

Enabling the Net-Zero Transition: Integrating Complex Multiphysics Efficiently at the Design Optimisation Level

Student: Dylan Rubini^{1,†} and Principal Investigator: Budimir Rosic^{1,‡}

¹Oxford Thermofluids Institute, Engineering Science Dept., University of Oxford, Oxford, UK

[†]Corresponding Author: dylan.rubini@eng.ox.ac.uk

[‡]PI: budimir.rosic@eng.ox.ac.uk

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1. Introduction and Motivation

Decarbonising high-temperature industrial heat within fossil-fuel-fired furnaces is the “grand challenge” of energy engineering, and is a critical hurdle in the development of a net-zero society. Greenhouse gas (GHG) emissions from high-temperature heat ($T > 400^\circ\text{C}$) alone account for more than 10% of the global total. For low-temperature heat, various mature low-carbon technologies already exist. However, high-temperature sectors have been plagued with techno-economic hurdles. To address this, Fig. 1 showcases the revolutionary new turbomachine called the turbo-reactor proposed as an efficient, effective and financially attractive solution for decarbonising over 40 hard-to-abate sectors. By replacing the surface heat exchange energy transfer mechanism within a furnace with direct mechanical energy transfer to the fluid within the turbo-reactor, the power density can increase by 50 to 500 times (Fig. 1), while simultaneously improving the quality of the process. This is enabled by a new turbomachinery principle, in which all mechanical energy transferred to the fluid is converted into kinetic energy and subsequently into internal energy of the fluid, rather than pressure.

This research focuses on endothermic chemical reaction applications of the turbo-reactor (*e.g.*, hydrocarbon cracking, seen in Fig. 1) as they pose a unique set of new requirements for the turbomachinery design. For the first time in turbomachinery, the working fluid chemically reacts along most of the bladed path. Therefore, to design the aerothermal bladed path to optimise the

