SAQN Scoping Study End of Project Report

Project Title	
Emulating the Chemical mechanism through Machine Learning to speed up the real time Air Quality Prediction (ECheMLAQ)	
Project Team	
Name	Role (PI / Co-I)
Dr. Raj Tiwari	PI
Dr. Barry Latter	Co-I
Dr. Vera He	Co-I (Planned but left)
Proposed activities (copy from your project proposal)	
Chemical transport models (CTMs), which simulate air pollution transport, transformation, and removal, are computationally expensive, largely because of the computational intensity of the chemical mechanisms: systems of coupled differential equations representing atmospheric chemistry. Here we investigate the potential for Machine Learning to reproduce the behaviour of a chemical mechanism, yet with reduced computational expense.	
Please report on the activities completed in the project	
We have developed the ML algorithm and tested it against the model generated results and then replaced the chemical mechanism with ML to perform simulations over UK. We have compared the time gain for developed ML method with respect to traditional WRF-Chem	

model simulation and it is noticed that ML approach provides 1.9 times faster simulation time than the traditional approach. Further we have investigated how well the new approach captures particulate matter and NH3 over UK for the year 2016. It is found that ML based framework is in good agreement with satellite derived NH3.
What are the next steps for this research? Will you be applying for further funding? What will you need to continue researching this topic?
We will follow up this work and results from this initial study will be used as proof of concept to allow this group to continue developing the next generation Air Quality Forecasting Systems (AQFS). Once the ML based system is sufficiently developed, it will enable scientists and prediction centres to implement in their AQFS and achieve orders of magnitude speed up in prediction with reduced computational time and cost. Yes, we need funding support (for proof of concept work and joint studentship) to extend this work with UH, RAL and STFC.
Please outline the role of STFC in this project
We have used STFC facilities for e.g., atmospheric dataset has been used from BADC-CEDA, Satellite data from RAL and JASMIN for testing the ML approach.
Please list a brief list of all outputs and impacts below. These may include papers, articles or blogs, presentations at events or conferences, meetings about future plans for the research. Please include links wherever possible
We will soon be submitting a conference paper in “13th International Conference on Air Quality – Science and Application”. The link for the conference is https://www.herts.ac.uk/airqualityconference
Were there any unexpected outcomes as part of the project?
Vera’s unavailability: She left the project before the actual project work started and that has made project to go beyond its initial agreed timeline. We have requested for no cost extension, and it was kindly agreed and helped us to complete the work.
What are your plans to share the outcomes of this research with others? (Give details of any future meetings, conferences, papers or other dissemination planned)
We will be sharing the detailed outcomes of this research work through an international peer reviewed journal article.
Project Impact: What is the most significant output/impact from this project?
Our initial study demonstrates the potential for Machine Learning to reproduce the behaviour

of a chemical mechanism, yet with reduced computational expense.