

# Full Injector Simulations of ECN Spray C

Mathis Bode<sup>\*,1,2</sup>

<sup>1</sup>Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

<sup>2</sup>RWTH Aachen University, 52056 Aachen, Germany

\*Corresponding author: [m.bode@itv.rwth-aachen.de](mailto:m.bode@itv.rwth-aachen.de)

## Abstract

The Engine Combustion Network (ECN) has defined several spray cases over the last years in order to increase the knowledge of physical processes related to injector flows. After heavily studying the Spray A case for many years, which was designed to suppress cavitation, the newer Spray C case moved into the main focus of interest recently. It has one hole and features cavitation inside the nozzle under diesel operation conditions. This work employs a high-fidelity simulation framework allowing one simulation featuring all different processes during the atomization process including nozzle flow. The simulation considers the real injector geometry evaluated with X-ray measurements. Gas effects inside the nozzle, such as cavitation or dissolved gases, are modeled with a homogeneous equilibrium model (HEM). To resolve the wide range of different length and time scales, a data-driven approach, called physics-informed enhanced super-resolution generative adversarial network (PIESRGAN), is used.

## Keywords

Engine Combustion Network, Spray C, Large-Eddy Simulation.

## Introduction

Reactive sprays are important for many industrial applications. Therefore, it is essential to fully understand all physical and chemical processes involved and derive accurate models for predictive simulations. The Spray C case defined by the Engine Combustion Network (ECN) [1] uses a 1-hole model injector for diesel injection under high temperature and high pressure conditions. The fluid is driven by a large pressure difference between upstream in the injector and downstream in the combustion chamber. As a consequence, typically high Reynolds numbers occur for diesel injection and the fluid becomes turbulent. In contrast to the Spray A case, also defined by the ECN, the Spray C case features cavitation in the nozzle, resulting in a tilted spray plume. Furthermore, the Spray C nozzle exit diameter is larger than the Spray A nozzle exit diameter, and the flame sits further downstream.

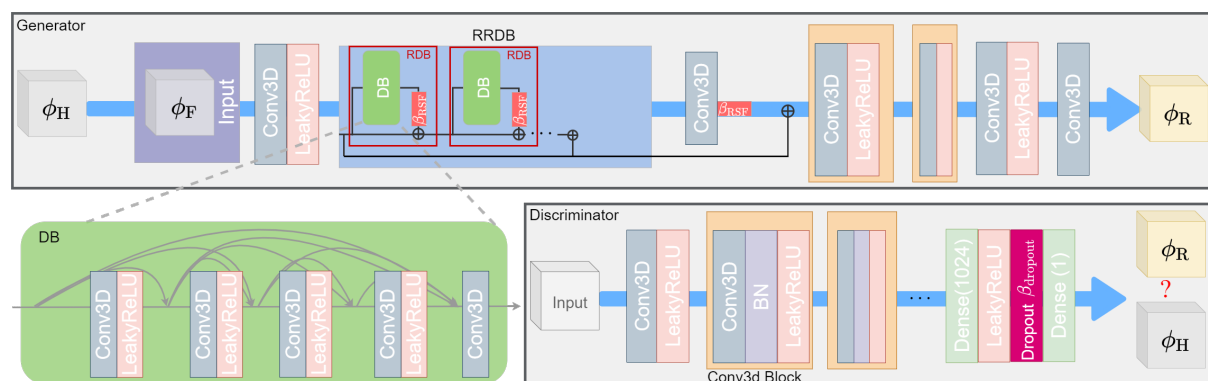
Simulations need to be able to accurately describe the flow of the fuel in the injector. Due to the shape of the injector, this includes the formation of cavitation. Furthermore, additional non-condensable gas is usually present in the nozzle either as it was originally dissolved in the fuel or as it penetrates the hole from the combustion chamber. Outside of the injector, the continuous liquid fuel breaks up into smaller ligaments and small droplets. These disperse droplets start evaporating, and the resulting vapor forms a reactive mixture with the ambient gas. Finally, combustion occurs, and the fuel oxidizes. The more the evaporation process and combustion are spatially separated, the more is the resulting combustion similar to classical non-premixed combustion.

