperature [17]. As a consequence, the viscosity level may vary up to four orders of magnitude between different stages of the pulping process [3]. During spraying, the viscosity is approximately 30–260 mPas at typical conditions [3]. In addition, black liquor may exhibit non-Newtonian behavior, i.e. the viscosity may depend on the shear rate, in certain high-shear conditions [2].

Motivated by the important role of viscosity in liquid spraying, and the connection between the viscosity and the Reynolds number, Publications I-II focus on the effect of the Reynolds number on the nozzle flow and the subsequent spraying process. Furthermore, the high viscosity level is often reduced by heating the liquid. If the temperature of the liquid exceeds its atmospheric boiling point, flash boiling may occur inside the nozzle and within the spray. This influences the breakup process heavily. In order to gain insight in such injection conditions where gas is present inside the

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1Reprinted from Maakala et al. [18] with permission from Elsevier.
2Reproduced based on the illustration in Ref. [6].
Figure 1.3. (a) The large-scale asymmetric swirl atomizer geometry studied in the present thesis. (b) A schematic of a symmetric simplex nozzle with fully developed air core and hollow cone liquid film. (c) Spray development stages in a typical simplex atomizer as the Reynolds number is increased: (1) the dribble stage, (2) the distorted pencil stage, (3) the onion stage, (4) the tulip stage, and (5) the fully developed hollow cone spray.

1.3 Swirl atomizers

This thesis focuses on pressure-swirl atomizers. Due to the relative large desired droplet size, the atomizer discharge orifice diameter is large compared to typical swirl nozzles (centimeter vs. millimeter range) [19, 20]. In fact, the size of the generated droplets scales with the orifice diameter. The nozzle size sets the liquid film thickness, which in turn, directly influences the subsequent ligament and droplet sizes in the atomization process [21]. In addition, the harsh boiler conditions necessitate robust and simple nozzle designs which are durable, easy to manufacture, and resistant to wear and clogging. One such design, which is studied in detail in this dissertation, is shown in Figure 1.3 (a).

To describe the main operating principles of a pressure-swirl atomizer, let us consider a more typical design depicted in Figure 1.3 (b). The schematic illustrates a so-called simplex atomizer. Typically, the liquid is supplied to the atomizer through multiple tangential inlet ports near the walls of the swirl chamber in order to create a swirling flow. With increasing injection

1Reproduced based on the schematic presented in Ref. [22] with permission from Taylor and Francis.
### Table 1.1. Examples of CFD studies with focus on annular liquid sheet dynamics (Film) or internal flow in swirl nozzles (In-nozzle).

<table>
<thead>
<tr>
<th>Author</th>
<th>Year</th>
<th>Focus</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuster et al. [23]</td>
<td>2009</td>
<td>Film</td>
<td>Validation of a geometric VOF method with adaptive mesh refinement on a conical swirling jet.</td>
</tr>
<tr>
<td>Galbiati et al. [24, 25]</td>
<td>2016</td>
<td>Film</td>
<td>Mesh refinement study and jet instability/ligament analysis of a simplex atomizer using a geometric VOF method.</td>
</tr>
<tr>
<td>Ding et al. [26]</td>
<td>2016</td>
<td>Film</td>
<td>Injection pressure sweep of a simplex atomizer using an algebraic VOF method.</td>
</tr>
<tr>
<td>Shao et al. [27]</td>
<td>2017</td>
<td>Film</td>
<td>Effect of turbulent inlet conditions and study of the recirculation zone of an annular swirling jet using a mass conservative level-set method.</td>
</tr>
<tr>
<td>Dash et al. [28]</td>
<td>2001</td>
<td>In-nozzle</td>
<td>Study of the air core in simplex and open-ended atomizers using an algebraic VOF method.</td>
</tr>
<tr>
<td>Yeh [29, 30]</td>
<td>2007-2008</td>
<td>In-nozzle</td>
<td>Effect of turbulence models on simplex atomizer flow in a 2d axis-symmetric domain using VOF.</td>
</tr>
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<td>Mandal et al. [31]</td>
<td>2008</td>
<td>In-nozzle</td>
<td>Non-Newtonian flow inside a simplex atomizer in a 2d-axis-symmetric domain using a geometric VOF method.</td>
</tr>
<tr>
<td>Renze et al. [32]</td>
<td>2011</td>
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<td>Non-Newtonian flow in simplex and asymmetric atomizers using an algebraic VOF method.</td>
</tr>
<tr>
<td>Fu [33]</td>
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<td>Effect of oscillating ambient pressure on an open-ended atomizer in a 2d axis-symmetric domain using a geometric VOF method.</td>
</tr>
<tr>
<td>Galbiati et al. [34]</td>
<td>2016</td>
<td>In-nozzle</td>
<td>Testing of turbulence models and comparison to correlations for a simplex atomizer using an algebraic VOF method.</td>
</tr>
<tr>
<td>Maly et al. [35]</td>
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<td>Internal flow and air core dynamics in a simplex atomizer in a 2d axis-symmetric domain using an algebraic VOF method.</td>
</tr>
<tr>
<td>Vashahi et al. [36]</td>
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<td>Internal and external flow of a simplex atomizer using a VOF method.</td>
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<tr>
<td>Tonini et al. [37]</td>
<td>2019</td>
<td>In-nozzle</td>
<td>Effect of nozzle geometry on a simplex atomizer flow using a VOF method.</td>
</tr>
</tbody>
</table>
pressure, and therefore the Reynolds number, the spray pattern undergoes various development stages as illustrated in Figure 1.3 (c). At certain Reynolds number, the rotational motion is strong enough that air from outside the atomizer is drawn in to the low-pressure region at the center of the vortex and an air core is formed. Due to the gas core and the tangential velocity of the liquid film at the orifice, a hollow cone type spray is formed. After exiting the nozzle, the liquid film extends radially, grows thinner and undergoes primary breakup into ligaments and droplets. Further aspects of swirl atomizer characteristics are provided in Publications I and II.

Due to their practical importance, swirl atomizers have been extensively studied by experimental, analytical and numerical methods. Recent overviews on the subject can be found in Refs. [38] and [39]. With relevance to the present work, previous numerical studies on swirl nozzle internal flow and scale-resolving simulations of annular liquid sheet dynamics are listed in Table 1.1.

1.4 Computational fluid dynamics and fluid flow phenomena

In Publications I-III, computational fluid dynamics (CFD) methods are utilized to study liquid injection. In CFD, information about the behavior and evolution of fluid systems is obtained through the numerical solution of the governing Navier-Stokes equations. Here, CFD methods are applied to immiscible two-phase gas-liquid flows which pose versatile flow physics. In the following, some fluid dynamical phenomena and concepts essential for the present research topic are shortly introduced.

