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Data Driven Design of Flow Blurring Atomizer

Cihan Ates[1], Abdallah Alshanawani[1], Rainer Koch[1], Hans-Jörg Bauer[1]
1. Institute of Thermal Turbomachinery, Karlsruhe Institute of Technology, Karlsruhe, BW, Germany.

Abstract
Liquid atomization relies on a variety of forces that disturb the surface of the liquid. In the case of flow-blurring (FB) atomization, turbulent structures are induced within the liquid channel to achieve this effect. It is known that the transition from the conventional flow-focusing (FF) pattern to the flow-blurring regime occurs at a specific geometric configuration and gas-to-liquid ratio (GLR). This transition causes the gas phase to flow partially upstream into the liquid channel, creating a back-flow mixing region. The behavior of internal recirculation is characterized by the gas penetration depth, GLR, and the geometry of the system. However, the dynamic nature of the turbulent structures responsible for generating transient micro-scale ligaments is still unclear, particularly in regards to the evolution of three-dimensional (3D) gas phase structures at the interface and their correlation with the shear acting on the liquid surface. To address this knowledge gap, the current investigation aims to establish a database of the transient nature of gas phase coherent structures across a range of operating conditions and nozzle designs. The primary objective is to shed light on the momentum transfer mechanism that underpins this process. For that purpose, a 3D computational domain for the FB nozzle geometry is prepared, and alternative modelling strategies for gas phase turbulence in the COMSOL Multiphysics® environment were tested on the high-performance computer system, BW UniCluster 2.0. Preliminary analysis was followed by a second grid refinement study for the selected large eddy simulation (LES) model configuration. In the next phase of the work, the gas phase flow at different phases of the cyclic FB atomization process was modelled, considering various operating points and geometric configurations. Flow asymmetry and the 3D nature of the flow structures were assessed using similarity-based methods and recurrence plots. The transient shear distribution on the liquid surface and its dependence on flow regime shifts and geometry were quantified. By placing virtual pressure sensors in the annular region during the simulations, different machine learning (ML) models, such as Lasso, Support Vector Machines (SVM), Random Forests, and Artificial Neural Networks, were trained and tested. The aim was to explore the optimal sensor configuration for capturing informative signals and determine whether it is possible to estimate surface shear using simple pressure measurements in a real setup. The analysis revealed that it is not only possible to characterize the flow regime shifts with a single pressure sensor but also estimate the shear acting on the surface. Moreover, the use of multiphysics software like COMSOL® enables the creation of a digital twin of the complex process, which can be leveraged for designing a test rig. Overall, this study contributes to a better understanding of the intricate dynamics involved in flow-blurring atomization. The outcomes have implications for optimizing atomizers in various applications, such as combustion systems and spray coating processes. Additionally, the integration of machine learning techniques and simulation tools opens up possibilities for improving the efficiency of atomization simulations and guiding future experimental investigations.
Keywords: Flow-Blurring, Computational Fluid Dynamics, Machine Learning, Simulation, Data Analysis, Large Eddy Simulation.

Introduction
Fossil fuels have been the primary energy source for electricity and combustion-based transportation since the 1900s. However, their limited supply and environmental impact have necessitated efficient and sustainable utilization. Long-distance air travel relies on kerosene combustion in jet engines. Enhancing combustion efficiency through atomization, the process of breaking liquid into smaller droplets, is crucial for reducing emissions and fuel consumption. This research focuses on pneumatic "flow-blurring (FB) atomizers" and aims to optimize air velocity and gas-to-liquid ratio (GLR) to improve atomization efficiency, thereby addressing environmental concerns and promoting sustainable aviation.
FB atomizers rely on the formation of a turbulent flow in the liquid, which is caused by incoming air at high velocity and the geometry of the atomizer. The incoming air velocity and gas-to-liquid ratio (GLR) are the two parameters that are controlled to achieve higher atomization of the fluid. Larger atomization leads to smaller droplet size and therefore higher combustion efficiency. This research paper aims to improve the atomization through geometry and constant real-time optimization of the atomization through changes in the air inlet velocity. The geometry of FB atomizers will be investigated through computational fluid dynamics (CFD) simulations to find out the optimal geometry for the best atomization efficiency. The CFD simulation results will be processed and relationships between the shearing of the liquid and pressure waves in the atomizer will be extracted.

