

Developing an Ecosystem for the Efficient Design and Modelling of Novel Catalytic Systems

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1 The Big Picture

Catalytic chemical processes are already ubiquitous across engineering systems (*e.g.*, ammonia production, naphtha reforming, automotive catalytic converters); however, with the urgent demands of the energy transition, the role of catalysis in engineering is poised for significant further growth. For example, in synthetic feed/fuel production, CCUS, and hydrogen production, catalysis plays a vital role in the overall performance and cost of these systems. However, the development of effective heterogeneous catalytic systems faces two key challenges.

First, realistic and accurate numerical modelling of highly complex and strongly interacting fluid dynamics, gas-phase chemical kinetics, and surface kinetics is computationally intractable. The problem applies universally across all reacting flow modelling systems; however, it is exacerbated for catalytic reactors because the characteristic length scale (or feature size) found in porous catalytic structures can be very small. Therefore, very high mesh densities are necessary to numerically model the flow. In addition to this, for realistic predictions of the yields (the key metric of interest), detailed kinetic models must be solved. Consequently, designers and numerical modellers of catalytic systems typically resort to using porous media models and applying simplified (but inaccurate) kinetics. This makes it difficult to improve catalytic performance and minimise pumping losses beyond the status quo.

Second, conventional manufacturing constraints have prevented the implementation of exotic internal catalytic structures to maximise surface-area-to-volume ratio while minimising pumping

power penalties (*i.e.*, pressure losses). Even if these constraints were lifted, the aforementioned numerical modelling deficiencies would prevent proper exploitation of the design space.

To this end, we hope to apply our new design and modelling ecosystem, developed for various applications, to aid accelerating the design, modelling and optimisation of novel catalytic systems. This ecosystem has three components that will be addressed separately in this report.

1. *Accelerated aerochemical modelling*: to alleviate the cost of modelling complex kinetic models, we introduce an machine-learning-assisted efficiently coupled aerochemical modelling methodology (called **ChemZIP**) to accelerate reacting flow modelling by three orders of magnitude. This is achieved whilst retaining a completely viscous 3D fluid flow model and without the kinetics imposing any time-step restrictions on the fluid side. Our approach features a intelligent strategy to overcome the training-data-generation bottleneck.
2. *Accelerated multiscale flow modelling*: within porous flow structures there are two well defined scales: the small-scale flow structures of the order of the feature size of the porous media, and large-scale base flow variations covering the domain. In many scenarios where the small-scale flow structures are repeating, this two-scale nature of the flow can be exploited to accelerate computation fluid dynamic simulations. A small number of fine mesh blocks can be distributed in targeted regions of the domain, while the remaining space is filled with a significantly coarser mesh. This approach enables considerable computational acceleration. To capture the effects of unresolved scales on the coarse mesh, source terms are used to globally propagate information from the fine mesh blocks.
3. *Flow-oriented TPMS devices for heat and mass transfer*: a new framework is developed to design additively manufactured heat/mass transfer devices using topology optimisation. This unlocks a new design space for tailoring the internal catalytic structures to be aligned nicely with the flow, leading to a so called “flow-friendly” device. Therefore, pumping losses can be minimised whilst maintaining good mass/heat transfer effectiveness.

The following three mini-reports will further elaborate on each of these features of the overall workflow. It is emphasised that although this methodology is discussed in the context of catalytic systems, it could also be applied more generally, for example, for designing, modelling and optimising novel micromix combustor technologies.

Bringing Aerochemical Modelling to the Design Optimisation Level – Dylan Rubini

2 Bringing Aerochemistry Coupling to the Design Level

2.1. Executive Summary

The role of the chemical industry in modern society is rapidly evolving; on the one hand, it must develop novel technologies based on the new requirements for the energy transition, and on the other hand, it must decarbonise, transform and modernise an existing asset base of chemical process. These existing assets, including hydrocarbon cracking units, hydrogen production plants, ammonia production facilities, etc., rely on fossil-fuel-combustion-based furnaces to supply energy to the chemical process. Radically new technologies are necessary to decarbonise these processes efficiently while maintaining profitability. On top of this, the energy transition unlocks a wide variety of opportunities for the industry, such as carbon capture, electrochemical process (*e.g.*, electrolyzers), synthesising sustainable feedstocks & fuels, and many more. Given the urgent climate emergency, these developments need to be accelerated.

However, a key bottleneck in designing, developing and optimising these new technologies and chemical processes is aerochemically coupled numerical simulations using detailed, comprehensive (and accurate) chemical kinetic models. Large kinetic models are often required for accuracy (consisting of $\mathcal{O}\{1000\}$ species and $\mathcal{O}\{10,000\}$ reactions). But the price paid is an acute increase in computational overhead, as CPU time scales cubically with the number of species $\mathcal{O}(N_{\text{species}}^3)$. Therefore, this places a heavy burden on accurate, but time-consuming and costly, physical experiments in order to reduce uncertainty and risk.

To address this, this work proposes a new methodology to mitigate this computational bottleneck. We will demonstrate that it is now possible to accelerate reacting flow numerical simulations by two to three orders of magnitude, while accurately capturing the response dynamics of a *detailed* chemical kinetic model and maintaining a high-fidelity 3-D viscous aerothermal fluid flow model. This new methodology is an automated approach that leverages machine learning to uncover preexisting low-dimensional latent spaces hidden within the governing physics.

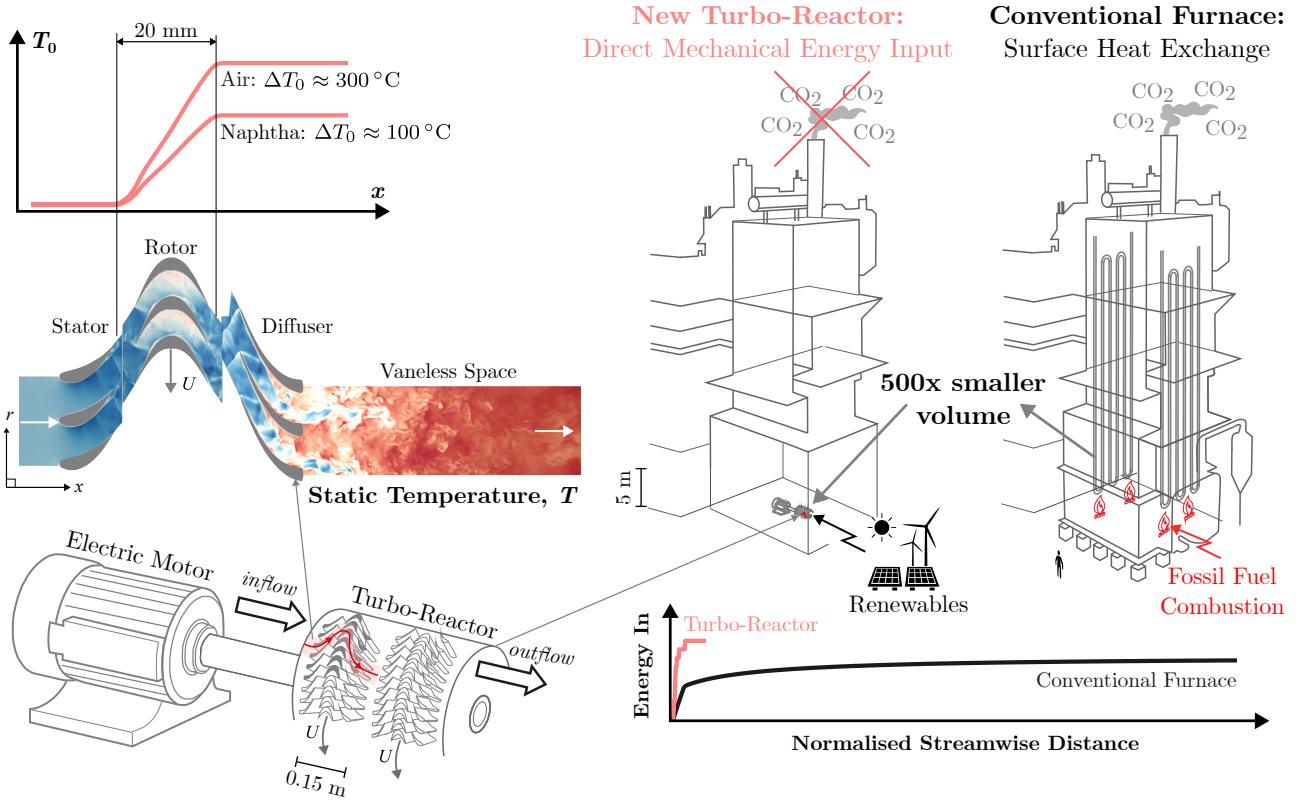
In this report, this methodology is explained in the context of a new turbomachinery concept that can decarbonise endothermic chemical reaction processes such as steam cracking. This is an ideal test bed because (1) the flowfield is highly complex and there are unique aerochemical

