EPSRC Centre for Doctoral Training in Aerosol Science

Annual Conference 2024

Poster Presentation

Disease Transmission

Investigation of novel methods to study the survival of foot-and-mouth disease virus in aerosols

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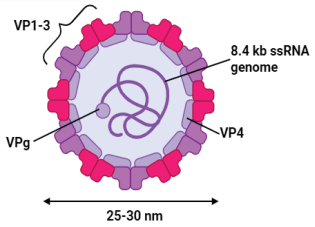
1. Foot and Mouth Disease Virus

- Non-enveloped, icosahedral +ssRNA picornavirus, as seen in diagram
- Infects cloven-hooved animals
- Endemic to Africa, Asia, the Middle East, and South America
- Highly transmissible – up to 100% morbidity



- A vesicular disease typically transmitted via direct contact, however a low probability-high consequence transmission event is via aerosols
- Highly economic disease; annually, the cost of FMDV is approximately £5.4-17.3 billion

2. CELEBS Instrument

- Controlled Electrodynamic Levitation and Extraction of Bioaerosols onto a Substrate
- Environmental conditions (e.g., temperature and relative humidity) can be controlled using the airflow within the instrument
- Individual aerosols can be generated, maintained under chosen conditions, and deposited into appropriate media

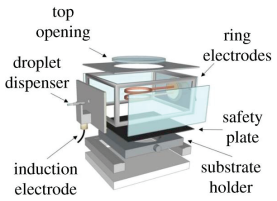


Figure 1: The CELEBS instrument

3. Gaps in Current Knowledge

- The effects of relative humidity, temperature, and pH on the survival of FMDV within aerosols - research that has been completed is significantly outdated, e.g., humidity effects studied over 50 years ago
- Investigation of aerosolised FMDV using updated instrumentation (CELEBS)
- Investigation of contemporary strains of aerosolised FMDV (most up to date strains housed at the Pirbright Institute)

4. Project Aims

Set-Up

1. Build a CELEBS instrument suitable for a SAPO4 virus
2. Establish levitation and subsequent survival assays using a surrogate BSL-2 virus with this CELEBS instrument

Investigating FMDV

3. Culture and titre contemporary FMDV strains
4. Investigate optimal survival of each strain using methodology developed in set-up
   a. Vary temperature during aerosolisation while controlling other environmental conditions
   b. Repeat, varying RH and controlling other environmental factors
   c. Repeat, varying pH of the droplet the virus particles are suspended in

Analysis

5. Establish survival parameters for each environmental condition for each strain
6. Investigate links between strain survival (virulence, evolutionary similarity)

5. Methodology

- At SAPO4, FMDV particles will be aerosolised into droplets of 5-10 µm radius for 5 s – 20 min and collected into 6 mL 2% FBS MEM culture media
- This will be added immediately to 60 wells seeded with LFBK-αVβ6 cells for a 3–5 day incubation
- Microscopy will be used to determine cytopathic effects – how well has the virus maintained its infectivity after levitation within aerosols?
- Poisson statistics will describe the specific number of infectious particles
- Staining will additionally be used to determine infection using plaque counts

- This can be repeated with varying temperature, relative humidity, and pH of droplet media for each contemporary strain under investigation to determine unique survival parameters

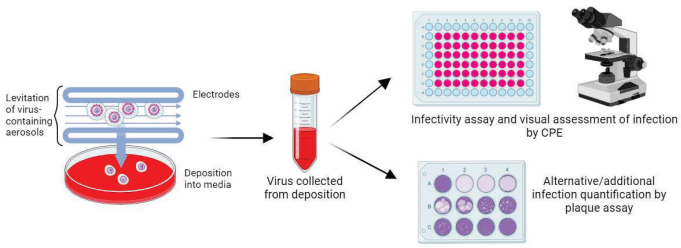


Figure 2: Workflow for determination of infection from levitation using CELEBS instrument.

6. Responsible Innovation

- There always must be the consideration of dual use research concerns when working with a highly transmissible pathogen, primarily use as a bioterrorism agent
- Strains are housed at the Pirbright Institute with security and biosafety procedures in place, and containment protocols are activated if FMD is suspected on a farm

7. Policy and Scientific Innovation

- The CELEBS instrumentation was only introduced in 2019, and has not yet been applied to picornaviruses
- New survival parameters for contemporary strains could inform updated quarantine policy, taking into consideration certain environmental conditions allowing greater distances to be travelled in the aerosol phase

Key References

- Brown, E., et al., *Airborne Transmission of Foot-and-Mouth Disease Virus: A Review of Past and Present Perspectives.* Viruses, 2022. **14**(5).
- Oswin, H.P., et al., *Measuring stability of virus in aerosols under varying environmental conditions.* Aerosol Science and Technology, 2021. **55**(12): p. 1315-1320.
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Transmission of bacterial resistance genes in aerosols

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Summary

- Investigate how bacteria carrying genes for antibiotic resistance spread through the aerosol and what factors influence the spread of these bacteria through the air, employing the innovative CELEBS technology.
- Enhance our comprehension of the factors that influence the dynamic of gene uptake by bacteria in air, providing strategies for mitigating the dissemination of antibiotic resistance dissemination in aerosols.

Introduction

- Abuse of antibiotics leading to the rise of antibiotic resistance (AMR), becoming a global health concern.
- Airborne ARGs, exhibit a broader transmission range and diverse sources[1], are affected by many factors, pose a threat to human and animal health[2].

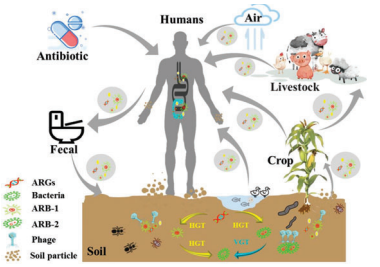

Figure. 1 Transmission of antibiotic resistance genes [1]

- Little investigation to identify the process of ARGs transmission in the aerosol directly.

Objectives

- Demonstrate that the high salt concentration in a droplet, coupled with its rapid dilution following deposition into a solution, will mitigate gene uptake by the bacteria present.
- Explore the fundamental processes that limit and accelerate this process, variables such as salt type, environmental relative humidity, and aerosol dispersal time.

Methods

Preparation of competent bacterial cells and bacterial transformation

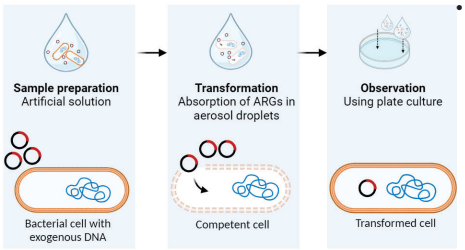

Figure. 2 Diagram of chemical transformation process in aerosol

- Competent cells are cells that have been treated to can take up exogenous DNA more easily and can induce corresponding changes in genotype and phenotype[3].
- Step 1: Prepare for the plasmid with ARGs and target bacterial.
- Step 2: E.coli treated with Ca2+ solution becomes cells that are easily transformed by plasmid DNA, ARGs are mixed with competent cells.
- Step 3: Using laboratory technique to observe the transfer of genetic information and the appearance of new heritable traits in the cells.

Controlled electrodynamic levitation and extraction of bioaerosol onto a substrate (CELEBS)

- Produce and levitate a population of aerosol particles (1 to >100) containing a known number of microorganisms (1 to >1000) with known (and indeed chosen) chemical and biological composition in a highly-controlled environment.

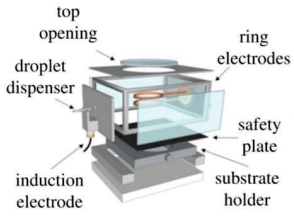

Figure. 3 Schematic diagram of main components of the CELEBS apparatus[4]

- Probe microbe viability in the air as a function of environmental factors.
- In this study, CELEBS is used to quantify ARGs transfer in the aerosol phase, provide evidence of ARGs in aerosol uptake by bacteria is quantified, aiming to identify the parameters.

Antimicrobial susceptibility testing (AST)

- Identify bacterial strains that carry resistance genes against specific antibiotics by testing aerosol samples.
  Disk Diffusion Method (Kirby-Bauer Method)
- Step 1: the isolated bacterial colony is selected, suspended into growth media, and standardized through a turbidity test.
- Step 2: the standardized suspension is then inoculated onto the solidified agar plate, and the antibiotic-treated paper is tapped on the inoculated plate. The disc containing the antibiotic is allowed to diffuse through the solidified agar, resulting in the formation of an inhibition zone after the overnight incubation at 35 °C.
- Step 3: the size of the inhibition zone formed around the paper disc is measured; the size of the inhibition zone corresponds to the concentration of antibiotic.

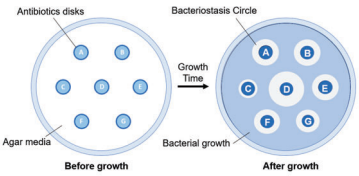

Figure. 4 Diagnostic diagram of the disk diffusion agar method test

Anticipated outcomes

1. Uncover the fundamental mechanism underlying bacterial resistance gene transmission in aerosol.
2. Elucidate the potential of aerosols to facilitate the spread of bacterial resistance genes, thereby contributing to combat the amplification and perpetuation of antibiotic resistance.
3. Understand the roles of aerosol in AMR transmission in human, animal and global ecosystems.
4. Aid in the prevention of the airborne spread of pathogens or source identification with the knowledge of the transportation of bacteria by air currents.

Reference

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The impact of environmental conditions on the prevalence and aerosol transmission of *Streptococcus pyogenes*

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Background

Previous studies show that exposure to pollutants significantly increase infection rates, however there is an indication that the structure and viability of airborne bacteria are also being impacted by the presence of pollutants.

- Nitrogen dioxide (NO_2) and ozone (O_3): increased susceptibility to serious infections[1]; compromise epithelial cells in respiratory tract and suppress the immune response[1].
  - NO_2: exposure causes increased viability of airborne bacteria[2].
- $PM_{2.5}$: has the ability to absorb bacterial cells and deposit them within the lungs[1]; bacteria growth pattern changes after exposure[3].

Motivations and Aim

Scarlet fever, a superficial infection caused by *S. pyogenes*, has increased dramatically in the UK in the last 10 years (Fig. 1). $M1_{UK}$, a novel strain, is a concern because it is causing increased scarlet fever and invasive *S. pyogenes* infections within England[4].

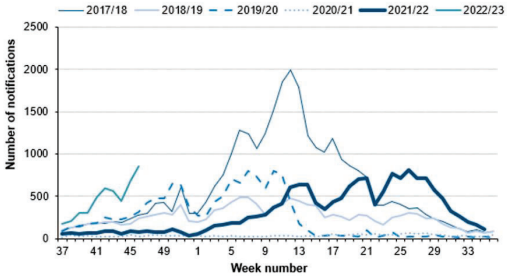

Figure 1. Scarlet fever notifications in England from 2017/2018 season onwards[4].

There is evidence that increased scarlet fever cases may be linked with high concentrations of NO_2, O_3 and $PM_{2.5}$[5], but epidemiology studies are unable to identify exactly how pollutants or certain environmental conditions allow for an increase in *S. pyogenes* infections.

This project aims to determine how the airborne viability of *S. pyogenes* is impacted by ambient conditions, such as gas and aerosol pollutants, temperature and relative humidity.

Proposed Research Strategy

1. Assembly of a CELEBS instrument to allow for: bioaerosol suspension; addition of pollutants; control of temperature and relative humidity
2. Development of methods for evaluating *S. pyogenes* viability with different pollutants and environmental conditions
3. Evaluation of how the viability of different *S. pyogenes* strains changes after exposure to different environmental factors

Experimental Technique

The Controlled Electrodynamic Levitation and Extraction of Bioaerosols into a Substrate (CELEBS) instrument (Fig. 2) is the primary method that will be used in this project because:

- It has a relatively low collection velocity[6]
- There is a 100% sampling efficiency[6]
- External gases can be added into the instrument[6]
- Temperature and relative humidity can be altered[6]

Challenges

The main challenge to overcome in this project is the adaptations of the CELEBS setup as aerosol pollutants have not been added to the instrument before.
This will likely be done with the addition of a nebuliser to the airflow inlet.

Responsible Innovation

As scarlet fever primarily effects children, communication of results need to be done in a clear manner to allow parents and carers to fully understand the findings and avoid misinterpretation.

Policy Implication – Outbreak Management

Guidance for managing scarlet fever within schools and nurseries is based around strict cleaning. This research could highlight the importance of adding face-masks and social distancing to this guidance if the viability of aerosolised *S. pyogenes* is found to be increased.

Policy Implication – ULEZ Zones

The effectiveness of these clean air zones at decreasing the concentration of air pollutants has been demonstrated by the introduction of the Ultra-Low Emission Zone in central London.

This research could show the importance of implementing these clean air zones and demonstrate why more Ultra-Low Emission Zones should be created across the UK.

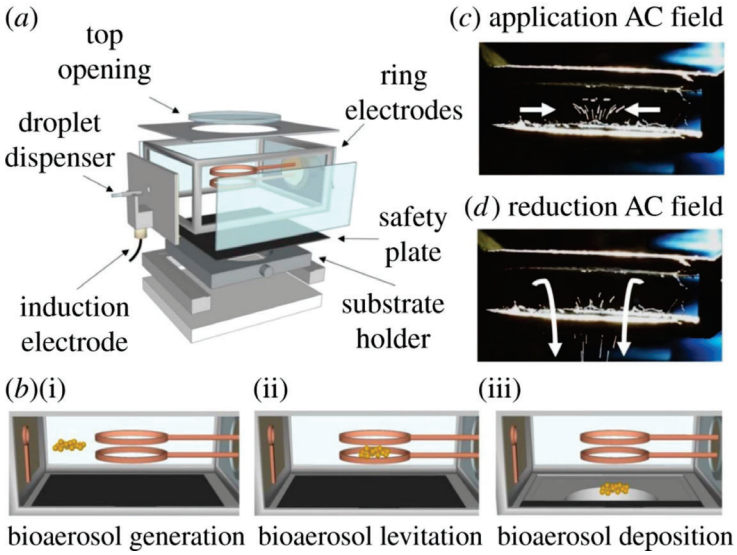

Figure 2. Schematic of the typical CELEBS setup and operating stages (a, b), images showing the levitation (c) and deposition (d) of a bioaerosol[6].

References

1. Pompilio, A. & Di Bonaventura, G. (2020). *Crit. Rev. Microbiol*. 46 (5), 600-630.
2. Mancinelli, R. L. & Shulls, W. A. (1978). *Appl. Environ. Microbiol.* 35 (6), 1095-1101.
3. White, J. K et al. (2020) *Int. J. Hyg. Environ. Health.* 230, 113608.
4. UK Health Security Agency (2023). Group A streptococcal infections: report on seasonal activity in England, 2022 to 2023 [Accessed 26/01/2024].
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Optimising the performance of air cleaning technology for mitigation of infection in hospital environments.

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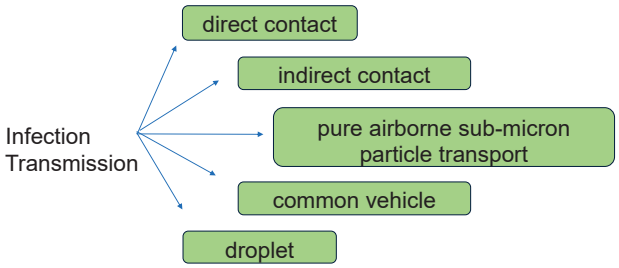
Background and Motivation

- People are exposed to significant amounts of particles that contain microbial material, also known as bioaerosols [1]
- We cannot eliminate the production of bioaerosols but we can certainly implement mitigation strategies to reduce the effects caused by it.
- People with low immune systems form the major fraction of people affected by inhalation of bioaerosols. Therefore, the risk of infection is at its highest in a hospital environment [2].
- There are several routes for infection transmission in a hospital [3].



- One of the most reliable and feasible ways to reduce exposure is the introduction of air-cleaning technology [2].
- Air Sentry, the industrial partner of this project, manufactures air cleaning devices that have been installed in the NHS and the private healthcare sector since 2000.

Methodology

- A series of experiments and modelling will be used to fulfil the objectives of this project.
- The project's novelty lies in the collection of spatial and temporal data under realistic conditions of a hospital ward.
- The experiments will be conducted in the bioaerosol chamber in a controlled environment at the University of Leeds.
- The experimental setup would be similar to [3] as seen in Figure 2 [3] and the methodology will resemble that described in [4].
- For modelling, computational fluid dynamics (CFD) would be used to understand the airflow of the room.
- The TBS will help understand atmospheric chemistry mainly focusing on chemical oxidation.

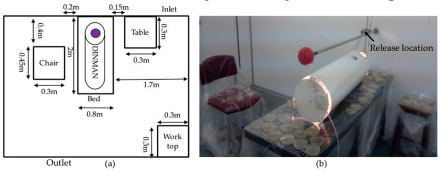
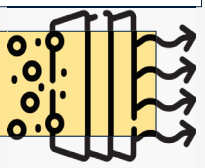


Figure 2. (a) Experimental layout in the chamber for hospital room; (b) Photo of furniture, DIN manset-up and release location.

Responsible Innovation and Policy

- Air cleaners could soon be placed in all public places and installed in offices, like the ventilation system.
- It is our responsibility to put forward the pros and cons of using these devices.
- Clean air will have a positive impact on the healthcare, education, residential, and commercial sectors.
- Innovation and development in this area possess the potential to impact a large section of society by improving indoor air quality, promoting health and safety, and enhancing overall quality of life.
- We can expect that policies related to accepted bioaerosol concentrations, certain regulations for manufacturers, sufficient ventilation in hospitals, and others could be implemented.

Will air-cleaning technology become the one-stop solution for achieving cleaner and risk-free air soon?



Objectives

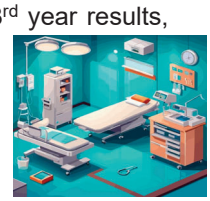
- The project intends to study and optimise the use of air-cleaning devices within hospitals. The aims are as follows:

a) To understand the interaction between the design of the air cleaners and the room flow.

b) Assess mitigation strategies for surface contamination.

Depending on the outcomes of the 2nd and 3rd year results, one or both objectives may be achieved,

1. Simultaneous removal of gaseous and particle contaminants from the air.
2. Incorporating smart action within the device.



Challenges

- As this project focuses on a sensitive area like a hospital, creating a realistic environment is difficult.
- The absence of standardized protocols for testing and reporting air cleaners makes comparing them difficult.
- Finding a common ground between the academic and industrial agenda is important to maintain a balance between the two sectors.

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Assessing the impact of aerosol degradation on microbial detection in air samples.

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Introduction

- Environmental air sampling is performed for a range of public health and biodefence applications (figure 1).
- Exposure to outside air may lead to irreversible changes to cell surface antigens and the nucleic acids of microorganisms.
- Detection of microorganisms within the environment may be impacted by the stresses imparted on the airborne microorganism.

Project Aim:

Develop a clearer understanding of how the aerobiological pathway (figure 2) impacts microbial detection in air samples.

Research Questions:

1. What effect does aerosol generation and collection (table 1) have on microbial biodetection targets?
2. What implications do these structural and genomic effects have for the detection and identification of microorganisms in collected air samples?
3. Are these effects altered or exacerbated in presence of outside air or simulated environmental stressors (figure 3)?

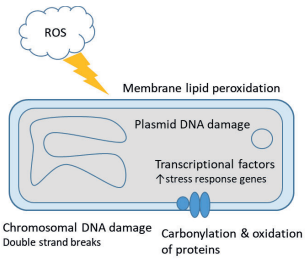

Figure 3. Oxidative stress in airborne bacteria

Scientific impact

- This project will develop multidisciplinary approaches to begin to empirically understand how microorganisms respond to the stresses associated with aerosol transport.

Responsible innovation

- The implications of this work have been thoroughly considered against the objectives and purposes of the Biological and Toxin Weapons Convention (BTWC).
- Any work which will be published in the public domain will undergo thorough review from both technical and security perspectives.
- Periodic review throughout the lifecycle of the project will also be carried out.

References
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(2) Kulmala M, Vesala T, Wagner PE. 1993. An analytical expression for the rate of binary condensational particle growth. Proc R Soc A Math Phys Eng Sci 441:589 – 605.

Figure 1. MOD personnel performing environmental air monitoring (1)

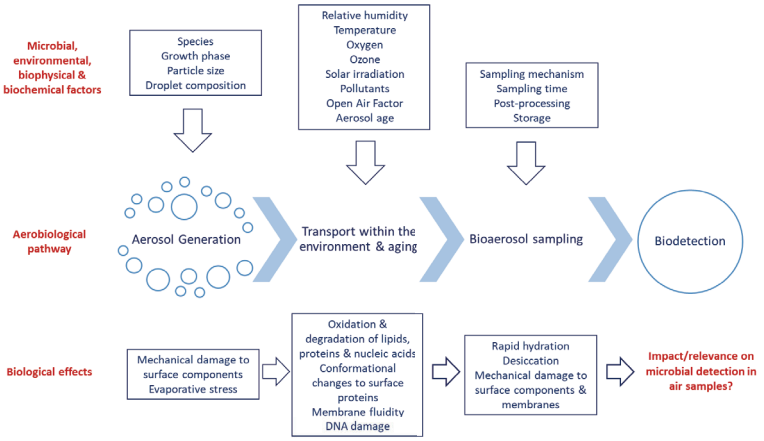

Figure 2. Project overview

Experimental Methodology

Assessing aerosol generation and collection methodologies

Table 1. Experiential considerations of various aerosol generation and collection mechanisms

Mechanism	Examples	Experimental considerations
Aerosol generation		
Reflux nebulisation	Collison, Wells, Aeroneb	Two fluid atomiser. Generally used for liquids. Small particle size. Operates via Venturi effect & wall impaction. Increasing jet number and pressure increases aerosol output and recirculation. Reservoir evaporation can occur over time. Forces associated with reflux nebulisation can damage bacteria/viruses
Non-reflux nebulisation	PFA nebulisers, SonoTek	No wall impaction or recirculation.
Aerosol sampling		
Impingement	AGI30, AGI4, SKC biosampler	Aerosol is accelerated through a critical orifice causing inertial impaction into collection fluid. Efficiency is affected by physical parameters. Reaerosolisaton can occur. SKC biosampler possesses angled nozzles, creating gentler swirling motion of bioaerosol during collection
Impaction	Andersen, Burkard	Air flows through orifices causing inertial impaction of particles too large to remain entrained in airflow. Size fractionation possible. Collection onto a range of different substrates possible. Substrate choice can affect collection efficiency. Particle bounce can be problematic.
Filtration	Gelatin, glass fibre	Good physical sampling efficiency. Biological sampling efficiency may be lower due to sensitivity of collected microorganisms to air drawn past filter. Elution of material from filter surface can affect efficiency

Simulating bioaerosol transport within the environment

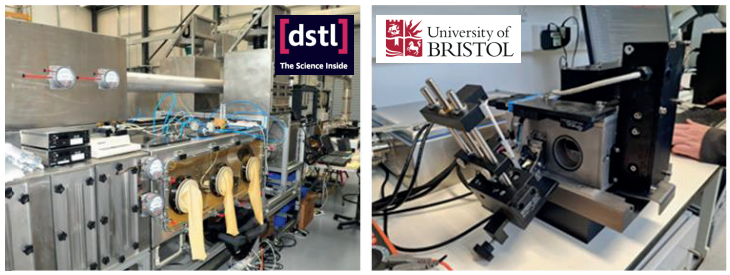

Figure 4. Dstl ACS wind tunnel & the CELEBS electrodynamic balance (University of Bristol)

Dstl Aerosol Challenge Simulator (ACS) wind tunnel

1. A variety of aerosol generators, monitoring/sizing equipment and air samplers can be incorporated
2. Outside air can be introduced
3. Background aerosols (bacteria and pollen etc.) and pollutants can be introduced

Electrodynamic balance (CELEBS)

1. Microenvironment heterogeneity occurring within individual aerosol droplets can be determined
2. Droplets can be levitated for seconds to days
3. The surrounding atmosphere (RH/temperature) can be accurately set and maintained

Characterising the damage occurring to cell surface structures and nucleic acids

Changes to nucleic acids
DNA integrity assays
DNA quality assays
Real-time qPCR
Flow cytometry
Microscopy & specific dyes
Gel Electrophoresis
Next Generation Sequencing
Nanopore Sequencing
Molecular Beacons

Changes to cell surface structures
Fluorescence
Microscopy & specific dyes
Immunoassays e.g. ELISA, Western blotting
Impedance flow cytometry
Cell membrane permeability assays
Cell membrane potential assays
TOF Mass Spectrometry (TOF-MS)
IR spectrometry
Raman spectrometry
Matrix-Assisted Laser Desorption/Ionisation
Nuclear Magnetic Reasonance

Figure 8. Tools/techniques for assessing damage to cellular surface structures and nucleic acids

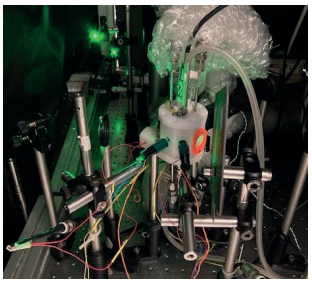

Figure 6. The concentric cylindrical electrodynamic balance

Bacterial metabolism of culture media influences its hygroscopic properties

- The comparative kinetic electrodynamic balance approach (figure 6) was used to determine the hygroscopic properties of spent and freshly prepared bacterial culture media.
- Measurements of the corrected radius over time were converted into droplet mass using density parametrisation and the mass flux as a function of time was calculated. Water activity at the droplet surface was determined using the mass and heat transfer equation (2).
- Spent culture media showed differing hygroscopic properties compared to controls (figure 7).

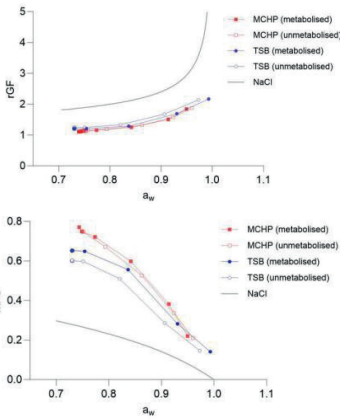

Figure 7. Hygroscopicity with variation in solution water activity (a_w), presented in terms of radial growth factor (rGF) and the mass fraction of solute (MFS) (n=6). The predicted curves for NaCl (grey line) are also shown.

Conclusions

- Metabolism of culture media likely alters solute composition/conc. and thus the water content of the droplet.
- At 35% RH, metabolism altered the solute concentration sufficiently enough to prevent the concentration surpassing supersaturation for efflorescence

Assessing the airborne stability of influenza A virus

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1. Introduction

- Influenza A virus (IAV) is a **major respiratory virus** which in the last 105 years has caused four pandemics and is responsible for annual influenza epidemics in the U.K. [1].
- Evidence that **airborne transmission** is a prominent transmission route for IAV (**Figure 2**) [2].
- Seasonality of IAV infection potentially linked to seasonal fluctuations in climate [3].
- Reported levels of IAV inactivation under different atmospheric conditions are inconsistent between studies. [4]
  - Inconsistencies hinder effective public health interventions for virus outbreaks.

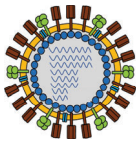

Figure 1: Diagram of the structure of IAV.

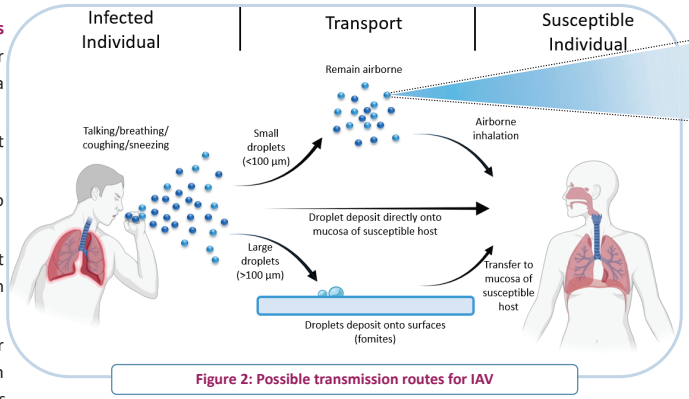

Figure 2: Possible transmission routes for IAV

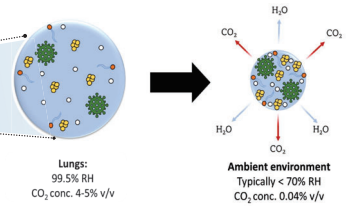

Figure 3: Equilibration of respiratory droplet with ambient environment. Depicts flux of CO_2 and water from respiratory droplet.

- Physicochemical changes in respired aerosol droplets may result in harmful microenvironments in which suspended pathogens must remain viable to transmit (**Figure 3**).
- Potential mechanisms of IAV inactivation include increased **solute concentrations** (e.g. salts or proteins), droplet **phase changes** and aerosol **pH changes** [5].

2. Objectives

1. To elucidate the influence of relative humidity (RH), temperature, and gas phase composition on IAV airborne viability
2. Identify the **mechanisms of IAV inactivation** in the aerosol phase

3. Methodology

Controlled Electrodynamic Levitation and Extraction of a Bioaerosol onto a Substrate (CELEBS)

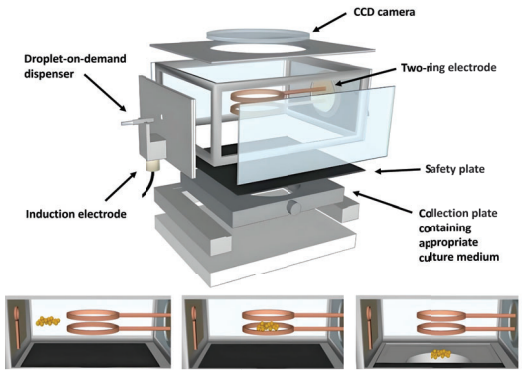

Figure 4: General configuration of the CELEBS device. Gas inlet (not depicted) allows control over environmental conditions experienced by trapped droplets.

- Allows the influence of environmental conditions (i.e. temperature, RH, and gas airflow composition) on virus viability to be investigated.
- Simulates the aerosol phase by levitating droplets in an electromagnetic field produced by two concentric ring electrodes (**Figure 4-5**)
- Atmospheric conditions experienced by the pathogen are controlled by a laminar airflow which is passed over levitated droplets
- After exposure to a desired atmospheric condition droplets are deposited into cell tissue growth media and the impact on virus viability is assessed using an infectivity assay.

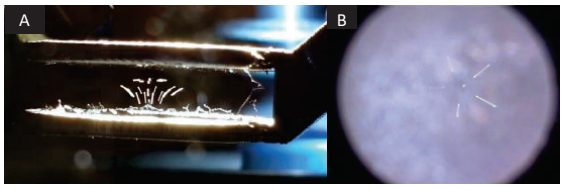

Figure 5: CELEBS generated droplets levitated in electromagnetic field. A) Side view of a population of droplets levitating in the CELEBS device. **B)** Overhead view of five droplets levitating in CELEBS device

Detection and quantification of single infectious particles following levitation

- Due to the small volume (around 100 pL) and low number of droplets produced by the CELEBS device the number of virions per levitation can be as low as 1 virion. Therefore, a **highly accurate and sensitive** method of quantifying infectious virions is required.
- Plaque assays are one of the most accurate methods for direct quantification of infectious virions
- Plaque assays use an overlay to localise virus spread, resulting in the formation of visible zones of cell death termed plaques (**Figure 6**) . Each plaque is assumed to be a result of a single virus infection.
- Here we use a **modified plaque assay** to quantify infectious virions post -levitation in the CELEBS device (**Figure 7**).

