New software to predict mass spectral fingerprints of atmospheric aerosol particles, key determinants of climate change and air-quality

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Introduction

Aerosol particles are ubiquitous components of the earth's atmosphere. They affect the earth's radiative balance through scattering and absorption of radiation, and are also widely acknowledged as key determinants of air quality. Comprised of both inorganic and organic material, the latter could *potentially* comprise millions of compounds. With this enormous number of compounds that are present, how do we quantify the evolving chemical composition of these particles and thus quantify how this dictates environmental impacts?

It is impossible to measure every compound in the particle even if we can predict compound-by-compound speciation. In light of this, analytical techniques have been developed that derive a chemical signature of the whole particle, such as complex Electronic Ionisation Mass Spectra and Proton Nuclear Magnetic Resonance Spectroscopy (HNMR).

How useful is this information?

Project Description

Mechanistic mathematical models of atmospheric aerosol particles track the concentration of the millions of compounds expected to condense from the gas phase, through gas-to-particle partitioning. This evolving chemical composition, and particle size, dictates the role of aerosol particles in climate change and air-quality. How do we know our models are accurate? How do we quantify the ability to accurately predict the chemical composition of aerosol particles through gas to particle partitioning? This is where we need to utilise the mass spectral fingerprints introduced earlier.

Degrading both measurements and model output to simple top-down metrics such as the oxygen to carbon (O:C) ratio (Aitken et al. 2007), does not provide the ideal constraint of speciated models. But, what if we could predict these mass spectral fingerprints, and thus directly compare model and measurement output? This forms the main crux of this PhD: to develop informatics software for predicting what an instrument might determine from sampling the condensed phase, based on mechanistic model outputs. Specifically, you will focus on deriving response functions for the Aerosol Mass Spectrometer (AMS) and Proton Nuclear Magnetic Resonance Spectroscopy (HNMR). Both techniques are widely used in aerosol science and offer complimentary insights. There is no known response function available for the AMS, and scarcely tested routines for HNMR.

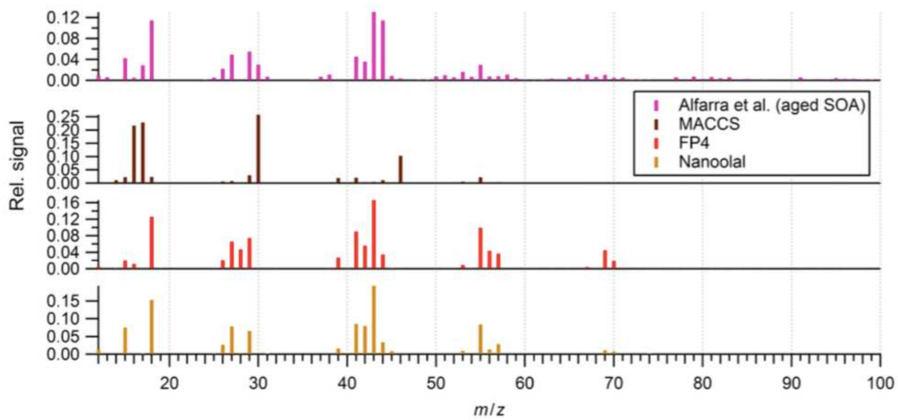

Figure 1. Measured mass spectra [top] versus proof of concept predicted mass spectra [other] for a biogenic aerosol particle.

To construct this new software you will investigate the ability of a wide range of machine learning platforms in building an accurate predictive model. Your work, based in the Python programming language, will follow on from our existing proof of concept work recently published (Topping et al 2016, 2017). You will work with co-supervisors in designing experiments in order to build up a database from which these models can be trained. Once constructed, your models will be validated in new laboratory experiments from the atmospheric simulation chamber in our centre (http://www.cas.manchester.ac.uk/restools/aerosolchamber/). This validation will be conducted by connecting your models to output from a separate model that predicts the evolving chemical composition of aerosol particles in these experiments. Thus, your work will provide and evaluate a novel and unique tool for interpreting the chemical evolution of an important component of the atmosphere. You will have the opportunity to share your work through software sharing platforms and through international partners.

Who are we looking for and why should they apply?

The project is multidisciplinary and will easily accommodate students from a wide range of backgrounds (our group already includes students with degrees in physics, chemistry, biology, geography and mathematics). We are looking for someone who is enthusiastic to build software engineering skills whilst appreciating the science that underpins the role of aerosol particles in climate and air-quality. We are not expecting you to start with all the required skillsets. A PhD is also the chance to build on your undergraduate training, and we will ensure you have the opportunity to do that in order to meet the project goals. You will work with local and international partners, gaining experience in a range of different environments. Your project partners and co-supervisors are all world leaders in their fields, giving you a rich environment across multiple disciplines. You will have the opportunity to travel to work with all partners, whilst presenting your work on the international stage at both EU and US conferences.

Software development and more broader data-science skills are becoming highly attractive to employers. In this project you will have the change to develop your own software, working with key partners in the fields of climate, air-quality, and data science. Through this process you will develop both ‘hard’ and ‘soft’ skills, with a demonstrable ability to adhere to best practices in software development and community engagement. This is often overlooked at the PhD level. Indeed, as a member of the Data Science Institute and through my active role within the local research software engineering community, I will ensure you get access to all relevant training to help you become a successful and skilled PhD candidate. On this, our DTP programme has a number of training modules that will allow you to build up skills within laboratory, computing and personal development arenas. This is an opportunity to develop as a scientist and individual. Get in touch if you would like to learn more.

References

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