Flow Blurring Atomization Concept
The roots of the flow-blurring concept date back to 2005, thanks to Ganan-Calvo's [1] pioneering research on FB atomization. This work unveiled a

key idea: when a crucial geometry factor, known as ψ = h/d, dips below 0.25, it triggers a fascinating effect. Backflow appears within the liquid jet, creating intense turbulence. FB atomization shares similarities with effervescent atomization, which involves injecting air into a liquid stream before ejection from the orifice. The mode of atomization is determined by the GLR ratio, which can range from internal bubbly flow at lower ratios for slug flow, and annular flow at higher ratios. Droplets can be produced at lower gas-to-liquid ratios than standard airblast atomization. FB atomization, like effervescent atomization, increases interphase mixing by creating a large gas-liquid contact area, which can benefit combustion applications.

The base geometry used in this work is depicted in Figure 1. Herein, the parameter ψ (i.e., h/d ratio) has been considered to be of critical importance, as it is one of the main factors that determines whether the flow exhibits a flow-focusing (FF) or FB pattern. In the early studies, having a value of ψ > 0.25 typically resulted in a flow-focusing pattern that leads to the formation of liquid micro-jets. In other words, the atomizer behaves like an airblast atomizer. When the value of ψ decreases below 0.25, the flow pattern at the feed tube's mouth underwent a significant divergence where the gas flow becomes radial, and a stagnation point forms between the feed mouth and the exit orifice [1]. As a result, the gas flows upstream into the liquid tube and mixes turbulently with the incoming liquid, creating a fine, mist-like spray plume [1].

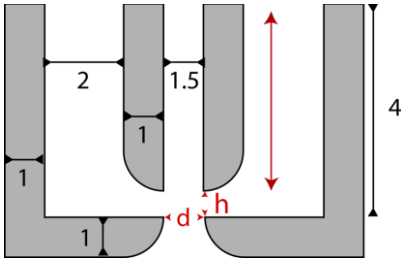

Figure 1: Geometry of FB Atomizers, scaled similar to the work of Ganan-Calvo [1].

Recent experimental and numerical studies further revealed that [2,3] transition from flow focusing to flow blurring is more intricate and influenced by factors like geometry, mass flow rates, gas-liquid ratio (GLR), and the h/d ratio. Ates et al. recently demonstrated a strong connection between coherent flow structures and the shape of the orifice, both inside and outside the nozzle [3]. Additionally, solely considering the h/d ratio or GLR is insufficient to classify the atomization process. In their test cases, among the nine expected flow-blurring scenarios, only one exhibited effective gas penetration and fine atomization within the nozzle, while the other eight resembled flow focusing atomization [3].

Objective of the Study

The core objective of this paper is to analyse how different geometries of FB nozzles influence atomization and to establish a data-driven method for predicting atomization. Currently, assessing atomization relies on high-resolution images to measure droplet sizes and spray angles, which is not requires complex measurement and post-processing techniques. As an alternative, in this work, we will combine the CFD and Machine Learning (ML) models to compare the atomization performances of alternative designs and operating conditions by analyzing virtual pressure probe readings within the nozzle. The aim is to uncover the relationship between the temporal pressure signals and shear acting on the liquid surface, and evaluate the similarities in pressure and velocity fields within different geometries via data driven techniques.

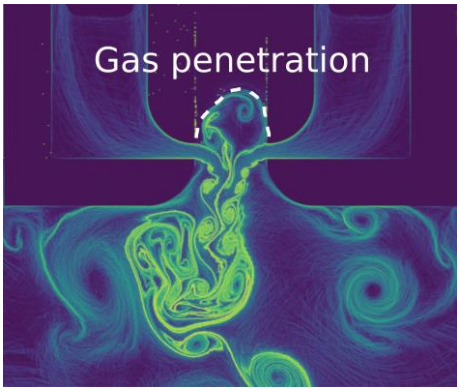

Figure 2: Curved surface of liquid from the work of Ates et al [3].

