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# Artificial Intelligence-Driven Surrogate Modelling for Nozzle Flow Simulation: A Review of Methods, Applications, and Challenges

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**Abstract**: *This review explores the transformative role of artificial intelligence in surrogate modelling for nozzle flow simulations, addressing the computational bottlenecks associated with high-fidelity computational fluid dynamics. Focusing on post-2020 advancements, the paper categorizes key methodologies into physics-based surrogates (such as Kriging and Radial Basis Functions), pure data-driven AI methods (including CNN-LSTM and Gaussian Processes), and AI-enhanced reduced-order modelling, such as Physics-Informed Neural Networks. Prominent applications are examined, ranging from high-precision flow rate prediction in sonic nozzles, achieving root-mean-square errors as low as 0.17%, to thrust optimization in aerospace components and real-time control of cold gas propulsion systems. While specific industrial cases have demonstrated significant speedup factors, significant challenges remain. These include data scarcity for specialized geometries, the difficulty of accurately resolving shock-wave discontinuities, and the inherent "black-box" nature of deep learning models, which complicates uncertainty quantification. The review concludes by identifying critical gaps in real-time industrial deployment and advocating for hybrid architectures that bridge the gap between data-driven flexibility and physical rigour to enhance model reliability in aerospace engineering.*

**Keywords**: Artificial intelligence, surrogate modelling, nozzle flow simulation, computational fluid dynamics, aerospace propulsion, flow prediction, reduced-order modelling

## INTRODUCTION

The design and optimization of nozzle systems for aerospace propulsion represent some of the most computationally demanding tasks in modern engineering. High-fidelity Computational Fluid Dynamics is essential for capturing the intricate physics of nozzle flows, which are often characterized by high-speed compressibility, complex shock-wave structures, and intense turbulence(Bernardini et al., 2021). While techniques such as Large Eddy Simulation and Direct Numerical Simulation provide unparalleled accuracy, their computational cost remains a significant barrier to iterative design cycles and real-time performance monitoring(Moldovan et al., 2022). For instance, simulating the transient dynamics of reactive flows in a rocket engine injector can require hundreds of high-fidelity simulations to explore even a small parameter space (Usandivaras et al., 2022).

To address these bottlenecks, the aerospace community has increasingly turned toward surrogate modelling as a means of providing rapid, cost-effective approximations of expensive numerical solvers. Traditional surrogate methods, including Kriging and radial basis functions, have been used for years to optimise nozzle shapes and injector designs (Krügener et al., 2022). However, these classical approaches often struggle to scale with the high-dimensional data generated by modern 3D flow simulations(Scherding et al., 2023).

The recent explosion in artificial intelligence and deep learning has introduced a new paradigm in fluid mechanics. Advanced neural network architectures, such as Convolutional Neural Networks and U-Nets, are now being deployed to learn the underlying physics of flow fields directly from Computational Fluid Dynamics (CFD) datasets (Usandivaras et al., 2022). These AI-driven surrogates can achieve remarkable speedups, sometimes accelerating the prediction of transient flows by a factor of 5 to 7 compared to conventional one- or two-equation turbulence models (Schmidt et al., 2021). By replacing traditional solvers with pretrained neural networks, researchers can now evaluate the performance of single expansion ramp nozzles and other complex geometries across multiple operating conditions in a fraction of the time previously required (Yang et al., 2024).

This review aims to fuse the latest advancements in this field, focusing on post-2020 methodologies that bridge the gap between pure data-driven models and physics-informed architectures.

