PhD Studentship for Home Student (3.5Y covering stipend and fees)

Hybrid ML-Physics Optimisation Framework for Pharmaceutical Reactors

Chemical flow reactors, especially crystallisation reactors, play a vital role in pharmaceutical manufacturing. Reactor geometry has a major influence on solute-solvent mixing, which directly affects product consistency, and ultimately drug quality. Yet high-performing reactor designs remain largely undiscovered as high-fidely models for so called 'many-query' problems are expensive for large-scale design space exploration.

This PhD project will develop a new multi-fidelity Bayesian optimisation framework for reactor design, enabling efficient exploration of complex design spaces while reducing computational cost. Computational fluid dynamics models have an unusually rich fidelity structure. Fidelity can vary continuously through mesh refinement, but also discretely through the choice of physical model, from simpler species transport descriptions to more advanced multiphase formulations. Existing optimisation approaches are not designed to handle both of these together. The project will address this gap by creating a computational framework that can learn across these mixed fidelity levels and use them to accelerate reactor design.

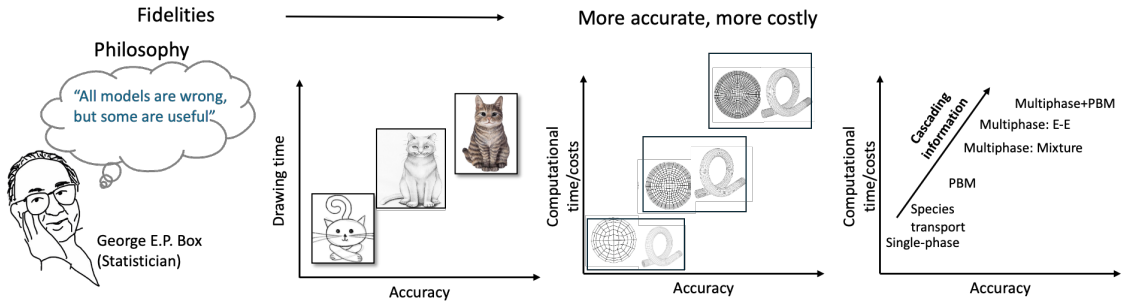
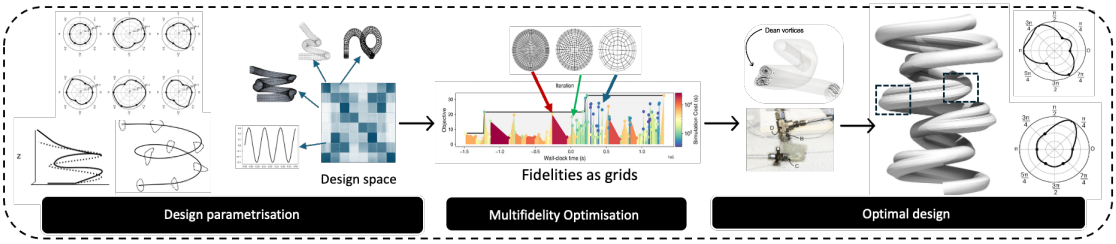


Figure 1. Explaining fidelities as cost vs accuracy in the computational models during evaluations for otpimisation



What will you do: You will develop Gaussian process surrogate models that can capture relationships across mixed discrete-continuous fidelity spaces. In practice, this means learning how inexpensive low-fidelity simulations, such as species transport models, can be used to improve predictions for expensive high-fidelity multiphase simulations. You will work at the interface of machine learning, computational fluid dynamics, and process engineering, developing both fundamental methods and design tools.

What we can offer:

- Dynamic and growing **Computational Design Intelligence** group where computational fluid dynamics, engineering design, and artificial intelligence converge to accelerate the discovery of next-generation chemical technologies
- Highly collaborative research environment spanning Chemical Engineering and Computing departments at Imperial College London
- Dedicated mentorship as well as the freedom to explore your own ideas
- By the end of this PhD, you will have developed a rare combination of skills: Bayesian machine learning, CFD simulations, and demonstrated ability to apply both to real world engineering design problems, a profile that is highly sought after in both industry and academia.

Eligibility: A First or Upper Second class (2:1) UK honours degree (or international equivalent) in areas such as Chemical Engineering, Mechanical Engineering, Aerospace Engineering, Physics, Mathematics, Computing, Data Science or a closely related subject. **Home students only**

Check out the group: https://nausheen13.github.io/nausheen-webpage/#/people

For more details contact Dr Nausheen Basha with your CV (nausheen.basha@manchester.ac.uk)