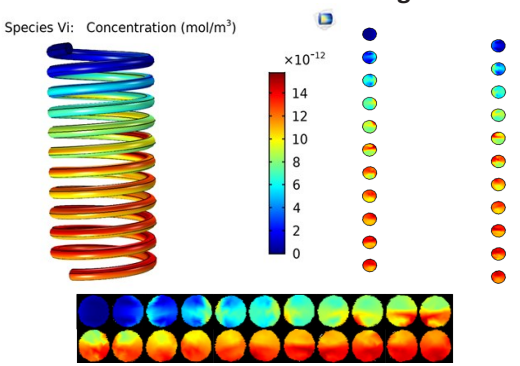
Machine Learning Methods for Accelerated Generative Equipment Design for New Medicines

Thomas Ralph

Introduction

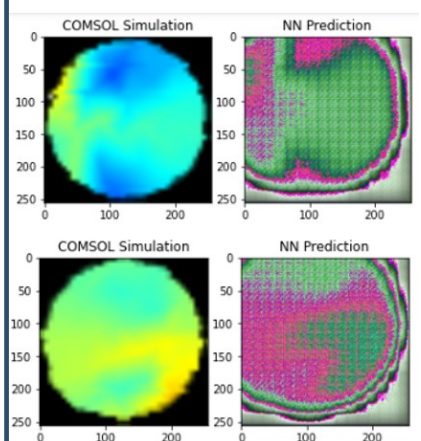
Simulation of the virus inactivation process within coiled reactors can be solved using multi-physics software such as COMSOL, Ansys Fluent, etc. These simulations can take up to weeks to finish processing, creating a bottleneck when trying to discover new medicines. The goal of this project is to design a variety of neural networks using machine learning which will aim to decrease virus inactivation simulation time.

Virus Inactivation Simulation Using COMSOL

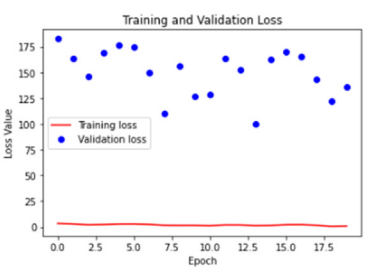


Virus inactivation is simulated within a coiled reactor using the multi-physics software COMSOL. The amount of inactive virus (Vi) is represented using colour. Once the 3D model is obtained, it is sliced through the centre by a plane which gives a series of circular images. The series of circles gives us a visual representation of Vi at different time intervals throughout the coil. Using Python, each circle can be extracted and placed into a large NumPy array. This array can then be organised so that a neural network can interpret each image. The neural networks purpose is to use few circle images, analyse colours and patterns, then predict images that occur next in the series.

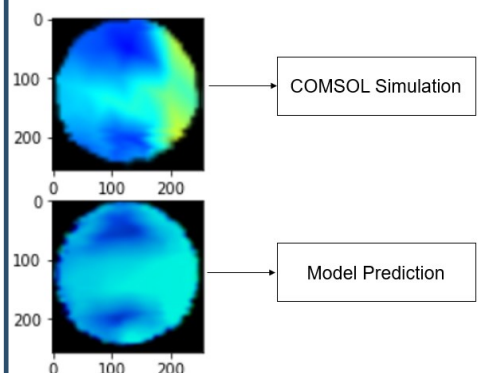
Transpose Convolutional NN Predictions



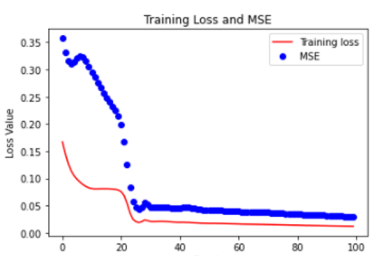
The initial network was tasked with analysing 20% of the data to train with, then asked to predict the remaining 80%. The results are expectedly bad, however the model managed to predict some of the patterns with some degree of accuracy.



Long Short Term Memory (LSTM) Model Predictions



The improved LSTM model proved to be far more effective in making series predictions. The overall shape and colour of the prediction is far more accurate as shown by the image and the graph of training loss and mean squared error (MSE). The next steps are to make the model recursive so that the model can use its own predictions to make further predictions.



Engineering and Physical Sciences Research Council
University of Strathclyde Glasgow
gsk
The University of Nottingham