## Fundamentals of Nozzle Flow Simulation

At the core of nozzle performance analysis are the governing equations of fluid dynamics, primarily the Navier-Stokes equations for viscous flows and the Euler equations for inviscid approximations. In the context of aerospace applications, these equations must account for the conservation of mass, momentum, and energy while accommodating the high pressure and temperature gradients found in convergent-divergent nozzles. Traditional CFD approaches rely on the discretisation of these equations across a mesh, a process that is inherently limited by mesh dependency and the iterative nature of convergence. For complex phenomena such as sonic fuel injection into supersonic crossflows, the interaction between the fuel jet and the Mach 3.8 flow creates intricate 2D flow fields where deep learning methods are used to predict the flow fields instantaneously (Akiyama & Ogawa, 2023). Furthermore, when dealing with transient flows relevant to flash boiling or two-phase jets, the simulation cost increases significantly due to the need for fine temporal resolution (Schmidt et al., 2021). AI-driven surrogate modelling seeks to bypass these limitations by training on "truth" data generated from Reynolds-Averaged Navier-Stokes or LES simulations (Krügener et al., 2022). By utilizing deep learning networks trained on datasets of high-fidelity simulations, such as a collection of 100 LES runs for a single-shear coaxial injector, surrogates can learn to predict global quantities and root-mean-square fields with high precision (Usandivaras et al., 2022). This transition from mesh-based solvers to data-driven inference allows for the rapid exploration of design parameters such as chamber diameter, recess length, and oxidizer-fuel ratios, providing engineers with local sensitivity analysis and insights that were previously too expensive to obtain at scale (Akiyama & Ogawa, 2023).

## Surrogate Modelling Techniques

The increasing complexity of nozzle designs and the high computational cost of traditional computational fluid dynamics have necessitated the development of surrogate models, which act as computationally efficient approximations of high-fidelity simulations, allowing for rapid design exploration and optimization without the prohibitive expense of full-order solvers (Bagy, 2020).

### *Physics-Based Surrogates*

Physics-based surrogates, often referred to as metamodels, utilize statistical and mathematical formulations to approximate the relationship between geometric parameters and flow responses. Response Surface Methodology has long been a standard approach, employing second-order polynomial approximations to represent the design space. However, while RSM is effective for certain applications, it may not be ideally suited for highly nonlinear responses Kriging models have emerged as a robust alternative to RSM in aerospace applications, particularly for the multidisciplinary design of aerospike nozzles (Simpson et al., 2001). Unlike simple polynomials, Kriging is a statistical-based method that provides both a global approximation and offers local error estimation (Simpson, 1998), (Hong et al., 2021; Simpson et al., 2001). In comparative studies involving aerospike nozzles, Kriging models using a Gaussian correlation function have been found to yield slightly higher accuracy than traditional second-order RSM (Simpson et al., 2001). Furthermore, Radial Basis Functions are increasingly recognized for their superior ability to capture the nonlinear characteristics of complex flow data, making them suitable for representing complex flow data (Hu et al., 2020). These methods are often integrated into adaptive sampling frameworks where the surrogate is iteratively refined to achieve a specified level of precision (Bagy, 2020).

### *Data-Driven AI Methods*

The shift toward data-driven artificial intelligence has introduced sophisticated architectures capable of predicting full flow fields rather than just scalar performance metrics. Gaussian Processes provide a Bayesian framework for inference, which is particularly advantageous when training data are limited (Roznowicz et al., 2024). However, as the dataset size increases, GPs can become computationally expensive, leading researchers toward deep learning architectures (Roznowicz et al., 2024). Neural networks, specifically Multi-Layer Perceptron, have demonstrated significant efficacy in aerodynamic data modelling by learning complex mappings from boundary conditions to steady-state flows (Hu et al., 2020). To handle the spatial and temporal complexities of nozzle flows, hybrid architectures such as the CNN-LSTM have been developed. In these models, Convolutional Neural Networks encode high-dimensional flow fields into a reduced-order latent representation, while Long Short-Term Memory networks predict the evolution of these fields over time or across varying pressure ratios (Liu, 2025). Studies have shown that these hybrid models can perform flow field predictions over 150 times faster than conventional pressure solvers while maintaining a high degree of accuracy (Liu, 2025). Recent advancements also include geometry-to-flow mapping, where networks use signed distance functions to better process complex wall boundaries and predict the resulting flow structures (Leer & Kempf, 2020).