interactions, and (2) this is the first time turbomachines have had to be designed to control and optimise chemical reaction dynamics along the bladed flow path; therefore, there is limited experimental data to guide the design process. By accelerating reacting flow simulations (100 to 1000 times) using this new methodology, it will be possible to perform aerodynamic optimisation early in the design cycle to maximise reaction efficiency and minimise coke formation rate (which are key design metrics of the process). To put into context the importance of tuning the chemical reaction through careful aerodynamic design, for a typical hydrocarbon cracking plant (with capacity = 1 million tonnes per year), a 10% improvement in reaction efficiency can increase annual profits for the plant operator by €90 – €110 million (as of 2024).

To further advance this methodology, we intend to generalise and modularise this numerical tool into a user-friendly platform that can accelerate chemical kinetic modelling for a wide variety of industry-relevant chemical reaction processes ranging from hydrogen production and synthetic fuel production to electrochemical reactions. A critical hurdle in generalising this methodology is the incorporation of catalytic surface reactions. Since catalysts dominate the chemical industry, *e.g.*, for synthetic fuel production, hydrogen production, etc., accelerating catalytic reactive flow simulations would be a game changer. A numerical tool that can accurately but highly efficiently predict yield and coking distributions in chemical processes will help produce more cost-effective designs, reduce dependence on costly physical experiments, and ultimately contribute to accelerating the net-zero transition.

2.2. 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 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



Turbo-Reactor Could Decarbonise More Than 40 Hard-To-Abate High-Temperature Industries

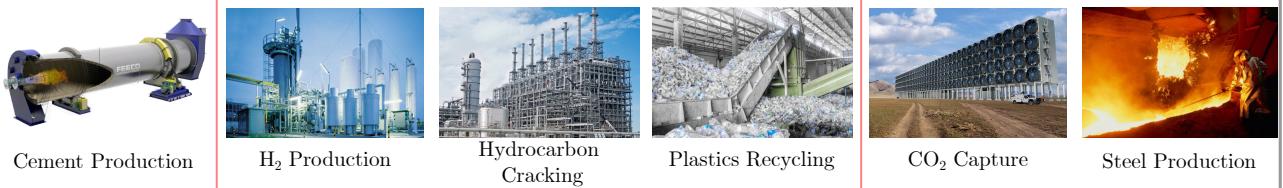


Figure 1: Electrified turbo-reactor could decarbonise many hard-to-abate industrial processes

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 chemical reaction dynamics, an accelerated aerochemically coupled numerical solver is required. This work introduces a multi-fidelity, efficiently coupled aerochemistry model, called **ChemZIP**, guided by machine learning (ML) to routinely bring reacting flow simulations into the early

design phases, rather than being “one-off” simulations.

2.3. Data-Driven Efficiently Coupled Aerochemistry Flow Solver

2.3.1. 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 characteristic 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, the highly efficient multi-fidelity ML-assisted ChemZIP methodology 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.

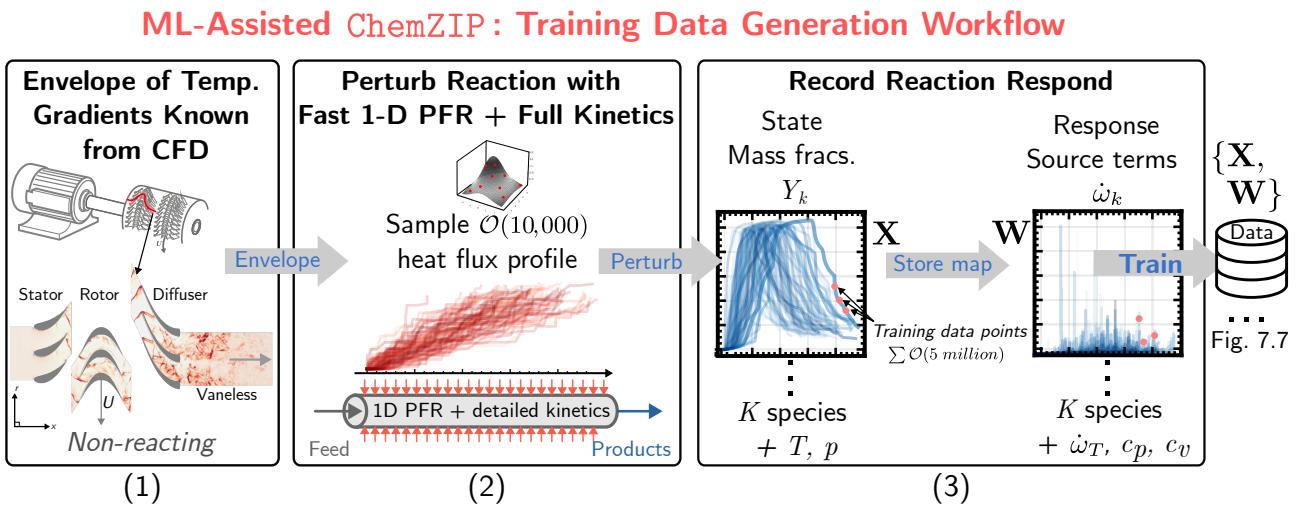
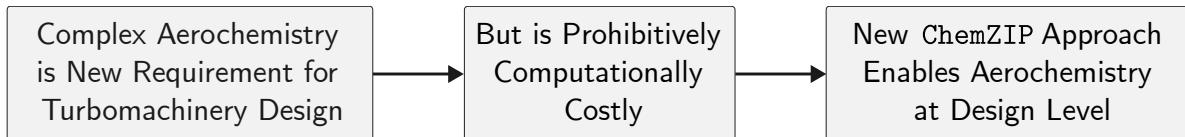


Figure 2: Multi-fidelity ML-assisted ChemZIP training database generation workflow

2.3.2. Methodology

Figures 2 & 3 outline the new multi-fidelity ML-assisted ChemZIP methodology to accelerate multiphysics numerical analysis of the turbo-reactor. First, 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 ChemZIP model (see Fig. 2(c)) with over 5 million samples. By simplifying the fluid dynamics (*i.e.*, by using a PFR) while retaining 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.