1.4.1 Turbulence

Turbulence is often described as chaotic fluid motion with vortical structures (eddies) occurring on a variety of length scales. In contrast, the flow can also be laminar with smooth and orderly nature. In fact, most flows of practical engineering relevance are turbulent. The distinction between turbulent and laminar flow is illustrated in Figure 1.4 (a). In between the two modes, the flow is in a transitional state where instabilities may trigger the onset of turbulence. The state of the system can be quantified by the Reynolds number:

\[
Re = \frac{UL}{\nu}
\]  

(1.1)

Above, \(U\), \(L\) and \(\nu\) are the characteristic flow velocity, length scale and the kinematic viscosity, respectively. As the Reynolds number expresses the ratio of inertial to viscous forces, high \(Re\) commonly indicates the predominance of inertial effects and high level of turbulence.

The energy cascade concept offers a qualitative description of the turbu-
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Figure 1.4. (a) Schlieren image of a candle thermal plume showing the transition from laminar to turbulent flow.\(^1\) (b) Typical spectrum of turbulent kinetic energy as a function of wavenumber \(k\). (c) Velocity field in RANS and LES of staggered turbulent jets.\(^2\)

Lent energy transfer process as first described by Richardson [40]. Kinetic energy is fed to the turbulent motions at the large scales comparable to the characteristic length \(L\). The large eddies interact, break down and the kinetic energy is passed down to smaller eddies. Thus, the energy is transported through the scales in a cascade process. Finally, at length scales where inertial and viscous forces are at balance, the kinetic energy is dissipated into heat by viscosity. These smallest eddies occur at the Kolmogorov scale [41]:

\[
\eta = \left( \frac{\nu^3}{\varepsilon} \right)^{1/4}
\]

and become continually smaller as the Reynolds number is increased. Above, \(\varepsilon\) is the dissipation which corresponds to the kinetic to thermal energy conversion power occurring predominantly on the smallest scales of the turbulent flow. The distribution of the kinetic energy among the scales can be quantified by the energy spectrum which is illustrated in Figure 1.4 (b). Most of the energy is contained at the low wavenumbers

\(^1\)Adapted from photograph by Gary Settles (CC BY-SA 3.0).
\(^2\)Based on the work of A. Laitinen on recovery boiler secondary air supply.
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\[ k = \frac{2\pi}{\lambda} \] (i.e. at large scales where wavelength \( \lambda \) is large), while dissipation occurs at high wavenumbers (small scales). Based on the classical theory of Kolmogorov [42, 43], the energy spectrum in the intermediate scales follows a power law, \( E(k) \propto k^{-5/3} \) [41].

In Publications I-III, the relatively low Reynolds numbers of the flows allow for directly resolving most of the flow structures. In general, this is not the case as the large scale separation between the smallest and largest scales of the flow complicates the numerical solution. Hence, different turbulence modeling approaches and models have been developed to emulate the convective and diffusive mixing effects on the unresolved scales. In direct numerical simulation (DNS) [44], all the relevant time and length scales of the flow are resolved. Hence, no modeling is required, but the approach is prohibitively expensive in most cases. In contrast, the effect of the entire turbulent spectrum is modeled in the Reynolds-averaged Navier-Stokes (RANS) equations [45]. RANS is computationally affordable, but involves sophisticated models that may be lacking in more complex flow scenarios. Large-eddy simulation (LES) [46], on the other hand, is positioned between the two approaches both in terms of resolution and computational cost. In LES, the motion of the large, energy-containing turbulent structures are resolved, while the effect of the sub-grid scale turbulence is modeled. Figure 1.4 (c) illustrates the distinction between a RANS and LES solution.

1.4.2 Primary atomization

Atomization refers to a liquid breakup process. Common examples of atomization include water sprinklers, hair sprays and water fragmentation from a garden hose. The overall atomization process is traditionally divided into the primary and secondary phases. Figure 1.5 (a) illustrates the phases in the case of liquid film disintegration. In primary atomization, the injected sheet undergoes breakup due to sheet instabilities and forms the first generation of ligaments and droplets. In secondary atomization, the generated droplets repeatedly breakup into smaller droplets due to aerodynamic forces. Finally, the breakup process ends when the droplets are small enough to be stabilized by the surface tension forces. In contrast to secondary atomization, primary atomization is strongly influenced by the flow configuration and other case specific details.

Primary atomization has been studied computationally in various canonical flow configurations, including round jets [47–50], planar liquid sheets [51, 52], and jets in cross-flows [53, 54]. In particular, liquid sheet breakup has close relevance to the present work. The breakup mechanisms include the wavy disintegration and perforation modes [21]. Primary atomization models are commonly based on the wavy disintegration mode [52]. Such models have been employed for example for multidimensional reacting
sprays [55].

The works by Dombrowski et al. [56, 57] were among the first to describe the wavy disintegration mode. The process is illustrated in Figure 1.5 (b). Aerodynamic interaction of the sheet with the surrounding gas results in an instability and growing waves on the sheet. Linear stability analysis has been used to identify the fastest growing, i.e. the most unstable, wave. In the inviscid analysis of a planar liquid sheet by Squire [58], the wavelength of the most unstable mode was determined to be:

$$\lambda = \frac{4\pi \sigma}{\rho_g U^2}$$  \hspace{1cm} (1.3)

where $\sigma$ is the surface tension, $\rho_g$ is the density of gas, and $U$ is the velocity of the sheet. Subsequently, Ponstein [59] carried out a similar analysis on a rotating annular jet, while analyses of planar sheets have been later extended to account e.g. for the liquid viscosity [55, 60]. The growing waves result in thickness variations of the sheet [61]. Due to the thinning, the sheet ruptures creating liquid structures of the size influenced by the wavelength. The structures evolve further under the action of surface tension and form ligaments. Finally, the ligaments break into droplets via the Rayleigh-Plateau instability [61]. It is well acknowledged that the onset of liquid instabilities in a primary breakup process can be sensitive to the incoming turbulence level and boundary conditions [49]. Furthermore, in certain conditions the most unstable mode may not be the mode finally leading to the disintegration of the sheet [52, 62].

Figure 1.5. (a) Atomization of a liquid sheet from a flat fan nozzle.\(^1\) (b) Schematic of the primary atomization process of a liquid sheet by wave disintegration.