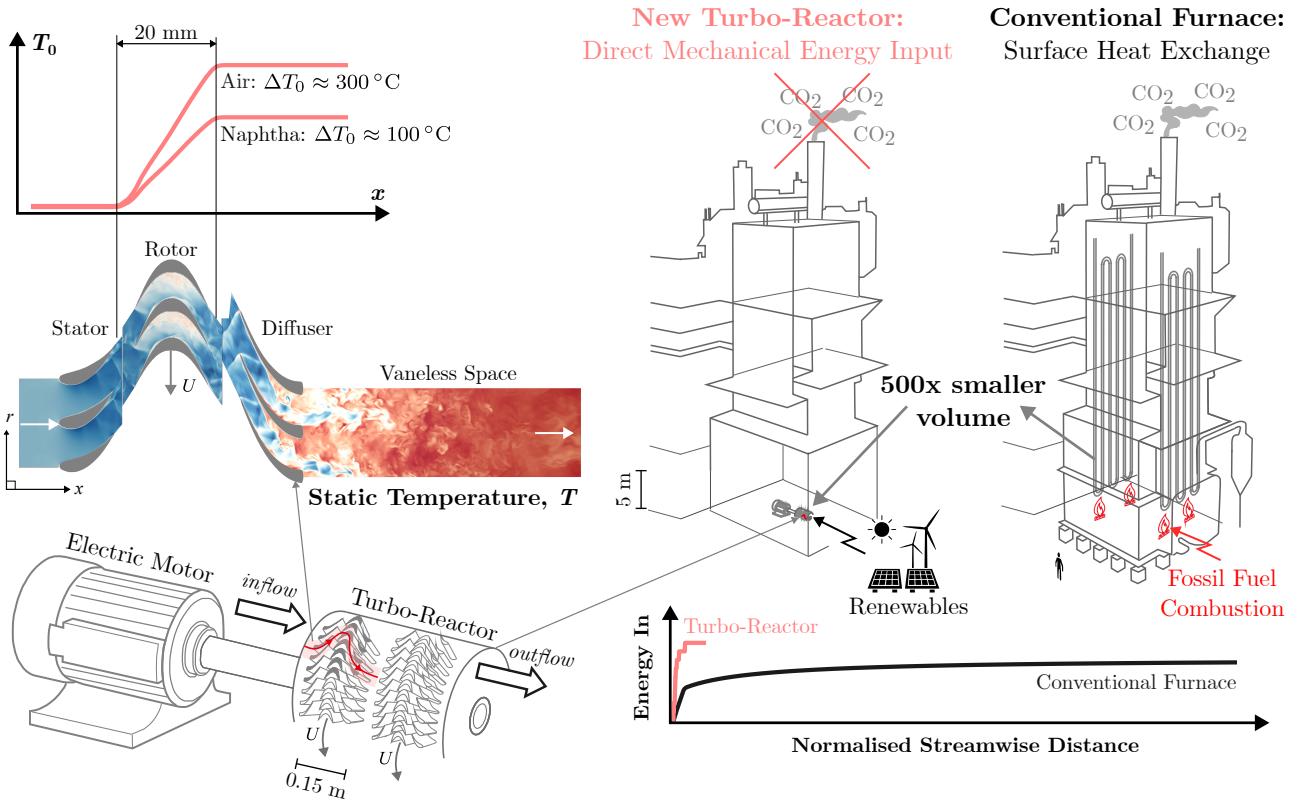


Figure 1: Electrified turbo-reactor could decarbonise many hard-to-abate industrial processes

chemical reaction dynamics, an accelerated aerochemically coupled numerical solver is required. This work introduces an efficient reduced-order model (ROM) guided by machine learning (ML) to bring aerochemically coupled numerical simulations to the design level.

2. Data-Driven Reduced-Order Aerochemistry Modelling

2.1. Importance

For applications of the turbo-reactor where the fluid undergoes a chemical reaction, in addition to power input requirements, the driving design metric is reaction efficiency rather than aerodynamic efficiency. The reaction efficiency is strongly affected by aerochemical interactions due to the complexity of the flow physics and the similarity of