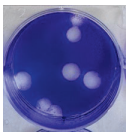

Figure 6: Example of plaques formed by IAV.

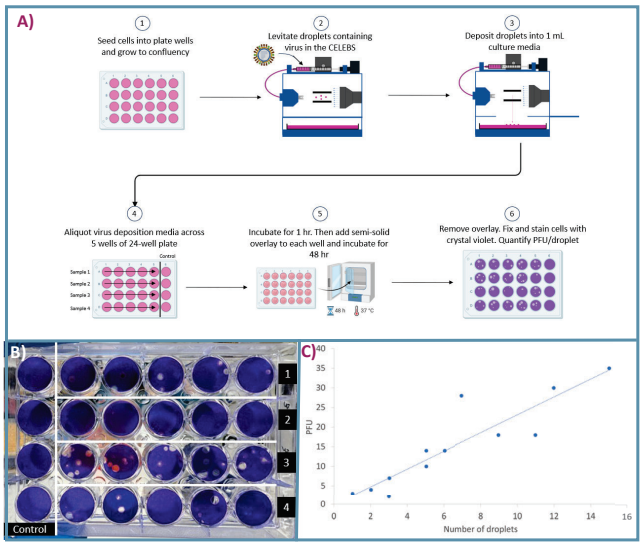

Figure 7: Plaque-based virus detection assay. A) Flow diagram of protocol to quantify infectious virions per levitated droplet after exposure to a desired environments condition. **B)** Plaques formed after 48 hrs by Influenza A strain WSN **C)** Correlation between the number of levitated droplets in the CELEBS and the counted PFUs.

4. Next Steps

- **Investigation of RH dependent decay profile for IAV.** Strains to be investigated include WSN, PR8, X31 and Udorn.
- **Investigate the effect of suspension medium composition on IAV viability.** Including altering salt and protein concentrations.
- **Effect of atmospheric CO_2 on the infectivity of IAV.** Previous research on SARS-CoV-2 demonstrates that atmospheric CO_2 concentrations play a significant role in controlling SARS-CoV-2 infectivity, possibly by altering aerosol pH (**Figure 8**) [7].
- **Identify the physicochemical changes occurring within aerosol droplets that lead to variations in IAV viability.**

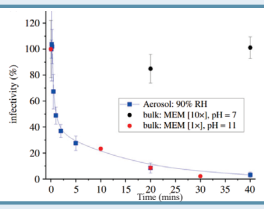

Figure 8: Comparison of the decay profile of SARS-CoV-2 in the aerosol phase (blue) with bulk solution measurements (High salt (black) and high pH (red)) [7]

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Digital Microfluidic Lab-on-a-chip for multiplex detection of biomarkers in Exhaled Breath Condensate

Daisy Ashton

Supervisors: Loic Coudron, Laura Urbano and Ian Johnston

Background

- Exhaled breath (EB) carries diagnostic biomarkers, which are biological indicators of infection and disease.
- Microfluidics is the science of miniscule volumes of fluid and its manipulation and the study of its behaviour.
- Digital Microfluidics (DMF) technology involves the manipulation of an ultra-small droplet on an array of microelectrodes.
- A lab-on-a-chip (LOC) device combines laboratory tests, such as blood analysis, ELISA assays and DNA amplification, all on a single miniature chip.
- Digital microfluidic multiplex LOC detection of lung disease biomarkers from EB can be carried out noninvasively and painlessly at point-of-care by the use of EB collection devices.

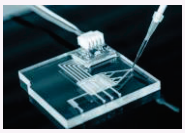

Figure 1: A digital microfluidic system (Berthier, 2018). Figure 2: A multiplex lab-on-a-chip device (Maxwell, 2016).

Motivation and Aim

- British Lung Foundation/Asthma UK states that 'lung diseases are responsible for more than 700,000 hospital admissions and over 6 million inpatient bed-days in the UK each year' and that 'somebody dies from lung disease in the UK every 5 minutes' (British Lung Foundation, 2017).
- 'It is thought that approximately 10% of the population have a needle phobia' (NHS Foundation Trust University Hospital Southampton, 2018). Therefore more non-invasive testing and diagnostic devices are necessary.
- At the end of this project, the goal is to have developed a fully automated multiplexed DMF system with bioprinted detection sites that can detect lung disease biomarkers at a low cost and at point-of-care. Beyond contributing to the progress of DMF technology in diagnostics, the project's results hold the potential for broader applications in fields such as agriculture and air quality monitoring.

Objectives

1. Biomarker selection
2. Selecting the most appropriate ink composition
3. Finding suitable geometric structures for separation sites on employing total extraction DMF approach
4. Selecting appropriate immunoassays for separation and detection
5. Creating artificial exhaled breath condensate

1. Biomarker selection

Table 1- Expected concentrations of chosen disease biomarkers

	8-isoprostane	IL-6	LB4
Control	7-64.23 pg/ml	1.5-5.1 pg/ml	7.9-53.6 pg/ml
Asthma	30.9-54.1 pg/ml	7.1 ± 1.1 pg/ml	88.9 ± 10.9 pg/ml
Chronic obstructive pulmonary disease	40 ± 3.1 pg/ml	8.0 ± 0.1 pg/ml	73.5-170.5 pg/ml
Cystic fibrosis	42.7 pg/ml	8.7 ± 0.4 pg/ml	N/A
Non-small cell lung cancer	N/A	9.3-11.4 pg/ml	24.2-61.5 pg/ml

2. Selecting the most appropriate ink

- To create the individual biosensing structures, a combination of printing methods including inkjet printing and extrusion 3D-bioprinting will be investigated.
- Inks will be initially selected based on their mechanical and rheological properties, wettability, printability, and of course their known compatibility with antibodies.
- The investigation will then consider two different avenues for functionalisation of the printed structure: (a) embedding antibodies within the ink itself or (b) using a post-functionalisation step of the pre-printed structure.
- Inks currently being investigated include: SU8, Mebiol and Gelatin Photogel.

3. Finding suitable geometric structures

- Inks can be printed in many different shapes and designs such as a pillar, a scaffold, a droplet shape, or simply a standard 2D spot.
- The geometry of the structure will affect its functionality, trapping and cleaning efficiencies.
- Fundamentally, the droplet must be able to detach from the structure. It is anticipated that droplet detachment will be correlated with the structure-to-electrode size ratio (area occupied by the structure footprint compared to the area of the electrode on the EWOD plate.
- Geometries will be coded using G-Code.

Figure 3: Geometries made using Tinkercad: (a) scaffold, (b) pillar, (c) droplet.

5. Selecting appropriate immunoassays

Table 2 - Standard assays for chosen biomarkers, their detection assays and specificities.

Biomarker	Standard Assay	Detection method	Sensitivity	Range
8-isoprostane	ELISA	Colorimetric	1 pg/ml	0.005 ng/ml – 5 ng/ml
IL-6	ELISA	Colorimetric	< 2 pg/ml	6.25 pg/ml – 200pg/ml
LB4	ELISA	Colorimetric	5.63 pg/ml	11.7 pg/ml – 3000 pg/ml

4. Creating artificial exhaled breath condensate

- Exhaled breath is composed of approximately 78% nitrogen, 16% oxygen, 4% carbon dioxide and 0.09% noble gases such as Argon, while the rest is made up of water vapour and over 3500 volatile organic compounds (Johnson, 2018).
- Would comprise of realistic ratios of the main components of exhaled breath in liquid form, salts, a buffer to ensure the stability of pH alongside, reported contaminants that are found in EBC samples and the chosen biomarkers.
- The components of the artificial exhaled breath will be mixed manually.

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Interaction of SARS – CoV2 and Influenza Viruses with Particulate Matter Air Pollution

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Prof. Alexandra Porter

IMPERIAL

EPSRC Engineering and Physical Sciences Research Council

There is evidence of higher transmission rates and worsening of disease outcomes for viral infection in more heavily polluted areas[1]. We hypothesise that fine and ultrafine Particulate Matter (PM) and viruse coinfection, increases viral infectivity and boosts the cellular inflammatory response, with varying PM chemistries triggering different inhibitory or protective immune responses.

1. Background

PM in our environment

Pollutant concentrations of Black Carbon (BC), PM 10, 2.5 and 1 (<10, 2.5 and 1μm) across 4 different London microenvironments[1]:
Park (**PK**), Indoor (**IN**), Traffic Intersection (**TI**), Street Canyon (**SC**)

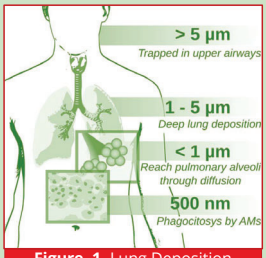


Figure. 1. Lung Deposition based on particle size [2]

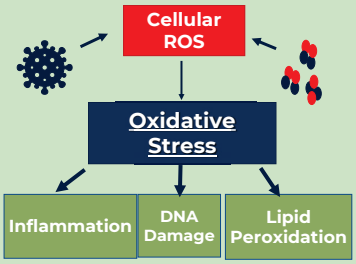
- **Sizes:** $PM_{2.5}$, PM_{10} and particle number counts were **TI > SC > PK > IN**. PM1 and BC was higher indoors.
- **Potentially toxic** trace transition metals including **Fe, Ti, Cr, Mn, Al and Mg** were detected at all sites.
- Same potentially toxic metals in the IN site as at the TI site- **Transport of PM indoors**
- Pollutant concentrations indoors followed the office time and work pattern
- Air quality **variation** at different MEs and reveals the **exposure inequalities** around the city

PM effect on viral infection

Virus Survival: Evidence that influenza can be deactivated by diesel emission particles[3]

Viral Cell Entry: PM known to upregulate expression of SARS-CoV-2 receptor, ACE-2. PM may also inhibit protective proteins in lung secretions[4]

Inflammatory Response: Persistent inflammation from chronic PM exposure, weaken immune response to viral infection. Overstimulation of immune response may occur through reactive oxygen species (ROS) and oxidative stress



Cytokine Storm

2. Statement of The Problem

- Direct visual evidence of interactions between virus and PM is yet to be demonstrated, as is the cellular inflammatory response to virus and PM acting together.
- The effects of specific PM chemical components on viral infectivity could be delineated.

3. Objectives

- To determine whether PM effects viral cell entry and intracellular trafficking
- To visualise virus and PM interactions within lung secretions
- To determine how PM affects viral cell entry and cellular inflammation in *in vitro* cell culture

4. Significance

- The outcomes will provide guidance around which polluted microenvironments are potentially most unsafe for infection
- Could shed light on new therapeutic interventions.

5. Methodology

- **PM** will be extracted from polyurethane foams and mixed with surrogate virus, **Psuedovirus,** to look for interactions using **Transmission Electron Microscopy (TEM)**
  - Developing and adapting new ***in situ*** **Liquid TEM** protocols (Fig.2) to image the mixtures of virus and PM in these media **real time**
- Using *in vitro* cell culture techniques, **human airway epithelial cells will be exposed to both PM and Pseudovirus** to measure:
  - **Virus/PM localisation and intracellular trafficking** (TEM)
  - **Cell death** (flow cytometry, plaque assay)
  - **Biomarkers of oxidative stress and inflammation** (Immunofluorescence, Reverse Transcription Polymerase Chain Reaction)
- **TEM** will be used to visualise virus and PM localisation within pre-prepared samples of **VeroE2 cells exposed to SARS-CoV-2 and PM from various sites** .

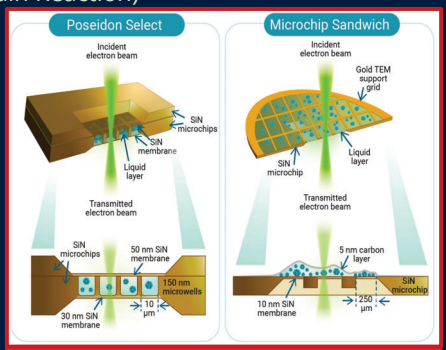
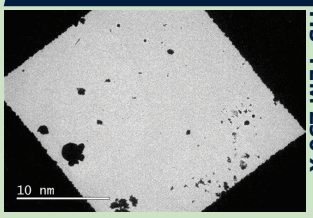


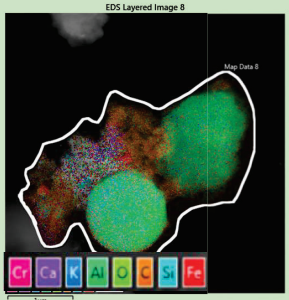
Figure 2. *Liquid TEM techniques. From* [5]

6. Year 1

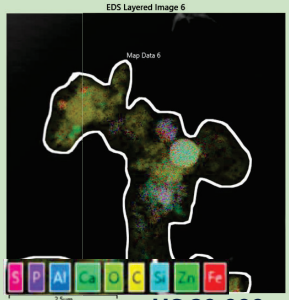


HS TEM 250 x

- TEM characterisation of PM10 collected at Marylebone Highstreet (HS) and Baker Street Tube station.
- Ongoing extraction of PM2.5 and PM1 from PUF collected IN, PK, GI and LU



HS 30,000 x



HS 20,000 x

STEM EDS layered Map Images

7. Responsible Innovation

- What research avenues should future work follow?
- How can the outcomes of these become entangled politically?

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The Structure of Exhaled Droplets and Aerosols – Preliminary Work

Engineering and Physical Sciences Research Council

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BACKGROUND

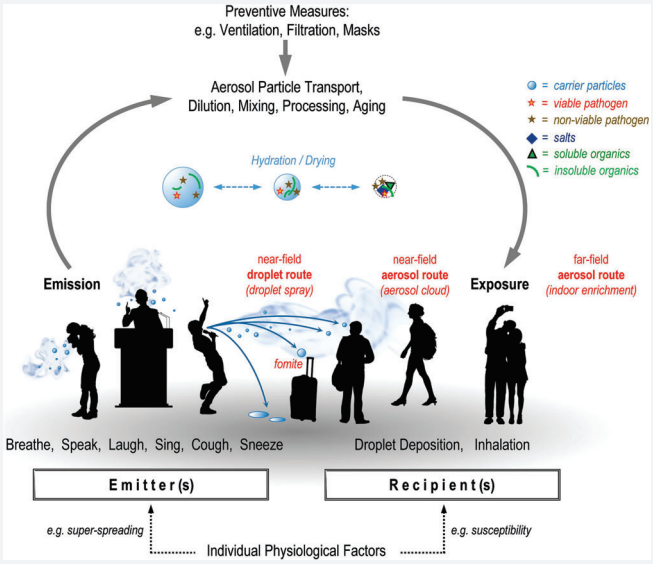

Figure 1. Illustrative representation of respiratory aerosol and droplet of disease transmission (Pöhlker et al. 2023)

- Exhaled aerosols are responsible for the transmission of many respiratory diseases and infections
- Droplet size and their suspension time in the ambient environment is dependant on their origin in respiratory tract
- Despite the prevalence of these sub-100 micron particles, **a detailed understanding of composition and structure of these particles is lacking**[3]
- **Limited characterization is reported**

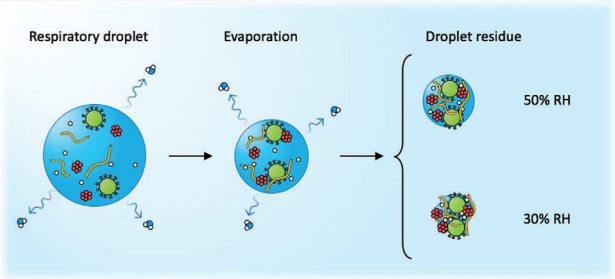

Figure 2. Drying process of a respiratory droplet. Image taken from (Božič and Kanduč 2021)

METHODOLOGY

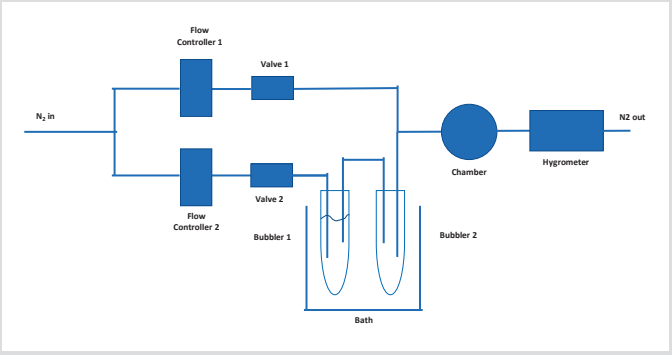

Figure 3. Schematic of the experimental setup

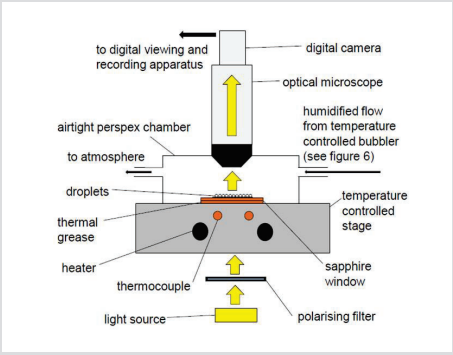

Figure 4. Schematic of the RH controlled chamber

- Relative Humidity (RH) was controlled in the chamber by the ratio of wet and dry flow
- Video were recorded on computer and were analysed
- Samples were also retrieved for SEM analysis (in process)

RESULTS

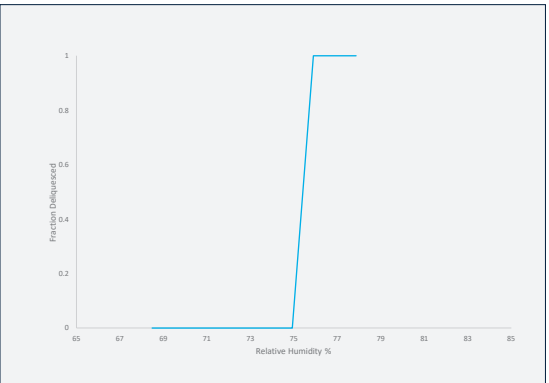

Figure 5. Deliquescence of NaCl

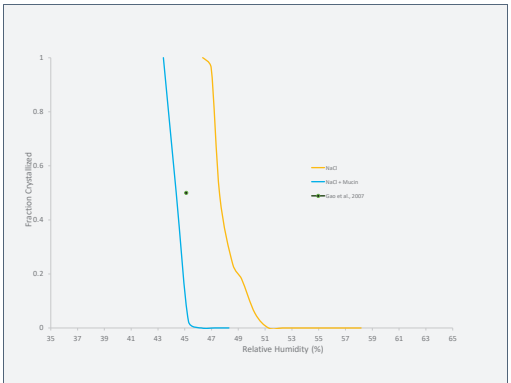

Figure 6. Efflorescence curve obtained from ramping experiment (~1% / 5 min)

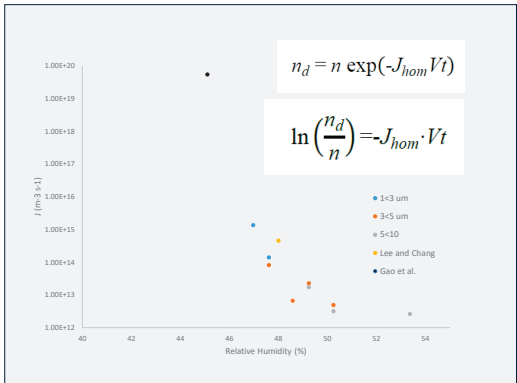

Figure 7. Homogenous nucleation of NaCl

CONCLUSSION

- The deliquescence is in accordance with literature
- The efflorescence of NaCl is in the same range as reported in literature
- The solution containing mucin has a lower efflorescence range than NaCl only
- Homogenous nucleation of NaCl is as expected with bigger droplets nucleating first and smaller later

FUTURE WORK

- Further experiments with different ratios of different components of the solution
- Making the solution more representative of lung fluid by adding other components (surfactants) to it to characterize the impacts on the crystallization of NaCl
- Sampling exhaled aerosol using a cascade impactors for characterization using various Electron microscopy techniques

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Drug delivery

High-dose Antibiotics Inhalers for Acute Lower Respiratory Tract Infections in Primary Care

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Supervisors: Bernardo Castro-Dominguez, Matthew Jones & Albert Bolhuis
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1. Background

- Acute lower respiratory tract infections (LRTIs) are a primary public concern with rapid morbidity and considerable mortality[1].
- LRTIs are one of the major lung diseases caused by pathogenic bacteria, viruses, which are mainly associated with pneumonia, bronchitis, influenza (Fig 1).
- Some environmental substances (tobacco smoke, air pollution, dust in Fig 1) could also cause inflammation, damage the lung cells and lead to the lung infections[2].

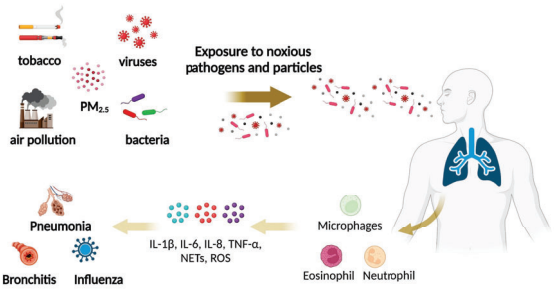

Fig 1. Schematic of development of acute lower respiratory tract infections (Biorender)

2. Problem Statement

- Dry powder inhalers (DPI) are devices for pulmonary drug delivery, which exhibit significantly advantages in delivering aerosolised drug particles into the deep lung.
- Particle flowability, drug payload, aerosolisation, controlled release and antimicrobial resistance pose significant challenges for the deployment of DPI formulations for lung diseases.
- Confinement engineering of the particles is required for pulmonary route administration.

3. Research Objectives

Objective 1- Design carrier-free pharmaceutical products, obtain high-dose antibiotic DPI formulations and explore their performance via the Orbital inhaler (Aptar).

Objective 2- Assess the performance of various excipients, polymers and surfactants to develop DPI formulations with sustainable release characteristics.

Objective 3- Design and optimise multidrug particles for enhanced therapeutic effect.

4. Methodology

Electrospray drying (ESD) is a versatile technique commonly used in producing the homogenous monodisperse particles under the electrostatic forces (Fig 2). The advantage consists of rapid, controlled disintegration of dry particles and particle size production at ambient atmosphere[3].

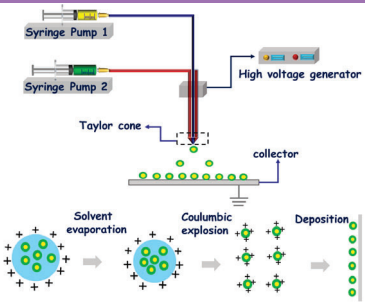

Fig 2. Schematic of electrospray drying

1. Materials synthesis and analysis

- Utilise ESD to generate inhalable monodisperse DPI of suitable & combination antibiotics with well-tuned and controlled physicochemical properties.
- Characterise physicochemical performance of DPI formulations like supramolecular structures, particle size & morphology, powder flowability, etc. Some of the common characterisation techniques are shown in Fig 3.

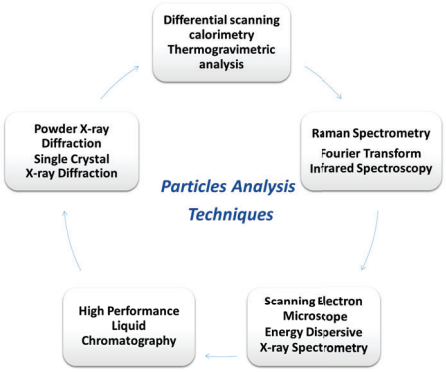

Fig 3. Common particle characterisation techniques

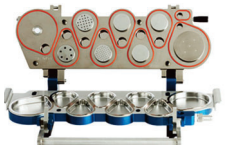

Fig 4. Schematic of Next Generation Impactor

2. In vitro pulmonary deposition

- Pulmonary aerodynamic deposition will be estimated via Next Generation Impactor (NGI) as present in Fig 4.
- Aerosols will be generated with the DPI using the Orbital inhaler device into NGI.
- Determine their aerosol performance via calculating emitted fraction, fine particle fraction and respirable fraction.

3. Antimicrobial activity determination

- The colony biofilms assay will be used to assess the antimicrobial activity (Fig 5)[4].

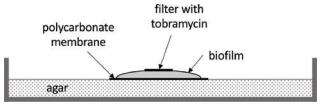

Fig 5. Schematic of the colony biofilm[4]

4. AI directed DPI formulations

- Machine learning (e.g. SVM, KNN, Random Forest, etc.) will be employed to optimise the process parameters.
- Predict and model the relationship between formulation variables.
- Optimise the critical quality attributes of the produced particles.

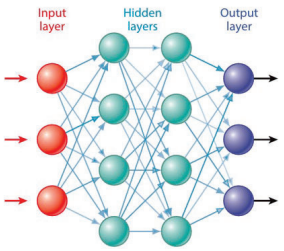

Fig 6. Example of machine learning model[5]

5. Responsible Innovation & Policy

- Formulate effective high-dose DPI products could alleviate acute airway infectious diseases and improve global healthcare in the future.
- Strengthen contemporary management practices and policies of antimicrobial drugs could contribute to reduce the antibiotic resistance.

6. Challenging

- Synthesis of pharmaceutical crystalline materials and determination of their supramolecular structures.
- Particle aggregation and aerodynamic deposition performance of DPI products.

[1] Flatby, H. M., et al., Risk of lower respiratory tract infections: a genome-wide association study with Mendelian randomization analysis in three independent European populations. *Clin Microbial Infec* **2022**, 28 (5), 732.e1-732.e7.
[2] Rahman Sabuj, M. Z.; Islam, N., Inhaled antibiotic-loaded polymeric nanoparticles for the management of lower respiratory tract infections. *Nanoscale Adv* **2021**, 3 (14), 4005-4018.
[3] Ee, L. Y., et al., Electrospray drying-mediated coating of cellulose nanocrystal. *Carbohydr Polym Technol Appl* **2023**, 6, 100345.
[4] Aljalamdeh, R., et al., The effect of particle size of inhaled tobramycin dry powder on the eradication of Pseudomonas aeruginosa biofilms. *Eur J Pharm Sci* **2021**, 158, 105680.
[5] Deng, X., et al., Emerging Applications of Machine Learning in Food Safety. *Annu Rev Food Sci Technol* **2021**, 12, 513-538.

Stability of dry powder formulations used in drug delivery to the lungs studied one particle at a time

Anna Catton
Supervisors: Prof Jonathan Reid (University of Bristol),
Dr Joe Takher-Smith (Viatris)

1. Background

- Drug suspended within a liquid droplet, or mixtures of dry particles agglomerated to carrier particles
- Carrier particles are sugars such as glucose and lactose
- Difficult to predict how drug separates from carrier particle
- Can use particle engineering to optimise physical properties

Powder Formulations | Dry Powder Inhalers (DPIs) | Thermo dynamics | Drug Deposition

3 essential parameters:
- Compliance of the system
- Ideal dispersion of fine particles
- Clinical efficacy

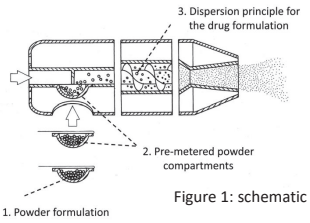

Figure 1: schematic of a DPI

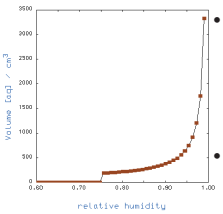

Figure 2: hygroscopic growth of NaCl with increased RH

- Hygroscopic growth occurs due to the increased RH (from 40 % to 99.5 %)
- Important for manufacturing process, storage, shelf life and delivery within the lung

Particle properties affecting deposition
- Size, shape, mass, morphology

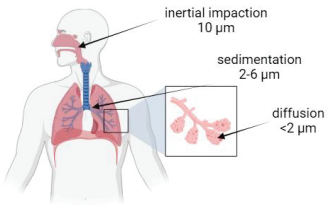

Figure 3: deposition location of particles

2. Statement of the Problem

- Study effects of RH and temperature on a variety of pharmaceutical formulations
- Understand effects of RH on manufacturing process, storage, shelf life and particle growth and deposition
- Understand how particle phase and moisture content vary particle to particle

3. Methodology

Electrodynamic Balance (EDB)

- Measure the forces upon a singular droplet suspended within an electric field
- Change in growth monitored by scattering of laser light
- RH and temperature can be altered

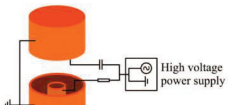

Figure 4: basic structure of an EDB experimental setup

Single Particle Electrodynamic Lung (SPEL)

- Two concentric cylinder electrodes
- Can suspend solid particles
- Can reach supersaturated condition
- RH and temperature can be altered

4. Objectives

1. To study the moisture resilience, clumping and coalescence of particles with respect to relative humidity.
2. To improve the stability and resilience of particles with respect to humidity.

2. Study the effects of relative humidity of specific drug formulations provided from Viatris.
2. To determine how the effects of relative humidity and temperature vary particle to particle within a sample.

3. Determine the optimum size, shape, mass and morphology of drug particles to control the dissolution rate.
2. Generate a predictive framework for the moisture response of APIs, carrier particles and engineered particles by spray drying

5. Responsible Innovation and Challenges

1. Am I using any propriety compounds? Who owns the IP?
2. What happens if I find a cure?
3. Is this process ethical?
4. How could this benefit the health service?

6. References

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Hygroscopic Dynamics of Solution Phase Aerosol on Generation and Inhalation to the Lungs

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BACKGROUND

- Soft Mist Inhalers (SMIs) deliver bronchodilators for COPD treatment, overcoming limitations of conventional inhalers such as coordination of actuation and environmental impact.
- Drug deposition profile of SMIs is a function of particle size distribution, with an optimal range of 1-5 μm for effective deep lung delivery.
- Hygroscopic growth of aerosol particles, influenced by the transition from ambient to lung relative humidity (RH) is poorly understood.

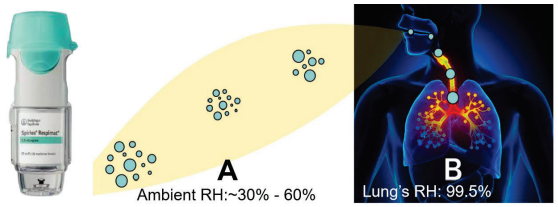


Figure 1: Diagram of droplet dynamics of SMIs on generation and inhalation to the lungs [1]

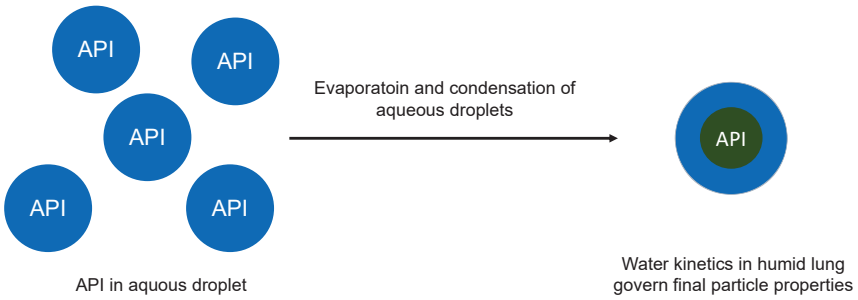


Figure 2: Aqueous aerosol production and dynamic aerosol processes occurring during inhalation of SMIs [2]

AIM

- To explore the impact of hygroscopic growth on particle size dynamics of aerosols from generation to lung deposition employing TAPS and CK-EDB.
- To revise current drug deposition models to include hygroscopic growth dynamics.
- To develope a Next Generation Impactor (NGI) simulator.

