Project Proposal

Physics-Informed Neural Networks for Modeling of Thermophysical Properties

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General Information

Type:	Master Thesis (30 ECTS)
Laboratory:	Laboratory for Applied Mechanical Design (LAMD)
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Background

Supercritical power cycles will play a key role in the energy transition towards renewable energies benefiting from higher efficiencies and higher energy density.
Supercritical fluids are fluids at higher pressures and temperatures where the ideal gas law does not apply. Supercritical fluids are subject to real gas effects, and non-linear thermo-physical proprieties. Accurate thermophysical properties are required to precisely model the non-ideal gas behaviour.
A major challenge for supercritical turbomachinery is condensation at the blade suction side due to a drop in static conditions resulting in a transition from the supercritical phase into the two phase domain. Figure 1 shows the relative Mach number showing flow acceleration along the suction side of an impeller blade.

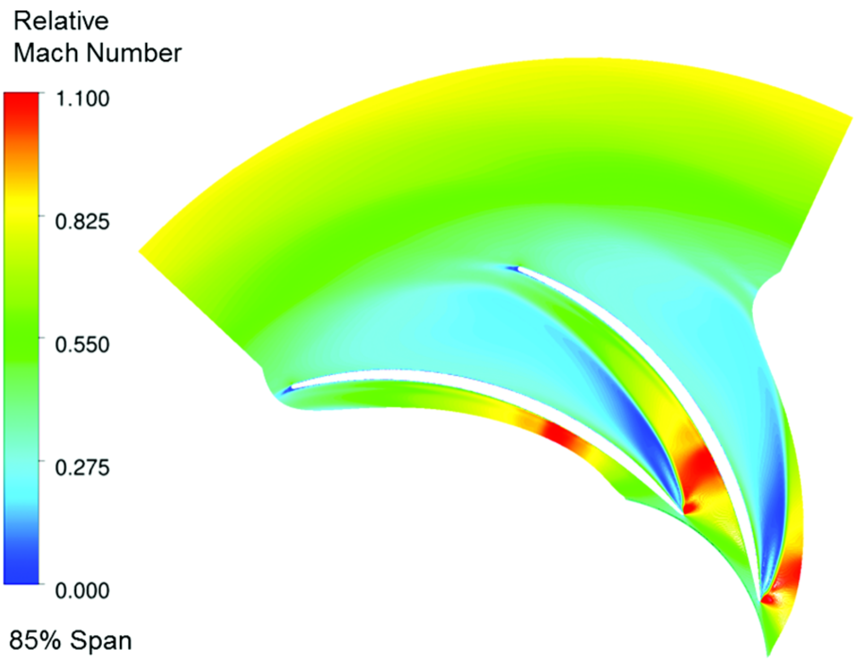

Figure 1: Relative Mach number within an impeller [1]

Due to the time delay for nucleation to occur (formation of liquid droplets), the supercritical phase transitions to a temporary metastable state (fluid within the two phase domain). The thermophysical properties within the metastable state remain largely unexplored and difficult to predict while playing a critical role in condensation prediction. Accurate thermophysical properties within the metastable state will allow for optimizing the design of power cycles leading to higher efficiencies.

A large variance in power cycle performance has been correlated to large variance in thermophysical properties of different fluids. Understanding which thermophysical properties leads to high power cycle performance is key in reducing emissions. Prediction of thermophysical properties of unknown fluids allows for fluid selection which deliver the highest performance. The extended corresponding states (ECS) model allows the prediction of thermophysical properties using 11 defining parameters. The ECS model has already been created. The model will be used as a tool and prospective students are not expected to develop it[2].

The ECS model, while robust, necessitates multiple invocations of the Refprop software, introducing a significant computational bottleneck for data-driven strategies in thermodynamics. This challenge underscores the imperative for a more efficient computational model. The proposed solution is the development of a surrogate model, leveraging Physics-Informed Neural Networks (PINNs), designed to expedite computations by several orders of magnitude and enable parallel processing. PINNs diverge from conventional neural network methodologies by embedding physical laws and governing equations directly into their structure. This integration not only ensures adherence to thermodynamic principles but also significantly enhances the model's efficiency, accuracy, and scalability. Specifically, PINNs promise to offer superior generalization across different thermodynamic states, optimize data utilization, provide insightful interpretations aligned with physical laws, and minimize the risk of overfitting. Moreover, their inherent robustness and capacity for handling multi-physics and multi-scale problems make them exceptionally suited for advancing thermodynamic simulations and predictions, potentially rendering Refprop computations more efficient or even unnecessary for a broad range of applications.

Objective

Creating physics-informed neural networks to obtaining thermophysical properties for a variety of fluids within different phases.

Tasks

1. Literature review of existing approaches.

2. Identification of data sampling approach.

3. Implementation of physics-informed neural networks.

4. Implementation of extended corresponding states model into physics-informed neural networks.

5. Validation of physics-informed neural networks.

NB: adjustments may be required according to progress, results, and project duration.

Prerequisite knowledge

1. Machine learning / neural networks
2. Programming (MATLAB / Python)
3. Thermodynamics (fundamental equations)

References

[1] Nikola D Baltadjiev, Claudio Lettieri, and Zoltán S Spakovszky. An investigation of real gas effects in supercritical co2 centrifugal compressors. *Journal of Turbomachinery*, 137(9):091003, 2015.

[2] Marcia L Huber and James F Ely. A predictive extended corresponding states model for pure and mixed refrigerants including an equation of state for r134a. *International Journal of Refrigeration*, 17(1):18–31, 1994.