### *Reduced-Order Modelling with AI*

Reduced-order modelling aims to lower the degrees of freedom required for flow simulation while preserving the underlying physics. A prominent technique is Proper Orthogonal Decomposition, which identifies the dominant modes of a flow system to construct a low-dimensional space for the solution

(Duthé et al., 2025; Witman et al., 2022). When combined with machine learning (Ali et al., 2025), POD modes can be used as coefficients for LSTM networks to predict transient phenomena, such as coolant jets in supersonic flows, with acceptable performance when at least 80% of the available data is used for training. Despite the efficiency of data-driven ROMs, they often lack physical consistency because they do not explicitly account for governing equations. To bridge this gap, Physics-Informed Neural Networks have been introduced to enforce conservation laws directly within the network's loss function (Renganathan et al., 2020; Zhao et al., 2021). By embedding the Euler or Navier-Stokes equations into the training process, PINNs can solve high-speed flow problems, including one-dimensional Euler equations and two-dimensional oblique shock waves, with significantly fewer data points than purely data-driven models (Zhao et al., 2021). This approach ensures that the surrogate predictions remain physically valid, even in regimes where training data may be sparse or noisy (Zhao et al., 2021). Recent frameworks also utilize neural basis functions to accelerate solutions for high Mach number flows, demonstrating the potential of AI to resolve complicated phenomena that traditional modal decomposition might miss (Witman et al., 2022).

## AI-Driven Applications in Nozzle Flows

The integration of artificial intelligence into nozzle flow research has transitioned from theoretical exploration to practical implementation across diverse engineering sectors. By replacing computationally expensive fluid dynamics simulations with high-fidelity surrogates, researchers can now perform complex design tasks in a fraction of the time previously required. This section provides an extensive review of AI applications in sonic nozzle prediction, geometry optimization, real-time control, and specific industrial and aerospace case studies.

### *Sonic Nozzle Flow Rate Prediction*

Sonic nozzles serve as high-precision standards for gas flow measurements, but manufacturing tolerances often compromise their performance, resulting in non-ideal geometries. Recent research has focused on developing surrogate models that can account for these deviations, such as local curvature radius variations near the nozzle throat (Weiß et al., 2025). For instance, a computational fluid dynamics-based surrogate model was developed to predict flow in parameterised non-ideal nozzle shapes, using a weighted non-linear least squares method to approximate real nozzle contours (Weiß et al., 2025). This approach demonstrated superior agreement with experimental data, achieving an average root-mean-square error of 0.17% across various test nozzles, compared to the 0.35% error associated with standard models (Weiß et al., 2025). Such advancements allow for individualised assessment of nozzle effectiveness in metrological applications without the need for exhaustive physical testing.

### *Optimization of Non-Ideal and Complex Geometries*

Shape optimization is a critical aspect of nozzle design, particularly for supersonic and aerospace applications where even minor profile adjustments can yield significant performance gains. Deep learning architectures, such as Convolutional Neural Networks, have been successfully integrated with genetic algorithms to optimize the shapes of supersonic nozzles for specific throat and outlet diameters (Zanjani et al., 2022). Furthermore, higher-order neural units and polynomial structures have been employed as approximators for the non-linear Navier-Stokes equations to optimize plane nozzle shapes, ensuring flow field uniformity and specific outlet conditions (Kovář & Fürst, 2024). In more advanced frameworks, deep reinforcement learning coupled with U-net surrogate models have been used to explore design spaces for rocket nozzles (Ma et al., 2024). Using B-spline-defined profiles and inference engines to calculate flow metrics, these models have achieved thrust improvements of up to 2.96% under practical conditions considering friction (Ma et al., 2024). Similarly, machine learning models have been applied to optimize fluidic injection parameters for Single Expansion Ramp Nozzles, improving the average thrust coefficient by 1.14% while drastically reducing the gradient computation time during optimization (Yang et al., 2024).