This research features several key objectives. Firstly, 3D nature of the flow structures is analysed in limiting case scenarios via similarity-based methods. This is done to assess the limitations of 2D transient simulations, and to decide the number and the location of the virtual pressure probe sensors for the flow regime classification. The second objective involves scrutinizing how distinct gas structures in different geometries affect the shearing of the liquid surface. For that purpose, ML techniques are used to create a data-driven model that uses pressure readings to predict shear forces acting on the liquid surface.

Problem Description

The high-level objective of this work is to examine how different nozzle geometries affect the atomization process for internally mixed-nozzles. The approach utilized to determine the optimal geometry involves conducting CFD simulations of the FB nozzle. Ideally, a two-phase simulation is employed, where the model simulates both the liquid, air, and their interaction, which enables the examination of droplet formation and shearing phenomena of the liquid surface that is occurring within the FB nozzle and downstream spray due to coherent turbulent structures. However, it should be

noted that conducting a two-phase simulation is associated with certain limitations, including prolonged duration and substantial computational resource consumption. The acquisition of accurate data on the two-phase flow necessitates the employment of accurate simulations, resulting in computationally intensive simulations. Given that the research also involves exploring different geometries, it is preferable to utilize less complex models to facilitate the exploration of a wider range of geometries. Furthermore, our previous analysis showed that the FB atomization process exhibits a cyclic two-phase flow behavior [3]. To facilitate the parametric study, we investigated two meta-stable ligament states, during which the liquid phase exhibit a pseudo-steady state behaviour at short time scales, and act like a "pseudo-wall" [3]. Specifically, the behavior of the liquid during FB is noted to exhibit a distinct ligament geometry: the gas-liquid interface is pushed inwards (Figure 2). Herein, the curvature depth is based on the work of Murugan and Kohle (2021) [2] based on the the Laplace Number.

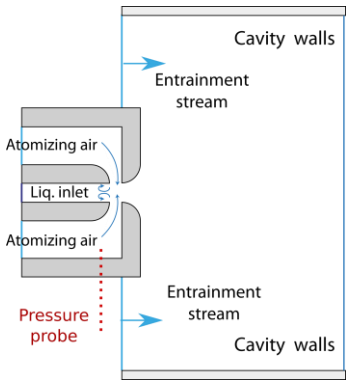

Figure 3: Simplified simulation domain.

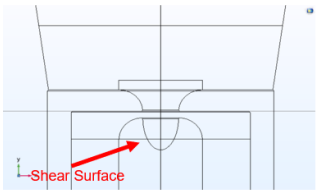

Figure 4: Pseudo-state surface of fuel with 1.5mm depth.

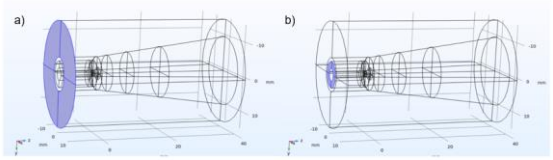

Figure 5a) Inlet for peripheral flow. 5b) Inlet for atomizing air.

In these limiting scenarios, the 3D transient gas phase flow at different phases of the atomization process is modelled via Large Eddy Simulation (LES). An overview of the boundary conditions and the location of the liquid surface in one of the limiting cases are shown in Figure 3 and Figure 4, respectively. 3D view of the inlet boundaries for the peripheral and the atomizing air is depicted in Figure 5.

Flow asymmetry and the 3D nature of the flow structures were by calculating Hellinger and Wasserstein distances between velocity and pressure distributions, along with using recurrence plots. Subsequently, we used the collected simulation data to train multiple machine learning-based predictors, including LASSO, Random Forest (RF), Support Vector Machines (SVM), and Artificial Neural Network (ANN), to evaluate the informativeness of virtual pressure probes. Scikit-learn and TensorFlow libraries are used for the shallow and ANN models, respectively.