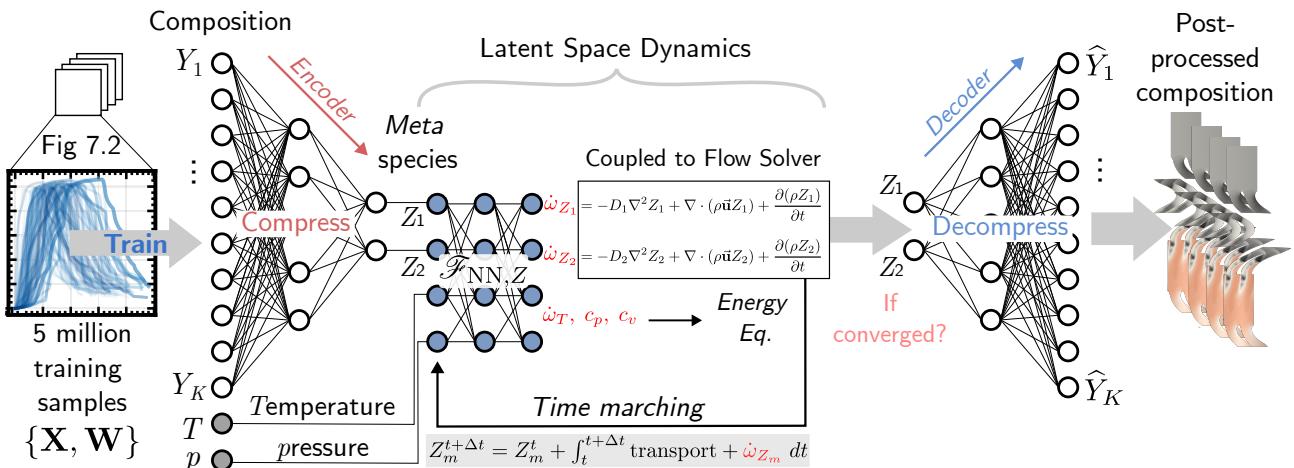


Figure 3: Multi-fidelity ML-assisted ChemZIP methodology overview

Subsequently, as shown in Fig. 3, a ML-assisted ChemZIP model 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.

Coupling the **ChemZIP** 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 pre-trained NN (see Fig. 3). A key feature of this methodology is that on the fluid flow modelling side, no new modelling assumptions are made, and its fidelity can range from RANS to high-fidelity LES modelling.

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) as shown in Fig. 3. This powerful methodology enables a speed-up of 100 to 1000 times relative to reacting flow CFD with detailed chemical kinetics, while maintaining high-fidelity aerothermal modelling and accurately capturing the dynamics of a detailed kinetic model. This will enable aerochemical optimisation to be brought to the design level for the first time.

2.3.3. 3-D Viscous Verification and Proof-of-Concept

To demonstrate the feasibility, success, and future potential of this new methodology, numerical predictions of the **ChemZIP** are compared with 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 as a verification test case (see Fig. 5). Crucially, Fig. 4 illustrates that the **ChemZIP** can achieve a two-order-of-magnitude speedup relative to a commercial solver with detailed kinetics.

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 **ChemZIP** can predict dry yields for both major and minor species within a few percent relative error compared to FLUENT. Over a long distance of 5 m the accumulation of errors for major and minor species is minimal, indicating robustness and ensuring accurate forecasts even over extended time intervals. Despite not being trained on any three-dimensional test cases (*i.e.*, all of the training data is from 1-D PFR simulations), the **ChemZIP** 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.

The toughest test of the **ChemZIP**’s capabilities is whether it can predict the spatial distribution of reaction rates, which are highly non-linear. Figure 6 shows that the **ChemZIP** is

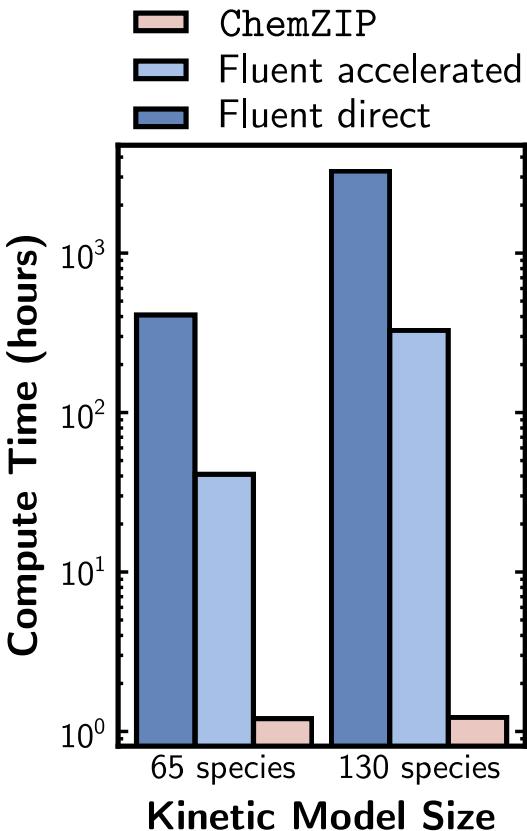


Figure 4: Computational speed of the ChemZIP relative to a commercial reacting flow solver FLUENT with a detailed chemical mechanism containing 65 species and 130 species

indeed successful in capturing spatial variability in reaction rates (induced primarily by temperature gradients). These factors support the generalisability and robustness of the ChemZIP given new and substantially different test data not seen during training. This strongly supports the feasibility of this new methodology.

As a proof-of-concept, the ChemZIP 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. Despite the highly complex nature of the flow relative to the more simplified training data provided, the reaction responds as expected to sharp and complex gradients in the temperature and reaction timescale. 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.