Due to the variety of different processes with varying length and time scales, it is very challenging to capture all processes with one model or even one simulation approach. Therefore, coupled simulations [2] have been developed, which employ different simulation approach for different parts of the domain, such as nozzle flow, formation of discrete droplets, and evaporation and combustion process. Depending on the goal of the simulation, it is also well established to map all nozzle and near-nozzle effects into mass flow rate and spray plume angle combined with a simple blob model for the initial droplet size distribution. This paper presents a

new data-driven approach, called physics-informed enhanced super-resolution generative adversarial network (PIESRGAN) [3, 4, 5, 6, 7] which uses the same neural network trained with different data to cover all injector domains.

## Methods

A data-driven approach based on generative adversarial networks (GANs) is followed in this work to resolve the wide range of scales in a full injector simulation. The recently developed PIESRGAN is used for the whole domain. PIESRGAN is trained with direct numerical simulation (DNS) data to close subfilter contribution terms in the large-eddy simulation (LES) equations. The network is sketched in Fig. 1. The key idea for PIESRGAN is to AI super-resolve filtered flow fields to get fields similar to fully resolved flow fields, which are then used to close the LES terms.



**Figure 1.** Sketch of PIESRGAN. "H" denotes high-fidelity data, such as DNS data, "F" are corresponding filtered data, and "R" are the reconstructed data. The components are: Conv3D - 3D Convolutional Layer, LeakyReLU - Activation Function, DB - Dense Block, RDB - Residual Dense Block, RRDB - Residual in Residual Dense Block,  $\beta_{RSF}$  - Residual Scaling Factor, BN - Batch Normalization, Dense - Fully Connected Layer, Dropout - Regularization Component,  $\beta_{dropout}$  - Dropout Factor. Image from [8].

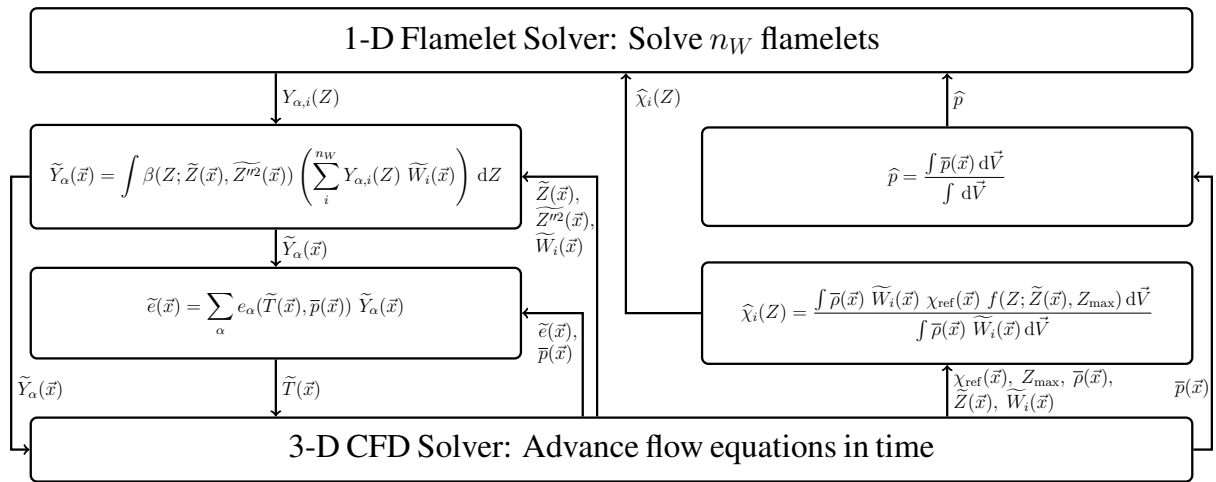
In general, PIESRGAN can be used with multiple combustion models and even finite-rate chemistry. The multiple representative interactive flamelet (MRIF) approach is used in this work. However, as pointed out by Bode [6], PIESRGAN is also used to replace the prescribed probability density function (PDF) approach for the distribution in mixture fraction space and the assumption for the scalar dissipation rate. The MRIF approach is sketched in Fig. 2, and a reaction by Yao et al. [9] was used for all simulations.

Furthermore, different physical models are employed either during runtime or for training of the data-driven approach. This includes a homogeneous equilibrium model (HEM) to consider the complex thermodynamic phenomena in the internal flow of an injector [10] and Volume-of-Fluid/Level Set methods for breakup [11, 12].