Modeling & Numerical Setup

Nozzle Geometries

We tested the base geometry initially proposed by Ganan-Calvo [1], along with three other derivatives. The main difference between the derivative designs are the cap, through which the air runs. The different geometries were assessed based on the shear acting on the pseudo-liquid surface. These geometries can be seen in Figure 6.

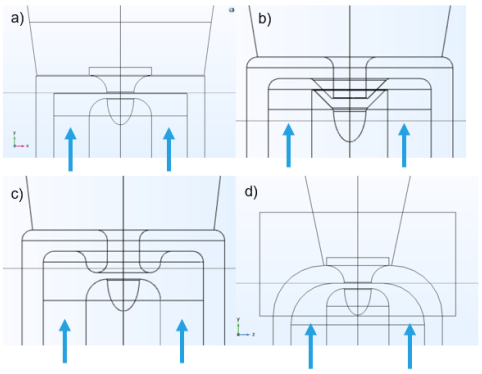

Figure 6a: Base Geometry. 6b: Case Geometry 1. 6c) Case Geometry 2. 6d) Case Geometry 3. Blue arrow represents airflow.

Operating Conditions

Prior research into FB technology predominantly concentrated on assessing the impact of GLR on atomization. Since the single-phase simulations employed here exclude the presence of liquid, the principal parameter under investigation is the inlet velocity of air.

The air inlet velocity is modeled based on the required airflow rates for combustion within jet engines. For the tested nozzle dimensions and h/d ratios, this is translated into air inlet velocities of 1.2 m/s and 2.8 m/s, which in turn leads to spray velocities of 52.8 m/s and 123.2 m/s, respectively (the velocity of air after exiting the nozzle). Velocities surpassing this threshold are not factored into the analysis due to limitations imposed by the simulation solver, which solely accommodates

incompressible flow. This velocity approximation remains reasonable, as air is deemed incompressible until it approaches a Mach number of approximately 0.3 [4], with the Mach number defined as the flow velocity divided by the speed of sound. In this scenario, simulations are conducted under ambient conditions with a temperature of 293.15 K and a pressure of 1 atm, equating to a speed of sound of 343 m/s. By reducing the inlet's cross-sectional area by a factor of 44, a corresponding increase in velocity is achieved, considering constant density. Dividing the two areas of the inlet and outlet area derives a cross-sectional area reduction factor of 44. As this simulation assumes incompressible flow, the initial velocities are augmented by a factor of 44, yielding velocities of 52.8 m/s and 123.2 m/s. In the context of the case study, nozzles experience a peripheral airflow at a velocity of $10 ms^{-1}$ (Figure 5). This airflow can significantly impact downstream spraying and lead to pressure waves propagating back into the FB nozzle. Atomizing air is introduced once the peripheral flow is developed.

Numerical Setup

CFD is a powerful tool for in-depth analysis of fluid behavior in diverse applications, ranging from aerospace to industrial processes. At its core, it leverages advanced numerical methods to solve the Navier-Stokes equations, which govern the intricate interplay of mass, momentum, and energy conservation within a fluid. Herein. the computational domain is discretized, employing sophisticated techniques such as finite volume, finite difference, or finite element methods. Through iterative procedures, CFD solves these governing equations to attain either steady-state or unsteady-state solutions, providing invaluable insights into the dynamic behavior of fluids.

For our CFD simulations, we employ COMSOL Multiphysics, specifically utilizing its CFD module. To enhance computational efficiency and reduce processing time, our simulations are conducted in parallel on high-performance computing cluster BwUniCluster 2.0. In tackling single-phase turbulent flows, we turn our attention to Large Eddy Simulation (LES). LES focuses on the larger turbulent structures, while efficiently modeling the smaller, sub-grid scales. This approach employs grid-based elements to simulate the dominant turbulent features directly, making approximations for the sub-grid scales. LES is particularly advantageous in complex scenarios, including those encountered in aircraft turbulence and combustion systems.