\(^1\)Photographs reproduced from Kooij et al. [61] (CC BY 4.0).
1.4.3 Two-phase flow regimes

Bubbly flow inside an atomizer is studied in Publication III with close relevance to gas-liquid flows in pipes. Such flows have been extensively studied [63–66] due to their practical importance e.g. in nuclear, oil and gas, and process industry sectors. Different flow regimes can be identified depending, for example, on pipe orientation and relative direction of phase velocities. As an example, Figure 1.6 shows the flow regimes present in vertical co-current pipe flow [67]. (1) In the bubbly flow regime, the gas is distributed as discrete bubbles in the continuous liquid. (2) In the slug flow regime, the gas accumulates into large gas slugs, called Taylor bubbles, which have sizes comparable to the pipe diameter. (3) In the churn flow regime, the flow enters an unstable and oscillatory regime with characteristics from both slug and annular flow. (4) In the annular flow regime, a continuous gas core is formed with annular liquid film on the walls. Liquid droplets may be entrained to the core. (5) In the wispy annular flow regime, significant amount of droplets are present in the core where they coalesce and form larger liquid wisps.

With relevance to liquid spraying, two-phase flow modes are utilized in effervescent atomization [68, 69]. In this technique, the liquid is aerated inside the nozzle and the resulting two-phase flow topology is used to destabilize the injected liquid stream, and thus, to enhance breakup. Publication III studies such flow conditions in the context of swirl atomizers. Effervescent atomizers have been studied both experimentally [70–72] and by numerical simulations [73–75]. More information about the relevant literature can be found in Publication III.

![Figure 1.6. Flow regimes in vertical co-current two-phase pipe flow.](image-url)
1.5 Research gaps and objectives

Based on the review of the relevant literature, the following gaps in the current knowledge are identified:

- Previous works on pressure-swirl atomizers have mainly concentrated on small-scale nozzles with symmetric designs. In contrast, here a large-scale nozzle with outlet orifice diameter of \( \sim 2 \) cm is studied. Additionally, the nozzle poses significant asymmetric features which distinguishes it from typical designs.

- Injection of biomass-based fuels is often characterized by the high viscosity of the liquid. Consequently, the Reynolds number of the flow is relatively low despite the large size of the used nozzles. Currently, full understanding of the atomizer flow dynamics and key parameters is lacking for the presently studied parameter range.

- In certain situations, gas bubbles may be present inside an injector. Based on the literature, it remains unclear how the bubbles interact with the flow in a complex swirl nozzle. Although the destabilizing effect of the inner-nozzle two-phase flow is utilized in effervescent atomizers, effervescent-swirl atomizers have remained relatively unstudied. Furthermore, studying a bubbly flow in an atomizer acts as a first step in understanding nozzle operation at flash boiling conditions.

The novelty of the present work lies in the application of scale-resolving numerical simulations to study a large-scale swirl nozzle of Figure 1.1 in parameter range and conditions relevant for industrial fuel injection. The main objectives of the work are: (1) to understand the atomizer flow physics, including both the inner-nozzle flow and liquid sheet dynamics, at a low-Reynolds-number range (Publications I and II), and (2) to explore the influence of bubbly flow to the swirl atomizer flow dynamics and initial sheet breakup (Publication III).

Additionally, the studies aim at providing quantitative information on the atomizer key parameters, such as the spray opening angle, discharge coefficient, and film velocity. Such information has practical relevance for example in the development of injection profiles for Lagrangian spray sub-models. In addition, the applicability of the present computational approach is assessed with sensitivity tests, numerical benchmarks and experimental validation.
2. Methodology

2.1 Governing equations

The numerical solution of the gas-liquid system is based on the one-fluid formulation [76]. The mass and momentum conservation equations for the flow system are written as:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]  

\[ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \rho \mathbf{g} + \nabla \cdot \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + f_\sigma \delta_s \]  

Above, \( \rho, \mathbf{u}, p, \mu, \sigma, \) and \( \mathbf{g} \) are the density, velocity, pressure, viscosity, and gravity vector, respectively. In the one-fluid formulation, a single set of equations is written for the mixture of the two fluids, while the capillary force, \( f_\sigma, \) present at the gas-liquid interface is included as a singular force [76]. The Dirac delta function, \( \delta_s, \) obtains value of 1 at the interface and 0 elsewhere.

In this work, the flow is assumed to be incompressible. The density in Equations 2.1 and 2.2 may vary within the solution domain and is allowed to be discontinuous (variable density flow). However, due to incompressibility, each individual fluid element retains its density as it is advected in the domain. This can be formally expressed as the material derivative of the density being zero:

\[ \frac{D \rho}{Dt} = 0 \]  

By combining Equations 2.1 and 2.3, the mass conservation simplifies to:

\[ \nabla \cdot \mathbf{u} = 0 \]  

Therefore, the same incompressibility condition as in single-phase flows holds for two-phase flows without mass transfer between the phases.
The gas and liquid phases are distinguished from each other by a discontinuous indicator function (Heaviside function):

\[
H(x, t) = \begin{cases} 
1 & \text{if } x \text{ in liquid} \\
0 & \text{if } x \text{ in gas}
\end{cases}
\]  

(2.5)

With the help of the indicator function, the fluid properties in the solution domain can be defined as \( \rho = H \rho_l + (1 - H) \rho_g \) and \( \mu = H \mu_l + (1 - H) \mu_g \). By combining the above definition of density with Equations 2.1 and 2.4, it is possible to write an evolution equation for the indicator function:

\[
\frac{\partial H}{\partial t} + \nabla \cdot (H u) = 0
\]  

(2.6)

Although the indicator function is deeply connected with the volume-of-fluid method, other methods for advecting different types of marker functions can be used in connection with the one-fluid formulation. Some of the most popular approaches include the volume-of-fluid (VOF) [77], level-set (LS) [78], front tracking (FT) [79] and phase-field (PF) [80, 81] methods. In addition, there exists multiple methods that combine characteristics of the aforementioned approaches, such as the conservative level-set (CLS) [82] or the coupled level-set and volume-of-fluid (CLSVOF) methods [83]. An overview of different schemes can be found for example in the review by Mirjalili et al. [84]. Next, the VOF approach utilized in this work is introduced.