the fluid and chemical timescales. However, up to now, these rich multiphysics interactions have been ignored due to the prohibitive

computational cost of fully-reacting flow simulations, making it challenging to perform design optimisation of the machine and thus meet reaction performance targets. To address this, a highly efficient multi-fidelity ML-assisted ROM is introduced to mitigate the computational burden of aerochemically coupled computational fluid dynamics (CFD) without sacrificing accuracy (see Fig. 2). Consequently, for the first time in turbomachinery, aerochemically guided optimisation can be incorporated at an early stage of the design, potentially facilitating a step-change improvement in reaction performance.

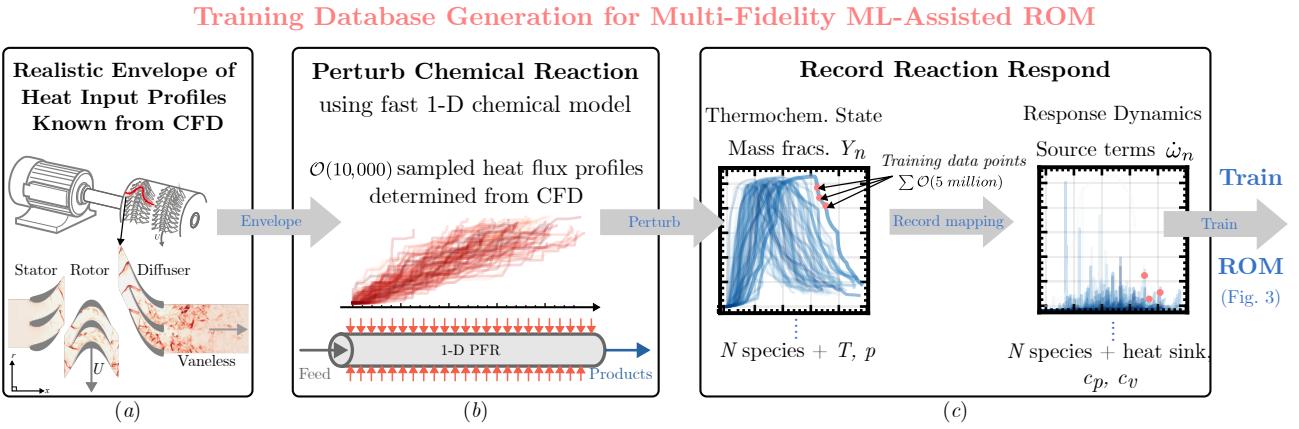
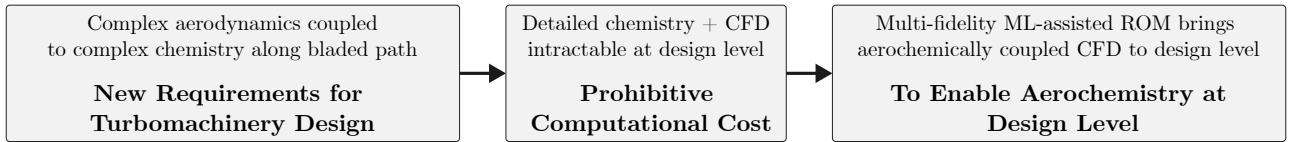


