

# Dataset Generation and Denoising Diffusion Probabilistic Model Training for Supersonic Flow Field Prediction in an Atomization Nozzle

## Master Thesis

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## Description

The aim of this master thesis is to generate a comprehensive dataset of the flow field within a supersonic atomization nozzle and to train a diffusion model to accurately predict this flow field. Gas atomization is a critical process in various industrial applications, including the production of fine metal powders for additive manufacturing, pharmaceuticals, and materials engineering. Understanding and predicting the supersonic flow behavior in atomization nozzles can significantly enhance process efficiency and product quality.

## Introduction

Gas atomization involves the breakup of a liquid into fine droplets through the interaction with a high-velocity gas stream. This process is pivotal for producing uniform particle sizes, essential for industries relying on high-quality powders. The complexity of supersonic flow fields within atomization nozzles poses significant challenges for traditional modeling techniques due to the intricate interactions of shock waves, turbulence, and phase transitions. This thesis proposes leveraging advanced data-driven methods, specifically denoising diffusion probabilistic models (DDPMs), to predict these complex flow fields accurately.

## Objectives

- **Dataset Generation:** Create a detailed dataset of the supersonic flow field within an atomization nozzle using computational fluid dynamics (CFD) simulations.
- **Model Training:** Train a diffusion model on the generated dataset to predict the flow field within the nozzle under various operating conditions.
- **Model Validation:** Validate the accuracy of the diffusion model against experimental data and CFD results.

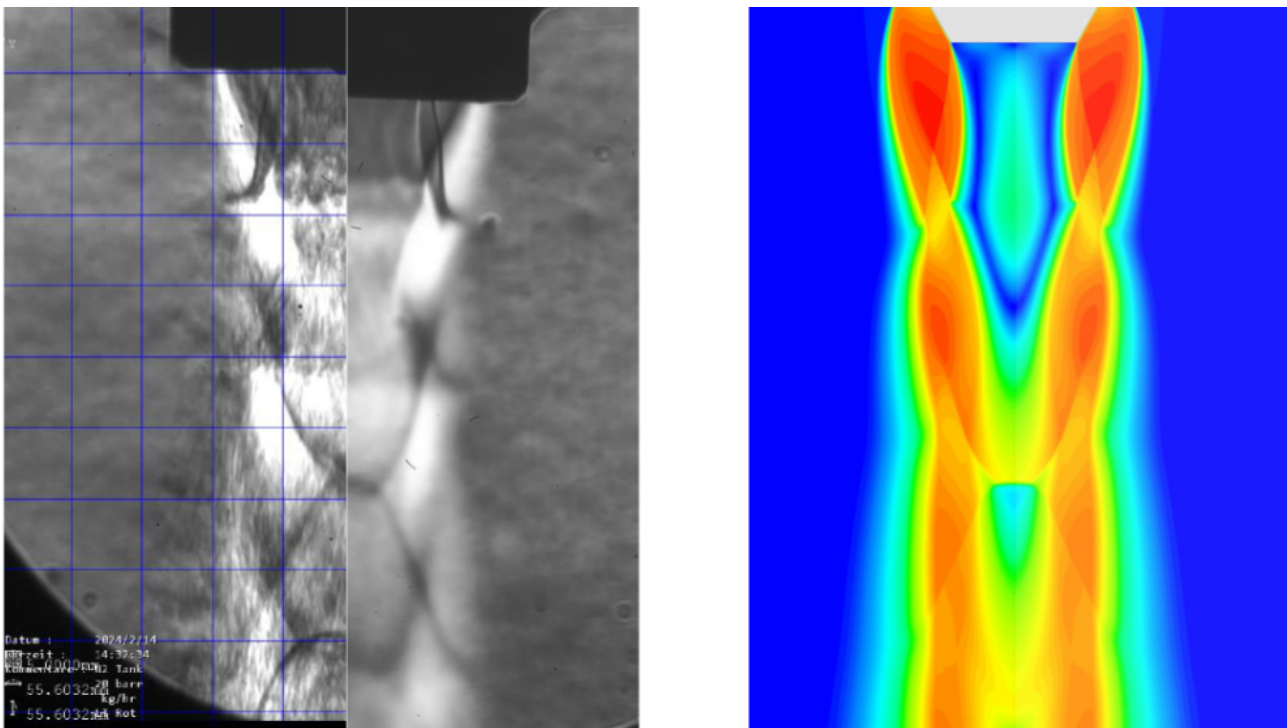
## Methodology

- **Literature Review:**
  - Review existing methods for modeling supersonic flow fields in atomization nozzles.
  - Assess the current state of diffusion models and their application in fluid dynamics.
- **Computational Fluid Dynamics (CFD) Simulations:**
  - Perform CFD simulations to model the flow using Ansys Fluent.
  - Validate simulation results with experimental findings to ensure accuracy.
  - Generate a diverse dataset encompassing a range of operational scenarios.
- **Dataset Preparation:**

- Preprocess the collected data to ensure consistency and remove noise.
- Annotate the dataset with relevant flow field characteristics (e.g., velocity, pressure, temperature).
- Split the dataset into training, validation, and test sets.
- Diffusion Model Training:
  - Develop a diffusion model architecture suitable for predicting complex flow fields.
  - Train the model using the prepared dataset, employing techniques such as data augmentation and regularization to enhance model robustness.
  - Fine-tune hyperparameters to optimize model performance.
- Model Validation:
  - Validate the trained model using the test dataset and experimental results.
  - Perform sensitivity analysis to evaluate the model's reliability under different conditions.

## Requirements

- Experience with Python.
- Basic understanding of CFD simulations.
- Basic understanding of Machine Learning.
- Ability to work independently and to learn new topics.



**Figure 1:** Left: Schlieren obtained from experiment. Right: Velocity-field obtained from CFD simulation.

Keywords: Supersonic Flow, Atomization Nozzle, Gas Atomization, Dataset Generation, Machine Learning, Diffusion Model, Computational Fluid Dynamics (CFD), Flow Field Prediction.