### 2.2 Volume-of-fluid method

The volume-of-fluid method is based on solving the evolution of the discontinuous indicator function according to Equation 2.6. Because the exact indicator function cannot be represented on a discrete grid, its numerical counterpart is formed by integrating \( H \) over the cell \( C_i \):

\[
\alpha_i = \frac{1}{V_i} \int_{C_i} H(x, t) dV
\]  

(2.7)

Above, \( V_i \) is the cell volume, and thus \( \alpha_i \) defines a cell-wise volume fraction of the liquid. In other words, \( \alpha_i \) is a volume-averaged representation of the indicator function \( H \). Unlike \( H \), the volume fraction may obtain values between 0 and 1 in cells where the interface is located. The distinction between the functions is illustrated in Figure 2.1 (a) and (b). Similarly, the cell-wise fluid properties may be defined based on the volume fraction:

\[
\rho_i = \alpha_i \rho_l + (1 - \alpha_i) \rho_g
\]  

(2.8)

\[
\mu_i = \alpha_i \mu_l + (1 - \alpha_i) \mu_g
\]  

(2.9)
Next, let us examine Equation 2.6 in terms of the volume fraction. By integrating Equation 2.6 over a cell volume and time interval \((t, t + \Delta t)\), the new volume fraction can be solved as:

\[
\alpha_i(t + \Delta t) = \alpha_i(t) - \frac{1}{V_i} \sum_{j \in N_i} \int_t^{t+\Delta t} \int_{F_j} H(x, \tau)u(x, \tau) \cdot dSd\tau
\]  

(2.10)

On the right hand side, Gauss’s theorem was used to transform the volume integral to a sum of surface integrals over the faces \(F_j\) the cell has with its set of neighboring cells \(N_i\). The integral

\[
\Delta V_j(t, \Delta t) \equiv \int_t^{t+\Delta t} \int_{F_j} H(x, \tau)u(x, \tau) \cdot dSd\tau
\]

(2.11)

gives the total volume of fluid entering/exiting the cell through the face in the time interval \(\Delta t\). It should be noted, that Equation 2.10 is exact, and the approximation of the integral of Equation 2.11 is the fundamental problem of the VOF approach [76, 85]. The value of \(\Delta V_j\) is very difficult to accurately estimate due to the sensitivity to the local distribution of the two fluids inside the cell and the relative orientations of the interface with the cell faces [85]. For example, if a planar liquid front reaches a parallel face, the integrated function is discontinuous and non-differentiable with respect to \(\tau\). For this reason, the advection problem is extremely challenging to solve with conventional tools of numerical analysis which rely on the existence of a Taylor series expansion (smooth functions) [85].

In practice, the aforementioned challenges lead to a question: how to advect a discontinuous function such that it remains sharp and bounded? Several approaches have been devised in order to achieve these goals. The schemes can be broadly divided into two categories: algebraic and geometric methods [84, 86]. In algebraic methods, conventional continuum-based discretization schemes are utilized. Such methods include, for example, the high resolution interface capturing scheme (HRIC) [87], the compressive interface capturing scheme for arbitrary meshes (CICSAM) [88], the tangent of hyperbola for interface capturing scheme (THINC) [89], and the multidimensional universal limiter with explicit solution (MULES) [90].
In contrast, geometric schemes take advantage of geometrical operations to approximate the solution of the VOF equation. In such methods, the sub-cell location of the interface is first reconstructed, and subsequently used in the advection step to approximate the face fluxes. For interface reconstruction, most of the current methods are variants of the piecewise linear interface calculation (PLIC) method in which the sub-cell interface is approximated with a line in 2d and plane in 3d (see Figure 2.1 (c)). However, several method options exist for finding the normal vector of the gas-liquid interface needed in PLIC, including Youngs’ method [91], the mixed Youngs-centered (MYC) method [92], and the efficient least-squares VOF interface reconstruction algorithm (ELVIRA) [93]. Similarly, there are multiple choices for the interface advection algorithm [92, 94, 95]. A review on geometric VOF methods on unstructured meshes is given by Marić et al. [86]. A fairly recent geometric scheme, named isoAdvector, is used in this work and will be introduced next in more detail.

2.3 isoAdvector scheme

The geometric volume-of-fluid method, isoAdvector, by Roenby et al. [85] is used to estimate the volume fluxes of Equation 2.10. As in other geometric VOF methods, the reconstruction and advection steps form the main body of the algorithm. The novelty of isoAdvector consist of (1) using an iso-surface in the sub-cell interface reconstruction, and (2) a straightforward method for flux estimation in the advection step. Due to the complexity of geometric operations on 3d unstructured meshes, geometric methods have been more commonly utilized on structured meshes [86]. The present procedure is fairly straightforward to implement on general unstructured meshes [85] and involves only a modest computational cost [96].

Following Roenby et al. [85], an overview of the isoAvector method is given in Algorithm 1. Next, the interface reconstruction and advection steps are described in more detail. The discussion follows Refs. [85] and [97], from where more information about the implementation can be found.

2.3.1 Interface reconstruction

The first step in a geometric VOF method is to find the sub-cell location ($x_s$) and orientation ($n_s$) of the phase interface based on the volume fraction values $\alpha_i$ available at the cell centers. The present method uses the concept of iso-surface to reconstruct this interface and to divide the cell into two parts: one fully immersed in liquid and the other in gas.

Standard iso-surface evaluation in a general polyhedral cell operates on vertex data. Therefore, the volume fraction values at cell centers are first interpolated to the cell vertices (inverse distance weighting). For a
Algorithm 1: isoAdvector

1 For all faces $j$, initialize $\Delta V_j$ with the upwind method
2 Find all surface cells $i$, i.e. cells where $\varepsilon < \alpha_i < 1 - \varepsilon$ (Here, $\varepsilon = 10^{-6}$)
3 for all surface cells do
   4 Reconstruct the sub-cell interface (Sec. 2.3.1)
   5 Execute the advection step to obtain $\Delta V_j$ for all the faces downwind of the cell (Sec. 2.3.2)
4 end
6 For all cells $i$, update $\alpha_i$ according to Eqs. 2.10 and 2.11
7 For cells $i$ where $\alpha_i < 0$ or $\alpha_i > 1$, apply a conservative bounding procedure to readjust $\Delta V_j$ and to recalculate $\alpha_i$. The step includes also an optional non-conservative clipping procedure to strictly enforce $0 \leq \alpha_i \leq 1$

Given iso-value $f$, the iso-surface intersects a cell edge, if the value $f$ lies between the interpolated vertex values $f_j$ and $f_k$. The intersection point $x_{cut}$ can then be calculated with linear interpolation as:

$$x_{cut} = x_j + \frac{f - f_j}{f_k - f_j} (x_k - x_j)$$  \hfill (2.12)

Above, $x_j$ and $x_k$ are the vertex coordinates. By applying the same procedure for all the edges of the cell, a set of points defining the iso-surface is generated as shown in Figure 2.2. Based on this information, it is then possible to calculate the volume of the sub-cell separated by the iso-surface. The volume evaluation is geometric and based on the division of the sub-volume using pyramid decomposition [97].