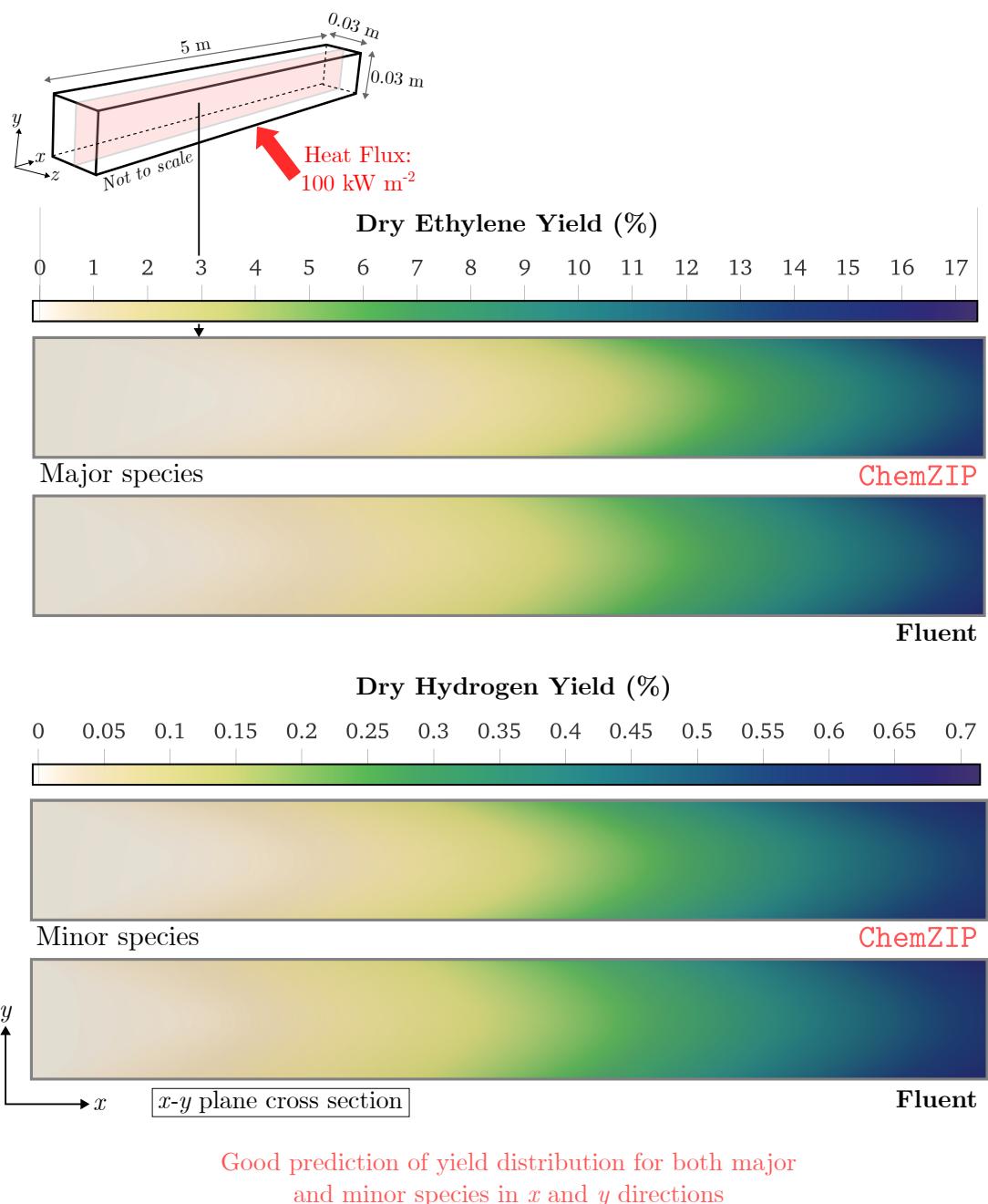


Figure 5: Verification of the ChemZIP against industry-standard commercial reacting flow solver FLUENT using a heated duct test case with a propane feedstock (65 species, 800 reactions): major and minor species mass fractions

2.3.4. 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 multi-fidelity ML-assisted ChemZIP methodology not only to gas-phase reactions (achieved during my Doctoral research) but also to heterogeneous catalytic surface-phase reactions. This will

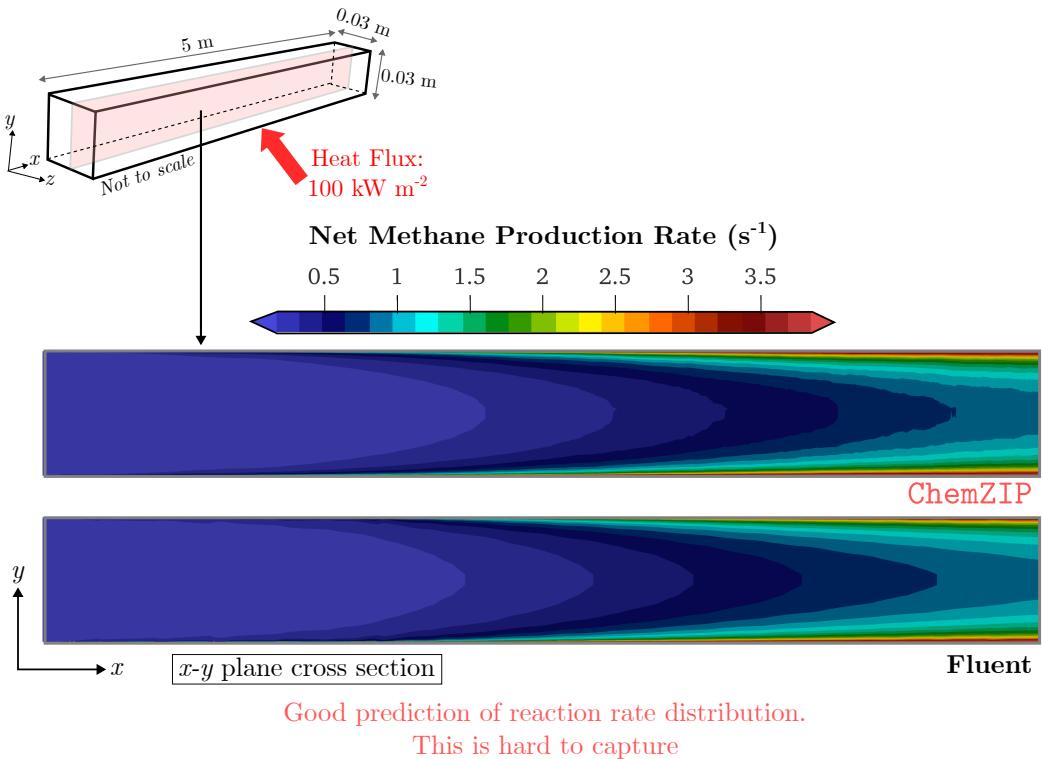


Figure 6: Verification of the ChemZIP against industry-standard commercial reacting flow solver FLUENT using a heated duct test case with a propane feedstock (65 species, 800 reactions): methane net production rates

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

1. incorporating catalytic reactions in the training database generation
2. training an autoencoder neural network similar to that developed in Sec. 2.3.2 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 evolution of active surface sites

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.

2.4. Summary

In summary, this work describes the development of a new multi-fidelity ML-assisted ChemZIP to provide an efficient solution to incorporate aerochemical interactions early in the design cycle.