In the simulations, we defined boundary conditions for walls, inlets, and outlets under standard conditions (1 atmospheric pressure and 293.15K), mimicking spray characterization experiments. The inlets of the peripheral airflow and the atomizing airflow are defined as the surfaces of the inlet, while the outlet is the surface parallel to the inlets, placed on the opposite side of the geometry (Figure 5). The walls are subjected to boundary conditions that are defined as follows:

1. The wall is assumed to be stationary.
2. The velocity of the fluid at the wall is zero, i.e., the no-slip boundary condition.
3. The temperature of the wall is constant.
4. The wall is impermeable, i.e., no mass or fluid can pass through it.
5. The wall roughness affects the flow in the immediate vicinity of the surface.

The initial conditions of the inlet velocities are set to zero to accommodate the complexity of the simulation at different time scales of the atomization process. To overcome this limitation, the inlet velocities for the peripheral air and FB nozzle inlet are introduced later in time using a Gaussian Step Function with smoothing, which is multiplied by the inlet velocities. Peripheral flow is introduced as soon as the simulation starts, while atomizing air will start at a time in the simulation when the peripheral air is fully developed.

Mesh Analysis

The accuracy of CFD simulations is influenced by the quality of the mesh, which includes the number of cells, their size and shape, and their arrangement. A well-designed mesh can ensure accurate and efficient simulations, while a poorly designed mesh can result in errors, instability, and longer simulation times. It is therefore important that the best mesh coarseness is chosen, one that is fine enough to capture the coherent structures, and coarse enough that the simulations are calculated in a reasonable time. In this work, the main regions of interest are the FB region in Figure 7, where air interacts with liquid, and after the nozzle, namely in the domain $-1.5mm < y < 4.0mm$. These are the regions that were analyzed for the best mesh size and should have the finest mesh. The mesh sizes are gradually increased in the direction of the jet flow.

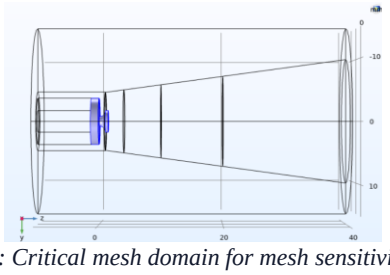

Figure 7: Critical mesh domain for mesh sensitivity analysis.

The whole mesh was created using tetrahedrons. Deployed mesh dimensions were found by a convergence analysis for the shear distribution on the pseudo-liquid surface.

For the mesh sensitivity analysis, 10 different cases were simulated. The table with the mesh dimensions is found in Table 1. The minimum and maximum dimensions of the mesh are listed in this table.

Additionally, the mesh growth along with the final number of elements that are found on the surface of the pseudo-state liquid. All these different models with different mesh dimensions were simulated using 5 nodes and 80 cores each, for 68 hours; from 0.03 seconds to 0.06 seconds. Table 2 shows a summary of the total number of elements, along with the real-time simulation and the mean shear that was calculated at the end. Finally, the mean shear for all simulations was calculated until 0.031697s as that is where the slowest simulation stopped. Cases 1-4 do not have information as they were stopped due to a lack of memory to support the simulation. They were eventually neglected because a convergence was already achieved. Therefore, all simulations will be run using the mesh dimensions of Case 7.

Case	Critical			
	Min (µm)	Max (µm)	Growth	Elements
1	5	45	1.04	25524
2	10	50	1.04	24706
3	15	55	1.04	15216
4	20	60	1.04	10640
5	25	65	1.04	7888
6	30	70	1.04	6080
7	35	75	1.04	5034
8	40	80	1.04	4064
9	45	85	1.04	3408
10	50	90	1.04	3000

Table 1: Cases 1-10 mesh sizes, critical domain.