METHODS

Tandem Aerodynamic Particle Sizers (TAPS)

- Measuring plume size distribution under varying relative humidity (RH)

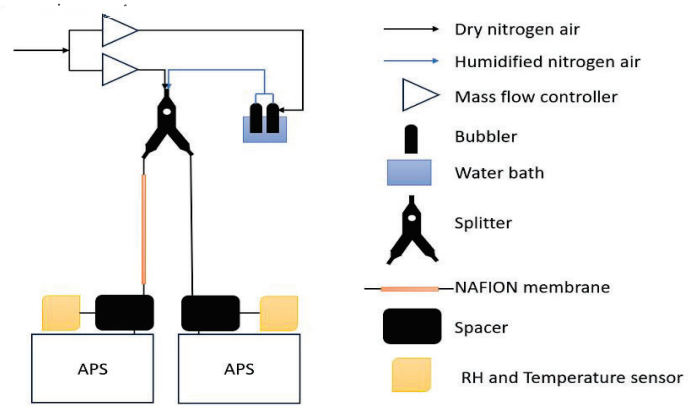


Figure 3: Experimental set up of TAPS [3]

Comparative Kinetics Electrodynamic Balance (CK-EDB)

- Studying hygroscopicity of single droplets to understand individual particle behavior.

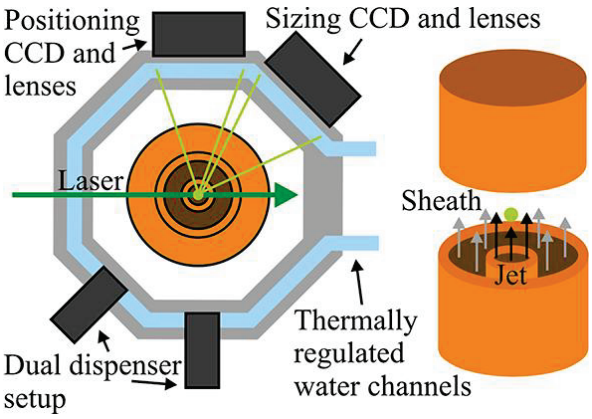


Figure 4: Experimental set up of CK-EDB [4]

MODELS

Models (E-AIM and AIOMFAC)

- Comparing experimental results with theoretical predictions to understand the hygroscopic dynamics of SMIs aerosols.

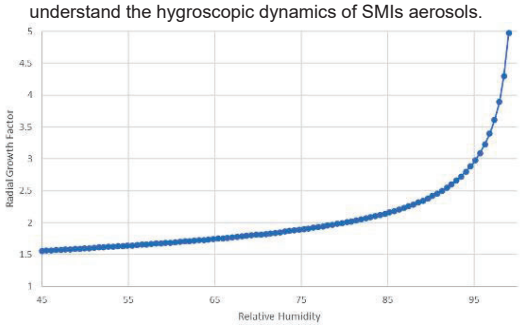
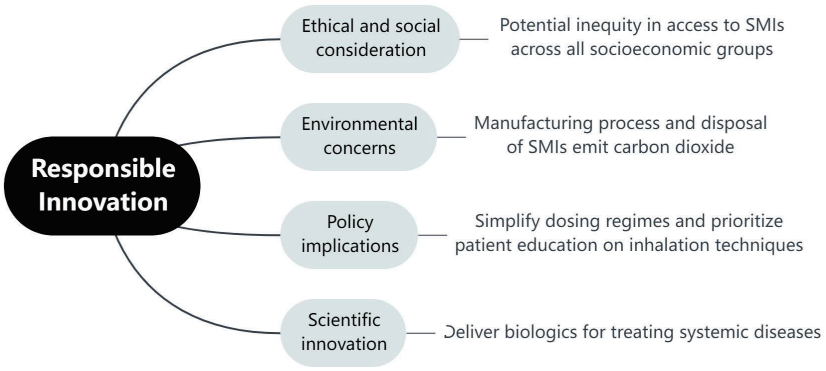


Figure 5: The radial growth factor curve for Sodium Chloride under RH from 45% to 99% determined by E-AIM model [3]

INNOVATION



CHALLENGES

- Specific setup of TAPS for SMIs requires a newly designed inlet and tailored splitter to ensure engineering precision and compatibility.
- Testing new APIs for SMIs presents formulation and financial challenges, including selecting appropriate ingredients, rigorous testing, and potential investment. In-house preparation of formulations carries risks, requiring careful implementation planning.

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2 NC Armstrong Green (2022). Dynamic Response of Hygroscopic Pharmaceutical Aerosol on Inhalation.
3 Jiang et al (2023). Drug Delivery to the Lungs, Volume 34.
4 Davies, J. F et al (2013). Simultaneous analysis of the equilibrium hygroscopicity and water transport kinetics of liquid aerosol. Analytical Chemistry.

Dry Water for Future Inhaled Medicines

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University of Hertfordshire UH

UKRI Engineering and Physical Sciences Research Council

Background

- Dry water (DW) is the stable dispersion of water in air. It is a are free–flowing dry powders that contain approximately 98% water.[1]
- DW is a method of coating water droplets with hydrophobic fumed silica particles to appear as a flowable powder, but it contains larger amounts of biologics trapped inside.[11]
- DW allows for the creation of unstable biological formulations, such as aerosols, which enhance thermostability, aerosol properties, and flexibility of administration. This could improve safety and efficacy and be beneficial for biological therapies. [2]
- Dry powder formulations, while freeing protein molecules from mechanical stress during aerosolization, may be unstable and more prone to degradation. DW formulations overcomes the issues of degradation in the dry powder state.[3]
- The drug delivery system involves the active release of a drug to achieve a desired therapeutic response. Upper airways deposit particle sizes 10 μm, the conducting airways deposit particle sizes 5 μm and respiratory airways deposit particle sizes 2 μm.[4]

1.Wang H, Fu Z, Ji X, Lu M, Deng L, Liu Z, et al. A general method for endowing hydrophobic nanoparticles with water dispersion abilities. Journal of Materials Chemistry B. 2023;11(35):8464-70. 2.Chhabra N, Arora M, Garg D, Samota MK. Spray freeze drying-A synergistic drying technology and its applications in the food industry to preserve bioactive compounds. Food Control. 2023:110099. 3. Williams III R. Improved Formulations to Enable Stable Delivery of Biologics. BioPharm International. 2022;35(7):46-9--9. 4.Ezike TC, Okpala US, Onoja UL, Nwike PC, Ezeako EC, Okpara JO, et al. Advances in drug delivery systems, challenges and future directions. Heliyon. 2023.

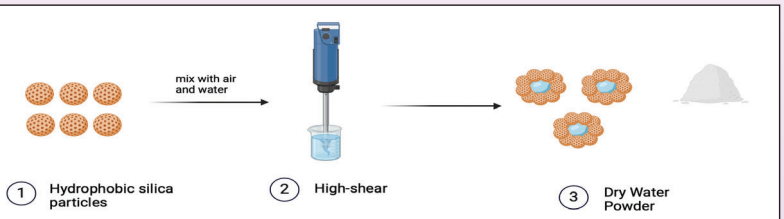

Figure 2. Mechanism of DW Formulations.[11]

11.Saleh K, Forny L, Guigon P, Pezron I. Dry water: From physico-chemical aspects to process-related parameters. Chemical engineering research and design. 2011;89(5):537-44.

Research Hypothesis and Objectives

DW is the stable dispersion of water in air. It proposes significant advantages in drug delivery as we can use DW to formulate biologics for drug delivery and delivering biologics such as proteins, which cannot be stabilised without water.

However, the formulation of stable powders of DW to the airways, which maintain sensitive therapeutic proteins in their native structure, remains unknown. Therefore, we hypothesise that if we can produce DW particles with an acceptable excipient toxicity profile, this would enhance aerosol drug delivery of challenging biological molecules.

This project aims to explore DW formulations for delivery to the airways by employing *in vitro* lung toxicology models to examine the toxicity and potential safety of hydrophobic silica colloids required for DW formulation. Furthermore, it will establish DW particle manufacturing approaches that prepare DW particles with appropriate physicochemical properties for aerosol drug delivery. Once the DW formulation has been established, we will examine the loading and liberation processes for DW particles and understand the particle structure and its impact on DW particle behaviour. Finally, we aim to examine the application of DW particle medicines in aerosol drug delivery.

Figure 1. Macroscopic demonstration of adhesion of hydrophobic particles.[11]

11.Saleh K, Forny L, Guigon P, Pezron I. Dry water: From physico-chemical aspects to process-related parameters. Chemical engineering research and design. 2011;89(5):537-44.

Programme and Methodology

DW excipient toxicity

- Toxicology assays determine the toxicology of excipient substances and formulations during processing, actuation, and liberation.
- MTT assays, which measure cell viability, cytotoxicity, and proliferation.
- LDH assay can detect cytotoxicity in alveolar epithelium cells.

DW manufacturing

- Aggregation of nanoparticles can significantly impact the size of DW formulations.
- Small-angle neutron scattering (SANS) aids in studying multicomponent complex structure through contrast variation and deuterium labelling.
- Laser scattering accurately determines the size of DW in various materials like liquids, solids, and aerosols.

Aerosolization of drug delivery

- DW would have a carrier–based formulation that will help improve DW flow properties. It will look at blends between silica particles and medications in order to aid dispersion.
- Next Generation Impactors (NGI) has seven stages and controls at any inlet flow rate between 30–100 L/min and a cut size ranging from 0.54 – 11.7 μm D_A at 30 L/min and 0.24 – 6.12 μm at 100 L/min.
- DW particle separation and sizing are achieved by increasing the velocity of the airstream as it passes through each stage by forcing it through a series of nozzles containing progressively reducing jet diameters

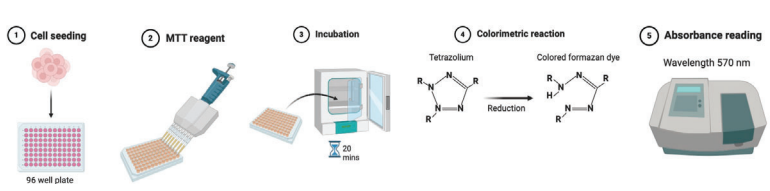

Figure 4. Schematic of MTT Cell Viability Assay Procedure

Responsible Innovation

DW, a novel pharmaceutical concept, requires accurate information and marketing to increase public awareness and receptiveness to its use in future inhaled medicines, enhancing effective healthcare.[5]

We still do not know if we can stabilize biologics that cannot be stabilized without water and can contain sensitive therapeutic proteins. However, DW formulation poses risks as bacteria or viruses can maintain their biological states.[6]

Transparency in new medicine development enhances drug access, promotes ethical practices, and increases trust, facilitating better decision-making and policymaking.[7]

Financial barrier to access for low-middle-income countries (LMIC), as the high costs make medication unaffordable.[8]

5.Smolynets I, Gutyj B, Petryshak O, Lytvyn R. Pharmaceutical marketing: objectives and types. Науковий вісник Львівського національного університету ветеринарної медицини та біотехнологій імені С3 Гжицького. 2016;18(2-4 (69)):151-4. 6.Tin D, Sabeti P, Ciottone GR. Bioterrorism: an analysis of biological agents used in terrorist events. The American Journal of Emergency Medicine. 2022;54:117-21. 7.Esfandiari A, Yazdi-Feyzabadi V, Zarei L, Rashidian A, Salari H. Transparency in public pharmaceutical sector: the key informants' perceptions from a developing country. BMC Health Serv Res. 2021;21(1):1316. 8.Leisinger KM, Garabedian LF, Wagner AK. Improving access to medicines in low and middle income countries: corporate responsibilities in context. Southern med review. 2012;5(2):3.

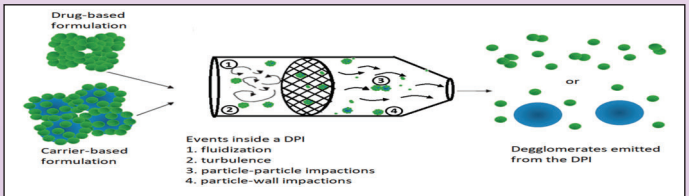

Figure 3. Schematic of DPI dispersion mechanism.[12]

12.Zheng Z, Leung SSY, Gupta R. Flow and particle modelling of dry powder inhalers: Methodologies, recent development and emerging applications. Pharmaceutics. 2021;13(2):189.

Scientific Innovation

DW is an innovative inhaled formulation for future biologics, enhancing patient adherence, as most biologics are delivered parenterally, with some exceptions being ocular or inhaled formulations. DW application aims to reduce incorrect inhaler usage and the need for trained professionals, enabling less trained professionals like teachers to administer drugs and use the application more efficiently.

DW application improves sterility and cost-effectiveness for LMICs by allowing storage in cool, dry places, reducing constant sterile conditions and improving inventory management, thereby enhancing patient care. DW increases access to medicines for low-income individuals by providing stable biologics and making them more cost-efficient, improving their quality of life and accessibility to DW applications.

9.Zhang C, D'Angelo D, Buttini F, Yang M. Long-acting inhaled medicines: Present and future. Advanced Drug Delivery Reviews. 2023:115146.
10.Yenet A, Nibret G, Tegegne BA. Challenges to the Availability and Affordability of Essential Medicines in African Countries: A Scoping Review. ClinicoEconomics and Outcomes Research. 2023:443-58.

Statement of the problem

Pulmonary toxicology of inhalable microparticle–based DW may be problematic in DW formulation as it consists of hydrophobic fumed silica particles. DW contains nanoparticles, it is unknown what impact this would have on pulmonary toxicity since they are formulated into microparticles.

Controlled drug release is important when it comes to DW; however, we are uncertain how the properties of the nanoparticles necessary to prepare DW particles impact the drug release rates and the potential control release.

To aerosolize DW formulation, it is important to consider designing it as micron–sized particles encapsulating or aggregated nanoparticles. Several challenges have arisen since DW has never been evaluated for respiratory drug delivery. Many DW formulations for inhaled therapy will be modelled with current dry powder inhaled therapy.

Challenges

Challenging areas of the proposed reach: DW formulation and device design application

- How can we prepare DW of the right particle size for this application?
- What particle size do we need for which application? Do we know from the literature that we can make DW particles in that range?
- What are the best devices to allow effective administration?
- How can the biologic be liberated from the DW after administration?
- Toxicology effects of the colloidal excipient

Next-Generation Nasal Drug Delivery Exploiting Non-Newtonian Fluids and Smart Thermoresponsive Materials

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[1]University of Hertfordshire, [2]University College London, [3]Bespak

Background

Systemic nasal drug delivery (NDD) as an alternative to oral and parenteral routes has been an area of interest due to its potential for delivery of vaccines and biologics such as proteins and peptides (1). However, there is a lack of literature studying the shear degradation of biologics during atomisation in nasal sprays. This is further complicated as the shear stress generated in unit dose nasal spray devices is not fully understood.

The aim of this study was to design a working computational fluid dynamics model to study the fluid flow and strain rates of simple Newtonian and non-Newtonian formulations in the NasaDose device, Bespak's proprietary unit dose nasal spray. This will be followed up by studying the shear rates in more complex formulations of interest.

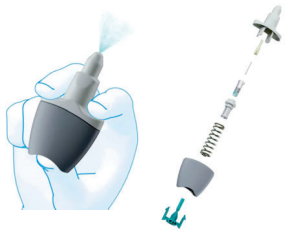

Fig.1. illustrates the Bespak NasaDose device (2)

Methodology

A computer-aided design (CAD) representing the internal geometry of the drug pathway in the NasaDose device was created (Fig.1)

Fig.2. Illustrates the CAD used in this CFD study

Next, the mesh was designed, a total of 4 mesh models were used in this study, [1] surface remesher, [2] automatic surface repair [3] Trimmed (hexahedral) volume mesher, [4] Prism layer mesher (Fig.3)

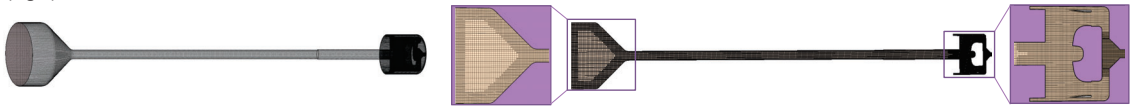

Fig.3. Illustrates the mesh operation used in this CFD study

The next step was setting up the physical models:

1. volume of fluid (VoF), a Eulerian multiphase model, was used as the main physical model (3).
2. Power-law viscosity model was implemented for non-Newtonian fluids.
3. Implicit unsteady flow model was used (4,5).
4. Convective and free-surface Courant-Friedrichs-Lewy (CFL) adaptive time step were also used (6).

Currently, the formulations tested include two Newtonian fluids, water and viscosity standard, 20cP silicone oil. Some aspects of this study were validated using experimental data from Proveris SprayVIEW and Malvern Spraytec.

Results & Discussion

Fluid flow

Here we look at the flow of a **Low-viscosity Newtonian** (water) and **High-viscosity Newtonian** (20 cP silicone oil) formulations in order of increasing solution time in the NasaDose device:

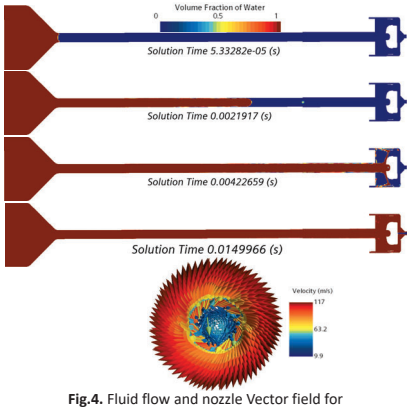

Fig.4. Fluid flow and nozzle Vector field for low-viscosity – water

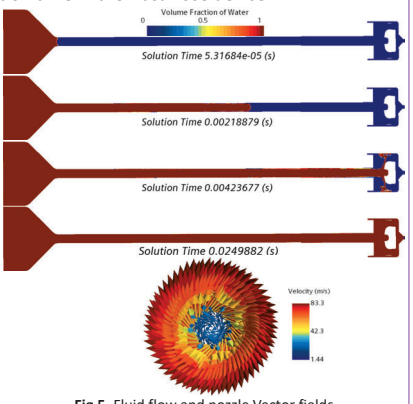

Fig.5. Fluid flow and nozzle Vector fields for high-viscosity – 20 cP silicone oil

As observed in Fig.4 and Fig.5, for low and high-viscosity formulations, it takes approx. 15 and 25 ms for the flow to fully develop at the spray nozzle. This is in line with high-speed video footage from Proveris SprayVIEW where it takes 10-30 ms from actuation to spray observation.

Fluid velocity

Here we will look at the velocity of **Low-viscosity Newtonian** (water) and **High-viscosity Newtonian** (20 cP silicone oil) formulations in the NasaDose device:

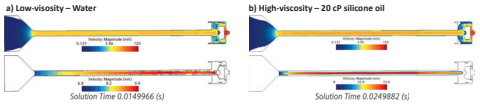

Fig.6. Velocity of formulations during atomisation

As observed in Fig.6, at the spray nozzle, the low-viscosity formulation reaches higher velocities. Additionally, the velocity near the wall is much lower with the high-viscosity formulation due to viscous drag.

However, surprisingly, the velocity of the high-viscosity formulation is slightly higher at the centre of the needle. This may be due to the fact that the Reynolds number at the needle for low-viscosity formulation is 3500, suggesting a transitional flow state while a laminar flow model was used in this simulation.

Additionally, considering the volume of the nasal spray model geometry is 18 µL, we can estimate that the average volumetric flow rate in the device is 18 µL/0.01s (or 1.8x10-6 m3/s). Thus, the average velocity would be 5 m/s which is in line with the velocity data observed in Fig.6.

Strain rate

Here we look at the strain rate of **Low-viscosity Newtonian** (water) and **High-viscosity** Newtonian (20 cPsilicone oil) formulations in the NasaDose device:

Finally, Fig.7 and Fig.8 illustrate that, formulations with higher viscosity will generally have a lower strain rate, this is specially visible at the nozzle spray. However, the exception to thisis at the centre of the needle where the strain rate was higher for the high-viscosity liquid.

In conclusion, VoF proves to be an effective tool for understanding the strain rate in a nasal spray device. However, the high velocity and shear rate of the high-viscosity formulation should be further explored as this is unexpected. Additionally, further research on implementing shear thinning formulation to these simulations is required.

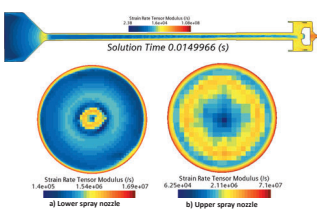

Fig.7. Strain rate of low-viscosity – water during atomisation

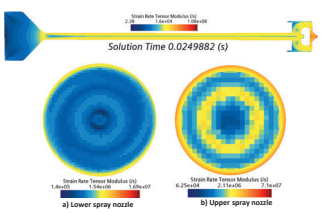

Fig.8. Strain rate of high-viscosity – 20 cP silicone oil during atomisation

Contact

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School of Life and Medical Sciences
Email: h.rasooli-nia@herts.ac.uk

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Synthesis of **PLGA nanoparticles** for alveolar **drug delivery**

By Melih Engur
Supervisor: Dr Jorge Bernardino

IMPERIAL
EPSRC Centre for Doctoral Training in Aerosol Science

Alveolar Basics and Surfactant

The alveoli have total surface area of ~70m2 with a respiratory barrier and diffusion distances as thin as 200nm(1,2,3). As demonstrated in *figure 1* surface area exponentially increases with each generation from the trachea, bronchi, bronchioles and finally the alveolar sacs (4, 5).

AT1 cells cover over 90% of alveolar surface area making them the gas exchange region of the lungs(6). AT2 cells secrete lung surfactant containing: surfactant proteins(SP) A,B,C and D and lipids. Surfactant is important as it prevent atelectasis by maintain surface tension(6).

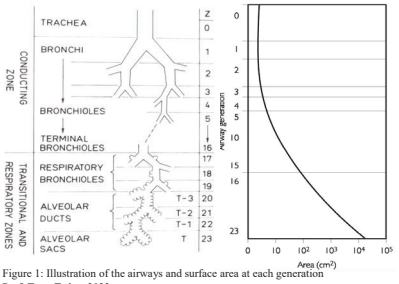


Figure 1: Illustration of the airways and surface area at each generation
Prof. Terry Tatley, 2023

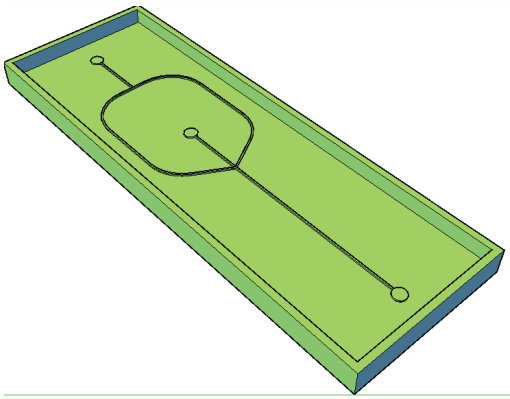


Figure 2: Master Mould for PLGA Synthesis

Statement of Problem

- Inhalable medicine is currently used to treat condition like COPD and asthma, however, these are not examples that demonstrate distal alveolar deposition
- PLGA nanoparticles are biodegradable whereby functional modifications can be made to optimise drug loading, bioavailability and immune-evasion.
- While PLGA has promise, there is only a handful of aerosolised examples, none intended for alveolar drug delivery.
- Later studies on PLGA for drug delivery had poor success due to reasons such as hygroscopic aggregation, instability during aerosolization and immune response
- Identifying the optimal PLGA nanoparticle formulation has the potential to combat these issues and undergo epithelial uptake.
- One example is the coating of the nanoparticle with polyethylene glycol to promote immune-evasion.

Objectives

- Primary Objective: Design and characterize a hydrodynamic flow focussing device to synthesise homogenous PLGA nanoparticle for alveolar internalizations*(figure 2)*.
- Secondary Objective: Characterise PLGA-Cell interactions to quantify NP internalization and cell response of PLGA particles on AT1 cell models.
- Tertiary Objective: Develop tumour like organoids and characterise cell penetration of PLGA NPs into organoids.

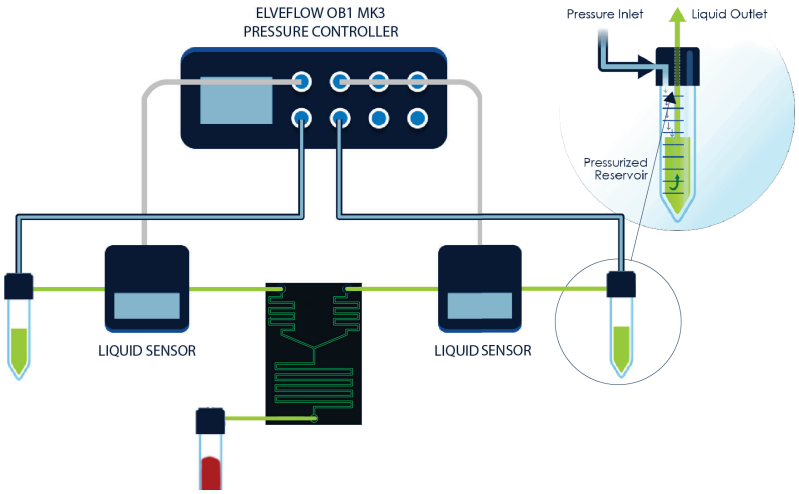


Figure 3: Microfluidic PLGA Synthesis Setup

Methodology

This study will use hAELVi cells which express tight cell junctions critical for air-lung modelling (12). PLGA nanoparticles will be synthesized using a hydrodynamic flow focussing chip to allow precipitation of homogenously sized nanoparticles.

We will deploy organ-on-chip (OOC) model to mimic in-vivo conditions (13). Customised PDMS chips will be developed within the lab seen in figure 4. PLGA nanoparticles will be functionalised with differing properties to identify optimal internalisation and stability formulations.

STED Inverted Confocal Microscope will be used to analyse cell response to formulations. Light Sheet Microscopy will be used to allow imaging of organoids and asses PLGA penetration into differently sized organoids which are meant to mimic cancer/tumorous cells.

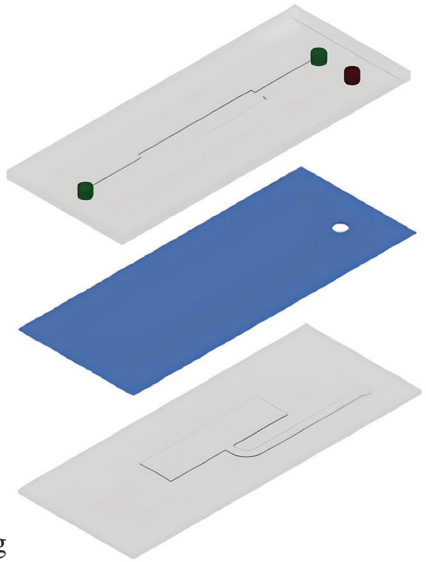


Figure 4: OOC Chip Design with Pneumatic Actuation
(by Joseph Xavier and Xiangxu Liu)

Conclusion

In conclusion, this study will deploy OOC model and advanced imaging techniques to assess varying formulations to optimise pulmonary alveolar-epithelial drug delivering.

Environmental

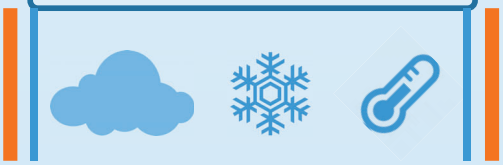
Ice Nucleation in Aerosols Containing Biomolecules

University of BRISTOL

Fraser Crawford

Supervisors: Jonathan Reid & Walther Schwarzacher

1. Why Study Ice Nucleation in Aerosols? [1]



The nucleation of ice in droplets is important for understanding:

1. Weather and meteorological models
2. Industrial processes such as flash freezing
3. The radiative forcing of clouds, and thus, climate models

Despite these applications, heterogeneous ice nucleation is still poorly understood, especially with respect to which properties of a material give it good nucleating ability.

2. Proposed Research Strategy

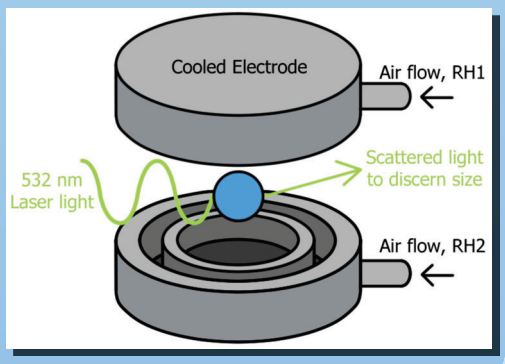
1. Construct an **electrodynamic balance (EDB)** suitable for examining the freezing behaviour of levitated single aerosol droplets. This should be able to explore micron scaled droplets

2. Using the EDB apparatus, explore the freezing behaviour of droplets containing the protein apoferritin/ferritin under different pre-treatment conditions: heat treatment, pH and concentration

3. Begin exploring droplets containing surfactants. Investigate different surfactant concentrations, droplet sizes and surfactants of different dimensions.

4. Continue with freezing experiments of droplets containing DNA origami sheets organised into wedges. By varying the angle between the sheets, explore substrate effects. Also conduct experiments with unannealed DNA.

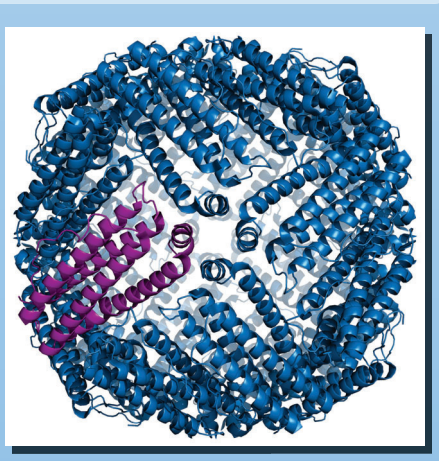
3. The EDB Design (TOP LEFT) [2]



The EDB uses a combination of AC and DC electric fields to levitate a single charged droplet in place. Using scattered light from a laser, the size of the suspended droplet can be found.

Conditions in the device can be varied using attached coolers/heaters and through running different humidity gases through the chamber.

The EDB benefits from droplets 100 to 1000 times smaller than droplet array methods leading to less contaminant driven nucleation.