It is important to note, that the appropriate iso-value $f$ is not known beforehand. For physical consistency, the value should be chosen such that the cell is cut in the proportion given by the cell volume fraction $\alpha_i$. By defining the cell volume fraction as a function, $\tilde{\alpha}(f)$, the correct iso-value $f^*$ should satisfy

$$\tilde{\alpha}(f^*) \equiv \frac{V_l(f^*)}{V_i} = \alpha_i,$$  \hfill (2.13)

where $V_i$ and $V_l$ are the volumes of the cell and the liquid sub-cell, respectively. Note that $f^*$ may be different for each cell which implies that the iso-surface between different cells may not necessarily be continuous.

In fact, Equation 2.13 represents a non-linear problem which requires finding a root $f^*$ using a properly chosen numerical method. In general, such a numerical procedure would require iterative evaluation of the function $\tilde{\alpha}$, which is expensive due to the repeated geometric calculation of the sub-cell volume. Fortunately, the process can be greatly accelerated by using additional information. First, it is advantageous to reorder the vertex values, $f_k \in \{f_1, ..., f_n\}$, in ascending order. Second, $\tilde{\alpha}(f) \in [0, 1]$ is a
monotonically increasing function in the interval \( f \in [f_1, f_n] \). And third, \( \tilde{\alpha} \) is a cubic polynomial of \( f \) in each sub-interval \( f \in [f_k, f_{k+1}] \) formed by two adjacent vertices. Therefore, the search for \( f^* \) can be restricted to a single sub-interval by first calculating \( \tilde{\alpha} \) at all the vertex values. In the sub-interval containing \( \alpha_i \), two additional \( \tilde{\alpha} \) evaluations at intermediate points are needed to solve the coefficients of the cubic polynomial. Finally, the polynomial can be used in conjunction with the iterative Newton’s method to efficiently solve for \( f^* \). If for some reason the polynomial coefficients cannot be determined, the algorithm can revert back to a more expensive iterative solution with direct geometric \( \tilde{\alpha} \) evaluation.

The overall purpose of the reconstruction step is to find the location \( (x_s) \) and surface normal \( (n_s) \) of the sub-cell interface. When the correct iso-value \( f^* \) is known, the appropriate iso-surface can be evaluated, and \( x_s \) and \( n_s \) can be estimated, thus completing the reconstruction step.

### 2.3.2 Interface advection

In the advection step, the reconstructed sub-cell interface is transported by the local velocity field during the time step \( \tau \in [t, t + \Delta t] \) which enables the estimation of the transferred volume of fluid \( \Delta V_j \). In practice, such velocity information is available at the cell centers (velocities, \( u_i \)) and at the faces (total volumetric fluxes, \( \phi_j \)). However, this information is only available at the start of the time step. Therefore, the following simplifying assumptions are made: (1) the velocity is constant during the time step, \( u(x, \tau) \approx u(x, t) \), and (2) the velocity at a face is constant and given by the face flux, \( u(x, t) \cdot dS \approx \phi_j(t) dS / S_j \), where \( S_j \) is the area of the face. With these approximations the integral in Equation 2.11 becomes:

\[
\Delta V_j(t, \Delta t) \approx \frac{\phi_j(t)}{S_j} \int_t^{t+\Delta t} \int_{F_j} H(x, \tau) dS d\tau \equiv \frac{\phi_j(t)}{S_j} \int_t^{t+\Delta t} A(\tau) d\tau \quad (2.14)
\]
Methodology

Figure 2.3. Sub-cell interface advection. (a) The face-interface intersection line (dashed line) sweeps a sub-area of a cell face (gray area) during a time step. (b) During each time interval \([t_k, t_{k+1}]\), the intersection line sweeps a quadrilateral. Here, the interval \([t_3, t_4]\) from (a) is shown.

Above, the integral \(A(\tau)\) denotes the submerged area of the face at the time \(\tau\). The time evolution of the submerged area is needed to evaluate the integral and, therefore, the transferred volume of fluid.

During the time step, the sub-cell interface is approximated to move with a constant velocity normal to itself. To estimate the interface velocity \(u_s\), the local velocity field is interpolated from the cell centers to the center of the interface \(x_s\). Additionally, the component normal to the interface is obtained by the dot product \(U_s = u_s \cdot n_s\).

The next step is to consider the evolution of the face-interface intersection line as visualized in Figure 2.3. As the interface moves with the velocity \(U_s\), it crosses the face vertices \(x_k\) in a certain order at time instances \(t_k\) estimated as:

\[
t_k \approx t + (x_k - x_s) \cdot \frac{n_s}{U_s}
\]  

(2.15)

In the time interval between two consecutive crossing times, the intersection line sweeps a quadrilateral area as shown in the figure. By including the time step beginning \((t_1 = t)\) and end \((t_{M+1} = t + \Delta t)\) to the set of times \(t_k\), and by excluding the vertices outside the interval \([t, t + \Delta t]\), the entire face area swept by the intersection line during the time step can be subdivided into \(M\) quadrilaterals. Therefore, the time integral of the submerged area can be subdivided as:

\[
\int_{t}^{t+\Delta t} A(\tau)d\tau = \sum_{k=1}^{M} \int_{t_k}^{t_{k+1}} A(\tau)d\tau
\]  

(2.16)

With this procedure, the time integral over the changing submerged part of a general polygonal face is reduced to multiple integrals over much simpler quadrilateral shapes. Furthermore, in each interval \([t_k, t_{k+1}]\) only one quadrilateral is filling/emptying, while the others are either fully submerged or empty.
The time integral over a changing quadrilateral area is calculated as follows. As shown in Figure 2.3 (b), such a quadrilateral is defined by the points $A$, $B$, $C$ and $D$. The location of the intersection points, $\tilde{C}(\tau)$ and $\tilde{D}(\tau)$, change in time and are approximated by linear interpolation similar to Equation 2.12:

$$\tilde{D}(\tau) = A + \frac{\tau - t_k}{t_{k+1} - t_k} (D - A) \quad (2.17)$$

$$\tilde{C}(\tau) = B + \frac{\tau - t_k}{t_{k+1} - t_k} (C - B) \quad (2.18)$$

Due to the linear dependency of the intersection line locations on $\tau$, the function $A(\tau)$ will be a second order polynomial. The polynomial coefficients can be directly solved by geometrical consideration of the quadrilateral area. When the coefficients are known, the time integral of Equation 2.16 can be analytically solved. By combining the results for the sub-integrals, the transferred volume of fluid $\Delta V_j$ is obtained thus concluding the advection step. It should be noted, that $\Delta V_j$ through a face is determined based on the motion of the sub-cell interface in the cell upwind of the face.