Case	Total Elements	Time Simulated	Shear Mean [N/m2]	Shear Mean until 0.031697
1	89756248			
2	73127484			
3	50768129			
4	38449074			
5	30632405	0.031697	1.43	1.43
6	24990166	0.032349	1.42	1.53
7	20884359	0.032757	1.4	1.52
8	17806401	0.032956	1.47	1.62
9	15372850	0.033845	1.63	1.82
10	13454701	0.035154	1.77	1.98

Table 2: Shear results cases 1-10 mesh, critical domain.

Simulation Results

In all simulations, 400 cores distributed over 5 nodes were used to run the 3D transient simulations. In the following sections, a thorough comparison of the planes within the 3D geometries and an examination of the impact of the different gas structures on the liquid surface's shearing will be presented. Moreover, we will explain how the pressure readings inside the nozzle are utilized to predict the shear, and establish a data-driven approach for improving the atomization efficiency. These results provide new insights into how we can use CFD and analyse informativeness of virtual sensor data to effectively analyse alternative geometries for potential applications.

Convergence of Peripheral Flow

During the peripheral flow simulations, which lasted 0.05 seconds and had a time step interval of 0.001 seconds, it is observed that the velocity of the flow is initially unsteady and requires the first 0.01 seconds to stabilize. Subsequently, the flow exhibits an expected oscillatory behavior, which reaches steady state at around 0.025-0.030 seconds and continues until the end of the simulation. Atomizing air is therefore introduced at 0.025 seconds with a smoothening Gaussian step function (Figure 8).

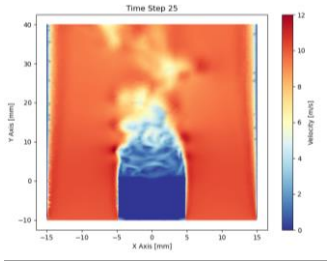

Figure 8: Peripheral flow at 0.025s.

Shear Distribution in Flow Focusing and Flow Blurring regimes

In this study, we first compared the mean shear curves of both the FF and FB regimes and observed a clear difference in both the mean values and the fluctuations of the mean and standard deviations (Figure 9). The results indicate that the FB regime exhibits more turbulent changes in the flow compared to the FF regime, which is evident from the mean shear plots. These findings are consistent with previous studies that have reported higher turbulence levels in the FB regime due to the unique atomization process, which involves the interaction of two liquid surfaces at high velocities.

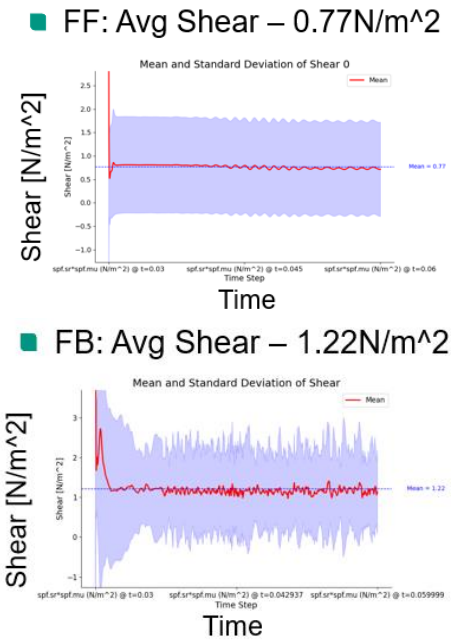

Figure 9: Shear graph over time of FF and FB results. Red line: mean shear. Blue region: mean +/- the 2nd standard deviation.

More importantly, shear distribution analysis revealed that the shift in the atomization mode from FF to FB atomization is very drastic (Figure 10). In the case of FF, the shear is acting on partial regions, which moves in angular symmetry. But the shape of the high shear region is persistent. In the case of FB

regime, however, the field is very dynamic and chaotic, and none of the two instances are alike (Figure 10).

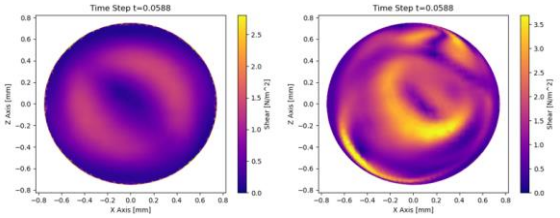

Figure 10: Contour plots of FF (left) and FB (right).

