Master Thesis Research Project Proposal

Machine-learning-assisted turbulence modeling in dense gas flows

Ecole Centrale de Lyon / LMFA / Queensland Univ. Tech.

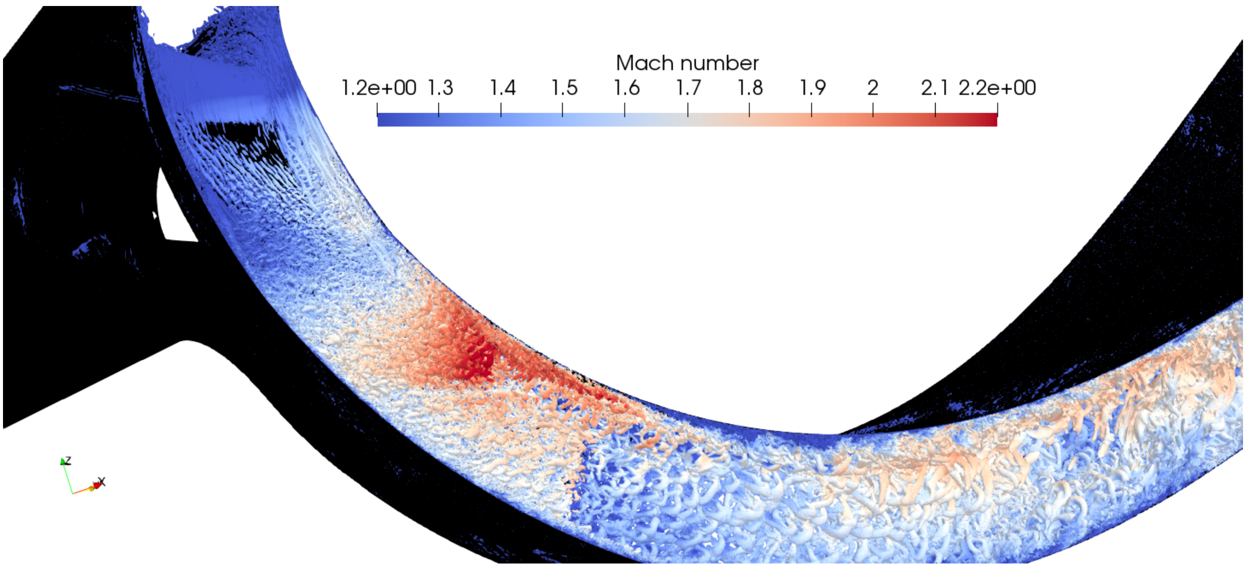

FIGURE 1 – Dense gas flow Large Eddy Simulation in a turbine. ANR-EDGES / PRACE Project – Isosurface of the Q criterion colored by the Mach number.

1 General Context

Dense gases are characterized by their large molar mass and heat capacities and are also known for their unusual thermodynamic behavior when their pressure, temperature and density are close to the saturation curve in the vicinity of the critical point. In this region, the fundamental derivative of fluid dynamics is lower than unity for dense gases, yielding a speed of sound decreasing with density, in opposition to the perfect gas behavior. Thanks to their peculiar properties, dense gases are used as working fluids in Organic Rankine Cycle (ORC) engineering systems harvesting thermodynamic cycles for the recovery of fatal heat. These ORC systems experience an accelerated development under the combined effect of the increase of the energy price and of the public awareness of climate issues. Companies developing such systems face numerous challenges among which some come from a lack of basic knowledge regarding the turbulent flows of dense gases in expanders. Indeed, to obtain efficient turbomachinery systems, numerous prototypes are designed on the basis of computer simulations, also known as Computational Fluid Dynamics (CFD) predictions, before being tested. Today, Reynolds Averaged Navier-Stokes (RANS) simulations have become a usual tool in the design phase of these machines, but the turbulence models upon which they rely were all developed in the context of perfect gases. Since it is estimated that the losses due to viscous effects can represent up to two third of the total losses in an ORC turbine stage, with dense gas effects tending to increase losses in supersonic wake flows, it can be therefore concluded that :

— turbulence models play a crucial role in the accurate prediction of friction losses at the walls and in the blades' wakes,

— it is essential to revisit turbulence models for dense gas flows [1]. The present Master thesis proposal addresses the design of accurate RANS models for compressible turbulent dense gas flows.