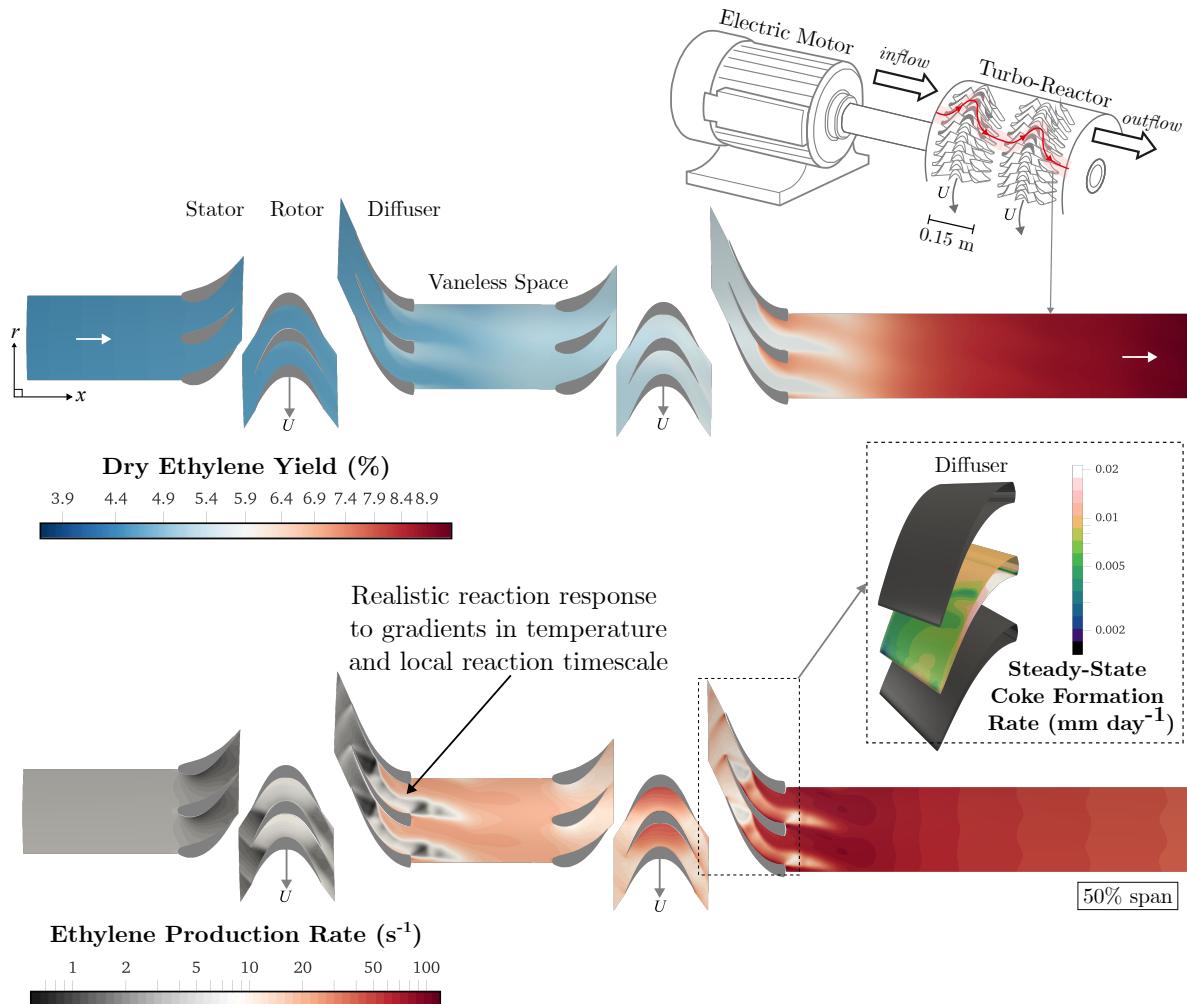


Figure 7: A proof-of-concept: first-ever numerical prediction of the chemical reaction yield, dynamics and coke formation rate predicted using the ML-assisted ChemZIP methodology for a multistage axial turbo-reactor architecture

This will enable detailed and comprehensive chemical kinetic models that accurately capture realistic reaction dynamics (but contain $\mathcal{O}\{1000\}$ species and $\mathcal{O}\{10,000\}$ reactions) to be compressed into a reduced dimensionality space, and coupled with a high-fidelity fluid solver at a computational cost 100 – 1000 times lower than state-of-the-art acceleration techniques in FLUENT. 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 new methodology will open up an entirely new design space for aerothermochimically optimising chemical catalytic processes—including carbon capture, synthetic fuel production, ammonia cracking, hydrogen production, and many more. Therefore, ChemZIP is a vital enabler for the development of novel processes for the next-generation low-carbon industrial sector.

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.

Nomenclature

List of Symbols

$\dot{\omega}$	Net species production rate (s^{-1})
\mathcal{O}	Order of magnitude (-)
\tilde{y}	<i>Meta</i> species mass fraction (%)
M	Total number of <i>meta</i> species (-)
N	Total number of physical species (-)
T	Static temperature (K)
Y	Physical species mass fraction (%)

Abbreviations & Acronyms

CFD	Computational fluid dynamics
LES	Large eddy simulation
ML	Machine learning
NN	Neural network
PFR	Plug-flow reactor
RANS	Reynolds-averaged Navier-Stokes
Subscripts	
\square_m	Species index of M total <i>meta</i> species
\square_n	Species index of N total physical species
Superscripts	
$\hat{\square}$	Reconstructed quantity
$\tilde{\square}$	Latent space quantity

Accelerating Multi-Scale Flow Modelling – Yueyun Xi

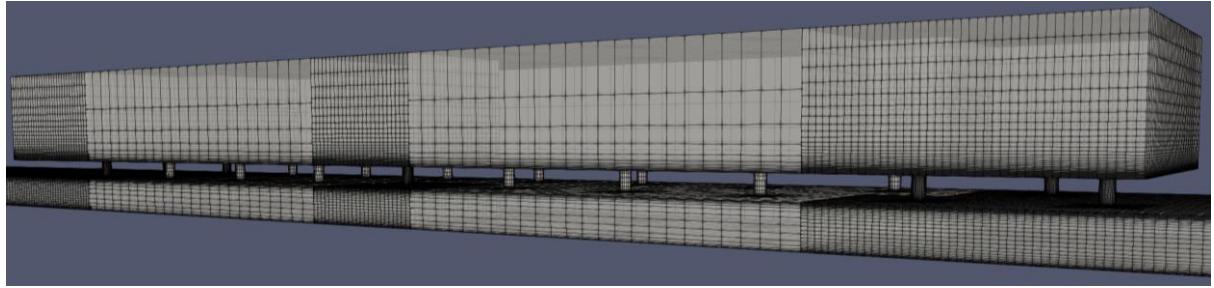
The multiscale nature in the flows in many engineering applications and in turbulent flows poses a big challenge for CFD. For local small-scale flow structures, fine spatial and temporal resolution is needed to resolve the local high gradient. To have a locally meaningful solution, local domain must be subjected to proper boundary provided by the global domain, leading to the cost of employing high spatial and temporal resolution in the entire domain.

This study tackles the multiscale challenge by

- (a) resolving the local flow fields with fine mesh blocks,
- (b) and propagating local flow fields to correct the global flow fields.

Two-scale mesh configurations

Fine-mesh blocks are deployed locally in the domain to capture the local flow physics. Coarse-mesh blocks are deployed in the rest of the domain to reduce the computation cost. Flow physics are resolved locally and propagated to the global domain.



Two-scale mesh configurations for impingement jets

Coarse-fine domain interface treatment

Small-scale fluctuations are introduced at the coarse-fine domain interface to initialise proper turbulent flow behaviour without violating the flux conservation. A flow variable at fine-mesh boundary is split into a coarse-mesh resolved base component and a fluctuation corresponding to fine-mesh resolution:

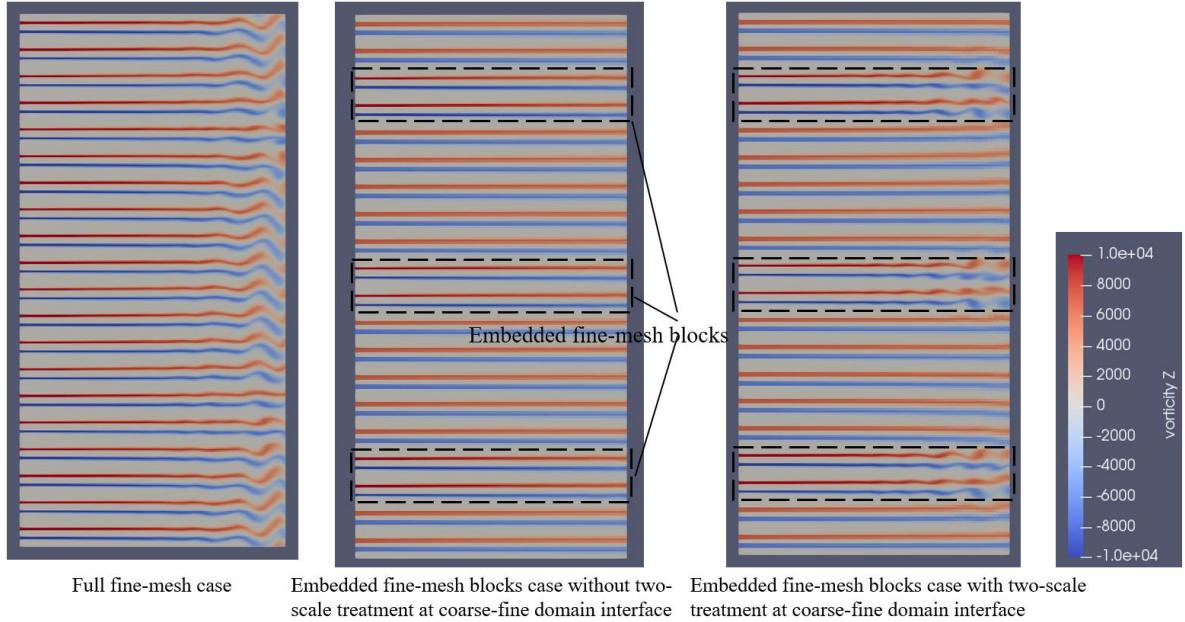
$$u_f = u_c + u'_f$$

Large-scale flow structures resolved by the global coarse-mesh blocks are interpolated at the coarse-fine domain interface to provide the base component boundary field using (flux-conservative) Galerkin projection.