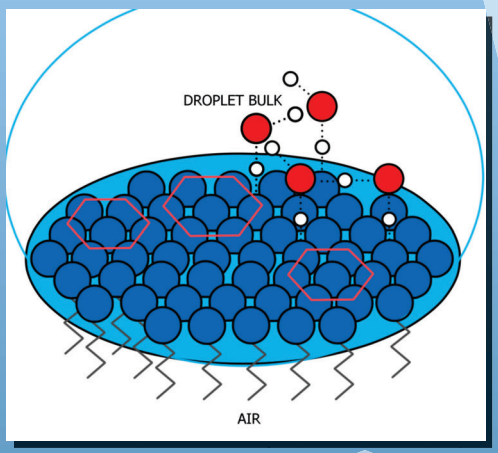


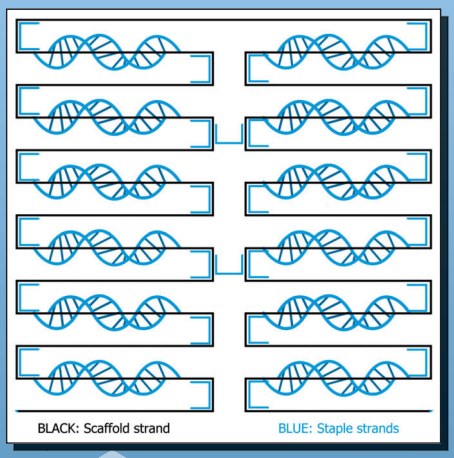
4. Apoferritin (TOP RIGHT) [3]

Apoferritin is a protein that stores iron. Despite this original evolutionary purpose, the protein is an exceptional ice nucleator.

The protein is believed to primarily nucleate ice growth through forming larger protein aggregates. Smaller droplets from the EDB provide a good environment to explore the effect of these rare structures.

The protein has a well studied structural behaviour under denaturing conditions such as at low pH and heat treatment. Exploring the ice nucleating ability of the protein under these conditions provides better insight into the biomolecule structures that best nucleate ice.





4. Surfactants [4]

Surfactant molecules in a droplet will generally accumulate at the air-water interface ie. The surface of the droplet.

Hydrophilic surfactant molecule heads (circles) pack in a hexagonal arrangement, similar to that of ice's crystal structure.

Different surfactant concentrations and molecules can be explored to see how parameters such as lattice matching effect the "scaffolding" of the ice and thus affect the nucleation rate.

5. DNA origami [4]

DNA by itself is a known ice nucleator but this ability can be augmented by changing the shape the DNA conforms to. Using a combination of long tailored DNA "scaffold" strands and shorter "staple" molecules, rigid 2D and 3D structures can be formed out of sheets of DNA.

By combining two sheets of this material, a wedge can be formed with a tuneable pitch angle.

Similar to the planar case from surfactants, the concave pit of the wedge can act to change the volume of the critical ice embryo, changing the rate of ice nucleation.

In these experiments, the angle between wedges can be varied, and this substrate effect can be explored.

Previous computational work has explored similar (though much smaller in scale) wedges formed from graphene and showed a large dependence between the interior angle and the rate of nucleation. [5]

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Aerosol Emissions from Future Generation Aircraft and Their Impacts on Climate

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Engineering and Physical Sciences Research Council

UNIVERSITY OF LEEDS

Background & Motivations

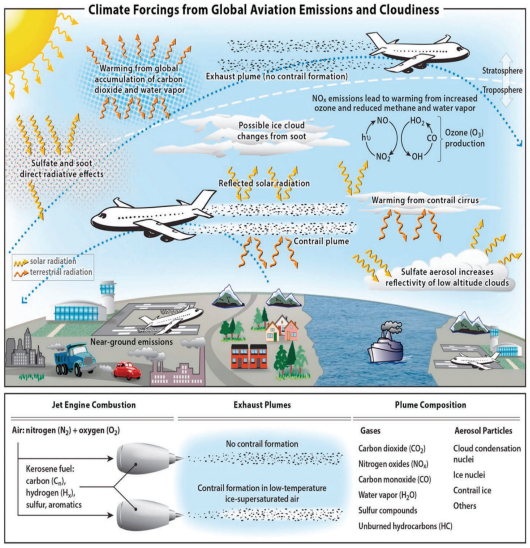


Figure 1. Schematic illustrating how aviation emissions affect the climate[1].

The aviation industry is thriving[1,2] but has a heavy realiane on fossil fuel.

A significant proportion of the aviation's climate impact (Figure 1) is caused by its non-CO_2 effects. Among them, **aerosol emissions present the greatest uncertainty**, especially in their role in influencing cloud formation[1].

There are still **no best estimates** for the climate impact due to aviation aerosol-cloud interactions[1] (Figure 2).

Key Challenges:

- The strong senstivity of the cloud radiative field to aerosol perturbations[1].
- The difficulty to simulate the impact of aerosol particles on ice nucleation[1].

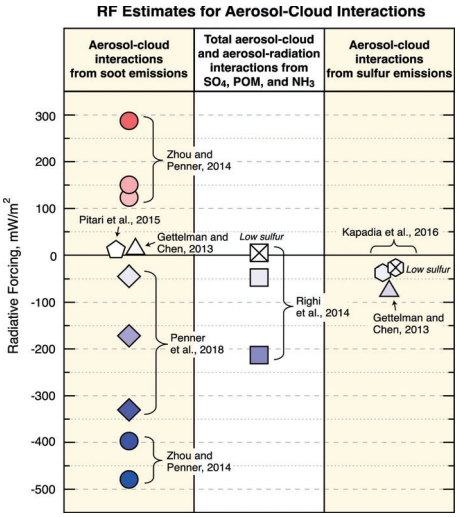


Figure 2. Summary of normalised radiative forcing estimates for aviation's aerosol-cloud interactions from various published studies[1].

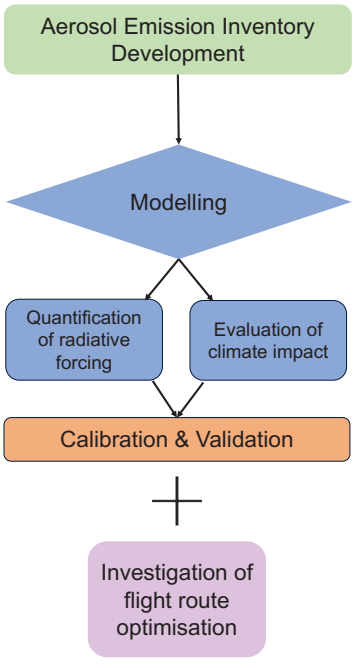
Objectives

Aim: investigate the impact of aviation aerosol emissions from both current and future generation aircraft and provide robust estimates for aerosol-cloud interactions.

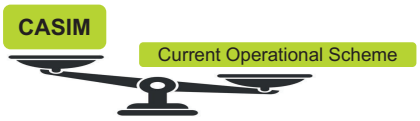
Objectives:

1. Assess global aerosol emissions from current and future aviation, considering different air traffic and aircraft technology scenarios.
2. Quantify the global radiative forcing of aerosol-radiation interactions resulting from both current and future generation aircraft.
3. Investigate present-day effects of aviation aerosol-cloud interactions in high air traffic regions.
4. Evaluate the global climate impact from both aerosol-radiation interactions and aerosol-cloud interactions under different scenarios.
5. Investigate the potential of flight route optimisation to reduce the climate impact of future generation aircraft aerosol emissions.

Methodology



This project will employ the state-of-the-art Met Office **Unified Model (UM)** that can address the current model challeges via improved aerosol microphysics scheme, **CASIM** (Cloud AeroSol Interacting Microphysics) and contrail cirrus scheme.



Multi-moment[3]	Single moment[3]
Represents cloud through **five species**[3]	Represent cloud through three phases[3]
Includes **aerosol processing** mechanisms[3,4]	No inclusion[5]

Can represent the response of cloud properties caused by changes in aerosols more accurately

Policy Implications

Insight into Aerosol-Cloud Interactions: Research highlights the the climate forcing term that is currently absent from assessments of aviation climate impact, enriching policymakers' understanding and enabling more informed mitigation strategy development.

Guidance for Sustainable Aviation: Assessment of diverse aircraft technologies offers valuable direction for emission reduction strategies, empowering stakeholders to make informed decisions and foster sustainable development in aviation.

Responsible Innovation & Challenges

RI: - Trade-offs between profitability and sustainability
- Equity and Justice in accessing air travel and sharing the costs of environmental mitigation measure

Ongoing dialogue and collaboration with stakeholders to integrate their perspectives into the research

Challenges: Limitations and uncertainties associated with modelling;

Calibration and validation, sensitivity analysis and parameter optimisation strategies

Reference:

1. Lee, D.S., et al. (2021). Contribution of global aviation to anthropogenic climate forcing for 2000 to 2018. Atmospheric Environment, 244, 117834.
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Developing and deploying new sensors for in-situ monitoring of clouds

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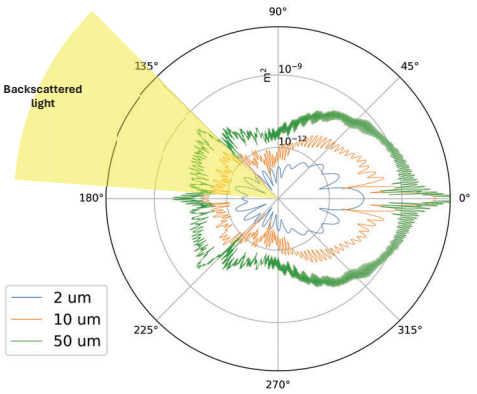
Background

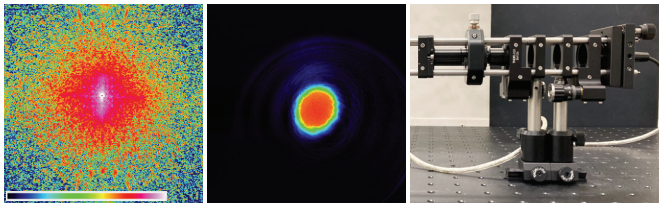
- Cloud droplet probes typically use forward-scattered light (from a laser) to measure cloud droplet size distribution.
- Backscattered light could provide means for a more practical measurement technique that (doesn't require a detector in front of the laser and) could be more easily used on non-specialist platforms e.g. commercial jets.
- **Research Aim:** Investigate feasibility of using backscattered light for accurate cloud droplet size distribution measurement.



'Phase' diagram for spherical water droplets – Scattered light intensity (differential scattering cross-section) over polar angle of an unpolarized 550nm beam (incident at 0°), spherical droplets scatter light symmetrically about the azimuth angle relative to the scattering plane.

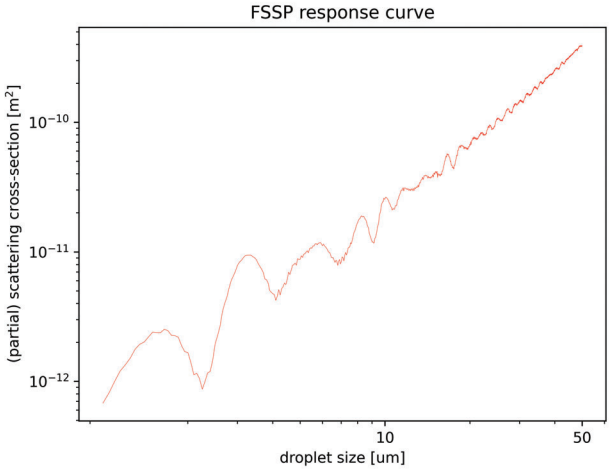
Method

- A model has been developed to produce droplet scattering 'response curves', for a collection optic displaced from an incident beam by a polar angle and will be used to inform optimum backscattering arrangements.
- An optical assembly is being developed to measure backscattered light experimentally and assess arrangements for droplet measurement.
- The assembly will consist of a laser source(s) directed at a scattering target and photodetector(s) that can be adjusted to assess different arrangements and parameters.

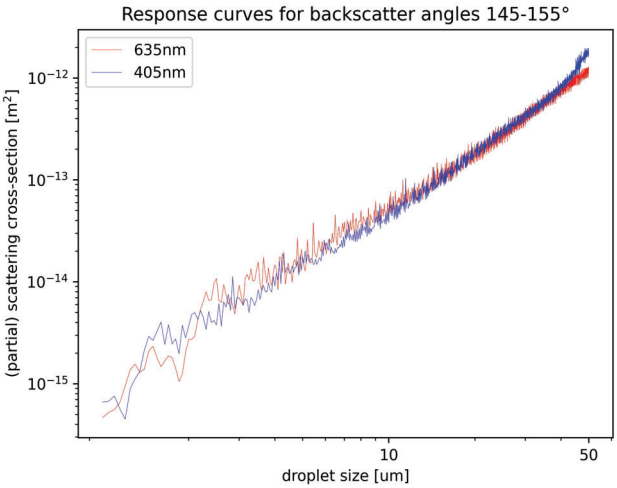


(L) Backscatter Cloud Probe (BCP) beam profile – The BCP is an existing backscatter instrument, but is limited for quantitative measurement [1]; variation of beam intensity within the sample area is one source of uncertainty.
(C) Beam profile produced by a spatial filter – A more confined and uniformly intense laser beam profile could help improve backscatter size measurement.
(R) Spatial filter and laser source – A spatial filter consists of three stages; an aspheric lens, a pinhole and a collimating (plano-convex) lens.

(Color maps to a linear intensity scale of greyscale pixel value from black to white)



Forward Scattering Spectrometer Probe (FSSP) response curve – The FSSP collects forward scattered light from a 632.8nm red laser between 4.6 and 12.8° polar angles using an annular photodetector and has been widely used in cloud droplet research; the instrument response curve used to measure droplet size is replicated by the model [3], (the model is implemented in Python and uses the Python module *scattnlay* to calculate scattering amplitudes [4]).



Backscattered light response curve – backscattered cross-section against droplet size, collected by an optic offset from the incident beam (0°) between 145 and 155° polar angles in red and blue wavelengths; non-monotonicity presents an uncertainty in the mapping of roughly ±2.5um.

Next Research

- A 'clean' spatially filtered laser beam could help define the sample area and reduce uncertainty due to varying beam intensity, which remains a challenge in single-droplet cloud spectrometers [2].
- Use of multiple wavelengths (sources) or detectors may also help define the sample area and reduce measurement uncertainty.
- Backscatter arrangements are being investigated experimentally that could be suitable for a compact instrument module.

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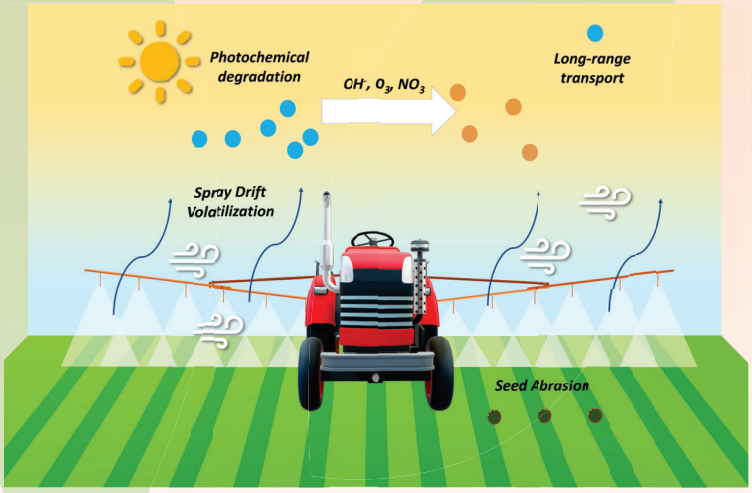
Towards a Better Understanding of the Lifecycle of the Pesticides in the Atmosphere

Ujjawal Arora
Supervisor: Prof. Hugh Coe
Co-Supervisor: Prof. Martin Gallagher and Dr. James Allan

The University of Manchester

1. Background

- Pesticides used to eliminate or control unwanted pests that can damage crops can be partitioned into the atmosphere, either in gas or particle phase by direct **volatilization**, or by **spray drift**, or can be degraded into the atmosphere either by reactions with $\mathbf{OH}$, $\mathbf{O_3}$, or $\mathbf{NO_3^\circ}$ or by direct **photolysis**[7]
- Agriculture contributes to feeding 8 billion people[3], leads to **Global consumption** of pesticides of around 2.66 million metric tons/year[2], causing an increased persistence in atmosphere. Their **Persistence** is highly dependent on vapor pressure, Henry's constant, and dry and wet deposition[1,6]
- According to FOCUS Air Report $V_p \geq 10^{-4}$(20°C) is considered to have potential of volatilization from surface and once suspended, it will distribute b/w vapour, aqueous and particle phases to reach equilibrium[5].



2. Statement of Problem

Limited understanding of **biosphere-atmosphere** of pesticides, their **transportation** mechanism, their conversion reactions, their persistence in the environment

Lack of standards to quantify direct surface **volatilization** of pesticides

Techniques to quantify range of pesticides is not well explored well to quantify **real-time** reactions and influencing **meteorological** parameters

3. Aim and Objective

The aim of this study is to determine **fluxes** of pesticides from the point of application to the **regional** scale, with the development of an **eddy covariance** (EC) system for both **gas** and **particle** phase characterization, with **HR-TOF-CIMS** in conjugation with a sonic anemometer.

- **Objective 1:** Development of system for **simultaneous** measurement of **scalar** quantity from HR-TOF-CIMS and the **vertical wind speed**
- **Objective 2:** Development of an eddy correlation system for both particle and gas phase species
- **Objective 3:** Deployment into the field at field scale first which can then be scaled to regional scale and for different range of environmental conditions and under **specific farming practices**. **Regional burden** of the pesticides may be examined.

4. Methodology

Eddy covariance flux measurements is based on determining **covariance** between changes in **vertical wind velocity** and deviations in **scalar quantity** such as mixing ratio of a trace gas or air temperature[8]

$$F_c = \overline{w'c'} = \frac{1}{n}\sum_{i=1}^{n}(w_i - \overline{w}).(c_i - \overline{c})$$

Sonic Anemometer (SA) with an operating frequency of 10 Hz in conjugation with **CIMS** would provide the Eddy Correlation fluxes, however further Correction are required.

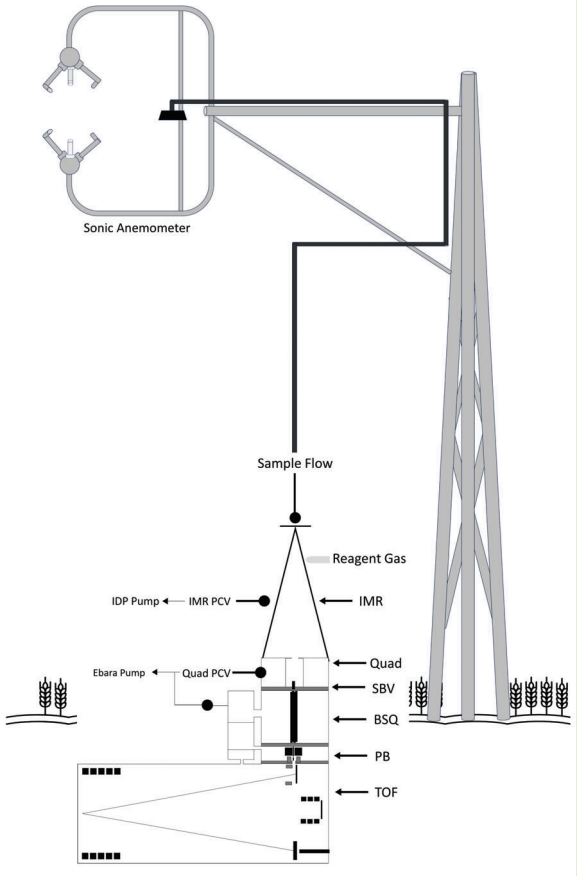
CIMS (Chemical Ionization Mass Spectroscopy) is capable of measuring pesticides in gas and particle phase because of its **reproducibility**, **minimum sample handling**, **high mass resolution** (m/Δm~4000-6000), **high time resolution** (1-10 Hz) allowing measurements of reactive compounds[4]

Consists of five main components:

- **VUV Ion source** which is a Krypton lamp
- Ion molecular Reactor (IMR)
- Big segmented quadrupoles to separate m/z
- An ion lens focusing region
- TOF mass analyzer

(I^- CIMS ionization mechanism) $I(H_2O)_n^- + M \rightarrow n(H_2O) + I(M)^-$

5. Proposed Setup



Site Specification
- **Homogeneous Terrain**[6] ($\frac{d\xi}{dx_1}$) & $\frac{d\xi}{dx_2}$=0)
- **No flow divergence and convergence**

Pre-Processing
- **Time Lag Analysis**
- **Data gap Filling**

Eddy-Pro for Flux Calculations and further corrections
- **Co-Spectra Analysis:**
- **Storage corrections** (during formation of nocturnal boundary layer)
- **Ogive Optimization**(to determine the averaging time interval)

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Fundamentals

Particle-surface adhesive forces and their role in resuspension phenomena

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Project Supervisors: Dr Matthew Jones, Dr Paul DeBank, Dr Anton Souslov, Prof. Jonathan Reid
DSTL Supervisors: Richard Thomas and Simon Parker

What is Resuspension?

Resuspension is when particles that are initially on the ground become entrained into the air flow

- A significant source of aerosol particles encountered on a daily basis can be attributed to this process, which poses a substantial health risk.
- Highly relevant and applicable across a range of disciplines:

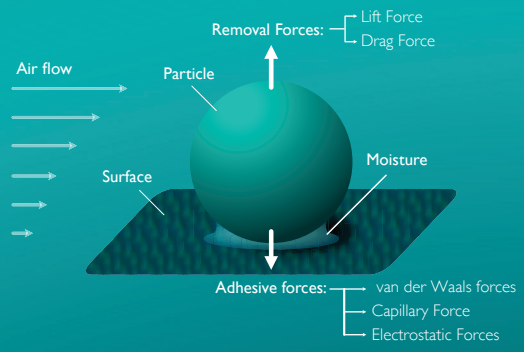
Biological	Chemical	Agricultural	Industrial	Nuclear
(eg. Virus droplets, pollen, spores)	*(eg. smoke, soot, fumes)*	*(eg. Pesticide spray, soil dust)*	*(eg. Metal, floor dust, pollen, spores)*	*(eg. Radioactive waste from power plants)*

- There are many factors influence resuspension, including (but not limited to):

Particle Morphology · Surface Material · Concentration · Wind Velocity · Temperature · Relative Humidity

Resuspension Theory

Whether resuspension of a particle happens depends on the balance forces:



Forces of adhesion are currently not well understood, with current models only applying in highly idealised cases. Capillary force equations have been shown to be inaccurate above 60% RH.

Rock 'n' Roll Model:

Proposed by Reeks *et al* in 1988 [1], the Rock 'n' Roll model offers a promising model for predicting the resuspension for a given set of input parameters.

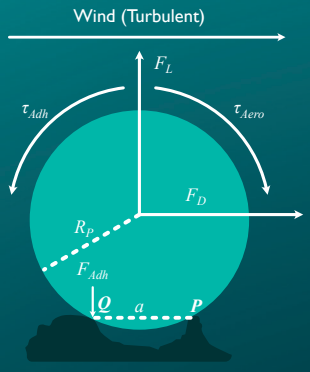


Figure 1 (Adapted from [3]): Schematic for a single particle in the Rock 'n' Roll model. A particle of radius R_P rests on 2 asperities separated by distance a, and the forces of adhesion are assumed to act at point Q. Torque imbalance arises about the pivot point P.

- It considers three forces - adhesion (F_{Adh}), lift (F_L) and drag (F_D).
- The lift and drag forces cause oscillatory motion about point P, providing the torque needed for the particle to either "rock" (oscillate) or "roll" over.
- Implemented by Biasi *et al* in 2001 [2] with a primary rate equation with constant p:

$$\frac{dN_R}{dt} = -p(F_A)N_R$$

- The macroscopic resuspension rate was solved numerically by integrating over time:

$$N_R(t) = \int_0^\infty \varphi(F'_A)e^{-p(F'_A)t}dF'_A$$

Limitations

The Rock 'n' Roll model in its current form includes many assumptions that limit the current predictive capability. These include (but are not limited to):

Particles are spherical and homogeneous; surfaces are smooth; only 2 or 3 asperities; log-normal force distribution, $\varphi(F'_A)$; over the surface; particles reside in a monolayer.

It's these assumptions the project aims to address using a variety of techniques.

Project Objective

The main objective of this project is to increase the accuracy of the model for resuspension, capturing a greater variety of realistic resuspension scenarios.

This can be broken down into 4 stages:

1. Produce a range of surfaces with increasingly complex chemistry and topology that mimic realistic surfaces
2. Measure adhesive force distributions between particles and these surfaces using Atomic Force Microscopy
3. Implement the Rock 'n' Roll model using empirical force data, thereby reducing the number of assumptions
4. Validate the Rock 'n' Roll model experimentally using a wind tunnel

The project aims to sequentially carry out these four stages and iterate the process, modifying one variable per iteration.

Methodology

Atomic Force Microscopy (AFM):

- Instead of incorporating an assumed force distribution into the model, the adhesive force distribution across surfaces and particles will be directly measured using colloidal probe Atomic Force Microscopy (AFM).

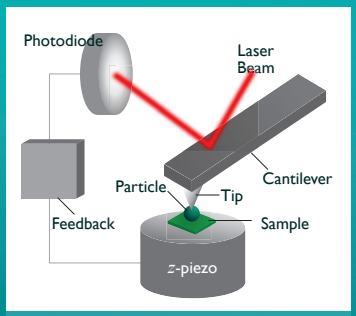


Figure 2 (Adapted from [4]): Schematic of a colloidal prove atomic force microscope.

- AFM uses a tip on the end of a cantilever to measure the force distribution across a surface.
- The cantilever will vertically deflect in accordance with the force applied [4]:

$$F = -kz \qquad k = \frac{3EI}{L^3}$$

- Particle will be securely adhered to the end of a cantilever.
- Particles chosen will have a known morphology such as salt, sugar and sand granules.

Custom 3D Printed Surfaces:

- The project will aim to print surface substrates with controlled topology, morphology, hydrophobicity, and surface energy, aimed at mimicking realistic surfaces.
- Surfaces to be modelled using 3D software such as Blender®.
- Complex techniques such as nano-lithography to be employed for even finer control.

Wind Tunnel:

Recent work by Vincent *et al* (2019) [3] at DSTL, has given shown promising validation of the Rock 'n' Roll model.

- Involved a wind tunnel experiment involving glass beads in a monolayer and carefully controlling environmental conditions.
- The model and experiments generally agree for low RH, although the trend line is imprecise, especially for large RH.
- This project aims to take this work further by using a similar wind tunnel at the University of Bristol. Force data from the AFM used in the Rock 'n' Roll model can be directly compared against.

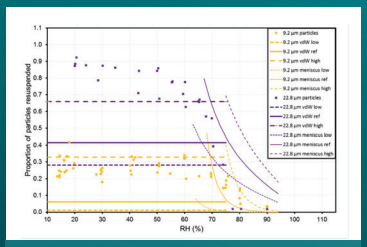


Figure 3 (From [3]): Plot of resuspension amount against relative humidity for 2 particle sizes. Curves represent the Rock 'n' Roll model, whereas points represent wind tunnel experiment results.

Responsible Innovation

Due to the project's close ties with a variety of different fields such as industry, agriculture, healthcare, etc., it's important that research into resuspension is brought into the wider context.

Accuracy	Ethics	Policy	Innovation
• Research findings must be accurate, reproducible, and reliable. • Clarity of communication to ensure findings aren't misinterpreted.	• Ties to industries, all of which have a vast potential on human health. • Objective is to improve human health through mitigating risk	• Potential for results to be implemented within an industrial setting as part of a protocol. • Results must therefore be heavily validated.	• Potential for novel technologies including surface coatings and filtration systems • Remote sensing technologies, assisted by novel technologies such as AI

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3. Vincent, J.C., Hill, J., Walker, M.D., Smith, S.A., Smith, S.E. and Cant, N.E., 2019. Towards a predictive capability for the resuspension of particles through extension and experimental validation of the Biasi implementation of the "Rock'n'Roll" model. Journal of Aerosol Science, 137, p.105435.
4. Piontek, M.C. and Roos, W.H., 2018. Atomic force microscopy: an introduction. Single molecule analysis: Methods and protocols, pp.243-258.

Model systems for exchange of liquid between different aerosol sources

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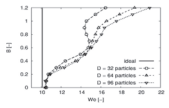
UNIVERSITY OF BATH
EPSRC
Engineering and Physical Sciences Research Council

Aims of Project

Much work has gone into understanding the coalescence of aerosol droplets and the different conditions that two droplets need to be under to result in this phenomenon. These have especially been understood on a droplet-to-droplet basis, but less work has been done on a larger scale to understand the product of two aerosol clouds interacting.

This project aims to develop a model that deciphers whether there are instances where every droplet from stream A coalescences with a droplet from stream B and the resultant droplet has parts of each stream in it.

We also aim to explore different parameters that would affect successful collision rate such as viscosity of droplets and there is also potential for experimenting with relative humidity in this experiment.



Experiment composition

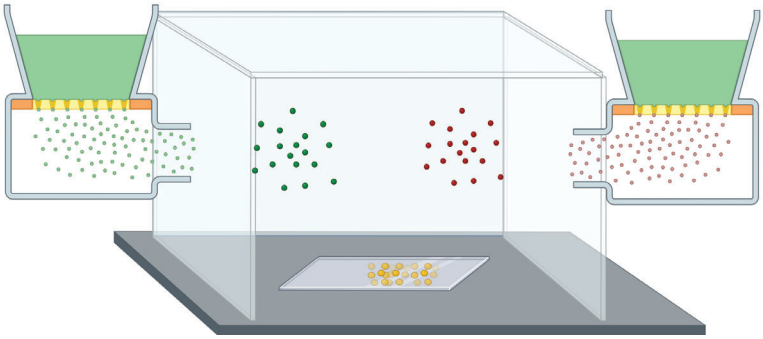


Figure 1: A figure showing a basic representation of the main experiment that we are looking to run

Explanation

Water clouds will be shot out of the ultrasonic nebulisers at the same rate and towards each other so that they meet in midair and collide.

This should hopefully make some yellow droplets that would settle onto the slide to be observed over different periods of time

Third hole for humidity monitoring possibly

Objectives

Objective 1:
This project aims to choose which modelling style is most appropriate then develop a fundamental model that explores whether there are instances where aerosol exchange between two streams is a complete process for each resultant droplet

Objective 2:
Construct and experiment that can verify the model that was created for this particular mechanism with two clouds of water that are dyed different colours.

Objective 3:
Use the findings from the original experiment to apply the mechanism to more realistic particles like known lipids e.g. lung surfactants and see whether results vary, and which points particles stop coalescing

Methodology

Modelling

COMSOL will probably be the programme of choice, but time will need to be taken as the initial calculations to display the trajectory, velocity and concentration of particles will need to be done as well as the properties of the chamber that the droplets will be modelled in.

Lattice Boltzmann Modelling (LBM) is a very good mechanism to use for a project like man as it has a great proficiency in modelling collisions and their behaviour in fluid flow simulations

Experimentation

This experiment will have different components which involve construction and purchasing of items as well as different experimental techniques. The chamber will need to be modelled and 3d printed

Fluorescent marking, microscopy and high-resolution imaging will also need to be utilised in order to quantify the results collected

Potential Challenges

One of the main challenges in this project would be the making of this model with its complexity and my personal proficiency with modelling. With models, they can also have many errors so it could potentially take a lot of time to create a model that works and that can have results that can be backed by the experiments that will be run.