Figure 2: Multi-fidelity ML-assisted ROM training database generation workflow

2.2. Methodology

Figures 2 & 3 outline the new ML-assisted ROM methodology to accelerate multiphysics numerical analysis of the turbo-reactor. Non-reacting CFD of the turbo-reactor establishes a realistic envelope of energy supply profiles into the chemical reaction (see Fig. 2(a)). From this envelope, thousands of energy supply profiles are generated and applied to a detailed chemical kinetic model in a 1-D plug-flow reactor (PFR) environment (see Fig. 2(b)). These randomly generated energy supply profiles (within a realistic envelope) lead to a broad spectrum of reaction perturbations for which the thermochemical state (*e.g.*, Y_n & T) and response dynamics (*e.g.*, $\dot{\omega}_n$) can be recorded. This forms a large database for training the ROM (see Fig. 2(c)) with over 5 million samples. By simplifying the fluid dynamics (*i.e.*, by using a PFR) while retaining the detailed kinetics, this methodology provides an elegant solution to rapidly generate a training

database that densely and widely covers the relevant region of the thermochemical space in only a few hours.

Multi-Fidelity ML-Assisted ROM Methodology

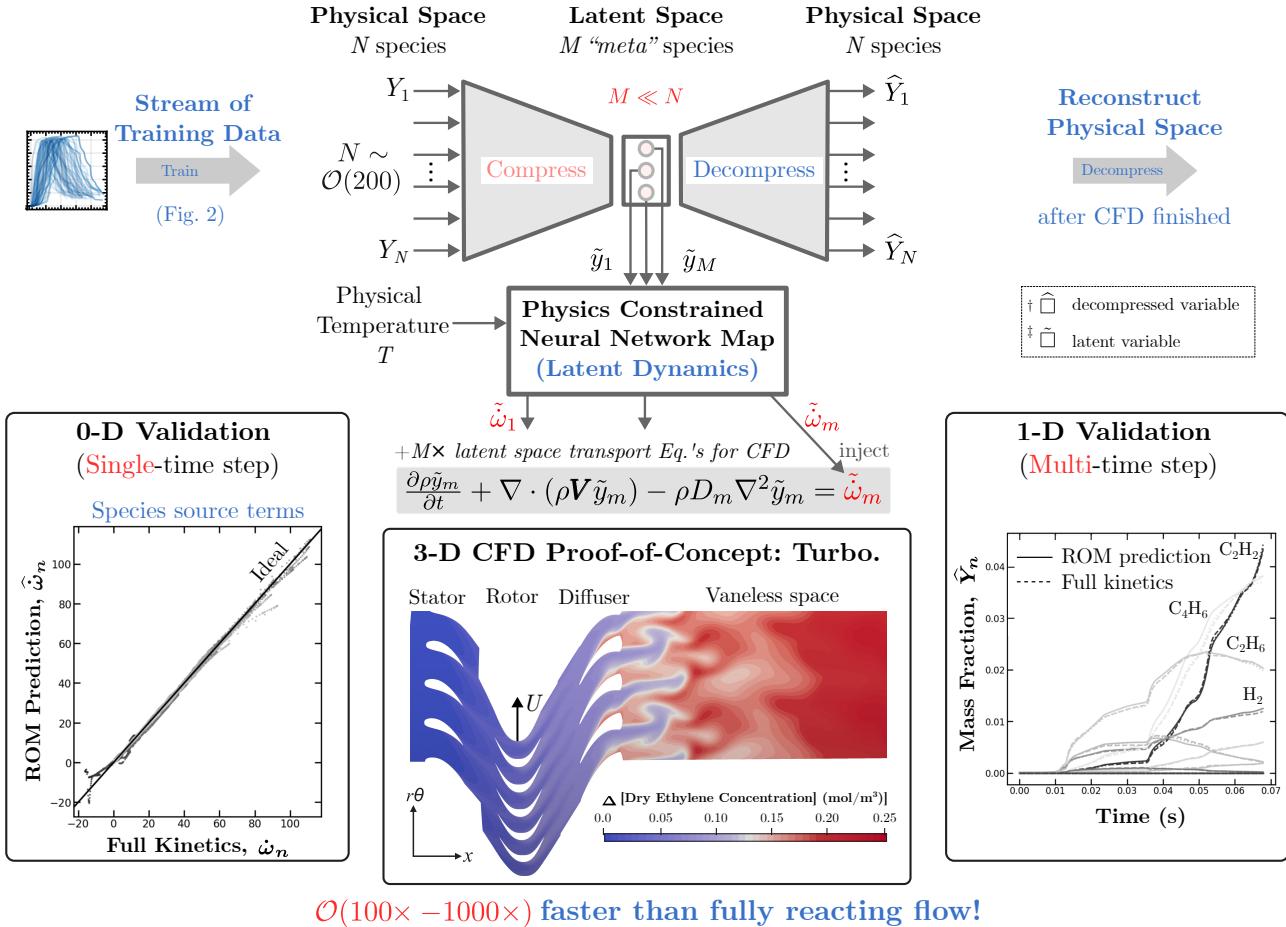


Figure 3: Multi-fidelity ML-assisted ROM methodology overview

Subsequently, as shown in Fig. 3, a ML-assisted ROM is developed using an autoencoder neural network (NN). This NN architecture compresses the high-dimensional thermochemical space ($\mathcal{O}\{200 - 1000\}$ chemical species and $\mathcal{O}\{1000 - 10,000\}$ reactions) into a substantially lower-dimensional latent space ($\mathcal{O}\{3\}$), where a reduced set of “meta” species \tilde{y}_m are mapped to their corresponding source terms $\tilde{\omega}_m$. These source terms represent the dynamic response in the latent space. In effect, the training procedure described above produces a “custom compression algorithm” that uncovers preexisting low-dimensional latent spaces hidden within the governing physics.

One-dimensional verification of the ML-assisted ROM, presented in Fig. 3, demonstrates accurate predictions compared to full chemical kinetics for both 0-D single-time-step and 1-D multi-time-step scenarios. The accumulation of errors for major and minor species is minimal,

ensuring accurate forecasts even over extended time intervals.

Coupling the ROM with a 3-D viscous CFD solver entails adding only three additional “meta” species scalar transport equations, where the dynamics are captured through source terms $\tilde{\omega}_m$ mapped by the trained NN (see Fig. 3). Once the CFD has converged, the high-dimensional physical space, consisting of $\mathcal{O}\{200 - 1000\}$ species mass fractions, can be reconstructed (*i.e.*, decompressed). This powerful methodology enables a speed-up of 100 to 1000 times relative to reacting flow CFD with detailed chemical kinetics. This will enable aerochemical optimisation to be brought to the design level for the first time.

2.3. 3-D Viscous Verification and Proof-of-Concept

To demonstrate the feasibility, success, and future potential of this new methodology, the numerical predictions of the ROM are compared against an industry-standard 3-D viscous reacting flow CFD solver FLUENT with a detailed chemical kinetic mechanism. A 5 m long heated square duct is used for the verification test case (see Fig. 5). Crucially, Fig. 4 illustrates that the ROM can achieve a two-order-of-magnitude speedup relative to a commercial solver with detailed kinetics.