The LMFA research team proposing this Master thesis together with QUT University has previously developed a strong experience in the analysis of turbulent dense gas flows using Direct Numerical Simulations as well as Large Eddy Simulations [2, 3, 4, 5, 6]. Figure 2 shows that the normalized momentum thickness growth rate of a dense gas shear layer at high convective Mach number (Mc=2.2) is significantly different from its perfect gas value, hinting peculiar turbulence characteristics for the dense gas flow and calling therefore for a dedicated effort towards the modelling of dense gas turbulence [7]. In the context of the ANR-funded EDGES project, our research

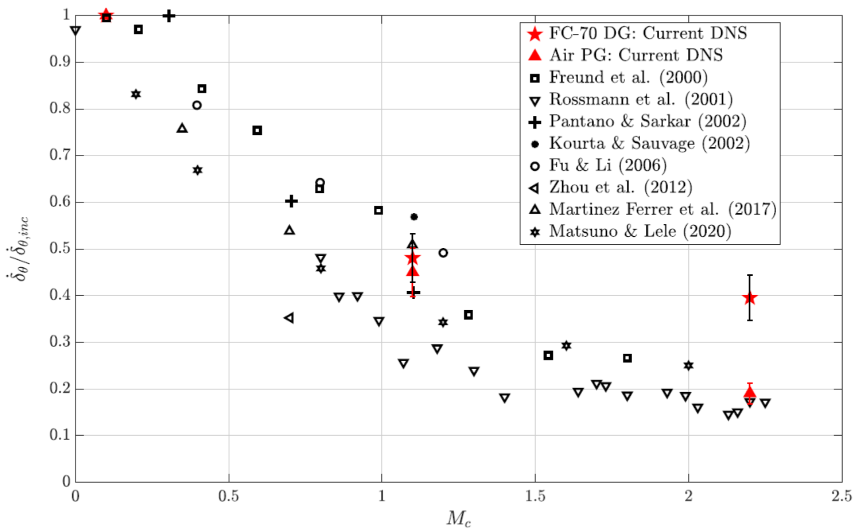

FIGURE 2 – Normalized growth rate of a compressible turbulent shear layer vs convective Mach number M_c. All DNS results are obtained in air (perfect gas) except red star symbols corresponding to the FC-70 dense gas DNS (Vadrot et al., Journal of Fluid Mechanics 2021).

team has used the DNS database produced at LMFA for several dense gas flows (homogeneous isotropic turbulence, shear layer, channel flow) to derive novel subgrid-scale models specifically dedicated to the Large Eddy Simulation (LES) of turbulent dense gas flows [8]. Because of the complex thermodynamic description of dense gases, it was found relevant to rely on Machine Learning in order to build such models. Figure 3 illustrates how an Artificial Neural Network can be trained using the computed DNS data so as to accurately predict LES closure terms for the filtered Navier-Stokes equations.

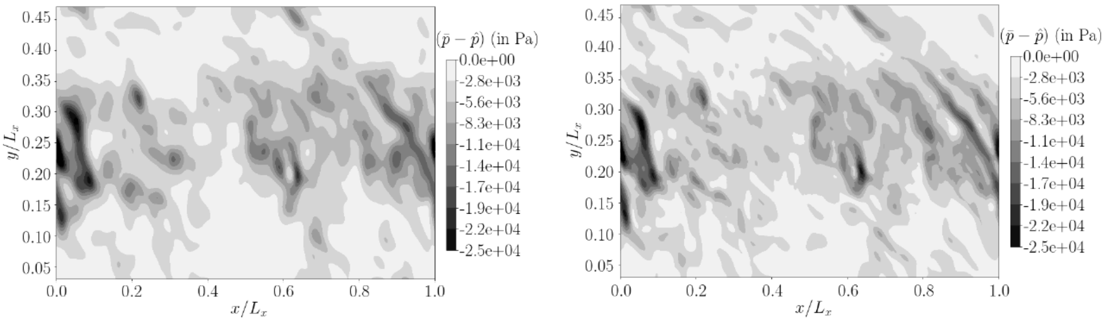

FIGURE 3 – Subgrid scale pressure term for the $M_c = 2.2$ dense gas shear layer. Left : true contours derived from DNS. Right : predicted values using ANN trained on DNS data (for other timesteps than the one assessed here). Taken from Vadrot PhD thesis (Oct 2021).