Another challenge with the model could be to use the correct model type to avoid wrong permutations and assumptions on the programmer's part. Work will need to be done to ascertain which model type would be best for this particle mechanism.

Another challenge would be with the slide. The question of how we can decipher whether droplets coalesced on the slide or in the air will always be there, so it needs to be looked into. A series of control experiments will need to be done with various time frames to also see to which degree that this could be a factor.

Because of the need for proficiency with the model, the experiment could have different conclusions to the model because of errors with the construction of the model.

Responsible Innovation

In future, this model could be very beneficial for understanding of aerosol exchange for more complex models that are more applicable to everyday human life. We could potentially see exchange between bioaerosols and pharmaceutical aerosols

We could also potentially see the exchange between rural air and urban air and explore the differences in air quality.

Dangerous advancements coming directly from this study are unlikely, but the step-up projects really could be used to make bioweapons and intentional cause adverse health to the public

Data-Informed Modelling of Aerosol Resuspension under Aerodynamic Loads

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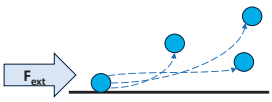
University of BRISTOL

Engineering and Physical Sciences Research Council

What is resuspension?

- Process through which **particles detach from a surface** to **become airborne**[1] through the action of **external forces**
- Ubiquitous applications:



Pollen, dust, sand, snow | Metals, fibres, pollutants | Virus, bacteria, bioaerosols | Pesticides, fertilisers | Brake, tyre & road/track wear

Problem statement

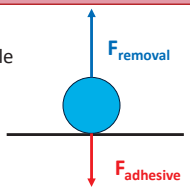
Current issues with existing resuspension model:

- Models are scarce and dated
- Mostly mechanistic and empirical
- Compromise between accuracy & computational cost
- Overall lack of data to perform numerical & analytical sensitivity

Need to investigate **novel solutions** to capture the complexity of the problem while enabling simpler and quicker steps towards resolution, combining accuracy and efficiency.
Can make use of **machine-learning techniques** to build on **numerical simulations** and **wind tunnel data** and enable useful **validation of existing models.**

Background

- **Rupture of the balance** between the forces moving the particle and those impeding its motion[1]
- Removal forces: unsteady fluid mechanics, mechanical & electrostatic forces, particle impaction and thermal gradients
- Adhesive forces: Van der Waals & electrostatic interactions, capillary forces, friction and chemical interactions
- 3 main resuspension modes: **rolling, sliding and lifting**



Resuspension mechanics: adhesive properties alter with complex interactions between

- **Particle properties**: size, shape (asperities), density, composition
- **Surface characteristics**: roughness, electrostatics, hydrophilicity
- **Flow conditions**: fluid velocity, Reynolds number and turbulence scale, boundary layer
- **Environment**: pressure, temperature, humidity

Some **existing models**:

- Detachment from surfaces with varying roughness in turbulent flow (Soltani et al, 1994 & 1995 and Ziskind et al, 1995 & 1997)
- RRH model: kinetic approach only considering lift and normal forces (Reeks et al, 1998)
- *"Rock'n'roll"* model[2]: rocking of a particle about an asperity (Reeks et al, 2001), later implemented by Biasi et al (2001)
- Recent model by Guingo and Minier (2008), enhanced by Henri et Minier (2014) has much greater complexity and requires more computational power.

Objectives

Evaluation of the feasibility and accuracy of **resuspension experiments** in a **controlled laboratory environment** for varying **particle sizes, surface topologies** and **flow conditions**

Investigation **of key parameters** influencing the resuspension mechanism and how they **interact** and **correlate** with each other

Application of **numerical** and **Computational Fluids Dynamics (CFD)** methods to solve scenarios of increasing complexity and gather data

Assimilation of **experimental** and **numerical data** into **machine-learning-based semi-empirical models** to achieve highly accurate **resuspension predictions** for a broad range of scenarios

Policy and Responsible Innovation

Policies:

- **Health and safety regulations**: evaluate resuspension hazards (e.g. dust & fibres in factories, viruses in hospitals)
- Adjust **tolerance thresholds** for particles highly prone to resuspend
- Regulate industrial **accidents** and sanction **malpractice**

Responsible Innovation:

- **AI training data-use**: use own data or get consent to use 3rd party's
- Model application: unethical and harmful usage very unlikely
- NN and CFD methods **environmental impact**: very computationally intensive, thorough planning required to limit footprint

Methodology and techniques

Phase 1: Experimental

3D printed wind tunnel, E. Neal [3]

- **Wind tunnel testing** to evaluate different resuspension scenarios
- Varying **particle sizes** and **surface morphologies**
- Variation in **fluid velocity** and **turbulence scale**
- Investigation of **time-varying effects**
- Instruments: **particle imaging** & **hot wire anemometry** to gather data (e.g. pressure & velocity fields, turbulence intensity, particle path, aerodynamic forces)

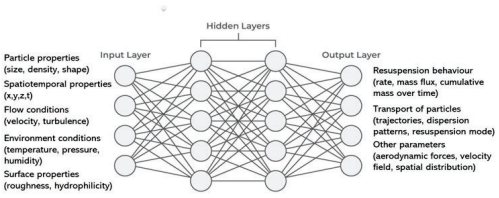
Phase 2: Numerical

Lagrangian particle tracking CFD simulation using Star-CCM+

STAR-CCM+

- Numerical methods to investigate resuspension
- **Computational Fluids Dynamics (CFD)**: analyse and predict flow & particle behaviour for complex scenarios
- Definition of **complicated geometries** to perform very **realistic simulations** with real-life-like conditions
- Modelling of **other phenomena**: fluid-structure interaction, multiphase, electrostatics, thermogradients
- High spatial & temporal resolution
- Cross-validation of phase 1, generation of additional data

Phase 3: Modelling



- **Physics-Informed Neural Networks (PINNs)**[4]: universal function approximator
- **Reduced-order** models
- Highly **modular** and versatile
- Powerful **data-driven tool** to model resuspension in a simplified and physics-accurate way

Challenges

Data management:

- Measurement errors/noise
- Sufficient scope and frequency
- PINNs overconstraining

PINNs convergence:

- Complex model, many layers
- Multiple parameters to predict
- Lengthy computations, no convergence guarantee

Model interpretability:

- NN seen as a "black-box" tool
- Lack of transparency
- Path to solution and output reasoning is not always clear

Computational needs:

- PINNs and CFD lengthy and expensive to run
- HPC facilities required
- Extensive planning ahead

[1] W. C. Hinds, 'Adhesion of Particles', in Aerosol Technology: Properties, Behavior, and Measurement of Airborne Particles, John Wiley & Sons, Incorporated, 1999.
[2] J. C. Vincent, J. Hill, M. D. Walker, S. A. Smith, S. E. Smith, and N. E. Cant, 'Towards a predictive capability for the resuspension of particles through extension and experimental validation of the Biasi implementation of the "Rock'n'Roll" model', J. Aerosol Sci., vol. 137, p. 105435, Nov. 2019
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Time-resolved Photochemistry of Organic Solutes in Aqueous Microdroplets

Engineering and Physical Sciences Research Council

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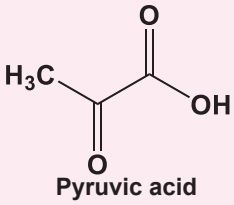
Background

- In the troposphere, **secondary organic aerosols** (SOAs) are a large proportion of organic aerosols, which contribute to global warming & climate change.[1]
- **Pyruvic acid** (PA) is an environmentally sensitive compound, which has a role in SOAs formation.[2]
- PA chemistry in the **gas phase**, aqueous **bulk**, and at the **surface interface**, is uniquely different.[3]



Pyruvic acid

Aims & Objectives

1. Conduct bulk solution **fluorescence/absorption lifetime spectroscopy** measurements on PA, exploring the **intermediates** and lifetimes of **excited states**.
2. Levitate droplets in a linear quadrupole electrodynamic balance (**LQ-EDB**) with initial **coupling to Time-correlated single photon counting**.
3. Vary the **environmental conditions** (pH & relative humidity) to measure the change in the photochemistry of PA.
4. Assess the suitability of **transient absorption spectroscopy** coupled to the LQ-EDB to study PA droplets.

TAS

Transient absorption spectroscopy (Figure 3) is used to observe the population of the short-lived excited states (a few femtoseconds) to long-lived photoproducts (a few nanoseconds) after **photoexcitation**.

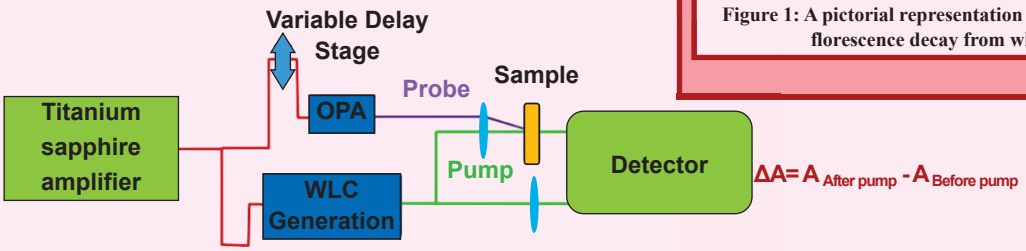


Figure 2: A schematic of the Pump Probe setup of TAS.[5]

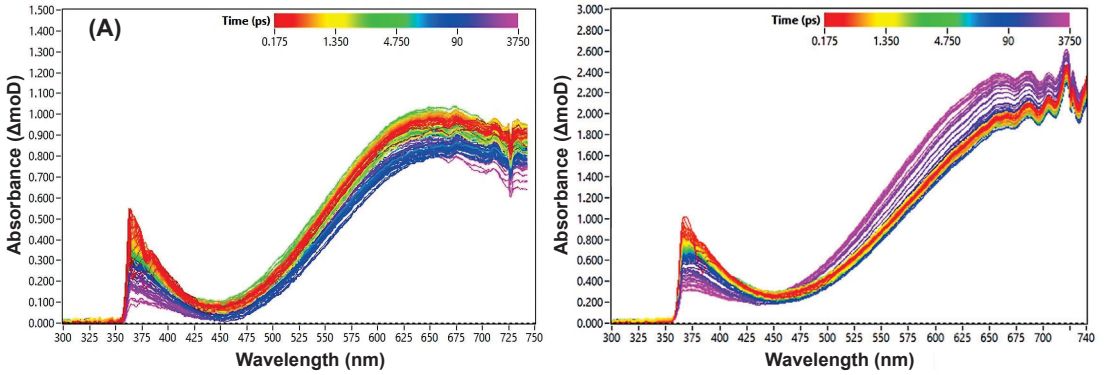


Figure 3: Transient Absorption spectra at 345 nm; (A) PA 1 molar in water, (B) PA 2 molar in water with 250 µm path length.

Key Questions

- **What are the excited states lifetimes that occur in PA droplets?**
- **How do the optical properties of a droplet affect the photochemistry of PA, compared to reactions in the bulk?**
- **How do the surface effects change the photochemistry of PA?**

TCSPC

Time-correlated single photon counting (TCSPC) exposes the sample to a UV or visible laser pulse to insight **excitation** and **fluorescence.** PA is excited at **345 nm** (within UVA range).

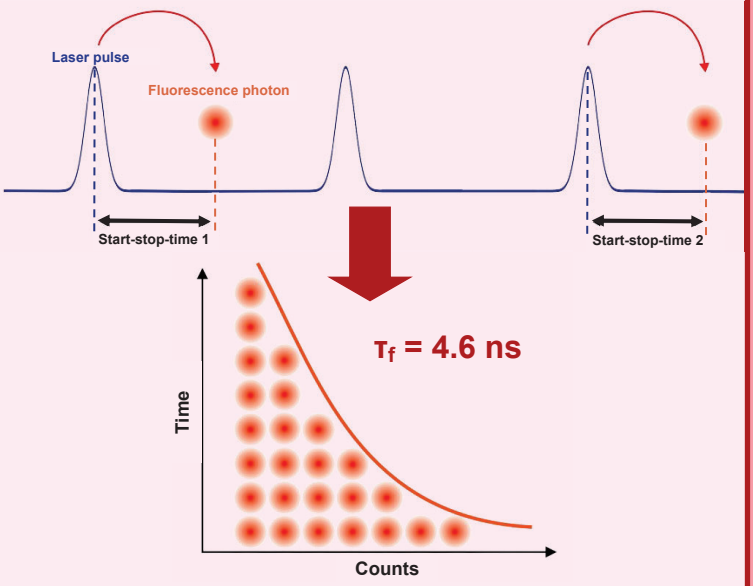


Figure 1: A pictorial representation of TCSPC and the histogram produced of the florescence decay from which a time constant is established.[4]

Future Work

TCSPC setup coupled with the LQ-EDB will allow for the individual droplets to be excited and retrieve the fluorescence of the droplets to compare to the bulk solution.

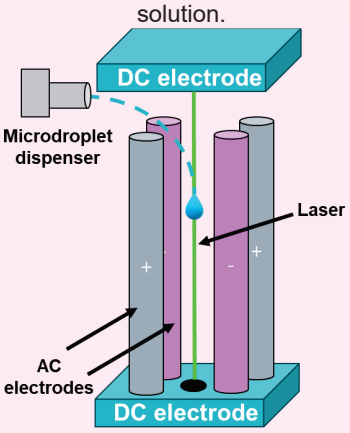


Figure 4: Schematic of the LQ-EDB.

References

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Responsive Aerosol: A Design Framework for Aerosol with Required Properties

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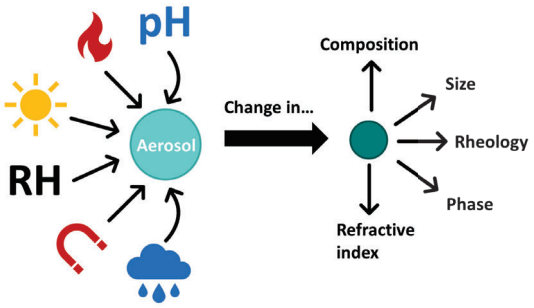
Prof. Jonathan Reid

University of BRISTOL

1. Background

Responsive aerosol

- Aerosols are responsive by nature, which provides an opportunity to design aerosol to have a desired response to a specified stimuli:



- Initially hydrogels are being used as the test system to explore aerosol with responsive properties.
- Hydrogels are three-dimensional polymeric networks that have hydrophilic groups attached to the polymeric backbone and can therefore swell to retain large amounts of water.
- Poly(N-isopropylacrylamide) (**pNIPAM**) and **Poloxamer-407**, both thermoresponsive hydrogels (Fig. 1), have been studied in the bulk phase and as single droplets.
- Both polymers exhibit a measurable response to temperature, moving from a solution to gel state as temperature is increased (Fig. 1).

Hydrogels

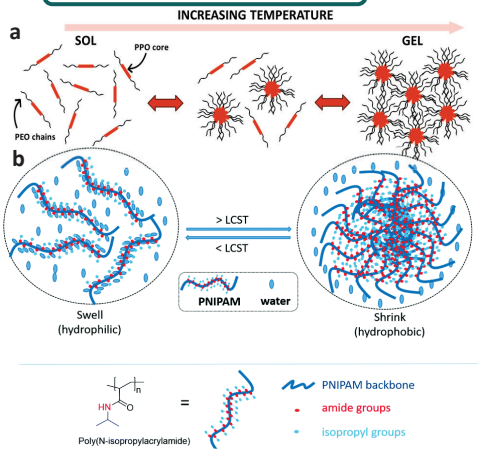


Figure 1—a) Solution to gel transition of P-407 b) Swollen and collapsed state of pNIPAM below and above the lower critical solution temperature (LCST). Figure taken from Doberenz et al.

2. Motivation

The ability to design an aerosol to have a required response to its environment has potential applications in many areas. For example, the aerosol could be used to report on changes in temperature, pH, or RH in the environment, and they could also be designed for controlled release of an API in aerosol drug delivery.

3. Aims

Characterise changes in an aerosol's properties in response to an external stimulus using two hydrogel systems.

Build a framework to allow the design of aerosol that have a desired response to stimuli.

Create a model to understand how changes in the environment can be detected from the corresponding change in size and rheology of the aerosol and to allow a prediction of one from the other.

4. Research Methodology

BULK PHASE:

- **A rheometer was used** to measure viscoelastic properties and a **bubble pressure tensiometer** was used to measure dynamic surface tension.

DROPLET PHASE:

Comparative-kinetic electrodynamic balance will be used to measure the size change of the droplets with respect to temperature and RH.

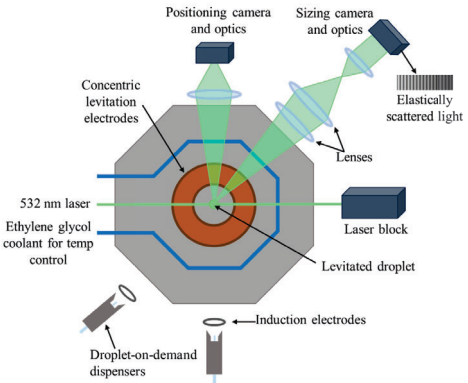
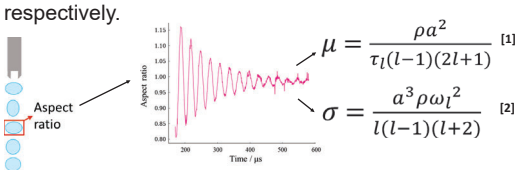


Figure 2—A schematic representation of a CK-EDB from a view looking down into the instrument.

Stroboscopic Imaging used to determine the surface tension and viscosity of the droplets phase from the droplet oscillation frequency and decay, respectively.



Equation 1 and 2– Viscosity and surface tension of the oscillating droplet, respectively, expressed in terms of the droplet radius, a, the fluids density, ρ, the decay time of the amplitude of the lth mode, τ_l, and the angular oscillation frequency of the lth mode, ω_l.

5. Results

Poloxamer-407 properties:

	Bulk		Droplet
Conc / wt%	σ_0 / mN m^{-1}	σ_{eqm} / mN m^{-1}	σ_0 / mN m^{-1}
0.5	61.1	42.5	61.4
1.0	60.1	41.0	60.5
1.5	59.4	40.6	59.2
2.0	59.1	40.1	59.3
2.5	58.1	39.3	58.5

Table 1—Surface tensions of Poloxamer-407 in bulk and droplet phase.

Bulk rheology studies:

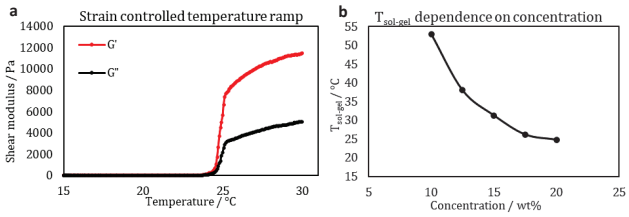


Figure 3- a) Example of a sol-gel transition of 20 wt% Poloxamer 407 exhibited by the extreme increase in storage and loss moduli. G' is the storage modulus (elastic component), and G" is the loss modulus (viscous component). In this case the sol-gel transition temperature is 24.5 °C. b) Sol-gel transition temperature of poloxamer 407 as a function of concentration. Each data point was found by plotting a strain controlled temperature ramp at varying concentrations.

Single droplet studies:

Temperature ramp on levitated droplets of poloxamer 407 and pNIPAM using the CK-EDB:

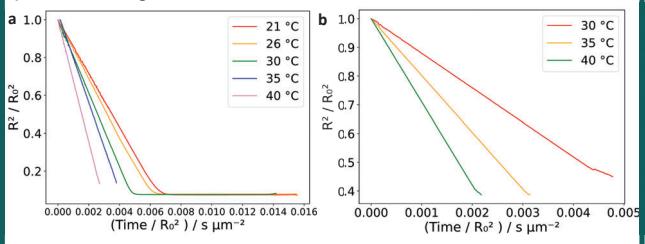


Figure 4—Normalised evaporation curves at different temperatures measured using the CK-EDB. a) 2.5 wt% Poloxamer 407 b) 0.2 wt% pNIPAM

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Triboelectric Charging of Aerosols:
Interpreting Measurements of Volcanic Ash

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EPSRC Centre for Doctoral Training in Aerosol Science


Fuego

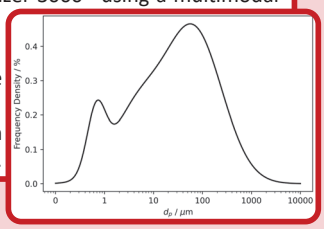
Introduction and Background


Pliny the Younger

- First documented by Pliny the Younger during the eruption of Mt. Vesuvius, **volcanic lightning** is a naturally occurring phenomena with poorly understood charging mechanisms.[1]
- Both material properties and environmental conditions have been shown to affect **granular triboelectric charging**, with the most common measurement technique being Faraday cups.[2]
- The charging of ash from the four volcanoes: Fuego, Grímsvötn, St. Helen's and Atitlán were measured using a **Faraday cup** and displayed a range of charging and trace shapes.
- Most current analysis of these charging traces would be to simply take the range of the charging but this doesn't separate the particle-particle (self-) and preexisting (pre-) charge, so this work develops a new model.

Size Distribution

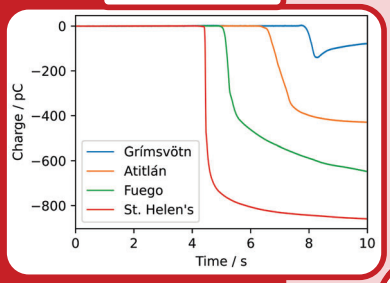
The following size distribution was fitted to experimentally obtained data from the Malvern Mastersizer 3000® using a multimodal lognormal distribution fit. This is the distribution for ash from Mt. St. Helen.

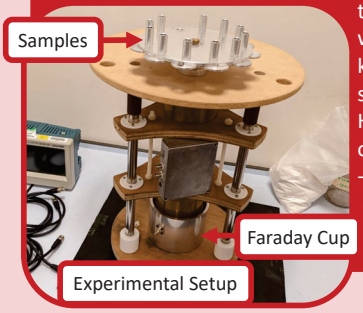


Charge Measurements

Charge measurement for ash of each type were taken using the rig shown below. The samples were left to equilibrate in grounded tubes before being dropped down a column into the **Faraday cup** which was hooked up to an electrometer. The voltage trace recorded by the electrometer was converted to charge using the know capacitance of the experimental setup of around 130 pF (top right). However, we don't know how much of this charging is arising from particle-particle (self-) charging or from charging whilst loading or with the walls (pre-charging).

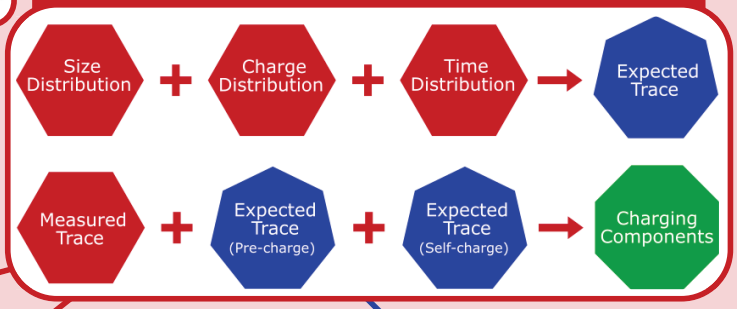
Charge Trace





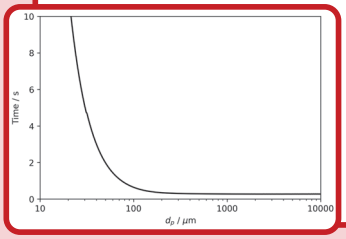
Modular Approach

- In order to separate out the charging contributions of the pre- and self-charging a model was devised as outlined below.
- Charge and time distributions as a function of size can be used with a size distribution to predict the expected trace shapes.
- The shapes of the expected pre-and self-charging can be fit to the experimental trace to estimate their relative contributions.



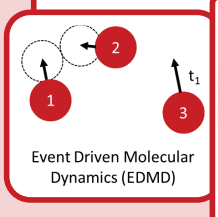
Time Distribution

A Newtonian particle dynamics model way used to calculate the expected time for particles to fall the 37.25 cm into the Faraday cup depending on their size. The drag force was calculated using equations for the Stokes and Intermediate regimes from work by Perry *et al.* Particles of d_p < 10 um were found to not settle in the given time.

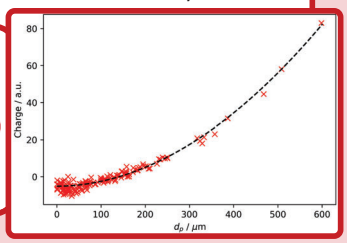


Charge Distribution

The shape of the charge distribution was estimated using an Event Driven Molecular Dynamics (EDMD) simulation of hard spheres. Where a single charge transfer in an excited state is transferred upon each collision then fit to: $y = ae^{bx} + c$.

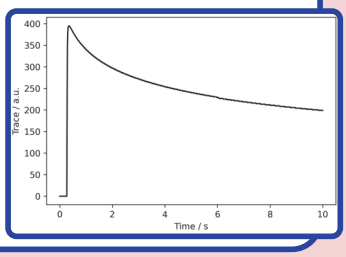


Event Driven Molecular Dynamics (EDMD)

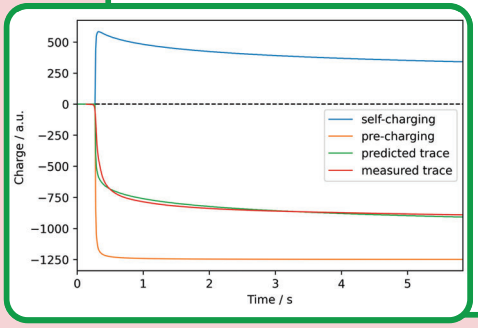


Expected Trace

The size and distribution and charge distributions were convoluted to give a charge frequency density distribution. This can be integrated from ∞ to each timestep to get the expected trace over time. The predicted self-charging trace for St. Helen's ash is shown. This is repeated for the pre-charging



Fitted Charging Components



By fitting the predicted self- and pre-charging components to the experimentally measured trace the ratio of self to pre-charging can be calculated. For St. Helen's ash it is 1 : 1.3 in this case minimizing the R^2 value of the fit.

Model Evaluation and Future Work

Strengths	Weaknesses
• The model is broadly generalisable to any insulating granular material • The modular approach allows any step to be substituted • Is an improvement on current Faraday cup powder charging analysis	• Approximation of the particles' aerodynamic diameters as optical diameters • Assumes the pre- and self-charging do not interact or impact each other • The charge distribution employs a highly simplified charging model

The next steps are to experimentally validate the model with a simplified validation cases of altered size distributions. This has begun using labradorite minerals, which show a good match with the X-Ray Diffraction (XRD) data from de Fuego ash.

1) Cimarelli et al., Bulletin of Volcanology, 84:78, 2022. 2) Lacks et al., Nature Reviews Chemistry, 3:465-476, 2019. 3) Perry *et al.*, Perry's chemical engineers' handbook, 8th ed., 2008 .

Health Impacts

Organ-on-chip, the end to animal testing?

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Supervisors: Dr Jorge Bernardino de la Serna

IMPERIAL

Motivation & Aims

$ 15 billion is spent on animal testing in the US every year with <10 % of drugs that pass animal testing, passing the first round of clinical trials. This project aims to develop a lung-on-chip with an aerosol delivery interface to improve pre-clinical drug screening procedures.

What is an Organ-on-chip?

An organ-on-chip aims to recapitulate organ-level function in a microfluidic device.

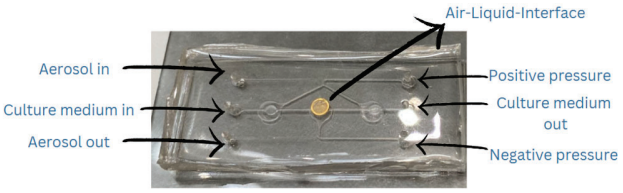

Figure 1: Illustration of the alveolus on a chip currently developed in the lab that will be used to interface with an aerosol delivery system.

Methods.

- Microfabrication of PDMS chip by 3D printing and soft lithography.
- Synthesis of hydrogel ECM mimic.
- Epithelial cell manipulation to express transmembrane protein GLP1-R, and seeding onto ECM mimic.
- Characterising the microfluidic chip by TEER and microscopy.
- Computational fluid dynamic, (CFD), model of aerosolised nanoliposomes through the chip.
- Interfacing the chip with aerosol delivery system.

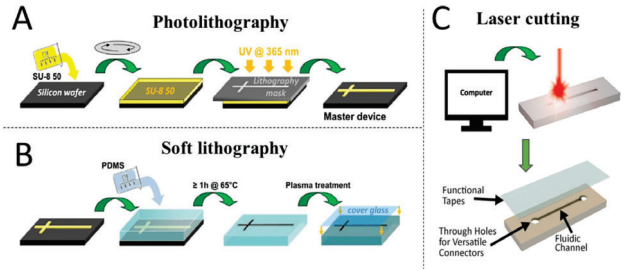

Figure 4: Fabrication methods of Organ-on-chips.

References

From First to Second to Future Gen.

Organ-on-chips have emerged out of advancements in tissue engineering, microfluidics and material science. The fisrt accepted organ-on-chip was developed by Huh *et al* at Harvard, Figure 2:.

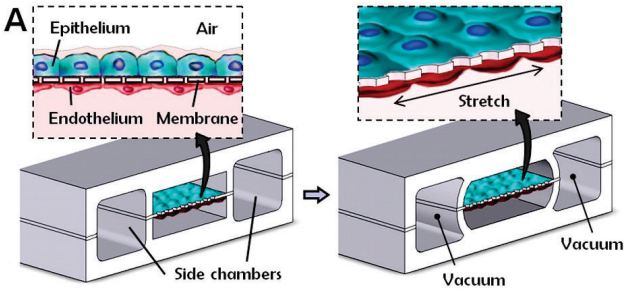

Figure 2: Huh *et al* First organ-on-chip, Emulate still use this design commercially. First generation design as the membrane only considers a single alveolar membrane as an extended structure.

This publication sparked the commercialisation of organ-on-chip technology with companies such as Emulate in the states and AlveoliX in Europe. Since, a variety of first generation chips have been produced. **First generation chips only consider the alveoli as an extended planar structure.**
More recently, second generation designs have been published. **Second-generation lung-on-chips consider an array of alveoli in 3 dimensions.** Allowing bidirectional airflow into and out of the alveoli to be modelled, as well as inter-alveoli interactions. Two notable designs by Zamprogano *et al.* and Huang *et al* are below:

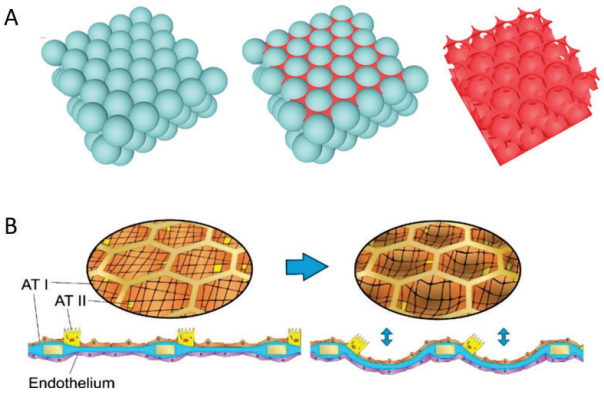

Figure 3: Second generation membrane designs for lung-on-chips. A) Reverse opal structure published by Huang *et al* [37] B) Zamprogano *et al* gold hexagonal mesh with collagen:elastin membrane.[29]

Chemical and Toxicological Properties of Aerosol Emissions Subject to Atmospheric Processing

Joseph Bainbridge
Supervisors: Dr James Allan, Prof. Gordon Mcfiggans

1. Motivation

The long term impacts of pollution sources on air quality and public health are of great importance in the transition to a net zero future in which secondary pollutants are expected to dominate as primary emissions are reduced. As characterisation and toxicology of secondary aerosols is limited there is a need to study chemical changes to inform chemical transport models and evaluate their health effects.