The fluctuation must be recycled or synthesised, two options are available:

- (a) For regular repetitive geometry, where we may define a proper counterpart interface for each coarse-fine domain interface. Galerkin projection is used to filter out the fluctuation (with zero net flux contribution) on the remote interface, and the fluctuation is recycled to provide the fluctuation component boundary field.

(b) For non-regular geometry, spectral information is collected at the coarse mesh side, and used to synthesize the turbulent content. The generated turbulent content filtered using Galerkin projection to get the fluctuation part (with zero net flux contribution).



Initialising proper turbulent flow behaviour at the interface by introducing small-scale fluctuations

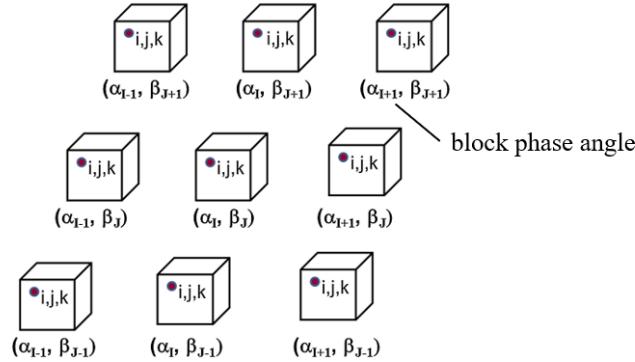
Target flow fields propagation

Time-averaged flow fields are collected at local fine-mesh blocks, and then propagated to the global domain as a target flow fields.

For the applicability on complex flow domain discretised by unstructured mesh, time-averaged fields are projected from fine-mesh block to a local pseudo-coarse-mesh block using 3D Galerkin projection.

After the fine-mesh fields are projected to a local coarse-mesh block, there are several options to propagate the local fields to the global domain:

(a) Provided the smoothness of the time-averaged flow fields, block spectral mapping can be adopted to propagate the target flow fields. The target flow fields is approximated by block-wise Fourier modes, and then propagated to the global domain.



$$(\mathcal{S})_{IJ} = \sum_{m=0, n=0}^{M, N} [a_{m,n} \cos(m\alpha_I) \cos(n\beta_J) + b_{m,n} \sin(m\alpha_I) \cos(n\beta_J) + c_{m,n} \cos(m\alpha_I) \sin(n\beta_J) + d_{m,n} \sin(m\alpha_I) \sin(n\beta_J)]$$

Propagating target flow fields using block spectral mapping

- (b) The target flow fields could also be propagated using reduced order modelling (ROM) techniques. Flow structures are captured and analysed at local fine-mesh block, and utilised to define the target flow structures at coarse-mesh blocks.

$$\frac{d}{dt} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_{n-2} \\ v_{n-1} \\ v_n \end{bmatrix} = \begin{bmatrix} \square & \square & \square & \dots & \square & \square \\ \square & \square & \square & \dots & \square & \square \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \square & \square & \square & \dots & \square & \square \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \square & \square & \square & \dots & \square & \square \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_{n-2} \\ v_{n-1} \\ v_n \end{bmatrix}$$

$$\frac{d}{dt} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_{n-2} \\ v_{n-1} \\ v_n \end{bmatrix} = \begin{bmatrix} \square & \square & \square & \dots & \square & \square \\ \square & \square & \square & \dots & \square & \square \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \square & \square & \square & \dots & \square & \square \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \square & \square & \square & \dots & \square & \square \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_{n-2} \\ v_{n-1} \\ v_n \end{bmatrix}$$

Propagating target flow fields using ROM

Base mesh domain solution with space-time source terms

To correct global coarse-mesh flow fields and provide proper boundary conditions for local fine-mesh domains, the propagated target flow fields at coarse-mesh domain are used to constrain the time average of the coarse-mesh fields. Space-time source terms are used to drive the coarse-mesh fields and to enable large-scale flow unsteadiness (which is important for the coupling between coarse-mesh domain and fine-mesh domain):

$$\frac{\partial U}{\partial t} + R(U) = R(U_{tgt})$$

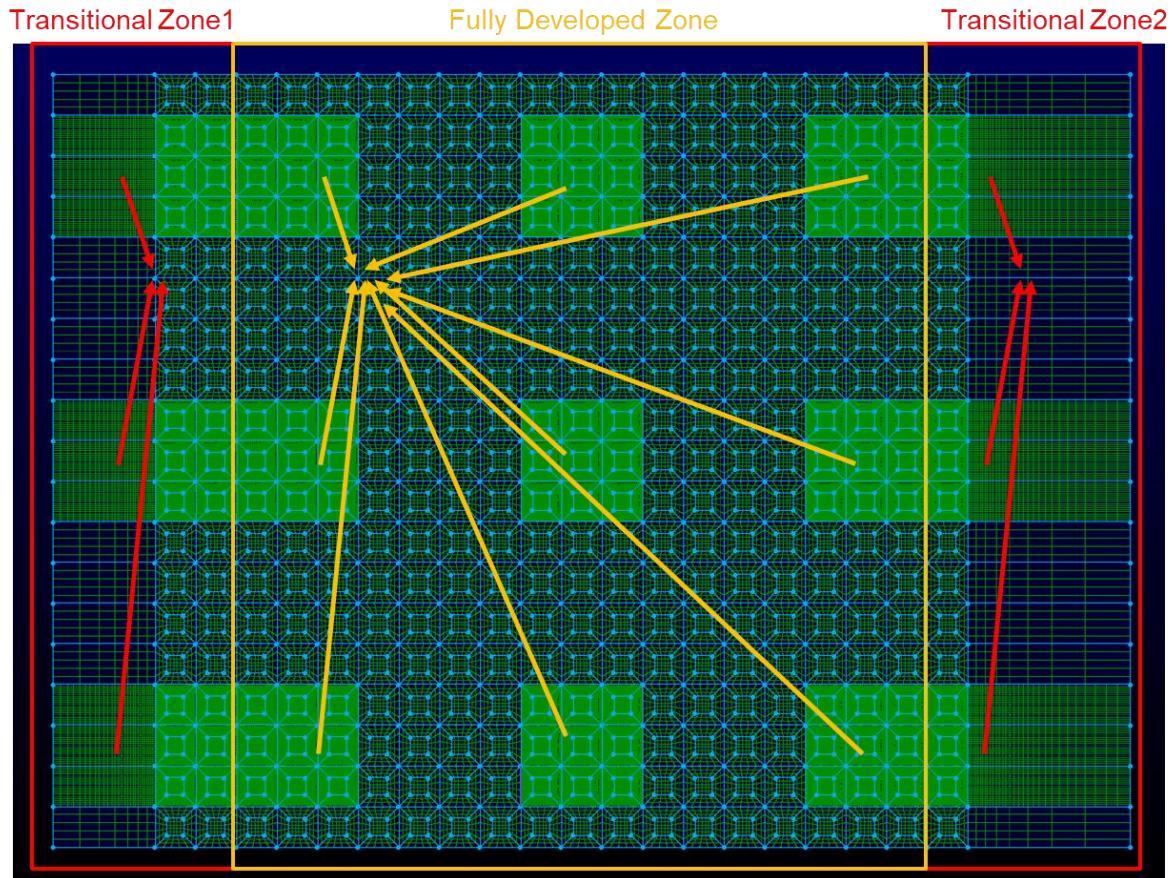
Time-averaging source term is introduced to correct nonlinear time-averaging effects for unsteady simulations:

$$\frac{\partial U}{\partial t} + R(U) = R(U_{tgt}) + \overline{R(U)} - R(\bar{U})$$