The recurrence plot (Figure 11) allows us to visualize the recurrence of states in the system over time and provides insight into the dynamics of the flow. The presence of many black-and-white areas in the FB simulation shows that the shear is highly fluctuating. These results suggest that there is high recurrence and fluctuation in the shear on the surface of the liquid, mainly in the FB regime.

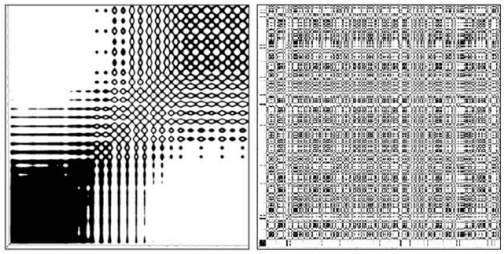

Figure 11: Recurrence plots of FF (left) and FB (right).

Effect of Nozzle Geometry

If we compare the mean shear curve of the base geometry to those of the four different geometries, it is seen that the base geometry and case 3 geometry outperform the others in terms of mean shear values, as observed on shear on the surface of the liquid. In fact, there is a factor of 3-4 difference in mean shear values than the other geometries on the curved liquid surface (Figure 12). This clearly shows the importance of the atomizing air entering the FB region perpendicularly. It is worth highlighting here that a small change to the geometry can drastically affects the mean shear that occurs on the surface of the liquid.

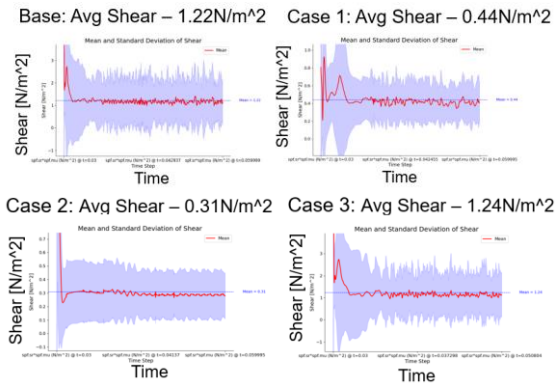

Figure 12: Shear graph over time of different geometries.

Velocity & Pressure Planar Symmetry

The main goal of this analysis is to investigate how many pressure measurements are required to reliably predict the shear on the liquid surface, as a preliminary step for an experiment design. In other words, comparing planes in the 3D model predictions enable us to identify (dis)similarities in different planes, and help us to determine the number and location of probes.

Figure 13 shows the velocity probability distributions at two different planes, where each curve denotes a different time step. The calculated Hellinger and Wasserstein distances between the planes at a given time t consistently yield negligible differences (<0.05), indicating that the instantaneous differences between the planes are not significant, and utilizing pressure sensors at one position can accurately represent the overall pressure distribution (Figure 14, 15).

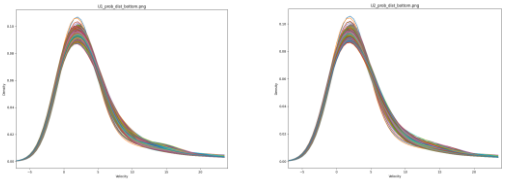

Figure 13: Velocity probability distribution of 2 different planes.

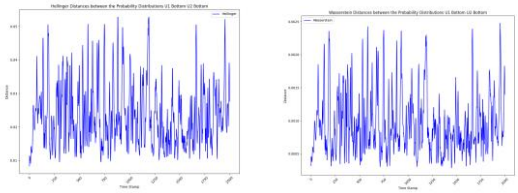

Figure 14: Hellinger and Wasserstein distance between velocity probability distributions. X axis denotes time step.