2. Hypothesis and Aims

The oxidation of primary aerosols will lead to the formation of secondary organic aerosols (SOA) with distinct physicochemical properties and an increased oxidative potential and therefore greater hazard.

1. **Establish a protocol** for the generation and quantification of secondary and aged primary aerosols from real-world sources
2. Record the **physicochemical properties** of SOA
3. Evaluate the **acellular oxidative potential** and **in vitro toxicity** of aged aerosols in epithelial and macrophage cells.

3. Ageing and Toxicity

- Biomass burning and diesel emissions contribute significantly to urban aerosol and cooking emissions supply over half of indoor aerosol.[1,2]
- The physicochemical properties of anthropogenic aerosol emissions are altered by chemical ageing, primarily due to oxidation by OH radicals. This can produce various radicals and redox active species.
- Respirable aerosols can penetrate deep into the lung and cause toxic effects when they interact with epithelial and airway macrophage cells.

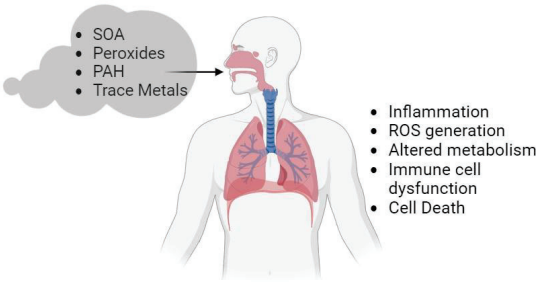

Figure 1: The Toxic effects of aerosols during ageing. Image was created on BioRender

4. Oxidation Flow Reactors

Oxidation Flow Reactors (OFRs) can simulate chemical ageing . A new commercial OFR developed by the Tampere University of Technology, Finland based on the design in figure 2 and produced by Dekati:

- Is **portable** and offers **short residence times** (<100s)[3]
- Is characterized by laminar flow resulting in **lower particle losses** compared to other ageing methods
- Is a widely available piece of equipment to generate SOA

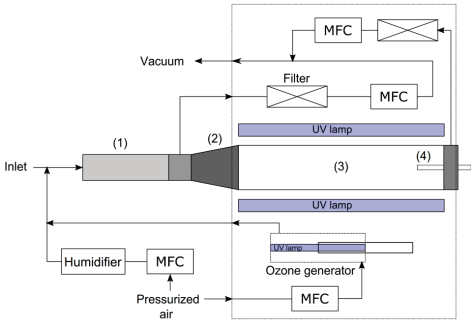

Figure 2: Design of a TSAR (TUT secondary aerosol reactor). Composed of (1) the residence time chamber, (2) the expansion tube, (3) the oxidation reactor and (4) the adjustable outlet. (3) and (4) are contained in a single housing.[3]

5. Methodology

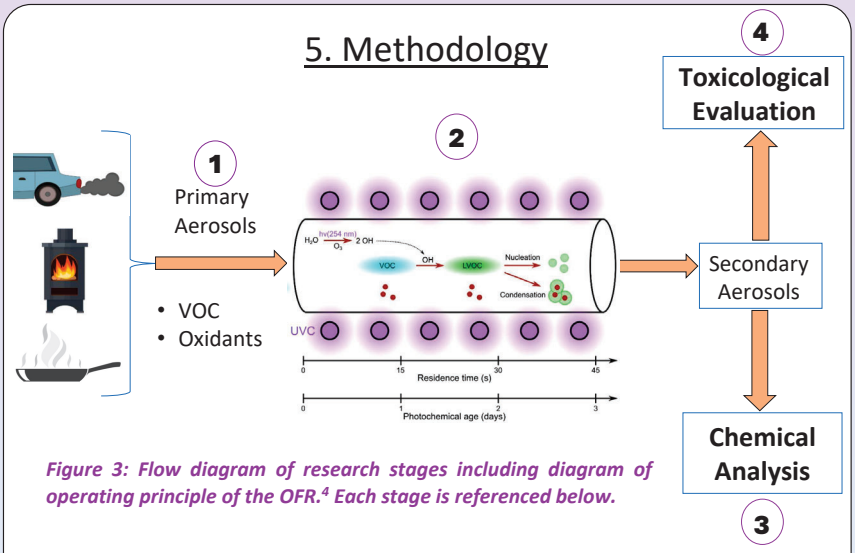

Figure 3: Flow diagram of research stages including diagram of operating principle of the OFR.[4] Each stage is referenced below.

Project is split into 4 steps to be repeated for each real-world source (wood burning, Euro 6 diesel engine, cooking emissions)

1. Generate and characterise primary emissions from the sources under relevant conditions to **establish a baseline** before ageing.

2. Optimise the **Dekati OFR** to be most representative of regional atmospheric ageing

3. Chemical analysis will involve the use of an **AMS** and **FIGAERO-CIMS** for chemical composition and volatility sets, **ICP-MS** to study the metal content, **FTIR** to identify organic functional groups of the bulk aerosol and **TSI SMPS** for aerosol counting and size distribution.

4. Oxidative potential will be determined in acellular models using the **DTT assay** and **synthetic respiratory tract lining fluid model.**[5] This is followed by an investigation into epithelial cell and airway macrophages with a focus on **cellular oxidative stress**, **inflammation** and **cell death**.

6. Policy and Scientific Innovation

- Use of OFR in standard emissions tests may result in new regulations and add to the body of evidence motivating induction of low emission zones (**LEZ**).
- An established protocol for the generation of SOA from real world sources using the OFR provides reproducible and reliable measurements when studying SOA.

7. Challenges

- May be issues with consistency of aerosol emissions
- Challenges with SOA capture - investigate the use of direct impingement onto tissue culture media vs. gas phase exposure in air lung interface.

8. References

1. Wang, G., et al., *Transport. Res. Transport Environ* 2009, 14 (3), 168-179
2. Klein, F., et al., *Indoor Air* 2019, 29 (6), 926-942
3. Simonen, P., et al., *Atmos. Meas. Tech.* 2017, 10 (4), 1519-1537
4. Dekati Ltd., DOFR™ User Manual 1.0, 2022
5. Ayres, J., et al., *Inhal. Toxicol.* 2008, 20 (1), 75-99

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Early Life Air Pollution Exposure and its Lasting Effects on the Lung

Armin Omidvar

UK Health Security Agency

Background

- Asthma attacks kill three people in the UK each day.
- Exposure to pollutants can induce asthma symptoms, exacerbations and decreases in lung function.
- Exposure to particulate matter (PM) during pregnancy can increase the risk of developing asthma.
- Lung epithelial cells and alveolar macrophages work together and remove inhaled PM.

Hypothesis

- Early life exposure to PM causes innate immune memory and contributes to asthma.

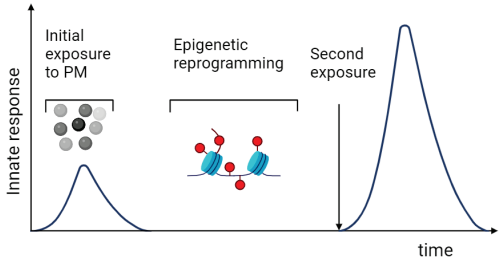
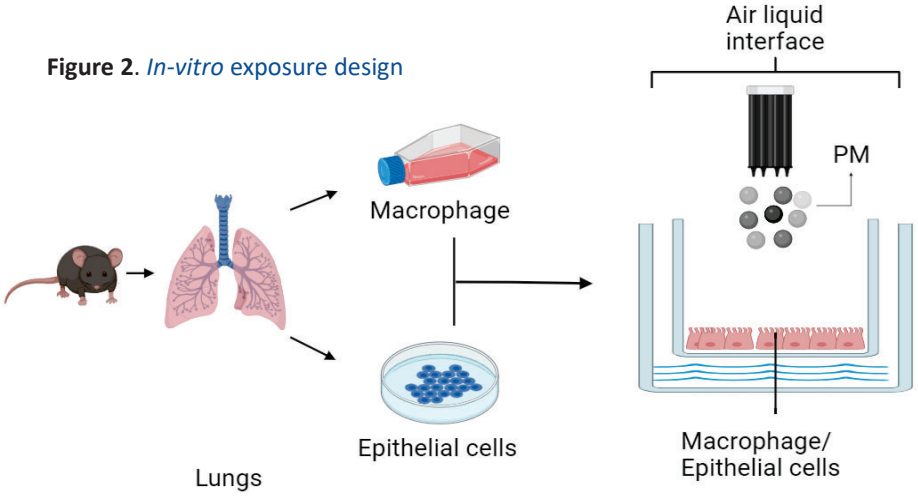


Figure 1. Trained immunity

Objectives

- **Objective 1**. To use particle sizing instruments for determining the particle size distribution in a liquid sample.
- **Objective 2**. To assess epithelial and macrophage *in-vitro* responses to primary and secondary stimulation with PM.
- **Objective 3.** To examine early life *in-vivo* responses to aerosol pollutant particles within the lung.

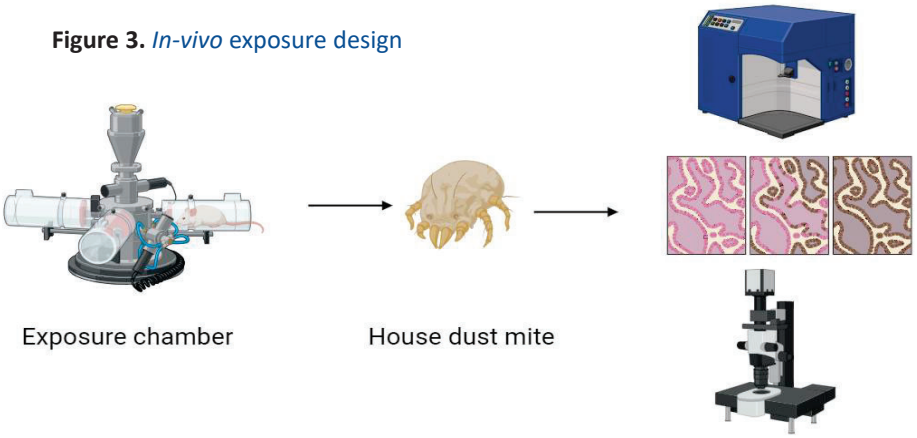
Figure 2. *In-vitro* exposure design



Objective 2

- The cells will be exposed to house dust mite (HDM) to induce asthma.
- The inflammatory cytokines produced will be checked using ELISA and QPCR.
- Epigenetic changes in cells will be analysed using ATAC sequencing.

Figure 3. *In-vivo* exposure design



Objective 3

- Neonatal mice will be exposed to PMs.
- Mice will be exposed to allergens such as HDM or extract of fungal products to induce asthma.
- Lung immune and epithelial cells will be isolated and analysed using flow cytometry, immunostaining, and microscopy.

Responsible innovation and policy

- Potential to lead to more evidence-informed public health guidelines and more effective prevention strategies against air pollution in relation to childhood asthma
- Adhesion to the Animal Rights Act of 1986, with Home Office project and personal licenses.
- Application of the 3Rs principle (Replace, Reduce, Refine) for animal research.

References

Materials & Aerosol

Field Effected Aerosol Assisted Chemical Vapour Deposition (FE-AACVD) of Thin Film Materials

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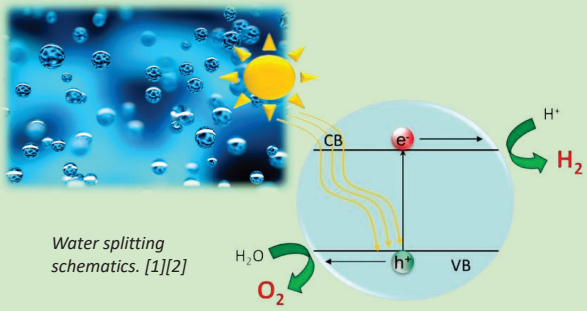
UNIVERSITY OF BATH



Water splitting schematics. [1][2]

1) Thin Films for Water Splitting

Photocatalytic water splitting aims to sustainably produce hydrogen, a fossil fuel alternative, from water and sunlight. Thin film semiconductors facilitate this via redox catalysis. Surface morphology and crystallinity of thin film materials can be tuned to increase their efficacy, stability and absorption range.

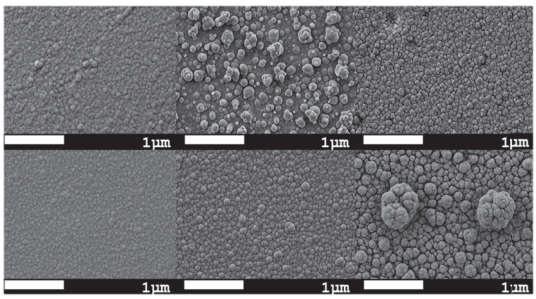
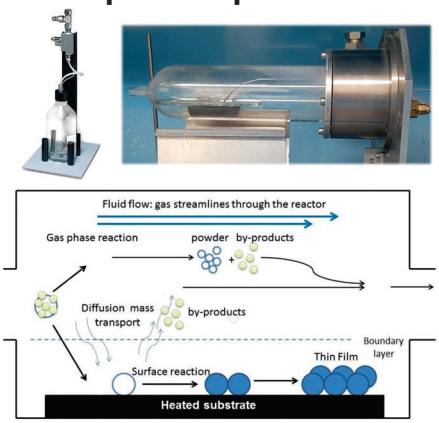


Figure 1: Scanning electron microscope images of tantalum oxide thin films, showing their differing degrees of crystallinity.

2) Aerosol Assisted Chemical Vapour Deposition

- Precursor solutions are aerosolised and transported to the reaction chamber
- Precursor aerosols deposit on the hot substrate and react
- Decomposition and evaporation of side groups generates a thin crystalline film of inorganic materials



Figures 2, 3 and 4: A TSI 3076 aerosol generator, and schematics of an AACVD reaction chamber. [3][4]

3) Chemical Precursors

- Need the correct elements to make the target thin film. No need for volatility but solubility is important
- Single source precursors are used to guarantee homogeneous films

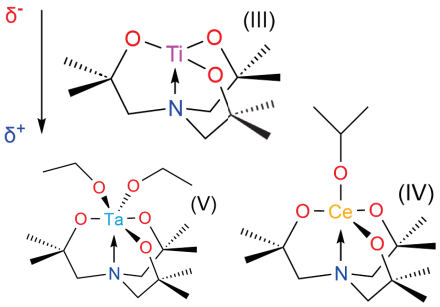
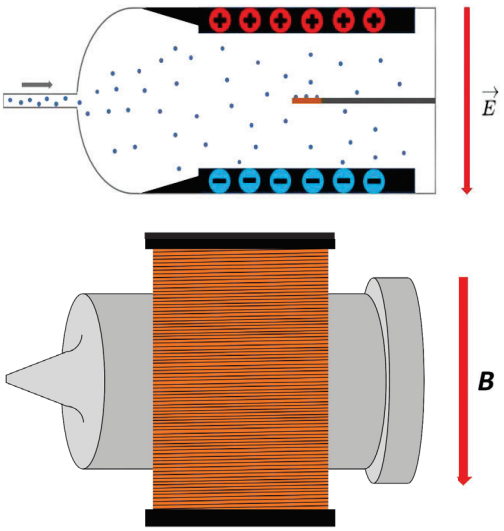


Figure 5: Examples of single source AACVD precursors possessing synergy with applied fields.

4) Directing Effects of Electric and Magnetic Fields

- Aerosols are affected by fields during transport and thin film synthesis
- Electric fields can direct charges and align dipoles on deposition
- Magnetic fields can direct paramagnetic species on deposition
- Crystallinity can be increased, and magnetic domains can be ordered



Figures 6 and 7: Example AACVD schematics configured to use electric field direction and magnetic field direction.

5) Challenges and Future Work

The work is among the first studies of electric field AACVD, and there is no literature precedent for magnetic field AACVD. The introduction of further variables to an already complex process means care must be taken to ensure both repeatability and reliability.

Two or more thin film layers are often needed for effective water splitting and research will be undertaken into stacking these. A corona discharge source will also be investigated to further alter aerosol properties and increase deposition efficiency.

[1] J. Zhang, C. Mück-Lichtenfeld and A. Studer, *Nature*, 2023, **619**, 506–513 [2] R. Marschall, *Eur J Inorg Chem*, 2021, **2021**, 2435–2441 . [3] TSI Instruments Ltd.
[4] L. Romero, PhD thesis, Queen Mary University of London, 2013.

Responsive Aerosol: A Design Framework for Aerosol with Required Properties

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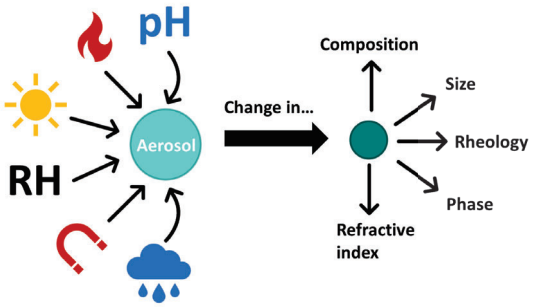
Prof. Jonathan Reid

University of BRISTOL

1. Background

Responsive aerosol

- Aerosols are responsive by nature, which provides an opportunity to design aerosol to have a desired response to a specified stimuli:



- Initially hydrogels are being used as the test system to explore aerosol with responsive properties.
- Hydrogels are three-dimensional polymeric networks that have hydrophilic groups attached to the polymeric backbone and can therefore swell to retain large amounts of water.
- Poly(N-isopropylacrylamide) (**pNIPAM**) and **Poloxamer-407**, both thermoresponsive hydrogels (Fig. 1), have been studied in the bulk phase and as single droplets.
- Both polymers exhibit a measurable response to temperature, moving from a solution to gel state as temperature is increased (Fig. 1).

Hydrogels

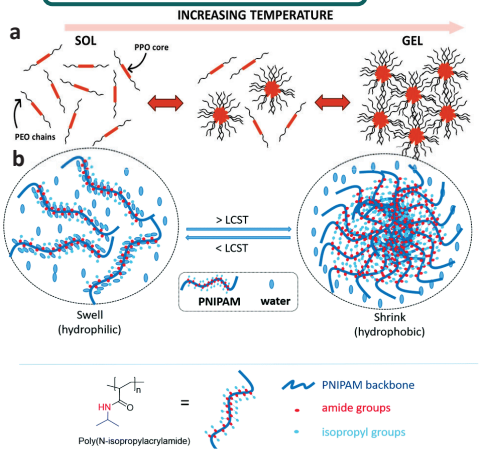


Figure 1—a) Solution to gel transition of P-407 b) Swollen and collapsed state of pNIPAM below and above the lower critical solution temperature (LCST). Figure taken from Doberenz et al.

2. Motivation

The ability to design an aerosol to have a required response to its environment has potential applications in many areas. For example, the aerosol could be used to report on changes in temperature, pH, or RH in the environment, and they could also be designed for controlled release of an API in aerosol drug delivery.

3. Aims

Characterise changes in an aerosol's properties in response to an external stimulus using two hydrogel systems.

Build a framework to allow the design of aerosol that have a desired response to stimuli.

Create a model to understand how changes in the environment can be detected from the corresponding change in size and rheology of the aerosol and to allow a prediction of one from the other.

4. Research Methodology

BULK PHASE:

- **A rheometer was used** to measure viscoelastic properties and a **bubble pressure tensiometer** was used to measure dynamic surface tension.

DROPLET PHASE:

Comparative-kinetic electrodynamic balance will be used to measure the size change of the droplets with respect to temperature and RH.

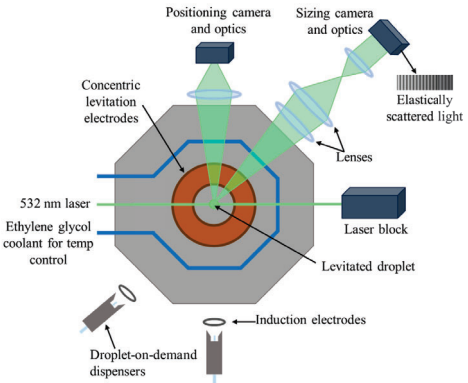
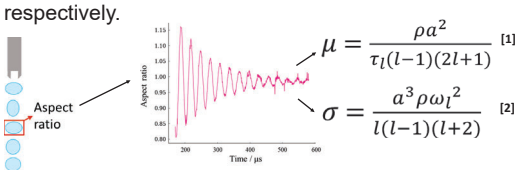


Figure 2—A schematic representation of a CK-EDB from a view looking down into the instrument.

Stroboscopic Imaging used to determine the surface tension and viscosity of the droplets phase from the droplet oscillation frequency and decay, respectively.



Equation 1 and 2– Viscosity and surface tension of the oscillating droplet, respectively, expressed in terms of the droplet radius, a, the fluids density, ρ, the decay time of the amplitude of the lth mode, τ_l, and the angular oscillation frequency of the lth mode, ω_l.

5. Results

Poloxamer-407 properties:

	Bulk		Droplet
Conc / wt%	σ_0 / mN m^{-1}	σ_{eqm} / mN m^{-1}	σ_0 / mN m^{-1}
0.5	61.1	42.5	61.4
1.0	60.1	41.0	60.5
1.5	59.4	40.6	59.2
2.0	59.1	40.1	59.3
2.5	58.1	39.3	58.5

Table 1—Surface tensions of Poloxamer-407 in bulk and droplet phase.

Bulk rheology studies:

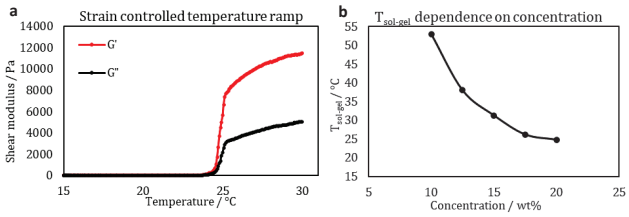


Figure 3- a) Example of a sol-gel transition of 20 wt% Poloxamer 407 exhibited by the extreme increase in storage and loss moduli. G' is the storage modulus (elastic component), and G" is the loss modulus (viscous component). In this case the sol-gel transition temperature is 24.5 °C. b) Sol-gel transition temperature of poloxamer 407 as a function of concentration. Each data point was found by plotting a strain controlled temperature ramp at varying concentrations.

Single droplet studies:

Temperature ramp on levitated droplets of poloxamer 407 and pNIPAM using the CK-EDB:

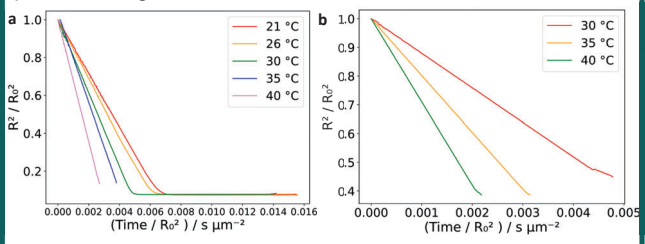


Figure 4—Normalised evaporation curves at different temperatures measured using the CK-EDB. a) 2.5 wt% Poloxamer 407 b) 0.2 wt% pNIPAM

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Measurements and Models

Development of a Novel Single Droplet Mass Spectrometry Approach to Investigate Interfacial Photochemistry in Aerosol Droplets

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University of BRISTOL

Supervisors:
Dr Bryan Bzdek
Dr Jim Walker

Sea spray aerosol; effects and composition

- Large uncertainties in cloud-aerosol interactions on radiative forcing in our atmosphere presents a need for an improved understanding of aerosol effects
- Around 70% of the earths surface is covered by ocean which produces 2000-10000 Tg/yr of sea spray aerosol (SSA) [1]
- 5-15 Tg/yr of organic material is contained within this SSA[1]
- Two-thirds of the fatty acid content of SSA is palmitic acid and steric acid [2]

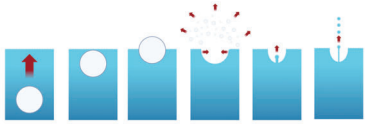


Figure 1. Mechanism for SSA generation

Why do we need this instrument?

1. These surface-active organics can have surface tension lowering effects, altering activation of SSA which can act as cloud condensation nuclei (CCN) [3]
2. Surfactants at the surface can undergo important, but understudied accelerated photochemical reactions at the interface when compared to the bulk [4]
3. Reactions with photosensitizers and light along with gases in the atmosphere including ozone cause breakdown of organics like palmitic acid into a range of products with differing properties[5]
4. The breakdown can affect many properties of SSA including lifetime, activation and optical properties

What sort of instrument is needed?

To probe these reactions an instrument that can isolate the surface and identify the constituent molecules is needed

Mass spectrometry – provides high resolution approach to detect small concentrations of organic molecules

Field induced droplet ionisation (FIDI) – Single droplet atmospheric ionisation approach that samples the surface of droplets via a very large electric field.

1. Perform FIDI on falling droplets

- The first step of the instrumental development process is to perform FIDI on free falling droplets
- Using larger droplets, ~200µm in diameter, with reduced surface tension (<40 mN/m) will be good candidates for the first attempts
- This phase of development is completed once droplets closer to 80µm in diameter have been reached.
- Going smaller requires more control over the droplet.

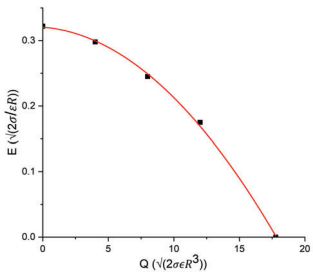
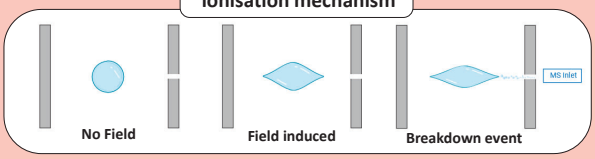
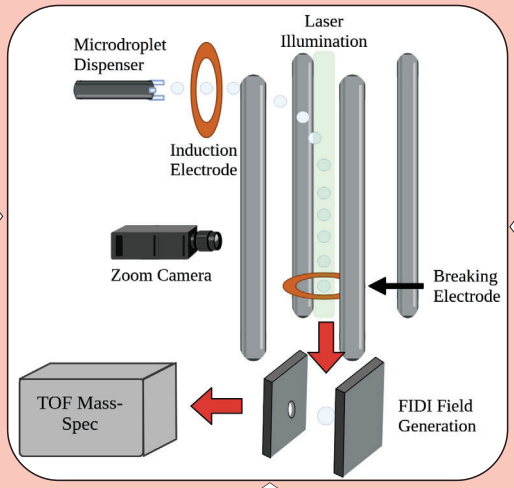


Figure 2. The field strength required to ionize the droplets can be calculated if a few characteristic parameters are known; Surface tension at the droplet interface, radius of droplet, amount of charge on the droplet [6]

Field-induced droplet ionisation mechanism





2. Couple FIDI with linear quadrupole

- The second phase consists of coupling the FIDI source to a linear quadrupole electrodynamic balance (LQ-EDB) to control the dispensed droplets
- This will allow the charged droplets to be trapped and released into the FIDI source when required
- During trapping the droplets can be evaporated to consolidate charge and move to smaller sizes, also allowing photochemical reactions to be performed

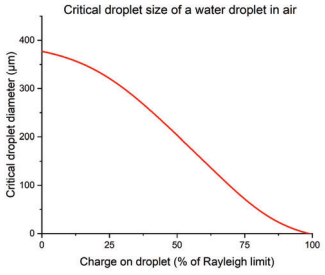
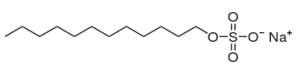


Figure 3. By increasing the amount of charge on the droplets relative to their Rayleigh limit smaller diameters can be ionized.

3. Test the surface selectivity of the instrument

- It has been demonstrated numerous times that FIDI is surface selective, but it is important to verify this for the smaller droplets being studied here [7, 8]
- This could be achieved by varying the ratio of two surfactants that are competing for the surface of the droplet and comparing MS spectra for the droplet bulk and the surface



Sodium dodecyl sulfate (SDS) – A well studied surfactant that is a strong candidate for testing surface selectivity

4. Perform experiments using the FIDI-MS instrument

Photosensitized reactions of lipids like POPC have been previously studied via FIDI-MS with great success but on much bigger droplets, 2mm. This reaction would be simple to execute and valuable to confirm the oxidation mechanisms on smaller droplets [9]

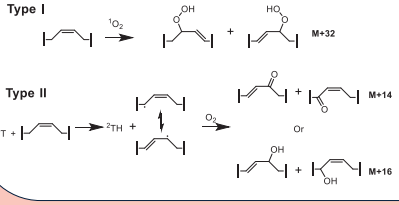


Figure 4. (Left) Photochemical oxidation of POPC with photosensitiser temoporfin

Moving forward the photosensitized reaction of palmitic acid would be a great choice for study due to its atmospheric relevance along with it being unstudied in the droplet environment [5]

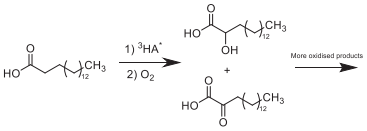


Figure 5. (Above) Photosensitized reaction of palmitic acid in the presence of humic acid

In the future this instrument my have scope to influence a wide range of fields including:

1. Drug encapsulation – Providing vital information on the composition of the interfaces of droplets containing drug molecules
2. Nano particle synthesis – Where droplet surface composition plays a large role in the dried materials shape, structure and composition
3. Synthesis chemistry – Where droplets act a micro reactors, accelerating reaction rates (by orders of magnitudes sometimes) compared to macroscopic solutions [4]

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9. C. Mu, *et al*, Angew Chem Int Ed, 2020, 59

HYDRA – Hydrogels for Aerosol Capture

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Supervised by Dr Michael Cook, Dr Loïc Coudron and Prof. Ian Johnston

Engineering and Physical Sciences Research Council

University of Hertfordshire UH

1. Motivation

- Airborne pathogens are a major issue for animal and plant survival and flourishment.[1] [2]
- Hence, we need more sensitive, autonomous and integrated collection and detection methods.
- Electrostatic Precipitator (ESP) aerosol samplers meet the needs given above, but sometimes suffer from low collection efficiencies.[3]

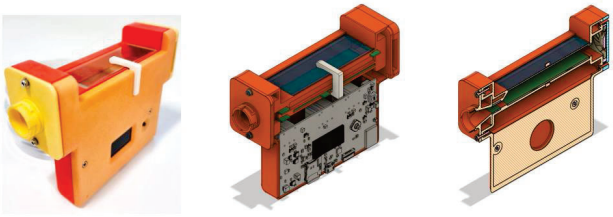

Figure 1: A portable electrostatic precipitator aerosol sampler in development at The University of Hertfordshire

2. Hypothesis

Inspired by the ability of mucus to capture and sustain some airborne pathogens,[4] this project aims to quantifiably test the hypothesis that hydrogels can be applied to develop a novel collection plate for an ESP to:

1. Enhance their collection efficiency.
2. Better protect the sample from factors that would result in pathogen death, such as osmotic shock.