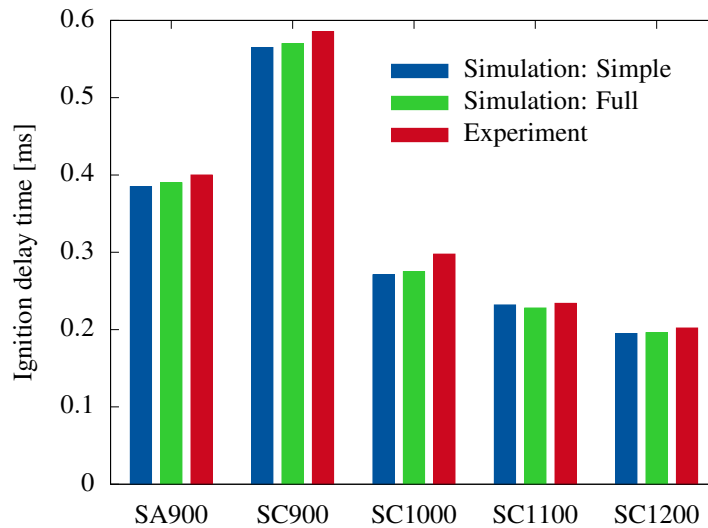
## Results and Discussion

The Spray C case was investigated at standard conditions with n-dodecane as fuel, 150 MPa injection pressure, 22.8 kg/m<sup>3</sup> ambient density, 15 % ambient oxygen concentration, 900 K ambient temperature, and 363 K fuel temperature. Furthermore, the ambient temperature was varied, resulting in a total of four cases with 900 K, 1000 K, 1100 K, and 1200 K ambient temperature. Moreover, one case was computed with the Spray A nozzle. The cases are denoted SA900, SC900, SC1000, SC1100, and SC1200 based on the used nozzle geometry and ambient temperature.

For all cases, two different simulation setups were computed and compared to experimental data. The simple setup only computed the flow outside of the nozzle using experimental data at the nozzle exit for initialization. The full setup computed the full injector employing pressure boundary conditions [13]. The results for the ignition delay time and lift-off length (LOL) are shown in Figs. 3 and 4.



**Figure 2.** Schematic representation of the MRIF approach. Tilde denotes Favre-filtered data. The overbar indicates Reynolds-averaging. The hat labels quantities in mixture fraction space.  $Z$  is the mixture fraction,  $W_i$  the flamelet weights,  $p$  the pressure,  $\chi$  the scalar dissipation rate,  $\rho$  the density,  $Y_\alpha$  the mass fractions,  $e$  the internal energy, and  $T$  the temperature.  $\beta$  denotes the presumed  $\beta$ -PDF, and  $f$  indicates the functional form of the scalar dissipation rate. The spatial coordinates are represented by  $\vec{x}$ , and integration over the volume of the full domain is described by  $\int d\vec{V}$ . All variables are time dependent, but  $t$  is omitted here for brevity. Image from Bode [6].



**Figure 3.** Ignition delay time for Spray A and Spray C cases.

The agreement for both simulations is reasonably well with the experimental data. Both ignition delay time and LOL are systematically underpredicted, which is probably due to the used reaction mechanism. For most cases, the full simulations are closer to experimental data, even though they use less information from the experiments.

## Conclusions

This short paper presents a data-driven-model-supported way to run full injector simulations of the ECN Spray C case. The results are in agreement with experimental data and do not require tuning or direct experimental input. Therefore, they are a very good basis to further understand processes involved or investigate the sensitivities of injection processes.