### 2.4 Surface tension and gravity forces

The surface tension force is handled with the continuum surface force (CSF) approach [98]. In CSF, the capillary force is expressed as:

$$f_\sigma \delta_s = \sigma \kappa \n \delta_s = -\sigma \kappa \nabla \alpha \quad (2.19)$$

where the latter equality follows from the properties of the Heaviside and Dirac functions [76]. Above, $\n$ and $\kappa$ are the interface normal and curvature, respectively, and the force expression is valid for constant surface tension $\sigma$. Here, a simple approach is taken to compute the curvature directly from the volume fraction field

$$\kappa = -\nabla \cdot \n = \nabla \cdot \left( \frac{\nabla \alpha}{|\nabla \alpha|} \right) \quad (2.20)$$

Other methods for determining the curvature include, for example, height functions (HF) [99–101] and the parabolic reconstruction of surface tension (PROST) method [102]. Accurate curvature evaluation is still an active research topic. For example the height function method, despite having good convergence properties, has been mainly utilized on Cartesian grids [103] and may need specialized treatment of under-resolved parts of the solution [104]. Recently, advances have been made to achieve HF like convergence on unstructured grids, however, these developments have been thus far applied only on 2d meshes [105].
To enable consistent treatment of the gravity and pressure gradient forces, the momentum equation is reorganized in terms of a modified pressure [103]:

\[ p_{rgh} = p - \rho g \cdot x \]  

(2.21)

With the modified pressure, the gravity and pressure gradient terms are expressed as:

\[ -\nabla p + \rho g = -\nabla p_{rgh} - (g \cdot x) \nabla \rho \]  

(2.22)

The final form of the momentum equation is obtained by inserting the CSF expression of the surface tension and modified pressure in Equation 2.2:

\[ \frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho uu) - \nabla \cdot \mu (\nabla u + \nabla u^T) = -\nabla p_{rgh} - (g \cdot x) \nabla \rho - \sigma \kappa \nabla \alpha \]  

(2.23)

In Equation 2.23, the terms on the right hand side should balance each other out when \( u = 0 \). To numerically achieve the balance, \( \nabla p_{rgh} \) and \( \nabla \alpha \) should be discretized consistently using the same numerical discretization [106]. The same applies to the gravity term because \( \nabla \rho = (\rho_l - \rho_g) \nabla \alpha \).

Methods that possess such discrete balance and recover the equilibrium solutions are often called well-balanced methods [103]. Well-balanced treatment of the gradient terms has been demonstrated for the numerical solution method used in the present work [90].

### 2.5 Flow solution

The solution for the system of Equations 2.4, 2.6 and 2.23 is obtained with a pressure-based, segregated solution procedure in the OpenFOAM framework. For the pressure-velocity coupling, the pressure implicit with splitting of operators (PISO) method [107] is used. An equation for the pressure is needed in the solution. Here, a semi-discrete equation is derived following Ref. [108]. First, the momentum equation (Eq. 2.23) is written in a semi-discrete form as:

\[ a_P u_P + \sum_N a_N u_N + E_P = -\nabla p_{rgh} + S_P \]  

(2.24)

where the subscripts \( P \) and \( N \) refer to the current cell and its neighboring cells, respectively. Above, the coefficients \( a_P, a_N \) and \( E_P \) depend on the velocities, but not on the to-be-solved velocities of the current iteration. Similarly, the coefficients \( S_P \) include the effect of the gravity and surface tension terms. By defining \( \mathcal{H}(u) \equiv S_P - \sum_N a_N u_N - E_P \), the velocity in cell \( P \) can be formally solved as:

\[ u_P = \frac{\mathcal{H}(u)}{a_P} - \frac{1}{a_P} \nabla p_{rgh} \]  

(2.25)
By taking the divergence of this equation and using the incompressibility condition of Equation 2.4 ($\nabla \cdot \mathbf{u}_P = 0$), a Poisson equation for the pressure is obtained:

$$\nabla \cdot \frac{1}{a_P} \nabla p_{rgh} = \nabla \cdot \frac{\mathcal{H}(\mathbf{u})}{a_P}$$  \hspace{1cm} (2.26)

With these ingredients, the solution process can be formulated.

The outline of the solution using the PIMPLE, i.e. PISO-SIMPLE, method of OpenFOAM is presented in Algorithm 2. As previously mentioned, the pure PISO mode is used here, and therefore, the number of SIMPLE iterations is set to $m = 1$. After the VOF solution and fluid property update, the PISO coupling is executed on lines 5-10. As the new pressure is not yet known in the momentum predictor step, the pressure from the previous time step is used to update the velocity. In this work, the optional predictor is not used. During the PISO iteration, the velocity is corrected with the new pressure obtained from the Poisson solution. Similarly, $\mathcal{H}(\mathbf{u})$ is updated before each pressure solution although the coefficients $a_P, a_N, E_P$ and $S_P$ remain unchanged. Small number of iterations, typically $n = 3 - 5$, is used in this work. More details on the exact discrete forms and solution procedure in general can be found, for example, in Refs. [90, 108, 109].

### 2.6 Other numerical details

Similar discretization schemes and solution methods are used in Publications I-III. Spatial derivatives are approximated with second-order schemes, while the second-order implicit backward scheme is used for time integration of the momentum equation. Multigrid solver with the Gauss–Seidel smoother is applied to obtain a solution of the pressure equation. Adaptive mesh refinement (AMR) has been utilized outside the nozzle to capture the liquid film dynamics in Publications I and II. In Publication
III, AMR was not used. For more information about the usage of AMR, the reader is referred to Publication I.

In the investigated cases, the inner-nozzle flow is in the low-Reynolds-number range. In most of the cases, the flow inside the nozzle is laminar and can be considered to be well resolved on the studied grid resolutions (see mesh sensitivity tests in Publications II and III). Even at the higher end of the studied range \((Re = 5300)\), the relatively low \(Re\) permits a scale-resolving simulation strategy. As such strategy, the implicit LES approach is used [110–112]. The convection term in the momentum equation is discretized with a non-linear flux limiter [113] to provide suitable numerical diffusion to account for the sub-grid scale turbulence. Similar approach has been used extensively both by the group and others in various flow scenarios and applications, such as homogeneous turbulence [111, 114], free shear flows [115, 116], wall bounded flows [117, 118], heat transfer [119, 120], and reactive flows [121, 122]. The flux limiter is also used in the laminar cases to provide the necessary numerical stabilization.