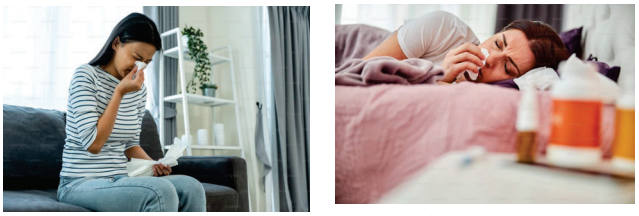

Figure 2: Public domain images of persons suffering from excessive mucus production.

3. Objectives

1. To synthesize a library of acrylate- and methacrylate-based hydrogels (figure 3, left) that is diverse with regards to conductivity, charge and acidity.
2. To evaluate the ability of these hydrogels to capture aerosols and identify the properties that result in optimal capture.
3. To develop a library of sustainable hydrogels (e.g. saccharide-based hydrogels – figure 3, right) that are optimised for aerosol capture.
4. To develop and evaluate an ESP incorporating a sustainable hydrogel collection plate (figure 4).

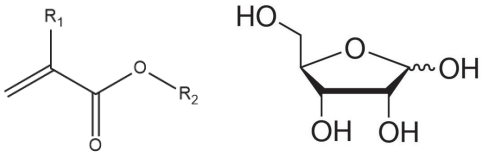

Figure 3: Chemical structure of acrylate (left, R_1 = H, R_2 = sidegroup), methacrylate (left, R_1 = Me, R_2 = sidegroup), and saccharide (right) monomers.

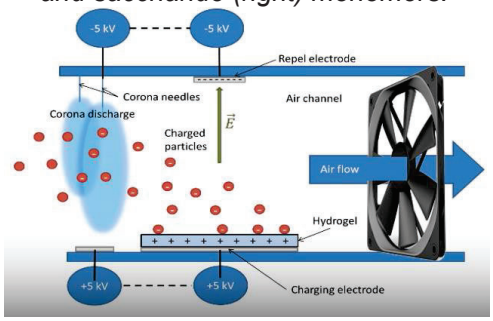

Figure 4: Proposed structure of portable electrostatic precipitator aerosol sampler incorporating a novel hydrogel collection plate.

4. Methods

This project aims to develop novel aerosol capture materials through use of the following main experimental techniques:

1. Synthesis
   a) Photo-initiated free radical polymerisation.
2. Characterisation
   a) Infrared Spectroscopy.
   b) Solid-state Nuclear Magnetic Resonance spectroscopy.
   c) Oscillatory rheology.
   d) Pycnometry.
   e) Volumetric analysis.
3. Evaluation of Aerosol Capture Efficiency
   a) Fluorescent microscopy.
   b) Solid-state Nuclear Magnetic Resonance spectroscopy.

5. Challenges

1. Determining the best method to evaluate aerosol capture given that microscopy of aerosol within a hydrogel substrate may be difficult.
2. Determining the optimal conditions inside the adapted ESP given that the high electrical current (10 kV) and flow rate (10 L/min) may have ramifications for hydrogel state and hydration, respectively.

6. References

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Improving aerosol and spray process computational fluid dynamics models with machine learning approaches

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Engineering and Physical Sciences Research Council

Background

Spray drying is a technique for transforming atomized slurries or solutions into powders. This process is behind commonly used products such as: **pharmaceuticals, milk powder, detergent powder, …**

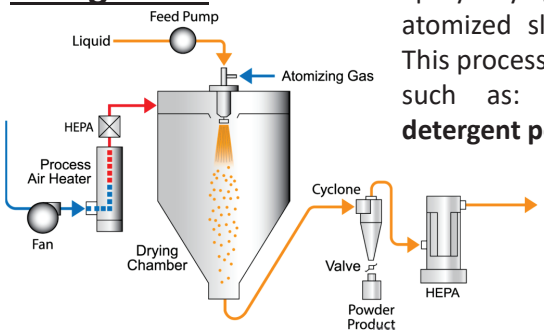


Figure 1: A schematic diagram of the spray dryer [1]

The drying process is complex

The characteristics of the powders produced, for example, density and porosity, **are significantly influenced by a range of factors**, including the diameter of the spray drying chamber, air temperature, air mass flow rate, and feed temperature.

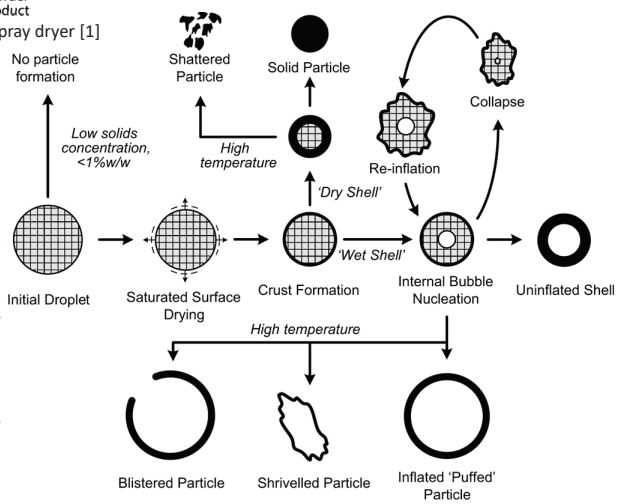


Figure 2: Different particle morphology determined by its drying history [2]

Statement of Problem

Computational fluid dynamics (CFD) models provides detailed information for identifying the optimal operating variables.

However, the drying models used in the CFD models are semi-empirical. This means they fall short of capturing the actual behaviours of droplets and the impact of drying history on particle characteristics.

Objectives

Speed-up of single droplet drying models

↓

Inclusion of more complex phase change physics

↓

Coupling of more complex single-particle drying models into spray dryer CFD models

Methodology

Physics-Informed Neural Networks

The learning process is to **minimize loss function** L

$$L = MSE_u + MSE_f$$

$$MSE_u = \frac{1}{N_u}\sum_{i=1}^{N_u}\left|\hat{u}^i - u(x_u^i, t_u^i)\right|^2$$

$$MSE_f = \frac{1}{N_f}\sum_{i=1}^{N_f}\left|f(x_f^i, t_f^i)\right|^2 \quad \textbf{PDE}$$

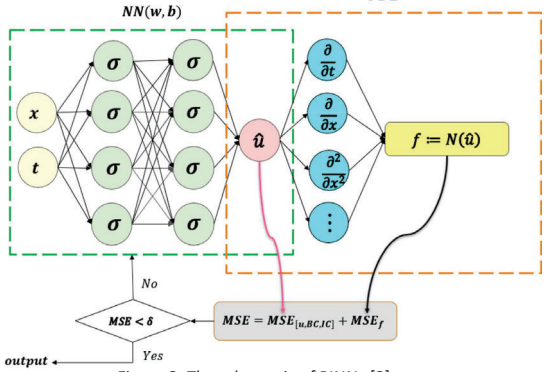
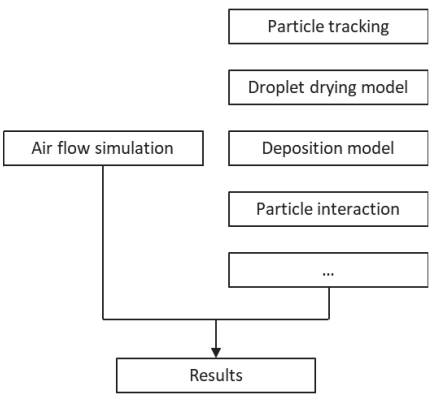


Figure 3: The schematic of PINNs [3]

Computational Fluid Dynamics

CFD model of spray drying



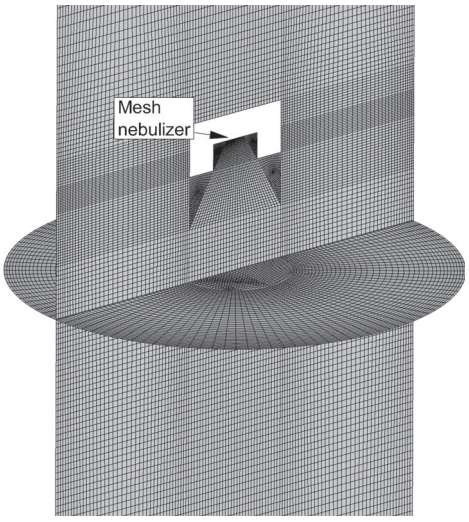


Figure 4: Hexahedral mesh of a spray dryer [4]

Eulerian-Lagrangian framework is employed in air flow simulations.

Eulerian approach calculates the continuous phase utilizing the Reynolds-averaged continuity equation and Navier Stokes equations.

Lagrangian approach applies Newton's Law to determine particles trajectories and velocity profiles

Responsible Innovation

- Integration of advanced models into Computational Fluid Dynamics (CFD) models for spray drying, addressing prolonged computational times due to complex model integration.
- Enabling quicker access to detailed information for scientists and engineers, facilitating the design of superior spray dryers.
- Enhancement of the capability to produce specially engineered particles and troubleshoot operational problems.

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Technical quantitative monitoring, modelling and classification of different agri-bioaerosol emissions

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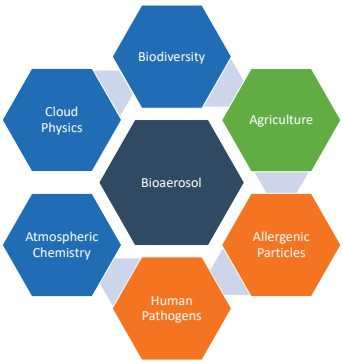
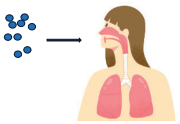
Bioaerosol Background

Bioaerosols, also known as primary biological aerosol particles (PBAP) Defined as suspended airborne particles that are emitted by living organisms. Contain diverse microorganisms such as pollen (10-100 μm), bacteria (0.2-10 μm), fungal spores (2-50 μm), viruses (< 0.2 μm), etc.
Through their extensive involvement in surface-atmosphere physic-chemical reactions affect the stability of the biosphere, climate change, and animal and human health.

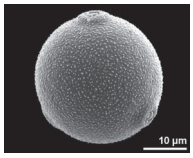


Research Motivations

Crops and different agricultural activities can be sources of Bioaerosols.



Pollen and other bioaerosols can be inhaled by human respiratory system, causing allergic reactions, etc.



Betula pollen SEM photo. From https://www.paldat.org/search/genus/Betula

Quantitative measurements of bioaerosol emissions can help farmers to set exposure standards and reduce the risk of hay fever. Also, monitoring bioaerosols for changes in distribution can guide land-use policies.

Challenges

Challenges in this experiment centred on methodological uncertainties, instrument construction and meteorological conditions:

- Low pollen and fungal spores concentration in the air >>> may not satisfy the resolution criteria for flux measurements.
- Varying atmospheric conditions, near-surface turbulence, etc., affecting data collection.
- Expensive detect sensors.

Aims

1. Determination of bioaerosol emission fluxes from agricultural crops using the Gradient-Flux and eddy-covariance methodology.
2. Measurement of the concentration of bioaerosols that may be generated during different agricultural activities as well as natural emissions during the growing seasonal.
3. Combining upon points, assessment of the accuracy of bioaerosol emissions will be conducted based on different meteorological case studies using the collected data.

Flux Calculation Theory

Aerosol flux measurements consist of two main methods, the Flux-Gradient measurement and Eddy Covariance measurement.

Flux-Gradient technique is a bottom-up measurement. Two aerosol monitoring instruments are fixed at two different heights. Equations below:

$$F = -K\frac{\Delta C}{\Delta z}$$

$$\begin{cases} \left(1-15\frac{z}{L}\right)^{-0.5} & L<0 \\ \left(1+5\frac{z}{L}\right) & L>0 \end{cases}$$

$$K=\frac{\kappa Z_m u_*}{\emptyset}$$

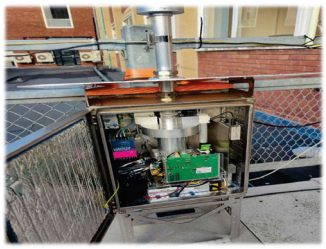
$$L=-\frac{{u_*}^3\,\overline{T}}{\kappa g\overline{w'T'}}$$

The eddy-covariance method is the direct way to measure the turbulent fluxes of momentum, temperature, trace gases, and particles between the land surface and the atmosphere.

$$F_x=\overline{w'c'}$$

By combining 3D sonic anemometers and pollen detect sensor, can calculate F_x through tools such as software EddyPro, Version7.

Instruments



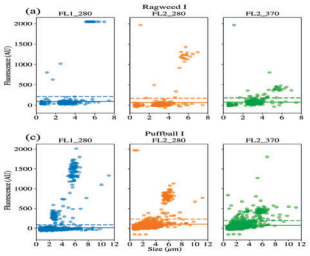
Swisens Poleno: Real time, speciated pollen concentration measurements. Using UV-LIF and holography camera to classification pollen species.

DMT WIBS-NEO: real-time, single particle measurement.
UV-LIF technology.

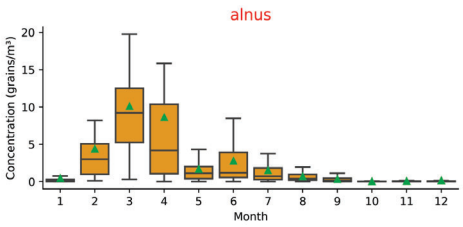
Plair Rapid-E+: Real time, single particle measurement.
Sigma-2 inlet; UV-LIF technology; GPU acceleration.

Research Innovations

For aerosol measurement fields, the real-time, high-temporal-resolution device allows capture of aerosol release processes in shorter time intervals. Bioaerosol identification of single particles is possible with UV-LIF technology(analysis of fluorescence spectra of bioaerosols). It can provide insights into previously poorly understood phenomena, such as wind–stamen interactions and the forces delivering pollen grains into airflows including rainfall events that generate sub PM2.5 pollen fragments and enhance certain fungal spore emissions.



An example of bioaerosols fluorescence response under different wavelengths.



After capture pollen emission we can draw plots like this to predict pollen seasons and provide guidance for farmers and other allergic group.

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Radioactive Aerosols in Wall-Bounded Turbulent Flow

Gregory Marsden, Dep. of Engineering, University of Bristol, Bristol, UK

What Are Radioactive Aerosols?

Sources of Radioactive Aerosols[1,2]

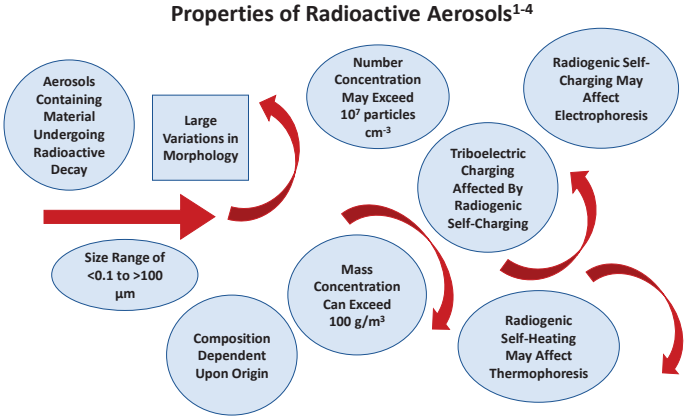
Laser Cutting & Ablation

Accidents & Incidents

Droplet Dispersion

Resuspension of Irradiated Material

Properties of Radioactive Aerosols[1-4]



Wall-Bounded Turbulent Flow[1-4]

Wall-bounded turbulent flow is characterised by **chaotic motion** and the formation of **eddies** of many different length scales, and depends upon the ratio of **inertial** to **viscous forces**. It may be found in:

Pipe Bends & Corners

Merging or Diverging Pipes

Narrowing or Expanding Pipes

Why Study Radioactive Aerosols?

'Evaluating the fate of these particles after their emission is one of the… key issues for these dismantling operations'

Dr. Thomas Gelain, Institut De Radioprotection Et De Sûreté Nucléaire (IRSN)[5]

Modelling is full of **assumptions** such as: spherical particles; absence of collision and coalescence mechanics; and the absence of electric fields. Consolidating, cataloguing, and combining data and techniques from various industries and disciplines may lead to a **new understanding** of the **microphysics** of radioactive aerosols in wall-bounded turbulent flow, and allow for **new large-scale correlations** to be discovered.

Reducing the **inherent risks** of nuclear decommissioning activities by allowing safe exposure times, distances, and appropriate levels of shielding to be **predicted**.

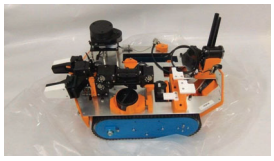


Fig. 1. In April 2022, the robot Lyra completed a survey of a 140m long radioactive ventilation duct below a disused laboratory at the Dounreay nuclear complex[6].

Assisting the use of **robotic** and **AI technologies** to solve challenges faced by the nuclear industry; for example, **identifying** radioactive **'hot spots'** where human access may be impossible.

How To Study Radioactive Aerosols?

Objectives

1. Create a **small-scale Lagrangian model** of the transport, deposition mechanics, and coupled physics of individual radioactive particles in wall-bounded turbulent flow.
2. Create a **large-scale Eulerian mode**l of the transport and deposition mechanics of a concentration of radioactive particles undergoing wall-bounded turbulent flow.
3. Apply **reduced order modelling** to the large-scale Eulerian model to decrease its' computational cost.
4. Validate approaches used to **reduce computational cost** across the stages of the project as modelling takes place.

Methodology

Computational Fluid Dynamics[1]

Computational Fluid Dynamics (CFD) provides a **virtual laboratory** in which problems involving fluid flows (e.g. aerosols transported through air) are solved using **numerical analysis** and **data structures.**

Lagrangian Modelling[1]

In the Lagrangian approach, the equations of motion of each individual particle are solved by the addition of all of the forces acting upon the particle, according to Newton's 2nd Law, $\sum \boldsymbol{F} = m\frac{d\boldsymbol{u}}{dt}$.

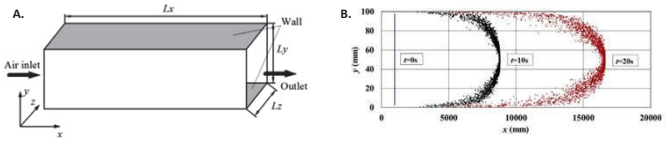


Fig.2. Adapted from Gu *et al.* A. An example of a computational domain used to model wall-bounded turbulent flow. B. The simulated distribution of particles in the x-y plane at t=0, 10, and 20s respectively[3].

Methodology (Cont.)

Eulerian Modelling[1]

In the Eulerian approach, the particulate mass conservation equation is solved, as opposed to solving equations of motion for individual particles. This can be expressed as the Aerosol General Dynamic Equation (ADGE).

The Aerosol General Dynamic Equation[1]

The aerosol general dynamic equation describes the conservation of particulate mass and is given by

$$I\left\{\begin{matrix}\text{Rate of}\\ \text{Change in d}V\end{matrix}\right\} = II\left\{\begin{matrix}\text{Transfer of}\\ n_i \text{ into d}V\end{matrix}\right\} + III\left\{\begin{matrix}\text{Rate of}\\ \text{Generation in d}V\end{matrix}\right\},$$

where n_i is the concentration of all aerosol particle n of species i in volume dV.

Reduced Order Modelling[7-11]

By reducing the degrees of freedom found within the original model, we can reduce the computational complexity of mathematical models. In this way, an approximation to the original ('full-order') model is created.

Numerous approaches have been used in other fields of study, such as in the modelling of coal and of haemodynamics, which could be adapted to this context, such as using look up tables to store key values, employing structured-tree models, and director theory.

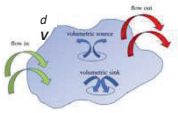


Fig.3. A schematic representation of a balance law in a volume dV [12].

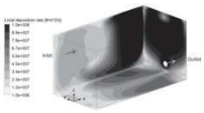


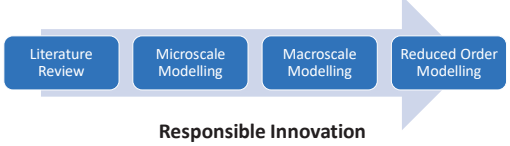
Fig.4. Adapted from Guichard and Belut. The computed local deposition rate of the CuO aerosol, given as an example of the desired use of CFD to identify the 'hot spots' of radioactive aerosol deposition[13].

How Will I Study Radioactive Aerosols?

Objectives

- The phenomena to be studied are of a **multi-scale** nature. The periods of time and dimensions of space to study within the remit of this project range from seconds to hours, and the size of models to be produced may vary from centimetres through metres to kilometres of pipe networks.
- Modelling the **wide range** of **morphologies** of radioactive aerosols and their **varying** size, volume, surface area, and mass **distributions** will prove challenging.
- Radioactive aerosols are often modelled as spheres of equivalent: surface area; volume; mass; or other parameters. Determining **which equivalent sphere** models have been **used** in comparing models to experimental evidence by whom, and **why**, will be a key outcome of the literature review.

Proposed Timeline of Research



Responsible Innovation

- The nuclear industry operates on long time scales; if the project is successful, the knowledge produced may be in use or development for decades.
- Unintended applications of radioactive aerosol modelling may be used to cause harm.
- Computational modelling of the cardiovascular system has been integrated into products for the clinical market. The feasibility and likelihood of this project leading to a commercial product or service is unknown at this stage of the project.

Desired Outcomes

Inform Pipe Network Design

Industrial-Academic Knowledge Transfer

Cardiovascular Modelling Crossover

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Digital Microfluidic Lab-on-a-chip for multiplex detection of biomarkers in Exhaled Breath Condensate

Daisy Ashton

Supervisors: Loic Coudron, Laura Urbano and Ian Johnston

Background

- Exhaled breath (EB) carries diagnostic biomarkers, which are biological indicators of infection and disease.
- Microfluidics is the science of miniscule volumes of fluid and its manipulation and the study of its behaviour.
- Digital Microfluidics (DMF) technology involves the manipulation of an ultra-small droplet on an array of microelectrodes.
- A lab-on-a-chip (LOC) device combines laboratory tests, such as blood analysis, ELISA assays and DNA amplification, all on a single miniature chip.
- Digital microfluidic multiplex LOC detection of lung disease biomarkers from EB can be carried out noninvasively and painlessly at point-of-care by the use of EB collection devices.

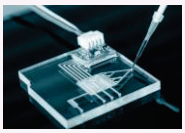

Figure 1: A digital microfluidic system (Berthier, 2018). Figure 2: A multiplex lab-on-a-chip device (Maxwell, 2016).

Motivation and Aim

- British Lung Foundation/Asthma UK states that 'lung diseases are responsible for more than 700,000 hospital admissions and over 6 million inpatient bed-days in the UK each year' and that 'somebody dies from lung disease in the UK every 5 minutes' (British Lung Foundation, 2017).
- 'It is thought that approximately 10% of the population have a needle phobia' (NHS Foundation Trust University Hospital Southampton, 2018). Therefore more non-invasive testing and diagnostic devices are necessary.
- At the end of this project, the goal is to have developed a fully automated multiplexed DMF system with bioprinted detection sites that can detect lung disease biomarkers at a low cost and at point-of-care. Beyond contributing to the progress of DMF technology in diagnostics, the project's results hold the potential for broader applications in fields such as agriculture and air quality monitoring.

Objectives

1. Biomarker selection
2. Selecting the most appropriate ink composition
3. Finding suitable geometric structures for separation sites on employing total extraction DMF approach
4. Selecting appropriate immunoassays for separation and detection
5. Creating artificial exhaled breath condensate

1. Biomarker selection

Table 1- Expected concentrations of chosen disease biomarkers

	8-isoprostane	IL-6	LB4
Control	7-64.23 pg/ml	1.5-5.1 pg/ml	7.9-53.6 pg/ml
Asthma	30.9-54.1 pg/ml	7.1 ± 1.1 pg/ml	88.9 ± 10.9 pg/ml
Chronic obstructive pulmonary disease	40 ± 3.1 pg/ml	8.0 ± 0.1 pg/ml	73.5-170.5 pg/ml
Cystic fibrosis	42.7 pg/ml	8.7 ± 0.4 pg/ml	N/A
Non-small cell lung cancer	N/A	9.3-11.4 pg/ml	24.2-61.5 pg/ml

2. Selecting the most appropriate ink

- To create the individual biosensing structures, a combination of printing methods including inkjet printing and extrusion 3D-bioprinting will be investigated.
- Inks will be initially selected based on their mechanical and rheological properties, wettability, printability, and of course their known compatibility with antibodies.
- The investigation will then consider two different avenues for functionalisation of the printed structure: (a) embedding antibodies within the ink itself or (b) using a post-functionalisation step of the pre-printed structure.
- Inks currently being investigated include: SU8, Mebiol and Gelatin Photogel.

3. Finding suitable geometric structures

- Inks can be printed in many different shapes and designs such as a pillar, a scaffold, a droplet shape, or simply a standard 2D spot.
- The geometry of the structure will affect its functionality, trapping and cleaning efficiencies.
- Fundamentally, the droplet must be able to detach from the structure. It is anticipated that droplet detachment will be correlated with the structure-to-electrode size ratio (area occupied by the structure footprint compared to the area of the electrode on the EWOD plate.
- Geometries will be coded using G-Code.

Figure 3: Geometries made using Tinkercad: (a) scaffold, (b) pillar, (c) droplet.

5. Selecting appropriate immunoassays

Table 2 - Standard assays for chosen biomarkers, their detection assays and specificities.

Biomarker	Standard Assay	Detection method	Sensitivity	Range
8-isoprostane	ELISA	Colorimetric	1 pg/ml	0.005 ng/ml – 5 ng/ml
IL-6	ELISA	Colorimetric	< 2 pg/ml	6.25 pg/ml – 200pg/ml
LB4	ELISA	Colorimetric	5.63 pg/ml	11.7 pg/ml – 3000 pg/ml

4. Creating artificial exhaled breath condensate

- Exhaled breath is composed of approximately 78% nitrogen, 16% oxygen, 4% carbon dioxide and 0.09% noble gases such as Argon, while the rest is made up of water vapour and over 3500 volatile organic compounds (Johnson, 2018).
- Would comprise of realistic ratios of the main components of exhaled breath in liquid form, salts, a buffer to ensure the stability of pH alongside, reported contaminants that are found in EBC samples and the chosen biomarkers.
- The components of the artificial exhaled breath will be mixed manually.

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IMPERIAL

Quantification of Microplastics in ambient air using Pyrolysis Gas Chromatography Mass Spectrometry (Py-GCMS)

Henry Blake, Email: HB1522@ic.ac.uk

Project supervisors:

Dr Stephanie Wright
Dr David Green
Nick Jones
Prof. Martin Gallagher
Prof. David Topping

1. Introduction

Airborne microplastics are particles of plastic >5mm that can be suspended in the air and have been detected in a range of environments from ~50n M^{-3} in mountaintops to ~9000n M^{-3} in urban apartment building. (Liao et al., 2021)
Historically airborne microplastics analyses have relied on visual identification and spectroscopy techniques such as Microscopy and Raman. However, these methods are generally: Slow, Difficult, Easily Biased, and Non-Quantitative, mainly producing particle counts instead of mass concentrations.

Pyrolysis 2-Dimensional Gas Chromatography Mass Spectrometry could help address some of these limitations. pyrolysis allows for the direct analysis of plastics by breaking polymers into smaller volatile marker compounds and providing a quantification of the actual polymer mass.
2-dimensional GC provides strong separation useful in complex mixtures like airborne particulate matter. (Milani et al., 2023)
An example case study using Py-GCMS to quantify PVC in $PM_{2.5}$ samples collected at an urban background site (Honour Oak Park, London) is provided here.

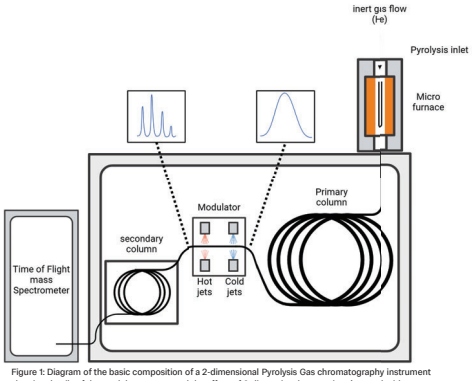

Figure 1: Diagram of the basic composition of a 2-dimensional Pyrolysis Gas chromatography instrument showing details of the modulator set-up and the effect of 2-dimensional separation. (created with Biorender)

2. Methods

Pyrolysis conditions:

Pyrolysis conditions	
Pyrolysis Temp.	650°C
GCxGC conditions	
1st column	HP5MS(Agilent), 30m x 0.25mm, 0.25um
2nd column	RXI17MS(RESTEK), 0.62m x 0.25mm, 0.25um
Oven temp.	50°C (2 min) → [10°C/min] → 250°C (0 min) → [20°C/min] → 300°C (15 min)
Inj. Temp.	300°C
Inj. Mode.	Split flow (50:1)
Carrier Gas	Helium
Column flow	1.4mL/min
Modulation period	3s
MS conditions	
Ionization	Emission current: 1.0mA Ion source temperature: 250°C Electron energy: 70.0eV Transferline heater Temperature: 300°C
m/z range	40 - 600

Table 1: Pyrolysis conditions used to analyse standards and samples gathered in this case study.

Samples were analysed by injection of 33.3% of collected filters in 4mm punches as detailed in Levermore et al's protocol (submitted). With a Thermal desorption (300°C) step prior to pyrolysis

Quantification was performed using an external calibration prepared from a commercially available 12 polymer standard mix.
The calibration standard was homogenised and diluted using a cryomill to improve reliability and lower the achievable calibration range to 165.47-1666.81ng.

3. Results

Three markers of PVC were compared for suitability (see Figure 2).

All three show strong linearity $R^2 \geq 0.98$.

Both Fluorene and Naphthalene show higher confidence intervals and worse linearity than Indene.

This suggests Indene is the most specific and stable marker. However, the factors influencing marker formation complicated and difficult to fully determine.

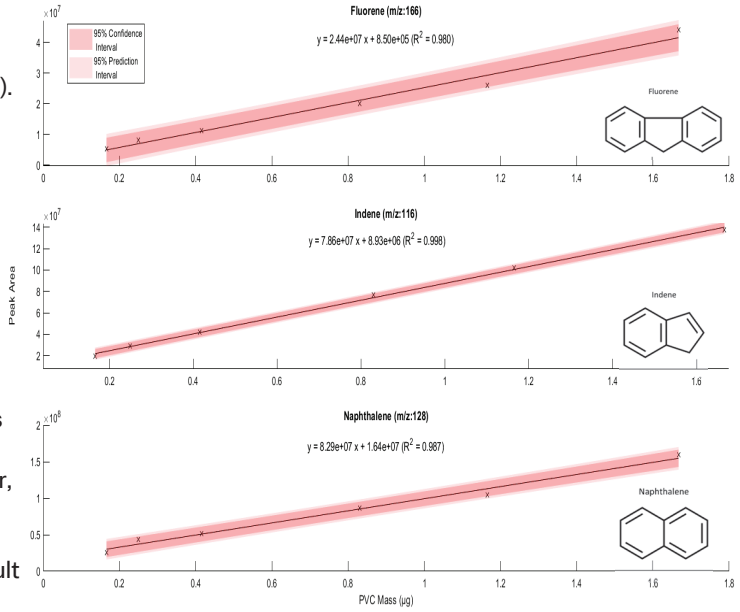

Figure 2: Averaged PVC calibration curves calculated from triplicate 6-point calibrations using the markers: Fluorene (m/z:166), Indene (m/z:116) and Naphthalene (m/z:128). Highlighted regions indicate 95% confidence (darker shading) and prediction (lighter shading) intervals.