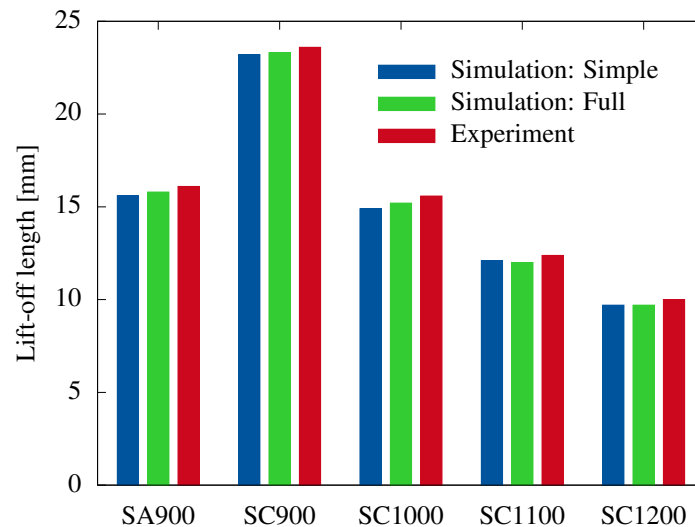


Figure 4. LOL for Spray A and Spray C cases.

### Acknowledgements

The authors acknowledge computing time grants for the projects JHPC55 and turbulencesl by the JARA-HPC Vergabegremium provided on the JARA-HPC Partition part of the supercomputer JURECA at Jülich Supercomputing Centre, Forschungszentrum Jülich, and funding from the European Union's Horizon 2020 research and innovation program under the Center of Excellence in Combustion (CoEC) project, grant agreement no. 952181.

### References

- [1] "Engine Combustion Network: <https://ecn.sandia.gov>." (2019). Accessed 2022-02-04, URL <https://ecn.sandia.gov>.
- [2] Bode, M., Falkenstein, T., Le Chenadec, V., Kang, S., Pitsch, H., Arima, T. and Taniguchi, H. "A New Euler/Lagrange Approach for Multiphase Simulations of a Multi-Hole GDI Injector." *SAE Technical Paper 2015-01-0949*.
- [3] Bode, Mathis, Gauding, Michael, Kleinheinz, Konstantin and Pitsch, Heinz. "Deep learning at scale for subgrid modeling in turbulent flows: regression and reconstruction." *LNCS Vol. 11887* (2019): pp. 541–560.
- [4] Bode, M. et al. "Development of Physics-Informed Enhanced Super-Resolution Generative Adversarial Networks for Subfilter Modeling." *arXiv preprint*.
- [5] Bode, M., Gauding, M., Lian, Z., Denker, D., Davidovic, M., Kleinheinz, K. et al. "Using physics-informed enhanced super-resolution generative adversarial networks for subfilter modeling in turbulent reactive flows." *Proceedings of the Combustion Institute Vol. 38* (2021): pp. 2617–2625.
- [6] Bode, M. "Applying Physics-Informed Enhanced Super-Resolution Generative Adversarial Networks to Large-Eddy Simulations of ECN Spray C." *SAE Technical Paper 2022-01-0503*.
- [7] Bode, M. *AI Super-Resolution: Application to Turbulence and Combustion, in: Lecture notes in energy: machine learning and its application to reacting flows*. Springer (2022).
- [8] Bode, M., Gauding, M., Lian, Z., Denker, D., Davidovic, M., Kleinheinz, K., Jitsev, J. and Pitsch, H. "Using physics-informed enhanced super-resolution generative adversarial networks for subfilter modeling in turbulent reactive flows." *Proc. Combust. Inst. Vol. 38* (2021): pp. 2617–2625.
- [9] Yao, T., Pei, Y., Zhong, B.-J., Som, S., Lu, T. and Hong Luo, K. "A compact skeletal mechanism for n-dodecane with optimized semi-global low-temperature chemistry for diesel engine simulations." *Fuel Vol. 191* (2017): pp. 339–349.

- [10] Bode, M., Maeda, K., Colonius, T. and Pitsch, H. “An equation-of-state tabulation approach for injectors with non-condensable gases: Development and analysis.” *10th International Cavitation Symposium* .
- [11] Le Chenadec, V. and Pitsch, H. “A 3D Unsplit Forward/Backward Volume-of-Fluid Approach and Coupling to the Level Set Method.” *Journal of Computational Physics* Vol. 233 (2013): pp. 10–33.
- [12] Le Chenadec, V. and Pitsch, H. “A monotonicity preserving conservative sharp interface flow solver for high density ratio two-phase flows.” *Journal of Computational Physics* Vol. 249 (2013): pp. 185–203.
- [13] Bode, M. and Schwarz, P. “On predictive nozzle simulations with advanced equations of state and pressure boundary conditions.” *SAE Technical Paper 2022-01-0504* .