2 Description of the work

The proposed Master thesis is focused on the development of novel turbulence closures for the Reynolds-Averaged Navier-Stokes equations applied to the description of dense gas flows in geometries of industrial interest (ORC turbines). This development will take advantage of the reference High-Fidelity Large Eddy Simulation results currently produced with the solver AVBP developed at CERFACS and including the ANN-based SGS models targeted for dense gas flows.

The first and main stage of the work will adapt to RANS modelling the supervised learning methodology previously developed and applied by the research team for LES. All RANS simulations needed to build models relevant for dense gas flows will be performed using the open-source SU2 solver.

In a second stage, an even more innovative approach will be tackled through the exploration of non-supervised learning. While most (if not all) methods currently proposed to improve turbulence modelling in Fluid Dynamics are intrinsically supervised in the sense that they require a form of high-fidelity results to be tuned, alternative methods exist which do not require supervision, among which Reinforcement Learning. In reinforcement learning the model consists in a policy which has to be learnt by an agent (see Figure 4). Depending on its choices, the agent modifies the

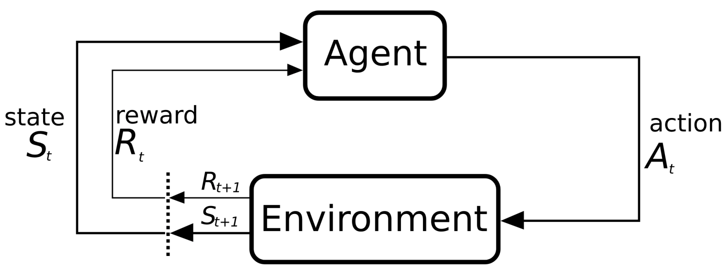

FIGURE 4 – Schematic of reinforcement learning technique.

environment in which it evolves. As the agent makes consecutive choices, it also gathers rewards from its environment. Those notions are perfectly fitted to applications such as self-driving cars or chess, and have led to impressive progress in these fields of application. They need to be properly transposed to the CFD domain, with the most promising property of reinforcement learning lying in the lack of supervision. Transposed to turbulence modelling, this could indeed mean the model could be learnt without the usually required set of high-fidelity data [9, 10, 11]. During this phase of research, some fundamental questions will be pursued such as the existence of a reward function devoid of high-fidelity simulation knowledge and yet capable of driving the agent towards an accurate representation of local turbulence statistics.

3 Master Thesis Advisors

Christophe Corre (Full Professor ECL) :

Christophe Corre joined Ecole Centrale de Lyon and the Fluid Mechanics and Acoustics Laboratory (LMFA) in 2014 within the Turbulence and Stability research group. His teaching activities address the numerical simulation of flows and engineering optimization. His research activities cover three main areas : (1) the development of efficient methods for the simulation of hydrodynamic or aerodynamic flows, (2) the robust simulation of complex (two-phase, non-Newtonian, dense gases) flows, and (3) the analysis and optimization of flows including uncertainties.

Alexis Giauque (Assistant Professor ECL) :

Since 2013, Alexis Giauque holds an assistant professor position at Ecole Centrale de Lyon. He is part of the LMFA turbomachinery research team and focuses his research on Large Eddy Simulation of secondary flows in realistic geometries. Since 2016, he has also started a new research initiative aiming at the precise modeling of turbulence in the context of turbulent dense gas flows for ORC turbomachinery applications.

Emilie Sauret (Full Professor QUT) :

Dr. Emilie Sauret is currently Professor in the School of Mechanical, Medical & Process Engineering, Queensland University of Technology (QUT), and an elected council member of the Australasian Fluid Mechanics Society. In 2013, she was awarded an ARC-DECRA and joined QUT where she teaches in the Mechanical Engineering degree. Dr. Sauret has extensive interdisciplinary research experience in computational fluid dynamics, applied mathematics and applied physics. Her current research focusses on the development of advanced computational techniques to accurately simulate complex non-ideal fluid flow behaviours that are critical for the rational design and robust optimisation of engineering applications, in particular in the field of energy and biomedical engineering.

4 Profile

This Master thesis research project (starting date April 2023) will be carried out in the Fluid Mechanics and Acoustics Laboratory (LMFA) at Ecole Centrale de Lyon (ECL). Since it involves both physical modeling of turbulence and numerical developments in machine learning, technical skills in fluid mechanics and applied mathematics are expected from the applicant. Prior knowledge in CFD and machine learning including supervised and non-supervised algorithms will be an asset.
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