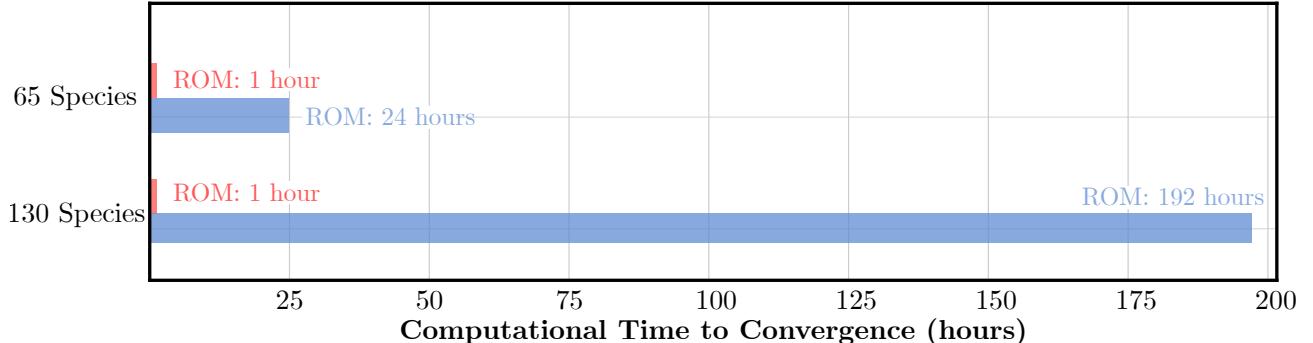
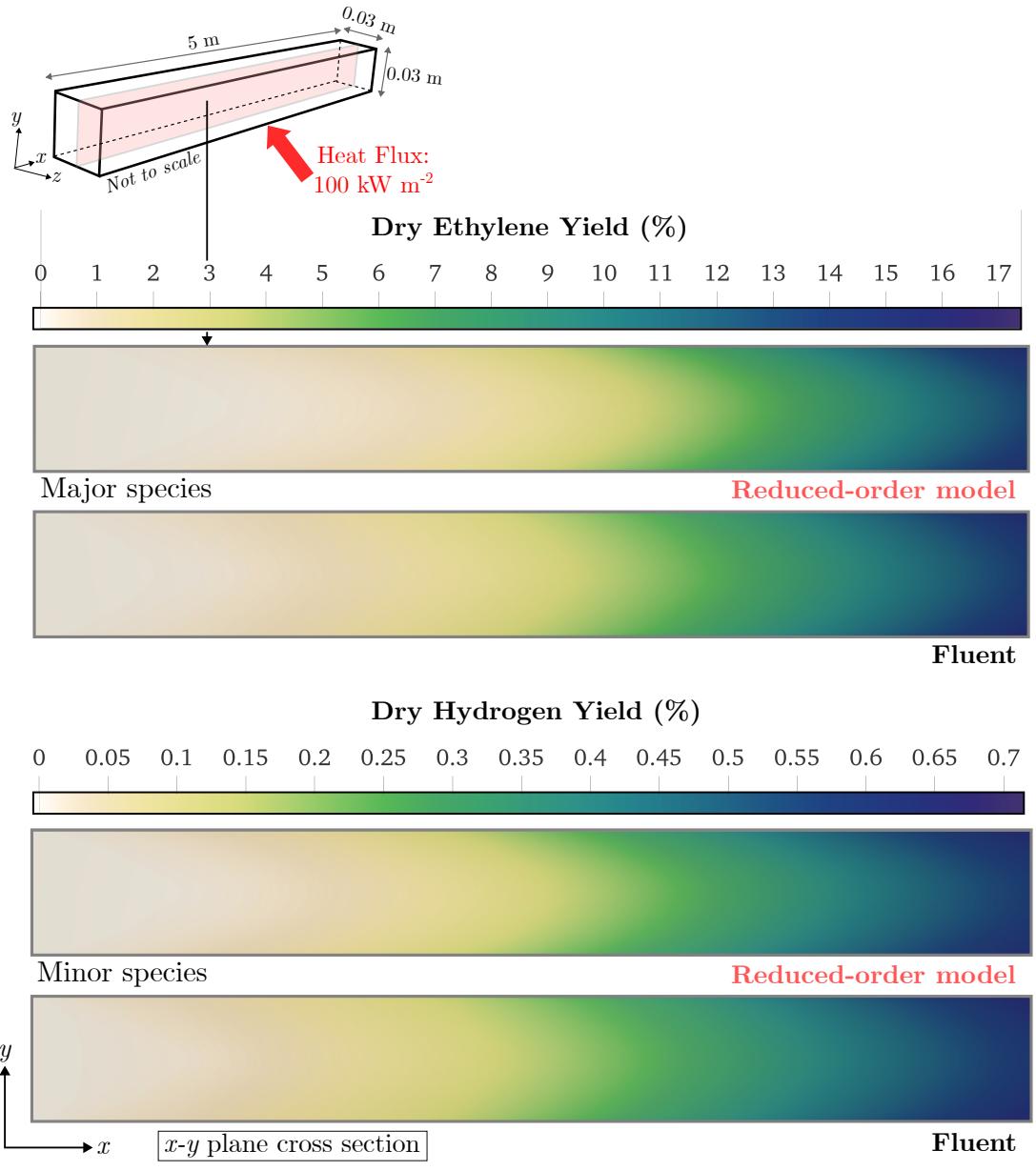