### *Real-Time Control and Monitoring*

The speed of AI inference makes it uniquely suited for real-time control and monitoring of nozzle systems. Feedforward neural networks have been implemented to predict thrust in cold gas thrusters with an accuracy of 0.98, leveraging operational parameters like storage pressure and propellant mass density (Farhid et al., 2025). These models can be integrated into graphical user interfaces for real-time estimation, simplifying the design and operational analysis of propulsion systems (Farhid et al., 2025). For dynamic flow environments, hybrid techniques combining Proper Orthogonal Decomposition and Long Short-Term Memory networks have been used to predict transient phases in coolant injections, though complexity in recirculation regions can lead to higher predictive errors in axial velocity (Ali et al., 2025). Additionally, deep reinforcement learning is emerging as a powerful tool for active flow control, enabling closed-loop systems that automatically optimize jet actuation based on real-time flow conditions (Montalà et al., 2025). These intelligent controllers can identify complex interactions between jets and the main flow, providing a more robust feedback mechanism than traditional open-loop strategies (Montalà et al., 2025)

### *Aerospace and Industrial Case Studies*

In the aerospace sector, AI-driven surrogates are now used for the design of rocket engine components, including coaxial injectors and combustion chamber elements (Usandivaras et al., 2022). Deep learning networks, specifically U-Nets and fully connected architectures, have been trained on large eddy simulation datasets to analyze the impact of design parameters such as recess length and fuel ratios on engine performance (Usandivaras et al., 2022). These models significantly reduce the number of experimental tests required, lowering overall development costs (Krügener et al., 2022). Industrial applications have seen similar breakthroughs, particularly in fuel injector and spray modelling. Machine learning emulators have been developed to predict spatiotemporal flow distributions in automotive injectors, achieving speedup factors of up to 38 million compared to traditional CFD approaches (Mondal et al., 2022). These emulators use autoencoders for dimensionality reduction and Gaussian process models to provide principled uncertainty estimates, which are vital for engine designers to determine the reliability of the data-driven predictions in specific design spaces (Mondal et al., 2022). Furthermore, artificial neural networks are being used to predict cavitation behaviour and steam generation in converging-diverging nozzles, offering a data-driven alternative to resolve the complex Multiphysics of high-pressure Venturi tubes (Lu et al., 2025).

### *Comparison of AI Applications in Nozzle Flow*

**Table 1: Summarizes Key Studies and Their Outcomes Across Different Application Areas**

| Application Area | AI/ML Technique | Key Outcome/Performance Metric | Reference |
|---|---|---|---|
| Sonic Nozzle Prediction | Parameterized CFD Surrogate | RMSE reduced to 0.17% for non-ideal geometries | (Weiß et al., 2025) |
| Supersonic Shape Optimization | CNN + Genetic Algorithm | Effective in optimizing nozzle geometries | (Zanjani et al., 2022) |
| Cold Gas Propulsion | FFNN | Accuracy of 0.98 for real-time thrust prediction | (Farhid et al., 2025) |
| Rocket Nozzle Design | DRL + U-Net ViT | 2.96% thrust improvement via profile optimization | (Ma et al., 2024) |
| Automotive Fuel Injectors | Bayesian Learning + Autoencoders | Speedup factor higher than traditional CFD | (Mondal et al., 2022) |
| Transient Coolant Jets | POD + LSTM | Prediction of transient mass fraction and pressure | (Ali et al., 2025) |
| Cavitation Modelling | Artificial Neural Networks | Modelling pressure drops and steam generation prediction | (Lu et al., 2025) |

## Challenges and Limitations

### *Data and Training Issues*

A primary obstacle in developing robust artificial intelligence surrogates for nozzle flows is the acute scarcity of high-quality data, particularly for rare or unconventional nozzle geometries. While standard convergent-divergent configurations are well documented, specialized designs for hypersonic or micro-scale applications often lack the extensive experimental or high-fidelity simulation datasets required for deep learning (Peyvan & Kumar, 2025). This data deficiency frequently leads to overfitting, where models achieve high accuracy on training sets but fail to generalize to high-dimensional flow features that were not explicitly included in the sample space (Chu, 2023). Furthermore, achieving generalization across varying Reynolds numbers remains a significant bottleneck. Most existing machine-learning models are trained on specific flow regimes and struggle when the physical parameters, such as the Reynolds or Knudsen numbers, deviate from the training domain (Taghizadeh et al., 2021). These models often act as interpolators rather than true physical predictors, which limits their utility in exploratory engineering design where new regimes are frequently encountered (Taghizadeh et al., 2021).