Further details on the used numerical methods, including information on the computational domains and grids, boundary conditions, complementary validation cases and sensitivity tests, can be found in Publications I-III.
3. Summary of results

The main scientific findings of the thesis are presented in the appended Publications I–III. Next, a summary of the results is given.

3.1 Publication I

In Publication I, a large-scale pressure-swirl atomizer was studied at $420 \leq Re \leq 5300$ by carrying out a viscosity sweep. The parameter range covers both laminar and fully turbulent inlet conditions relevant for high-viscosity liquid injection. Both the inner-nozzle flow and the onset of liquid sheet breakup were explored by the present simulations. Adaptive mesh refinement was utilized outside the nozzle to resolve the dynamics of the liquid sheet.

The four studied cases revealed a range of different flow conditions as summarized in Table 3.1 and Figure 3.1 (a). An S-shaped liquid film was observed for laminar flow ($Re = 420$), while the presence of a helical and rotating gaseous core resulted in a hollow cone liquid film at $Re \geq 1660$. The results indicate a liquid sheet of mixed type for $Re = 830$. The observed S-shaped mode was noted to differ from the regimes reported for typical pressure-swirl atomizers. The difference was explained by the asymmetry of the present nozzle design.

In addition, the gas core and the film thickness at the nozzle orifice were

<table>
<thead>
<tr>
<th>$Re$</th>
<th>$\mu_l$ [mPas]</th>
<th>Inlet pipe flow</th>
<th>Swirl chamber turbulence level</th>
<th>Air core</th>
<th>Near field spray pattern</th>
</tr>
</thead>
<tbody>
<tr>
<td>420</td>
<td>395</td>
<td>Laminar</td>
<td>Laminar</td>
<td>No</td>
<td>S-sheet</td>
</tr>
<tr>
<td>830</td>
<td>200</td>
<td>Laminar</td>
<td>Laminar, unsteady</td>
<td>No</td>
<td>In transition</td>
</tr>
<tr>
<td>1660</td>
<td>100</td>
<td>Laminar</td>
<td>Moderately turbulent</td>
<td>Yes</td>
<td>Hollow cone</td>
</tr>
<tr>
<td>5300</td>
<td>31.2</td>
<td>Turbulent</td>
<td>Fully turbulent</td>
<td>Yes</td>
<td>Hollow cone</td>
</tr>
</tbody>
</table>
Summary of results

Figure 3.1. Graphical summary of Publication I: (a) Overview of the liquid film and gas core characteristics at different $Re$. (b) The liquid film thickness at the orifice ($\delta$) agrees with correlations from the literature [123, 124], but exhibits large temporal fluctuations. (c) The mass flux ($j_m$) pattern becomes more uniform as $Re$ is increased.
observed to fluctuate significantly. As depicted in Figure 3.1 (b), the mean film thicknesses with respect to the orifice diameter were $\delta/d_o = 0.39$ and $0.35$ at $Re = 1660$ and $5300$, respectively. Similarly, the film thickness fluctuations were 25% and 18% of the mean. The large fluctuations may be explained by the helical structure of the gas core inside the swirl chamber. In contrast, for lower Reynolds numbers, the gas core was absent and the orifice was fully covered by liquid.

It was also established, that the uniformity of the mass flow pattern increases with the Reynolds number as shown in Figure 3.1 (c). The non-uniformity was attributed to the non-uniform velocity field at the discharge orifice due to the asymmetry of the nozzle geometry.

To conclude, Publication I provides a detailed description of the versatile flow physics occurring in the present swirl nozzle. The study covered a relatively wide Reynolds number range where the atomizer flow was found to be developing in terms of the turbulence level, gas core presence and spray pattern. In practice, the observation suggests sensitivity of the injection process to the exact spraying parameters in the present parameter range.

### 3.2 Publication II

Publication II continued the work of Publication I. A flow rate sweep was carried out to study a focused Reynolds number range of $600 \leq Re \leq 910$. The main objective of the study was to conduct a detailed comparison between numerical simulations and experimental measurements. The experiments were carried out by the co-authors using high-viscosity water-glycerol mixture and various measurement techniques, including laser-Doppler anemometry, high-speed imaging and pressure measurements. For the numerical solution, the same approach as in Publication I was utilized. In addition to evaluating the performance of the numerical method, the aim was to apply the complementary approaches of simulations and experiments in order to gain insight to nozzle flow phenomena at a parameter range relevant for high-viscosity liquid injection.

Consistent with the results of Publication I, laminar inner-nozzle flow and a relatively weak developing gaseous core were observed in the studied $Re$ range (see Figure 3.2 (b)). Outside the nozzle, the liquid film was continuous and of hollow cone type. The film was noted to be highly unstable in the present conditions where a developing gas core was present. The instability was apparent from the large temporal fluctuations of the tilt and opening angles of the spray. In addition, the film velocity was quantified and shown to depend linearly on the Reynolds number as depicted in Figure 3.2 (a).

Inside the nozzle, the numerical simulations were in agreement with
Summary of results

**Figure 3.2.** Graphical summary of Publication II: (a) The film velocity increases linearly with $Re$. (b) Time-averaged indicator field at the swirl chamber and below orifice. The gas core develops and the film uniformity increases with $Re$. (c) Simulated tangential mean velocity profiles inside the swirl chamber agree well with the measured ones. The profiles are taken at 10–30 mm from the chamber roof.
the experiments. Best correspondence was noted for the mean velocity profiles inside the swirl chamber as shown in Figure 3.2 (c). Outside the nozzle, the main liquid sheet features were correctly predicted despite small differences between the real and virtual nozzle geometries and the uncertainty of the experimental flow parameters. In addition, numerical sensitivity tests indicated that the solution was fairly insensitive to the mesh resolution and the exact inlet condition.

To conclude, Publication II extended the analysis of Publication I at a focused $Re$ range and presented new numerical and experimental results. The combined approach of simulations and experiments was found to be highly beneficial in analyzing the flow system. Moreover, the numerical method was validated against the experiments at the studied parameter range.

### 3.3 Publication III

In Publication III, a swirl atomizer with bubbly inlet flow was investigated. The study was a direct continuation to the previous publications as the single-phase inlet flow cases from Publication II were used as reference. In the present study, the gas-to-total volumetric flow rate ratio ($\beta = 0.07$, 0.20 and 0.33) and initial bubble size ($d = 5–15$ mm) of the bubbly flow were varied. The study targeted relatively large gas structures resolvable by the VOF approach. The aim was to investigate the atomizer flow in cases where considerable amount of gas is present inside the nozzle, for example, due to liquid aeration or flash boiling.

