Uncertainty Quantification of Model Extrapolation in Neural Network-informed Turbulent Closures for Plenum Mixing in HTGRs

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ABSTRACT:

Background: Advent of cheap computational resources has brought Data-driven machine-learning (ML) models to different engineering fields, including Nuclear Engineering . Within the spectrum of ML models, a class of models that mathematically replicates the connection between neurons within a brain are neural networks (NN). NN based models have been found to provide swift and accurate prediction of complex thermohydraulic phenomena and processes. At one end of the scale-spectrum, it can be used as a surrogate model for the entire process/cycle, e.g. integrated regenerative transcritical cycle, completely replacing the physics based model. At the other end, NN models are being used as turbulence closures to improve accuracy of large eddy simulations (LES) and RANS based CFD simulations. Despite their success, model extrapolation, that is the ability to predict accurately beyond the range of training data remain the primary constraint to their widespread adaptation, especially for nuclear systems where failure of a model can be catastrophic. Thus, from a regulatory standpoint it is essential to quantify the uncertainty in prediction of the NN models, in case the operating condition (e.g. transients during accidents) is outside the range of the training data set. In the proposed study we will systematically quantify the uncertainty in these situations, for NN-based turbulence closures used in conjunction with URANS based CFD for simulating complex thermohydraulic flows. Modeling turbulent phenomena in nuclear reactors is challenging as one needs to obtain high-accuracy models with a reasonable computational time to run realistic transients, which could last hours or days. Standard coarse-mesh RANS/URANS turbulence models are not able to provide the necessary accuracy, whereas the turbulence-eddy resolved direct numerical simulations (DNS) or high-fidelity LES simulations are computationally intractable. Hence, neither DNS/LES nor RANS/URANS is currently used for the regulatory licensing of advanced reactors. The proposed research will aim at solving this fundamental licensing problem. It will propose better neural network based turbulence closures for the URANS equations, which are informed by data from high-fidelity LES simulations, and it will also build a framework for quantifying uncertainties in these closures.

Objectives:

The objective is to quantify and understand the uncertainty (UQ) in turbulence predicted by neural network (NN) based URANS models, when the neural network models are operating beyond the range of conditions they have been trained for. The proposed UQ framework will be applied to

1. Different flow and thermal mixing phenomena, ranging from canonical buoyant-jets and T-junctions, to complex flows within the plenum of high-temperature gas reactors (HTGRs). Establishing the baseline for the framework to be applied at advanced reactors.
2. Both steady and transient flows observed in HTGRs, helping establish the uncertainties for the safety parameters of interest within the framework of regulatory licensing.