Figure 4: Computational speed of the ROM relative to a commercial reacting flow solver FLUENT with a detailed chemical mechanism containing 65 species and 130 species

This sizeable computational acceleration is achievable whilst maintaining a sufficiently good level of accuracy such that reliable design optimisation can be performed in the future. Figure 5 demonstrates that the ROM can predict dry yields for both major and minor species relatively accurately compared to the full-order model (FOM), *i.e.*, FLUENT. Despite not being trained on any three-dimensional test cases (*i.e.*, all of the training data is from 1-D PFR simulations), the ROM accurately predicts gradients in the yield perpendicular to the flow direction due to 3-D temperature non-uniformities (due to heated walls) and mass diffusion. Furthermore, Figs. 5 & 6



Good prediction of yield distribution for both major and minor species in x and y directions

Figure 5: Verification of the ROM against industry-standard commercial reacting flow solver FLUENT using a heated duct test case with a propane feedstock (65 species, 800 reactions): major and minor species mass fractions

suggest that chemistry-related modelling errors do not accumulate and the yield distribution is accurate over the full 5 m flow path length.

The toughest test of the ROM's capabilities is whether it can predict the spatial distribution of reaction rates, which are highly non-linear. Figure 6 shows that the ROM is indeed successful in capturing spatial variability in the reaction rates (induced primarily by temperature gradients). These factors support the generalisability and robustness of the ROM given new and