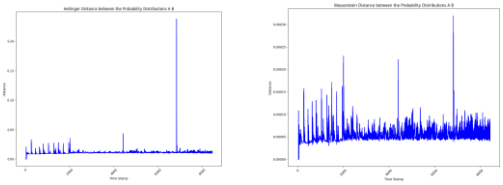

Figure 15: Hellinger and Wasserstein distance between pressure probability distributions. . X axis denotes time step.

Data-Drive Shear Prediction

Upon examination of the autocorrelation and partial autocorrelation plots, the partial autocorrelation plot indicated that a time window of 10 consecutive pressure readings should be employed to predict the instantaneous shear. For the regression analysis, Least Absolute Shrinkage and Selection Operator (LASSO), Support Vector Machines (SVM), Random Forrest Regression (RFR), eXtreme Gradient Boosting (XGBoost), and an Artificial Neural Network (ANN) were deployed. Performance of all the models on the test data were

found to be very similar, once the time series data with sliding windows are scaled and detrended (Figure 16). It is worth noting here that the ANN-based model was found to overfit, even with regularization, due to the limited amount of training data (Figure 17). The comparison showcases the value of shallow learners to achieve better generalization in the case of limited data.

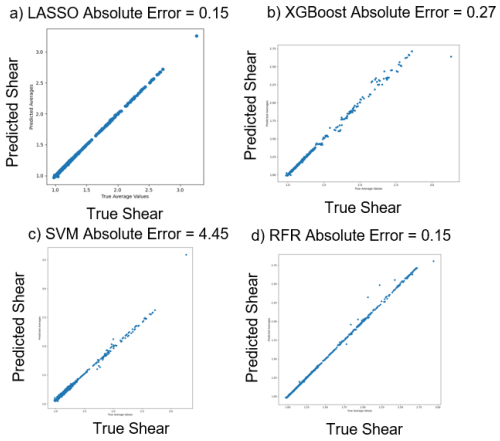

Figure 16. Results of the ML models for shear prediction.

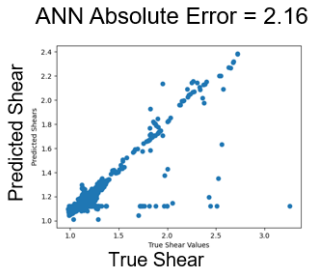

Figure 17. Results of the ANN for shear prediction.

The simpler ANN, with one hidden layer (3 neurons with ReLu activation functions) had a significantly increased performance. The optimizer used was an Adam optimizer and the loss function was a mean square error. The evaluation metric for the ANN was the mean absolute error. The final absolute error for all models was:

- LASSO: Absolute Error - 0.15
- RFR: Absolute Error – 0.27
- SVM: Absolute Error – 4.45
- XGBoost: Absolute Error – 0.27
- ANN: Absolute Error – 2.16

It is worth noting here that models with implicit feature selection capabilities such as LASSO has an advantage in sequence to target predictions, as it can learn to “pay attention” to most informative time steps of the (pressure) sequence.

Conclusions

This study aimed to investigate (i) the 3D nature of the gas phase structures in the nozzle at different operating regimes and (ii) the impact of different flow regimes and geometries on surface shear patterns and (iii) to predict shear using pressure readings at a single point through machine learning algorithms to quickly scan different nozzle designs in an experimental setup, without relying on complex measurement techniques. The results revealed that the FB regime exhibited more complex changes in flow than the FF regime, leading to higher atomization. Furthermore, the flow structures show a significant symmetry when we analyzed the flow focusing regime. The study also showed that the nozzle geometry has an impact on the shear distribution, and the shear distribution is influenced significantly with minor changes in nozzle curvature. Regarding the prediction of shear using pressure readings, the results showed that most models were able to predict shear to some degree for the raw data with minimal success. The reason for that is the high correlation between the parameters which necessitated the use of complex models to account for the nonlinearity and interaction between them. Therefore, by utilizing detrending methods, it was possible to use the predicted shear using pressure to a high degree with LASSO. The ANN had alternating results and prone to overfitting, even with regularization. The most successful ANNs were the simplest ones, mainly due to data limitations.

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