Micromixing in Turbulent Flows: A Literature Review of CFD Approaches and Neural Network Integration

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Abstract

Micromixing plays a crucial role in turbulent flow environments, particularly in fast chemical reactions where product selectivity is highly dependent on mixing efficiency. Traditional Computational Fluid Dynamics (CFD) approaches, such as Reynolds-Averaged Navier-Stokes (RANS) and Large Eddy Simulations (LES), struggle to accurately resolve micromixing dynamics due to their reliance on turbulence closure models. While Direct Numerical Simulation (DNS) provides the highest fidelity, it remains computationally expensive, especially for large-scale applications.

This study leverages Homogeneous Isotropic Turbulence (HIT) data obtained from DNS simulations to train machine learning models for improved micromixing prediction. We explore the use of Autoencoders, Convolutional Neural Networks (CNNs), and Physics- Informed Neural Networks (PINNs) as alternatives to traditional turbulence modeling approaches. These models are integrated into OpenFOAM, allowing for efficient predictions of scalar transport at micromixing scales.

The proposed methodology undergoes rigorous accuracy assessment using metrics such as Root Mean Squared Error (RMSE) and parity diagrams, ensuring reliable performance. Additionally, sensitivity analysis is performed to determine the required number of training samples for robust model generalization.

By combining high-fidelity CFD data with neural network-based modeling, this project aims to develop a scalable and computationally efficient framework for micromixing predictions. The findings contribute to improved industrial process optimization, particularly in chemical reactors, pharmaceutical crystallization, and environmental engineering applications.

Keywords: micromixing, turbulence, neural networks, machine learning, CFD, mixing.