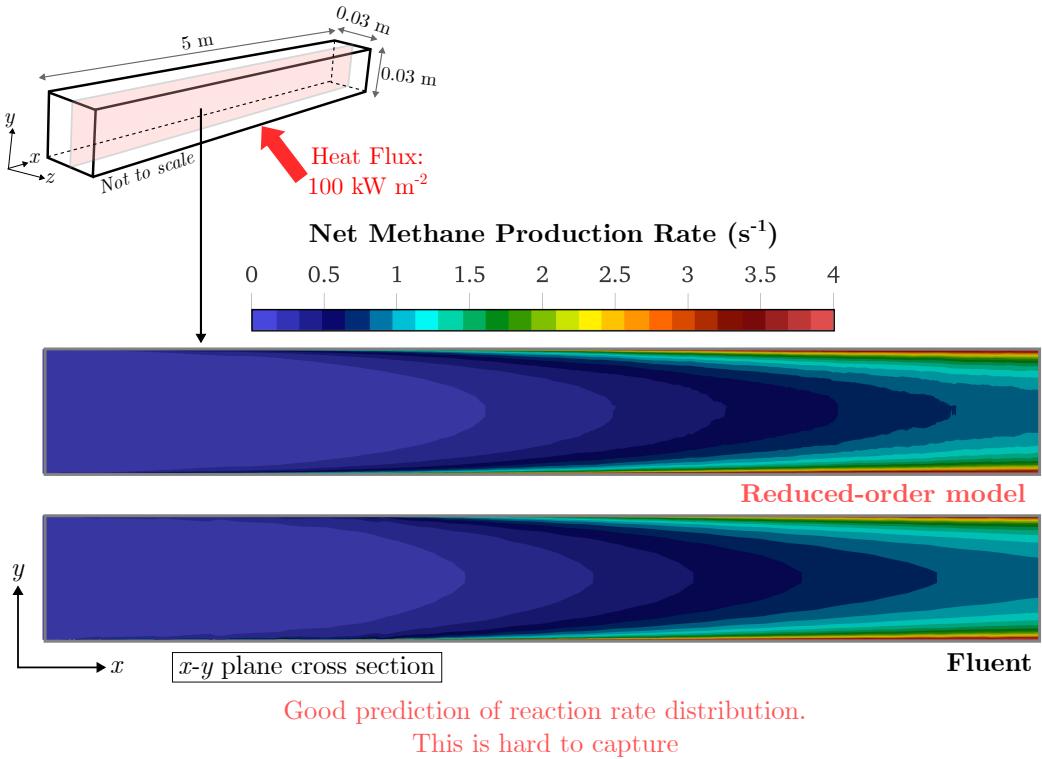


Figure 6: Verification of the ROM against industry-standard commercial reacting flow solver FLUENT using a heated duct test case with a propane feedstock (65 species, 800 reactions): methane net production rates

substantially different test data not seen during training. This strongly supports the feasibility of this new methodology.

As a proof-of-concept, the ROM is now applied to an engine-relevant multistage axial turbo-reactor architecture. Figure 7 shows the ethylene yield & production rate, as well as the steady-state coke formation rate on the surfaces of the diffuser blade. This is the first-ever numerical simulation performed of the turbo-reactor capturing aerochemical interactions. This will inform design decisions, facilitating aerodynamic design optimisation to improve reaction efficiency and mitigate coking.

2.4. Proposed Next Development Phase

In this next phase of methodology development and advancement, we intend to generalise, modularise and package this tool to be used universally across a range of industry-relevant chemical reactions and chemical processes. A first step towards this goal is to extend this ML-assisted ROM methodology to be applied not only to gas-phase reactions (achieved during my Doctoral research), but also to heterogeneous catalytic surface-phase reactions. This will