Automatic fine-mesh deployment based on flow fields probation

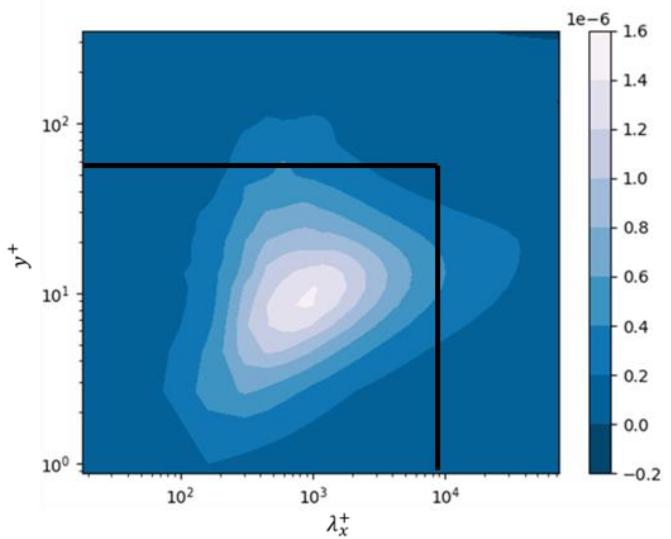
For simulation with practical interest,

- (1) Different flow patterns could coexist. The flow patterns need to be identified and different target fields collection and propagation schemes could be deployed.



Identification of different target fields collection and propagation schemes

- (2) The lengthscale of the fine-mesh blocks could be determined based on spectral information. The size of the fine-mesh block should be able to contain the local energy-containing flow structures.



Determining the size of fine-mesh blocks based on spectral information

Flow-Oriented TPMS Devices for Heat and Mass Transfer – Tom Merritt-Webster

Flow Oriented TPMS Devices for Heat and Mass Transfer

Combining parameterisable periodic lattice structures and design specific envelopes to design compact heat and mass transfer devices for complex assemblies.

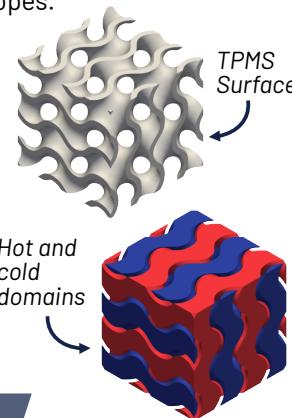
MOTIVATION

Additive manufacturing enables the creation of novel geometries which feature complex internal structures within almost any shape, allowing **design to be driven by performance rather than manufacturing limitations**.

However, design tools for heat and mass transfer devices that realise and exploit these possibilities are limited. The aim of this project is to develop an automated design platform that incorporates parameterised, flow-oriented internal structures into design specific envelopes.

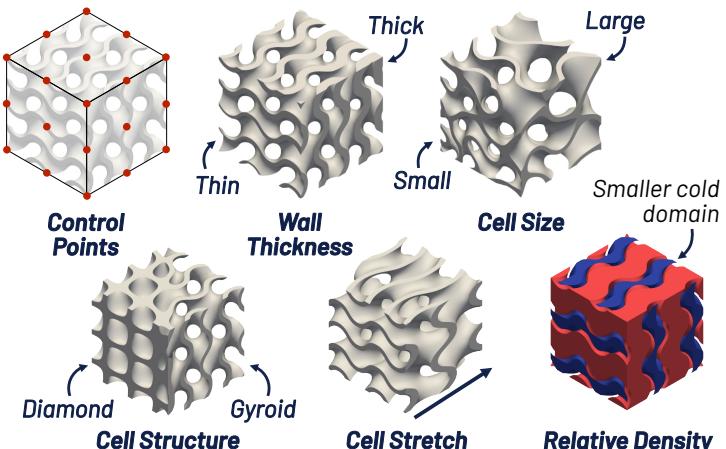
TPMS STRUCTURES

TPMS or Triply Periodic Minimal Surfaces are a family of analytically defined surfaces which are periodic in 3 directions. TPMS can be used to generate internal lattice structures that are ideal for transport processes: they divide space into **two interpenetrating domains**, have a **high specific surface area**, are **smooth** and can be **easily parameterised**.



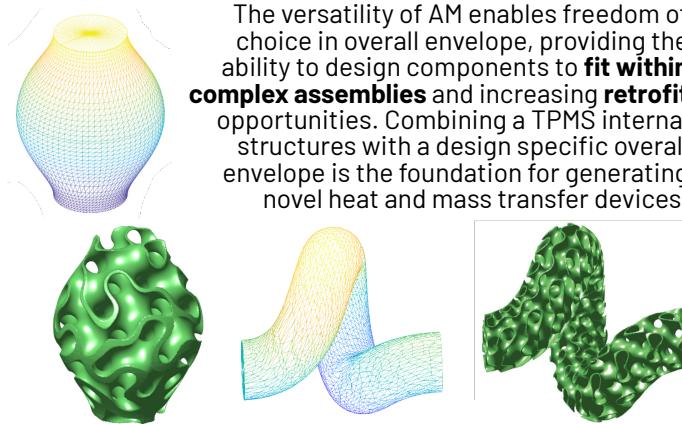
PARAMETER CONTROL

Parameters can be **smoothly and continuously adjusted** throughout the domain via control points to optimise the performance characteristics of the device.



FREEDOM OF ENVELOPE

The versatility of AM enables freedom of choice in overall envelope, providing the ability to design components to **fit within complex assemblies** and increasing **retrofit opportunities**. Combining a TPMS internal structures with a design specific overall envelope is the foundation for generating novel heat and mass transfer devices.

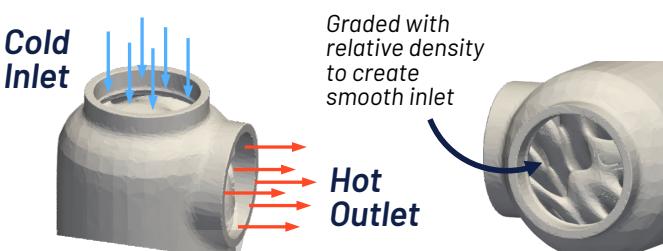


MANIFOLD PLACEMENT

The continuous nature of TPMS structures mean that hot and cold domains can be accessed from any surface, hence **manifolds can be placed at any orientation or position**. The opposite domain can be blocked off so the **manifold requires almost zero volumetric footprint**.