The inner-nozzle flow was found to be significantly affected by the value of $\beta$. As depicted in Figure 3.3 (a), the initially spherical gas bubbles deform and undergo breakup inside the inlet pipe and enlargement regions. Inside the swirl chamber, a bimodal bubble size distribution was observed consisting of both small and large gas structures. Both the size of the largest structures and the scale separation between the two size groups increased with $\beta$. In addition, the effective gas core diameter at the discharge orifice was noted to increase with $\beta$.

The liquid film outside the nozzle was also noted to be influenced by $\beta$. The near-orifice film was mainly continuous, and therefore, the total resolved interfacial area was used to quantify the films susceptibility to breakup. As shown in Figure 3.3 (b), the interfacial area depends strongly on $\beta$. At $\beta = 0.07$, 0.20 and 0.33, the area was observed to increase by 6%, 20% and 40% with respect to a corresponding case with single-phase inlet flow. Furthermore, the spray uniformity was enhanced at $\beta = 0.33$ compared to the corresponding single-phase case.

For the intermediate case $\beta = 0.20$, the exact bubble size at the inlet ($d = 5–15$ mm) did not have a significant effect on the flow characteristics. The
Figure 3.3. Graphical summary of Publication III: (a) Bubbly flow inside the inlet pipe section of the nozzle at various flow rate ratios ($\beta$) and inlet bubble diameters ($d$). (b) The increasing amount of resolved interfacial area in the near-nozzle spray indicates susceptibility to earlier breakup with increasing $\beta$. (c) The bubble size PDF inside the swirl chamber is insensitive to the exact inlet bubble size at $\beta = 0.20$. 
flow at the swirl chamber, discharge orifice, and the liquid film were shown to be fairly insensitive to the bubble size as demonstrated, for example, by the bubble distribution at the swirl chamber in Figure 3.3 (c).

The results of the study suggested that the liquid film is influenced, and its breakup may be controlled, by the amount of gas introduced to the inlet stream. On the contrary, the exact size of the added gas structures was shown to have a weaker effect at the studied parameter range.
4. Conclusions and future work

4.1 Conclusions

As presented in Publications I-III, scale-resolving numerical simulations were carried out to study two-phase interfacial flows in the context of liquid injection. The investigations featured a large-scale pressure-swirl nozzle with significant asymmetric features. The inner-nozzle flow and liquid sheet characteristics were studied at low-Reynolds-number conditions and with both single-phase and bubbly inlet conditions. Such flow conditions are relevant for injection of viscous liquids in industrial applications. The overall conclusions of the dissertation are as follows.

Detailed description of the atomizer flow dynamics was provided. The flow was noted to be highly dependent on the Reynolds number at the studied low-$Re$ range. Most noteworthy, $Re$ was shown to affect the gas core development stage and the spray pattern. S-shaped, transitional and hollow cone spray patterns were demonstrated as the Reynolds number was increased from fully laminar ($Re = 420$) to intermediately turbulent conditions ($Re = 5300$). Furthermore, the flow field inside the nozzle was observed to directly influence the liquid sheet dynamics. The film thickness decreased with increasing $Re$ in agreement with previous literature. In addition, the spray uniformity was noted to improve with increasing $Re$.

Bubbly atomizer flow was found to strongly affect the liquid film characteristics as well as the general nozzle flow dynamics. The film stability was highly dependent on the amount of gas in the bubbly inlet stream. On the contrary, the exact size of initial gas structures had only a weak effect on the flow characteristics.

In addition, several quantitative metrics, including the discharge coefficient, film velocity, spray opening and tilt angles, and the film thickness, were determined as functions of $Re$. Knowledge of such atomizer key parameters has practical relevance for example in developing injection sub-models to be used in other CFD investigations.
Finally, the requirements for scale-resolving simulations in the context of large-scale swirl nozzles were evaluated by numerical benchmark tests, sensitivity assessments and by validation against experimental measurements. The results indicated the applicability of LES in the present context. The problem, particularly liquid sheet breakup, is inherently unsteady, and therefore, a scale-resolving solution strategy is desired. However, such strategy requires considerable computational resources especially when film disintegration is considered. Yet with regard to the inner-nozzle flow quantities, a fairly coarse grid resolution was sufficient to capture the main characteristics of the present low-Re flows. Finally, the inner-nozzle flow dynamics were demonstrated to be connected to the evolution of the near-nozzle liquid film. Therefore, a coupled solution strategy is advised.

4.2 Suggestions for future work

The present work has primarily focused on the flow characteristics inside the swirl nozzle with simplifying assumptions made about the fluid properties. Several avenues can be pointed out for future studies to deepen the understanding on high-viscosity liquid injection.

First, high-fidelity simulations concentrating on the near-nozzle liquid film alone could bring further insight on the primary breakup. By excluding the nozzle, the computational resources could be focused specifically on the spray region. Furthermore, the solution domain would be simplified (a box) which would enable the use of VOF methods utilizing highly efficient adaptive mesh refinement strategies on structured Cartesian grids. However, as the present research points out, the internal flow in the nozzle has significant effect on the early liquid film dynamics. This effect should be incorporated in such simulations. One possibility could be through time dependent boundary conditions generated from separate preliminary simulations where the nozzle is included.

Second, the methodology presented in the thesis could be used to probe wide injection parameter ranges or in optimizing injector geometries. However, the relatively high computational cost of LES would be a prohibiting factor in such an endeavor. Nonetheless, even rather coarse simulations provide fairly accurate results on selected metrics as shown by the mesh sensitivity assessments of Publication II and III. Large number of such simulations could be carried out to extract trends over wide parameter ranges and to test the performance of various nozzle designs.

Third, flash boiling conditions may be encountered in certain injection applications. In such conditions, the spray breakup mechanisms change and the numerical solution method needs to consider variety of new factors. These include, but are not limited to, bubble nucleation, boiling mass transfer, coupled energy solution, and complex fluid properties. Numerical
methods capable of considering these aspects would be highly advanta-
geous in gaining new insights to nozzle flow phenomena and would greatly 
enhance the understanding of flash boiling injection from large-scale swirl 
nozzles.

Last, further experimental work would be beneficial to establish high-
quality validation data on large-scale swirl atomizers at wider parameter 
range and on additional metrics. Further validation data is especially 
important, and increasingly more difficult to obtain, when moving towards 
more complex fluid properties or boiling conditions. However, at these 
relatively unexplored conditions, such data is fundamental for proper 
validation of the possible computational approaches.
References


References

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