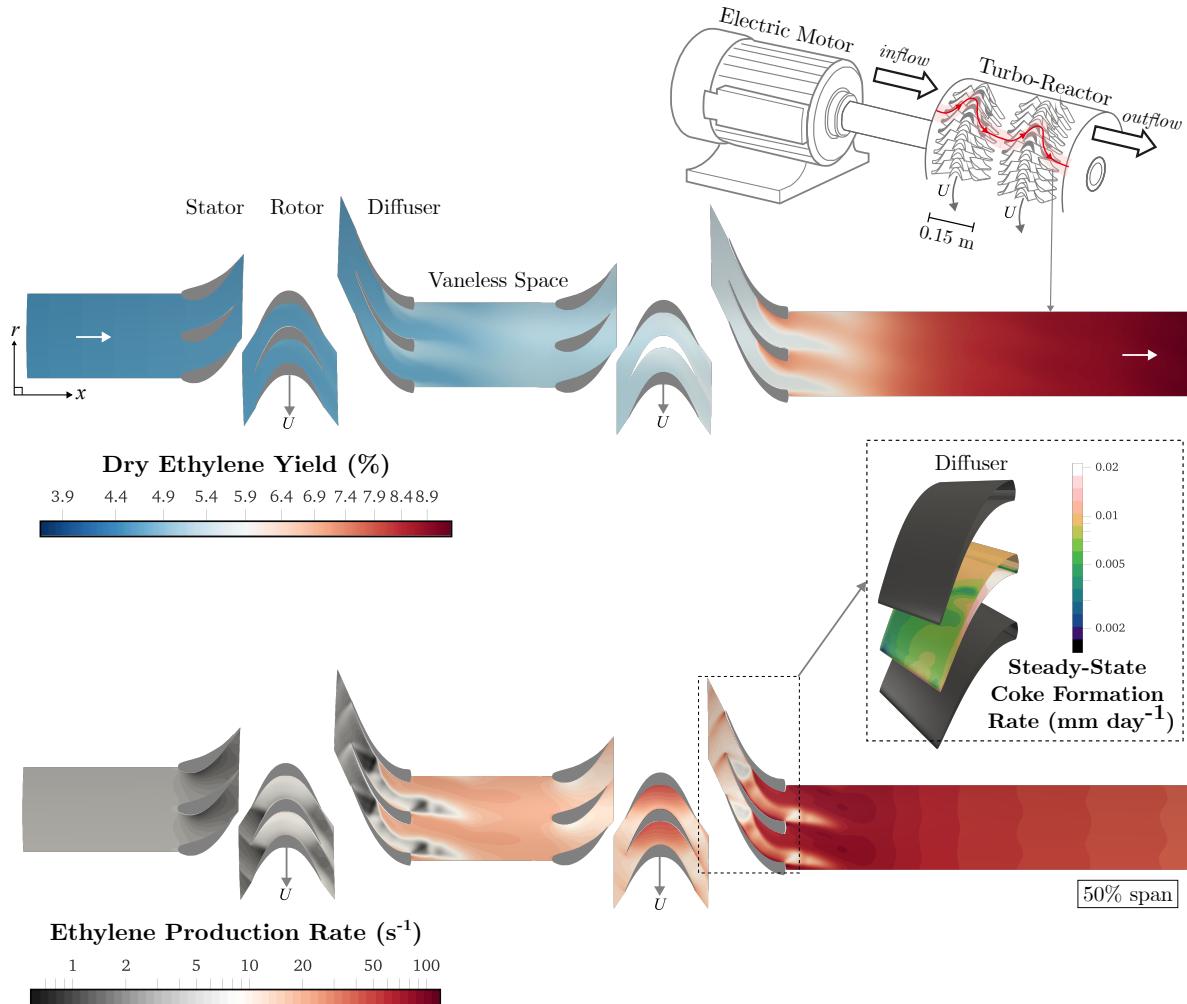


Figure 7: A proof-of-concept: first-ever numerical prediction of the chemical reaction yield, dynamics and coke formation rate predicted using the ML-assisted ROM for a multistage axial turbo-reactor architecture

substantially expand the applicability since many chemical processes feature catalytic reactions. This advancement in the ML-assisted ROM methodology would involve

1. incorporating catalytic reactions in the training database generation
2. training a autoencoder neural network similar to that developed in Sec. 2.2 to capture the dynamics of surface-phase reactions
3. developing an interface treatment to couple the surface- and gas-phase reactions
4. implementing additional transport equations in our in-house CFD solver for the surface species

Once this has been achieved, this methodology can be translated into a user-friendly platform that can be universally applied to industry-relevant reaction processes.

Commercialising a numerical tool developed in a research setting is always challenging. However, working in close collaboration with an industrial partner will help to efficiently guide this development process, maximising the user-friendliness and modularity of the tool, and ensuring the requirements of industry are embedded in the platform early in the tool development cycle.

2.5. Summary

In summary, this work describes the development of a new multi-fidelity ML-assisted ROM to provide an efficient solution to incorporate aerochemical interactions early in the design cycle. This will enable detailed and comprehensive chemical kinetic models that accurately capture realistic reaction dynamics (but contain more than $\mathcal{O}\{1000\}$ species and over $\mathcal{O}\{10,000\}$ reactions) to be compressed into a reduced-dimensionality space, and coupled with CFD at a computational cost 100 – 1000 times lower than the FOM. This is a vital step in designing a new class of turbomachines with the unique requirement of controlling reactions along the bladed flow path.

This step-change advancement in the field of computational science brings multiphysics from being “one-off” simulations to being exploited routinely at the design optimisation level. Whilst historically, this development cycle would require many physical experiments, now, by integrating complex multiphysics early in the design cycle, the burden on experiments can be reduced and costs saved, accelerating the net-zero transition.

We hope to collaborate closely with the chemical industry to develop a modular, production-ready platform for automatically accelerating high-dimensional reacting flow numerical simulations. Iterative feedback with industry will be vital for rapidly developing a user-friendly tool that meets the user specifications.