### *Accuracy versus Speed Trade-offs*

The fundamental promise of AI surrogates is the acceleration of computational fluid dynamics, yet this speed often comes at the expense of capturing critical discontinuous phenomena such as shock waves. Traditional numerical methods are computationally intensive but reliable for resolving shocks, whereas many deep neural networks tend to smooth out these sharp gradients unless specifically architected to handle discontinuities(Wassing et al., 2025). Recent developments like Weighted Essentially Non-Oscillatory Neural Networks and Physics-Informed Neural Networks have attempted to bridge this gap by providing sharper shock identification without the heavy computational overhead of traditional solvers (Liang et al., 2023; Montáns et al., 2023)However, turbulence modeling introduces additional complexity, as data-driven closures must balance mathematical tractability with the need to capture multi-scale turbulent structures (Raje et al., 2025). While surrogates for models like Spalart-Allmaras can offer speedups of up to 7 times, maintaining the same level of accuracy as two-equation models in transient flows remains a persistent challenge (Schmidt et al., 2021).

### *Integration Barriers*

Integrating AI models into existing industrial workflows is hindered by significant concerns regarding uncertainty quantification and the inherent "black-box" nature of neural architectures(Scillitoe et al., 2021). In engineering applications, the inability to verify and validate the internal logic of a model leads to a lack of trust among practitioners (Chu, 2023). This has sparked interest in explainable artificial intelligence and additive feature attribution methods to clarify the relationships between input features and flow outputs (Cremades et al., 2024). Moreover, the computational overhead required for the initial training of high-fidelity surrogates can be prohibitive, sometimes negating the time savings during the inference phase (Roohi & Mahdavi, 2025). Establishing a quantitative framework for AI in fluid mechanics requires not only better benchmarks for generalization but also interdisciplinary collaboration to ensure that learned models strictly adhere to known physical laws such as conservation of mass and momentum (Wang et al., 2024), (Buzzicotti, 2023). The future of nozzle flow simulation lies in the development of multi-fidelity surrogates that can leverage both low-accuracy, high-volume data and high-accuracy, low-volume data to create more reliable predictors(Xu et al., 2024). Transfer learning will play a pivotal role in this evolution, allowing models trained on simulated data to be fine-tuned with limited experimental results, thereby narrowing the gap between simulation and reality (Wang et al., 2024; Xie et al., 2023). Another promising avenue is the use of reinforcement learning to develop real-time adaptive models that can adjust mesh topologies or control parameters dynamically during a simulation(Huergo et al., 2025),(Wang et al., 2024). Hybrid AI-physics approaches, which encode fundamental physical laws directly into the neural network architecture, are expected to produce models that are more robust and physically consistent than purely data-driven methods (Roohi & Mahdavi, 2025; Wang et al., 2024). Finally, the establishment of open-source communities and standardized benchmarks will be essential for the systematic validation of these emerging tools across the aerospace and industrial sectors(Bosello et al., 2024; Ziaja et al., 2021).

## CONCLUSIONS

Artificial intelligence-driven surrogate models represent a transformative shift in the simulation of nozzle flows, offering the potential for significant reductions in computational cost and improvements in real-time monitoring. However, the widespread adoption of these technologies is currently constrained by issues related to data scarcity, the difficulty of capturing complex shock-turbulence interactions, and the need for greater model transparency. By addressing these challenges through hybrid physics-based architectures, multi-fidelity data integration, and advanced uncertainty quantification, the field can move toward more dependable and generalizable AI tools. Ultimately, the successful fusion of traditional fluid dynamics principles with modern machine learning techniques will be the key to unlocking new frontiers in nozzle design and aerospace engineering.

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