

## Faculty of Engineering

### Summer Research Program 2024-2025

Project Title: Explainable Artificial Intelligence in Kinetic Study of Sustainable Materials

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### Objective

Material sustainability is a key issue that our generation must address. This includes several heavy industries like iron, aluminum, and cement production, which together account for nearly 20% of carbon emissions. A common method to introduce sustainability into their processes involves solid-gas reactions. For example, in green steel production, hydrogen gas replaces coke to convert iron oxide into metallic iron. These reactions can be highly complex due to the variability of raw feedstock, complex boundary conditions, and intricate reaction mechanisms. In practical scenarios, the industry is likely to adopt empirical surrogate models rather than fully physical-based models. These surrogate models could be statistical, such as time series machine learning models.

In this project, we will explore the use of machine learning approaches to model time series data from reaction kinetics in the context of green steel processing. Our aim is to develop a new physics-informed, data-driven analytical pipeline for sustainable materials processing. We invite engineering students to join this proposal and explore this new opportunity together. Participating students will gain research experience in cutting-edge topics such as materials science, material characterization, and machine learning, preparing them for diverse career paths in engineering and academia.

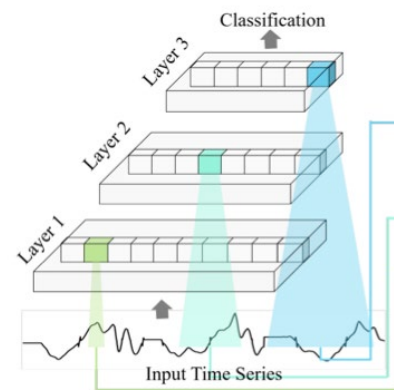


Figure 1 XAI for time series data modelling

### Project Details

The student will work with a synthetic dataset generated by a parametric kinetic model based on certain kinetic theories. This dataset serves as the ground truth, and we expect the explanations derived from machine learning to align with it. We will also utilize experimental data from the literature to derive initial insights under complicated reaction conditions. This synthetic data will be used for time series modeling within physically meaningful boundary conditions. A key task in this project is to identify the contributing factors to this reaction—to interpret the model's behavior accurately. Several explainability methods will be tested, ranging from post-hoc methods, such as local quantitative feature attribution analysis, to ante-hoc methods that reveal clearer causal relationships. The outcome of this project will be an in-house analytical pipeline that enhances our understanding of experimental data and potentially develops an active learning workflow for smart experimentation. This pipeline will enable us to develop reliable explainable artificial intelligence for the kinetic study of sustainable materials.

### Prerequisites

We encourage all students motivated by this project description to apply. The ideal candidate should possess expertise in materials phase transformation theory and machine learning. Students familiar with phase transformation kinetics, who also have experience in Python and popular machine learning packages (TensorFlow/PyTorch), will find it easier to begin this project. A key benefit of this project is that we will provide a subscription to GPT-4 for the year to help the team quickly flatten the learning curve.

### Additional Information

Please email Dr. Yuxiang Wu/Prof. Michael Preuss ([yuxiang.wu@monash.edu](mailto:yuxiang.wu@monash.edu) and [michael.preuss@monash.edu](mailto:michael.preuss@monash.edu)) for more details before applying. In your email, please explain (within 200 words): Why this project interests you? Which past experiences/knowledge prepare you for success in this project? Describe a scenario where you solved a hard problem from scratch?