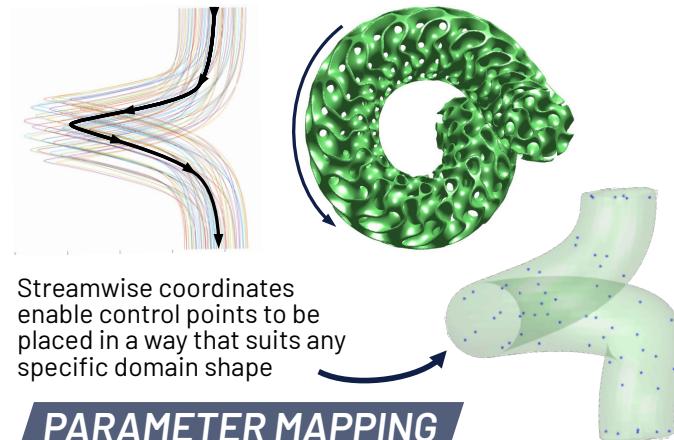


Control points placed around the manifold can alter the relative share to provide a smooth inlet or outlet, **reducing pressure losses** and enabling **fast flow distribution**.



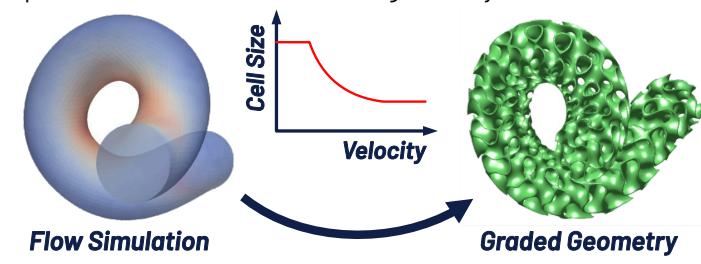
STREAMLINE STRUCTURES

Velocity data from an inviscid flow simulation can be used to produce **flow oriented TPMS structures** via streamwise coordinate system.



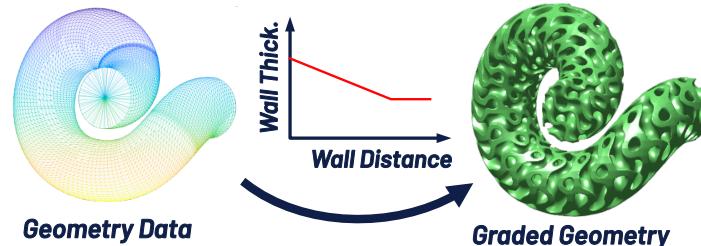
PARAMETER MAPPING

Flow simulation data can be mapped to specific parameter values to control the geometry.



Flow Simulation

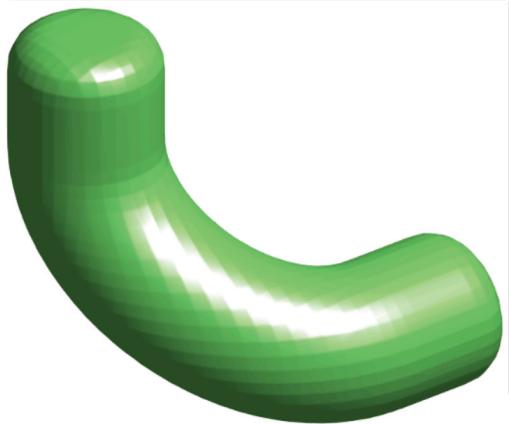
A mapping between geometrical characteristics (e.g. distance from wall) and parameter values can be used to control the geometry.



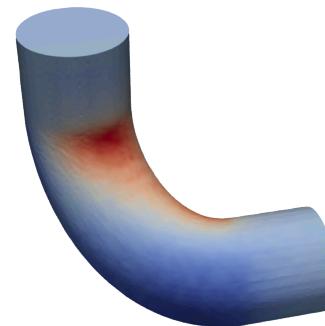
Geometry Data

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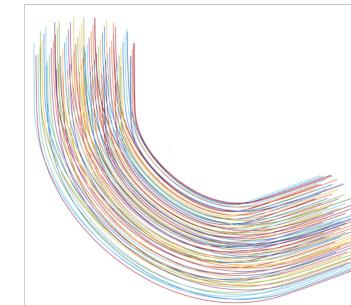
Example Workflow



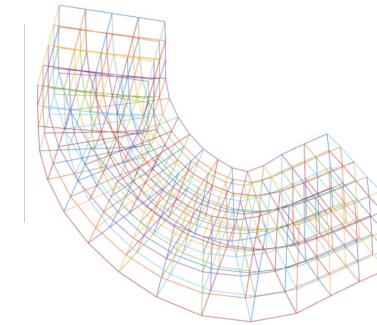
Arbitrary Input Geometry



Inviscid Flow Simulation



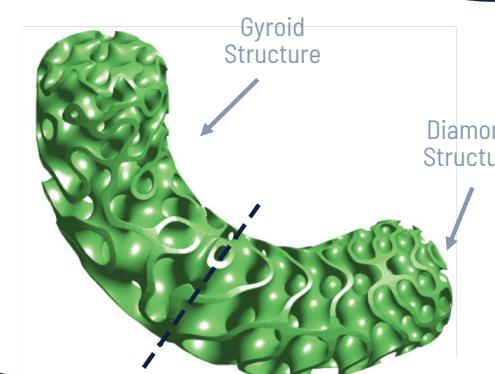
Extract Streamlines



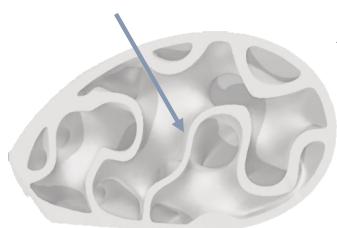
Create Streamline Coordinate System



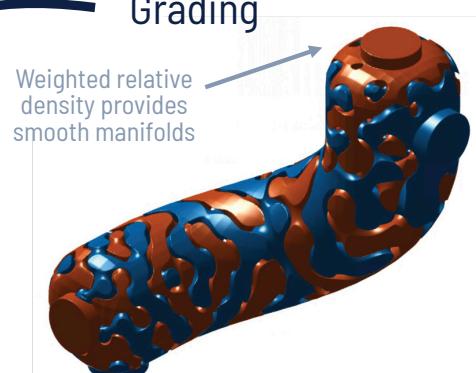
Cell Size Grading



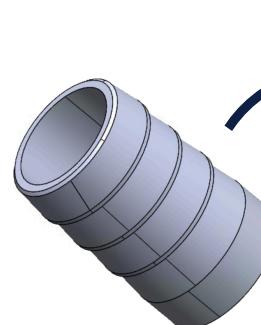
Core Structure Transition



Wall Thickness Grading



Manifold Positioning and Grading



System Integration
(E.g. hose connections)



Final Geometry



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OXFORD



OXFORD
THERMOFLUIDS
INSTITUTE

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3 Summary

In summary, this report has introduced three important components of an overarching ecosystem required to design and optimise novel catalytic systems for the energy transition. By leveraging machine learning and additive manufacturing, it is now possible to explore a much broader region of the design space using realistic compute resources. Ultimately, we hope to facilitate the design of more energy-efficient, more compact, and lower-cost catalytic systems within shorter turn-around times. We hope to work closely with industry to develop a complete platform in line with the requirements and specifications of the end-user.

Although this methodology and ecosystem has been discussed in the context of catalytic chemical systems, we are developing multi-fidelity and multiphysics strategies like those introduced here for a range of heat transfer, thermofluid and chemical applications.