SAQN Scoping Study End of Project Report

Project Title	
'Heterogeneous reactivity of Persistent Organic Pollutants' (SS2104)	
Project Team	
Name	Role (PI / Co-I)
Jamie Kelly	Co-I
Maxim Zyskin	Co-I
Andy Ward	PI
Alin M Elena	Co-I
Sanghamitra Mukhopadhyay	Co-I
Alexander James	Co-I
Stefano Rolfo	Co-I
Proposed activities (copy from your project proposal)	
The heterogeneous reactivity of POPs is to be explored by STFC laboratory experiments and modelling techniques. Andy Ward has already used CLF capability to explore heterogeneous reactions on aerosol in the context of atmospheric chemistry. Sanghamitra has expertise in exploring oxide ion dynamics and catalytic reactions using neutron spectroscopy, which can also be used for this research question. Both of these laboratory experiments will be funded by a separate application within this project. Alin Elena has expertise in using modelling techniques such as Density Functional Theory (as implemented in CP2K*) to investigate chemical reactions in clusters and bulk systems, but has not performed this in the context of air quality (e.g. POPs/aerosol). Here, DFT	

modelling will be performed to estimate molecular-level reactivity, by computing the energy barrier of the reaction and the Arrhenius law pre-factor. Multi-scale modelling, guided by experiment, will be performed to estimate droplet-scale reactivity and parameters essential in macroscopic modelling. For several of these STFC expertise and technical capability, it will be the first time that they are being applied to the field of air quality. Furthermore, these approaches give us an exciting opportunity to integrate data from both laboratory and modelling work, which could be highly complementary of one another.
Please report on the activities completed in the project
The team have conducted research which has informed two applications to the STFC Central Laser Facility to request access. The applications were to investigate the specific areas identified by the research namely the impact of persistent pollutants such as polyaromatic hydrocarbons undergoing heterogeneous reactions on aerosol in the context of atmospheric chemistry. Unfortunately, both applications were unsuccessful. We have also run DFT and MD simulations of pollutants diffusing in aerosol droplets.
What are the next steps for this research? Will you be applying for further funding? What will you need to continue researching this topic?
No further funding will be sought at this stage for experimental studies. Initial experimental studies and preliminary results are required to continue research.
Please outline the role of STFC in this project
STFC staff were involved with research to inform applications to be assessed by the STFC Facility Access Panel. Andy Ward is experience with performing such aerosol studies. Because the applications were unsuccessful no access to instrumentation was possible. Alin M Elena assisted Maxim Zyskin regarding discussions and modelling of aerosol containing pollutants
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
Two applications for access. An article in the SAQN newsletter on proposed activities.
Were there any unexpected outcomes as part of the project?
None
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)
No future plans have been made a present. As the modelling matures this may result in a publication.
Project Impact: What is the most significant output/impact from this project?

The MD simulation runs at temperatures of 10 and 50 K can tell us about diffusion rates, i.e., the time, for pollutant to migrate to the surface – see image. As we approached higher temperatures, the droplet itself seems unstable. The impact of such MD simulations comes when the predictions from modelling are compared compared to measured kinetics to confirm if a diffusional process of the PAH molecule (pollution) is significant. Ultimately this will determine the reactivity and the likely location of reaction, namely a bulk or surface reaction, which can influence the lifetime of the pollutant as an aerosol.