Using Indene as a quantification marker masses of PVC were determined and used to calculate mass concentrations.

Sample	Measured PVC Mass (ng)	Calculated PVC Concentration (ng M^{-3})
Week 1 Wed	149.84	18.40
Week 1 Thur	410.11	50.35
Week 1 Fri	249.16	30.59
Week 2 Thur	171.90	21.10
Week 2 Fri	253.96	31.18

Table 2: concentrations of PVC calculated from masses measured in the $PM_{2.5}$ air fraction sampled at Honour Oak Park air quality monitoring site.

These are somewhat consistent with a recent study by Chen et al., 2024, which measured the concentration of PVC in $PM_{2.5}$ as being between 0 and 1800ng M^{-3} with an average of 500ng M^{-3}
However, This study was performed on a university campus in Shanghai which may explain the higher plastic concentration.

%PVC contribution to total $PM_{2.5}$ concentration:

0.4-1.3%

This observed level of PVC is quite significant for an urban background site, which supports the hypothesis that microplastics are ubiquitous throughout urban air environments.

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EPSRC Centre for Doctoral Training in Aerosol Science

Imperial College London
imperial.ac.uk

References:

Liao, Z. *et al.* Airborne microplastics in indoor and outdoor environments of a coastal city in Eastern China. *J Hazard Mater* **417**, 126007 (2021).

Milani, N. B. L., van Gilst, E., Pirok, B. W. J. & Schoenmakers, P. J. Comprehensive two-dimensional gas chromatography— A discussion on recent innovations. *J Sep Sci* **46**, 2300304 (2023).

Chen, Y. et al. Quantification and Characterization of Fine Plastic Particles as Considerable Components in Atmospheric Fine Particles. Environ Sci Technol 58, 4691–4703 (2024).

Developing and deploying new sensors for in-situ monitoring of clouds

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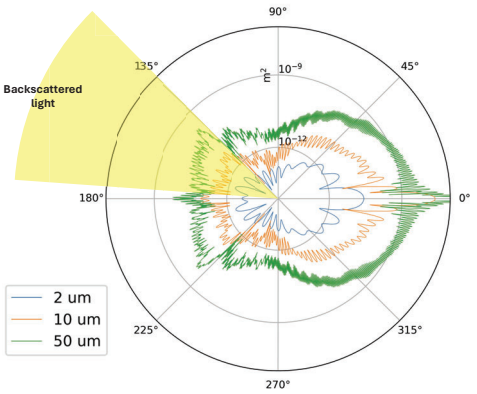
Background

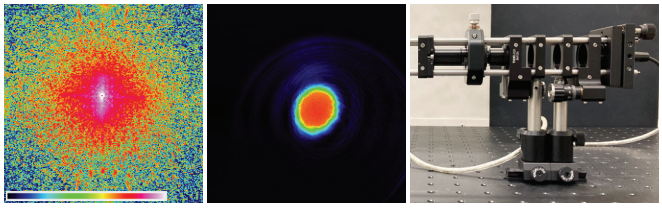
- Cloud droplet probes typically use forward-scattered light (from a laser) to measure cloud droplet size distribution.
- Backscattered light could provide means for a more practical measurement technique that (doesn't require a detector in front of the laser and) could be more easily used on non-specialist platforms e.g. commercial jets.
- **Research Aim:** Investigate feasibility of using backscattered light for accurate cloud droplet size distribution measurement.



'Phase' diagram for spherical water droplets – Scattered light intensity (differential scattering cross-section) over polar angle of an unpolarized 550nm beam (incident at 0°), spherical droplets scatter light symmetrically about the azimuth angle relative to the scattering plane.

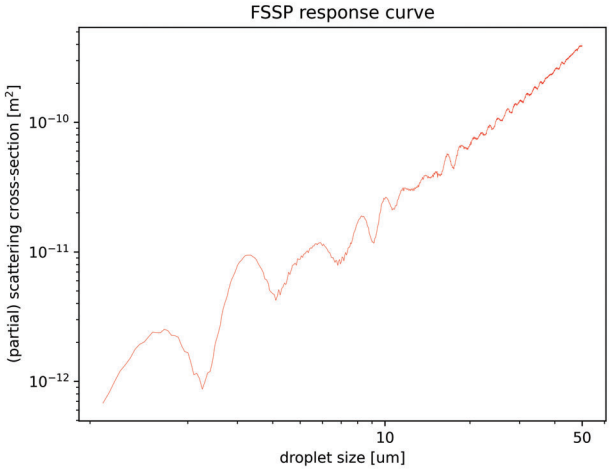
Method

- A model has been developed to produce droplet scattering 'response curves', for a collection optic displaced from an incident beam by a polar angle and will be used to inform optimum backscattering arrangements.
- An optical assembly is being developed to measure backscattered light experimentally and assess arrangements for droplet measurement.
- The assembly will consist of a laser source(s) directed at a scattering target and photodetector(s) that can be adjusted to assess different arrangements and parameters.

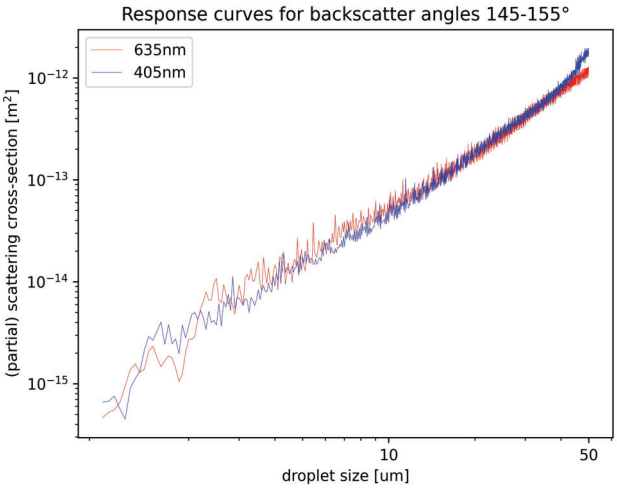


(L) Backscatter Cloud Probe (BCP) beam profile – The BCP is an existing backscatter instrument, but is limited for quantitative measurement [1]; variation of beam intensity within the sample area is one source of uncertainty.
(C) Beam profile produced by a spatial filter – A more confined and uniformly intense laser beam profile could help improve backscatter size measurement.
(R) Spatial filter and laser source – A spatial filter consists of three stages; an aspheric lens, a pinhole and a collimating (plano-convex) lens.

(Color maps to a linear intensity scale of greyscale pixel value from black to white)



Forward Scattering Spectrometer Probe (FSSP) response curve – The FSSP collects forward scattered light from a 632.8nm red laser between 4.6 and 12.8° polar angles using an annular photodetector and has been widely used in cloud droplet research; the instrument response curve used to measure droplet size is replicated by the model [3], (the model is implemented in Python and uses the Python module *scattnlay* to calculate scattering amplitudes [4]).



Backscattered light response curve – backscattered cross-section against droplet size, collected by an optic offset from the incident beam (0°) between 145 and 155° polar angles in red and blue wavelengths; non-monotonicity presents an uncertainty in the mapping of roughly ±2.5um.

Next Research

- A 'clean' spatially filtered laser beam could help define the sample area and reduce uncertainty due to varying beam intensity, which remains a challenge in single-droplet cloud spectrometers [2].
- Use of multiple wavelengths (sources) or detectors may also help define the sample area and reduce measurement uncertainty.
- Backscatter arrangements are being investigated experimentally that could be suitable for a compact instrument module.

[1] Beswick, K., et al. "The backscatter cloud probe–a compact low-profile autonomous optical spectrometer." Atmospheric measurement techniques 7.5 (2014): 1443-1457.
[2] Lance, Sara, et al. "Water droplet calibration of the Cloud Droplet Probe (CDP) and in-flight performance in liquid, ice and mixed-phase clouds during ARCPAC." Atmospheric Measurement Techniques 3.6 (2010): 1683-1706.
[3] Dye, James E., and Darrel Baumgardner. "Evaluation of the forward scattering spectrometer probe. Part I: Electronic and optical studies." Journal of Atmospheric and Oceanic Technology 1.4 (1984): 329-344.
[4] K. Ladutenko, U. Pal, A. Rivera and O. Peña-Rodríguez, "Mie calculation of electromagnetic near-field for a multilayered sphere," Computer Physics Communications, vol. 214, May 2017, pp. 225-230.

Optical Properties

The Impacts of Phase Separation and Particle Shape on Aerosol Optical Properties

By Ruaridh Davidson
University of Bristol

Introduction

- Aerosols in the atmosphere are known to regulate global climate through radiative forcing.
- The extent of this is poorly understood resulting in large uncertainties in climate models.
- A deep understanding of the **optical properties** of aerosols with diverse shapes and those of multiphase composition remains elusive.
- Understanding these optical properties can allow us to infer the physical properties, allowing refinement of climate models.
- Applications out with environmental science, such as investigation of multiphase bio-aerosol to understand disease transmissions.
- UV based sterilisation devices may also be designed to eliminate airborne pathogens in the environment at a high level of disinfection should their interaction with light be better understood.
- The development of innovative approaches like this to counteract quickly evolving superbugs is needed, where pathogens are becoming resistant to the standard chemical approach.

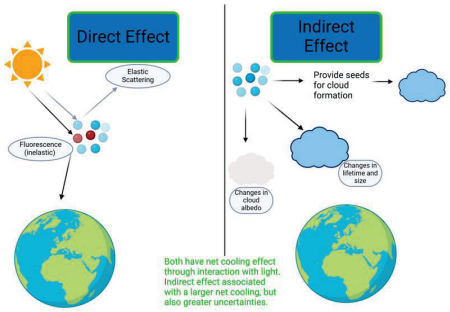


Figure 1 describing the direct and indirect effect of radiative forcing.

Methods

EDB Quadrupole

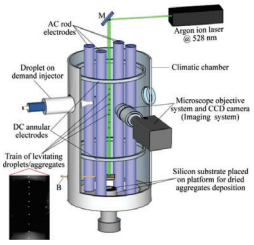
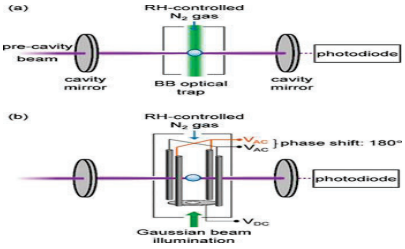


Figure 2 by Archer, Kolwas et al. 2019[1] *illustrating the components of a quadrupole electrodynamic balance.*

- The trap applies a DC voltage above and below generating a static electric field.
- Insufficient to hold levitated particles in place to allow for precise measurements.
- Quadrupoles apply AC voltage to generate an oscillating electric field.
- This field can respond to changes in the position of the particle in space, keeping the particle still in accordance with newtons second law.

SP-Cavity Ring Down Spectroscopy



$$\alpha_{ext} = \frac{L}{lc}\left(\frac{1}{\tau} - \frac{1}{\tau_0}\right)$$

c: speed of light
L: distance between the two reflective mirrors.
l: cavity length occupied by the sample

Figure 3 by Cotterall, Knight et al[2] showing a diagram of a SP-CRD spectrometer. Equation on how to calculate the extinction co-efficient from cavity ring down measurements.

- Two highly reflective mirrors flank optical cavity resulting in constructive interference.
- Light leaks out the back mirror, of which the intensity decays at an exponential rate.
- Referred to as the ring down time.
- Difference in ring down time of empty cavity and that with sample gives the above relationship.

Modelling Techniques

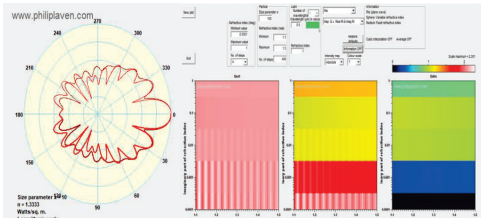


Figure 4 showing plots generated in Mieplot. The left-hand side shows a polar plot of intensity vs scattering angle (phase function). The right-hand side shows the refractive index(imaginary) vs the absorbance efficiency (Qabs).

- "Wet lab" techniques such as SP-CRDS will be used to retrieve the extinction cross sections and particle size may be retrieved using angularly resolved elastic light scattering.
- Complementary Mieplot software can then be used to retrieve phase state and particle shape.
- T-Matrix add on may be used for non-spherical particles (solids).

Workflow

Year 1
Non-Absorbing Particles During LLPS

Atmospherically relevant aerosol particle with core shell morphology.

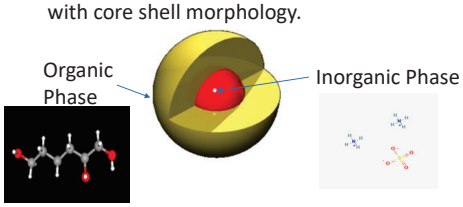


Figure 5 showing the core shell morphology adopted by many composite aerosols with both an organic and inorganic component.

Year 2
Absorbing Particles During LLPS

Refractive Index $m = n + ik$

$$n = \frac{c}{v}$$

- Where n is the real refractive index, and ik is the imaginary refractive index, measuring the attenuation of light by absorption.
- The real part refers to the speed of light in a vacuum over that in a medium, such as an aerosol droplet.

Year 3
Non-Spherical Particles (Solids)

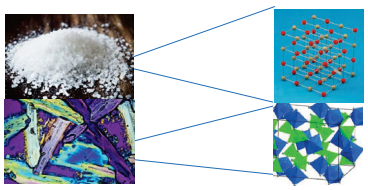


Figure 6. Unit cells of atmospherically relevant salts. NaCl(top) and ammonium sulphate(bottom)

References

1) Archer, J., et al. (2019). "Sodium dodecyl sulfate microaggregates with diversely developed surfaces: Formation from free microdroplets of colloidal suspension." The European Physical Journal Plus **134**.
2) Cotterell, M. I., et al. (2022). "Accurate Measurement of the Optical Properties of Single Aerosol Particles Using Cavity Ring-Down Spectroscopy." The Journal of Physical Chemistry A **126**(17): 2619-2631
3) Brunamonti, S., et al. (2015). "Redistribution of black carbon in aerosol particles undergoing liquid-liquid phase separation." Geophysical Research Letters **42**(7): 2532-2539

University of BRISTOL

Department of chemistry

University of BRISTOL

Photoinitiated Chemistry in Single Levitated Aerosol Droplets using Cavity Ring-Down Spectroscopy

Xu Zhang

Supervisors: Michael I. Cotterel, Anderw J. Orr-Ewing

Introduction

This project investigates the photobleaching kinetics of individual aerosol particles in the size range of 1-10 µm using a linear electrodynamic quadruple (LEQ) trap combined with cavity ring-down spectroscopy (CRDS), where the effects of particle size, viscosity, chemical composition and wavelength of illumination will be explored.

Background

Size dependent photochemistry:

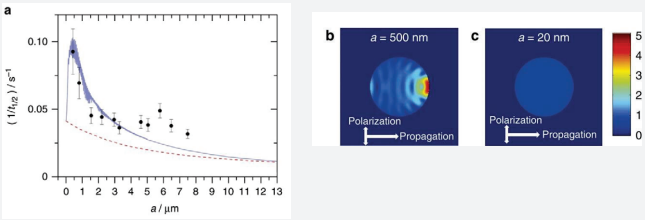
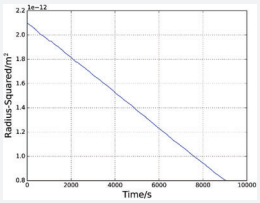


Figure 1 - (a) Inverse first half-lives as a function of the droplet radius for a laser power of 1 mW. Distribution of the light intensity inside droplets at t=0 s for (b) a 0.5 µm droplet and (c) a 20 nm droplet. The colour scheme is relative to an incident light intensity of 1. Figure is adapted from Ref.1

Droplets vapour pressure:

- Droplet vapour pressures, p, can be obtained by fitting the Maxwell equation to the time-dependent radius data.



$$\frac{da^2}{dt} = -\frac{2D_{ij}M_i p}{R\rho T}$$

D_{ij} = the gas diffusion coefficient of species i in the surrounding phase j

a = particle radius

M_i = molecular weight

ρ = density

T = temperature at droplet surface

Figure 2 – Time dependent radius change.

Interaction of aerosols with light :

- extinction cross section (σ_{ext}): quantifies how much power is removed from the incident light.
- σ_{ext} is a combination of the scattering cross sections (σ_{sca}) and absorption cross sections (σ_{abs}).
- The extinction cross section can be measured by many spectroscopic techniques, e.g. cavity ring-down spectroscopy (CRDS) .

$$\sigma_{ext} = \frac{L\pi w^2}{2c}\left(\frac{1}{\tau} - \frac{1}{\tau_0}\right)$$

L = length of optical cavity

w = beam waist at the cavity center

c = speed of light

t = ring down time

t_0 = ring down time for empty cavity

Methodology

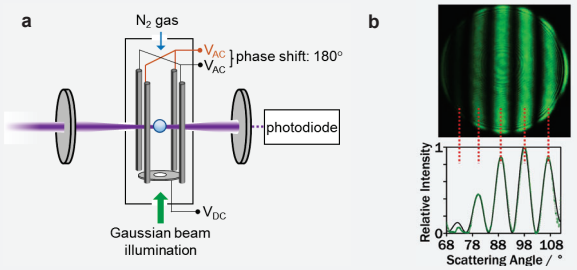
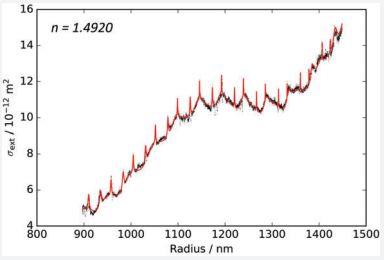


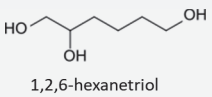
Figure 3 – (a) Schematic of CRDS and quadrupole electrodynamic trap. (b) Phase function of a single particle. Figure is adapted from Ref.2

- CRDS accurately measures the extinction cross-section of single particle, which indicates the chemical composition. And phase function measures the evolving size.

Results

Measurements on 1,2,6-hexanetriol:



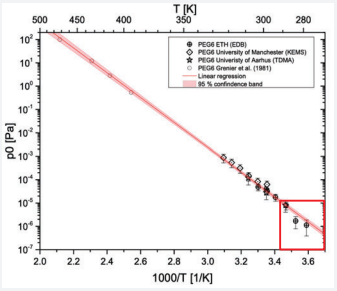


1,2,6-hexanetriol

- Non-absorbing at 405nm
- Relative low volatility

Figure 4 – Extinction cross-section measurement of 1,2,6-Hexanetriol as a function of particle radius. The red line shows the Mie theory prediction.

RI and vapour pressure of Hexaehylene glycol:



- n : 1.4796
- Vapour pressure : 1.534 E-05 Pa
- Temperature : 291K

Figure 5 – Saturation vapor pressures vs. temperature of hexaethylene glycol[3]. The red square marked the experiment point.

References

1. Cremer J W, Thaler K M, Haisch C, et al. Nature communications, 2016, 7(1): 10941.
2. Cotterell, M. I.; Knight, J. W.; Reid, J. P.; Orr-Ewing, A. J. The Journal of Physical Chemistry A 2022, 126 (17), 2619-2631.
3. . Krieger U K, Siegrist F, Marcolli C, et al. Atmospheric Measurement Techniques, 2018, 11(1): 49-63.

Transport Emissions

IMPERIAL AIRBUS

Using Experiments to Develop Understanding of Nanoparticle Activation to Inform Contrail Models

Emily Winter
Marc Stettler
Jey Williams

Engineering and Physical Sciences Research Council

Contrail Overview

Contrails are line shaped clouds formed from ice crystals. The distribution of contrail coverage is sensitively dependent on ambient conditions, seasonal effects, fuel and aircraft properties. [1]

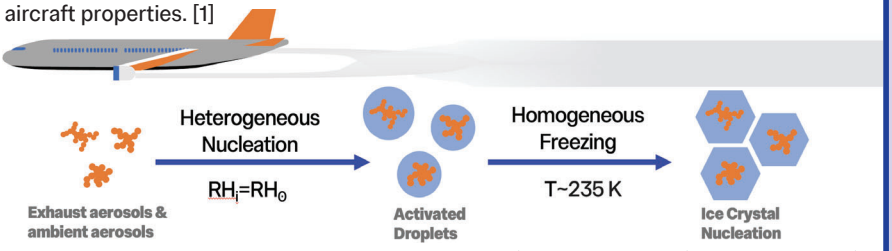


Fig 1. Schematic of contrail formation

Contrails form → plume conditions exceed water saturation.
Contrail persists → ambient air ice supersaturated.
Persistent contrails can spread to form contrail-cirrus. [2]

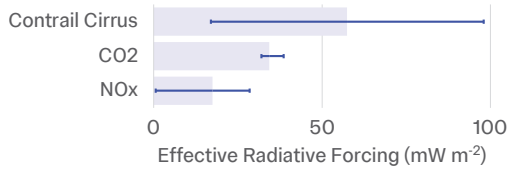


Fig 2. Aviation EFR adapted from Kärcher *et al.* [3]

Problem Statement

This project aims to measure the process of condensation onto nanoparticles, to better understand the relationship between the activation of emissions and the characteristics of AIC formed. Data collected will be used to address the current limitations of contrail models.

Specific Research objectives include:

- Produce and characterise nvPM and vPM (both externally and internally mixed)
- Activation measurements using CPC-based approach
- Parameterise the hygroscopicity of particles
- Implement the experimental data into models to assess how aviation climate impacts are impacted by uncertainty in emissions properties.

Short life-time of contrails makes them ideal for global warming mitigation efforts.

κ -Kohler Hygroscopicity

In 2007 Petter and Kreidenweis introduced a hygroscopicity parameter κ, which relates the uptake of water volume to a particles water activity. κ is determined experimentally by fitting CCN activity. [4]

Particle Type		κ	Ref
nvPM	Pure soot	0	[3]
	Coated soot particles	0.005	[3]
vPM	Sulfuric acid	> 0.6	[3]
	Lubrication oil	0	[1]
	Organic Compounds	0.0-0.5	[5]

Fig 3. κ values of different particle types

Proposed Experimental Method

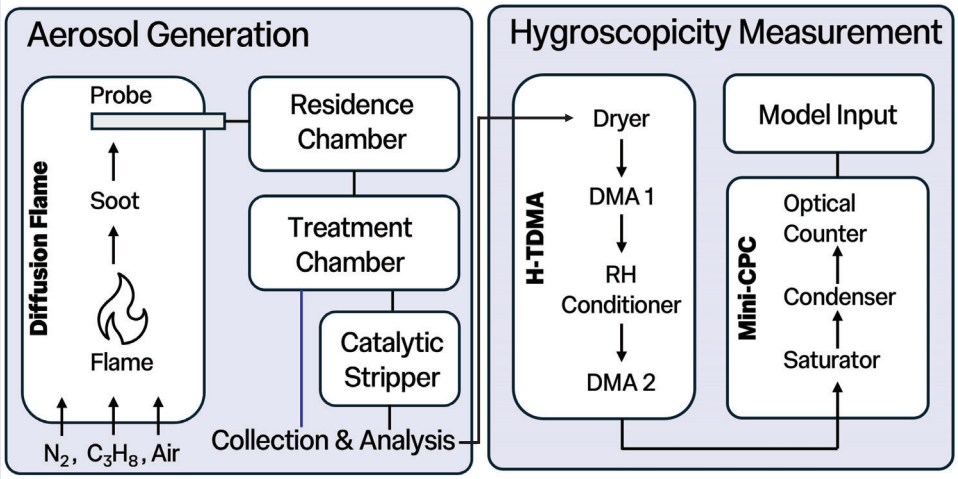


Fig 4. Schematic of proposed experimental set-up to parameterise hygroscopicity

1. An aerosol source will be obtained by a diffusion flame combustor [6]
2. The polydisperse aerosol will be size selected by a H-TDMA
3. The number concentration will be obtained by a mini-CPC [7]

Parameterised hygroscopicity will be used as input for the CoCIP model [2]

Policy Implications

In November 2023, supported by up to £1m of grant funding from the government Virgin Atlantic's Flight100 became the first commercial airliner to cross the Atlantic using 100% SAF.

By 2025, five commercial scale SAF facilities should be under construction in UK with £53m of funding between nine sustainable initiatives.

By 2030, 10% of all jet fuel in flights taking off from the UK to come from SAF. [8]

Mini-CPC

Low- cost optical particle counters (OPCs) normally detect particles with diameters d_p> 300 nm. Ultrafine particles common in exhaust and present in contrail plumes $d_p \leq 100$ nm. Using the mini-CPC diameter $d_{init,p} = 10$ nm can be detected. [7]

This device will be compared to other activation techniques e.g PINE chamber. [1]

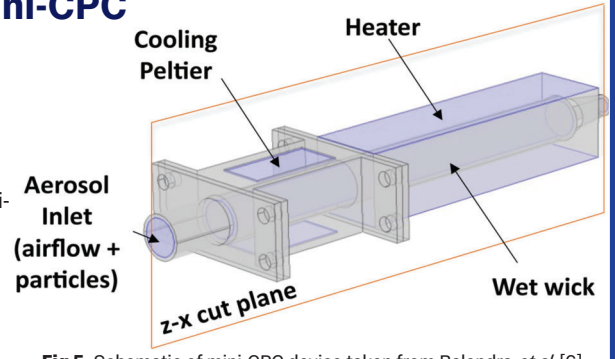


Fig 5. Schematic of mini-CPC device taken from Balendra *et al.* [6]

Acknowledgements

Funding is provided by the EPSRC Aerosol Science CDT and Airbus

References

[1] Ponsonby et al., 'Jet Aircraft Lubrication Oil Droplets as Contrail Ice-Forming Particles'.
[2] Schumann and Heymsfield, 'On the Life Cycle of Individual Contrails and Contrail Cirrus'.
[3] Kärcher, 'Formation and Radiative Forcing of Contrail Cirrus'.
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[5] Han et al., 'Hygroscopicity of Organic Compounds as a Function of Organic Functionality, Water Solubility, Molecular Weight, and Oxidation Level'.
[6] Stettler et al., 'Updated Correlation Between Aircraft Smoke Number and Black Carbon Concentration'.
[7] Balendra et al., 'Condensation Particle Counters'.
[8] Department for Transport, 'Supporting the Transition to Jet Zero: Creating the UK SAF Mandate'.

IMPERIAL

Even in ideal conditions only 53% of contrails can be seen in satellite images—but the ones that matter can.

Factors influencing contrail observation in satellite images

Oliver Driver (o.driver22@imperial.ac.uk)
Marc Stettler, Edward Gryspeerdt

Background

- Contrails cause more than half the warming impact of aviation (**Fig. 3**)
- Observations are needed for model validation, tactical avoidance, and mitigation trials.
- Contrails might be unobservable if they are narrower than the pixel resolution or are too optically thin to cause a strong signal.

Research questions

- Can geostationary satellites meet the observational need?
- How are observations limited?

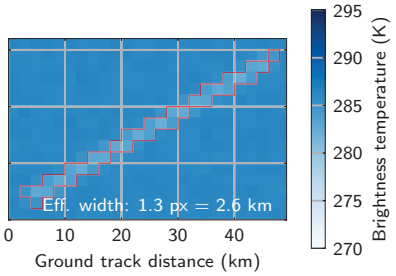


Fig. 1 A 2 km resolution simulated contrail image

Methodology

1. Test simulated satellite images of contrails (**Fig 1**) with a detection algorithm.
2. Vary the simulated contrail properties to build an observability threshold (**Fig. 4**).
3. Assess the observability of forming contrails using a modelled population of contrails.

Results

- Lots of contrails are unobservable; but strongly forcing contrails are much more accessible.
- A higher resolution satellite wouldn't be a huge win: the unobserved contrails are mostly too optically thin.
- Biofuel adoption decreases observability: contrail ice crystals have bigger effective radii. Climate benefit may be overstated.
- Observability has a characteristic time evolution, just like contrail properties (**Fig. 2**).

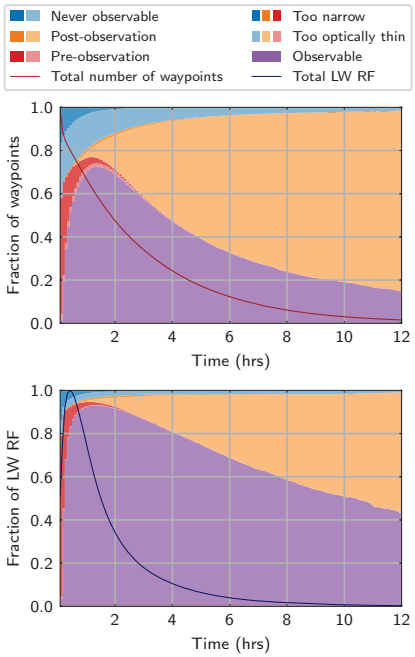


Fig. 2 The time-evolution of observability.

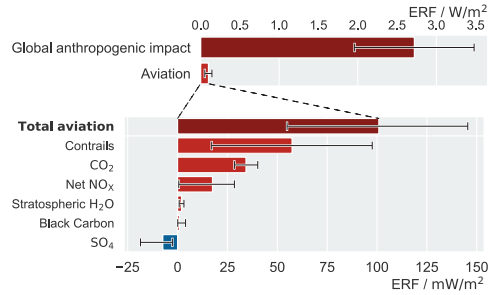
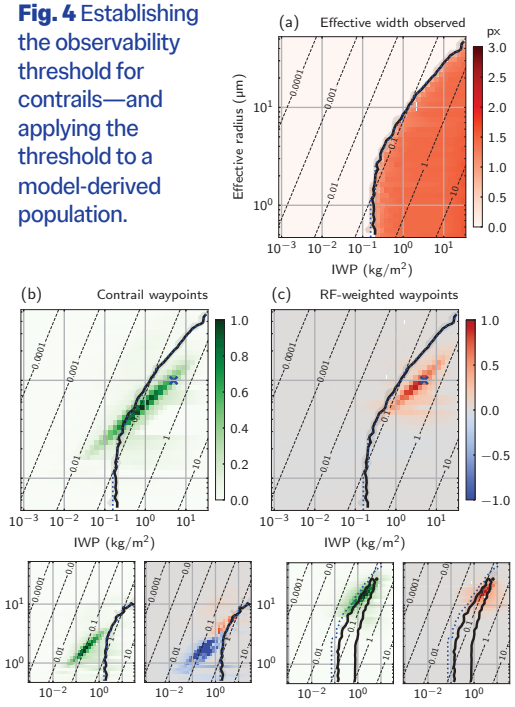


Fig. 3 The radiative forcing caused by aviation sources (Lee et al. 2021)

Fig. 4 Establishing the observability threshold for contrails—and applying the threshold to a model-derived population.



Scan for a scrollable version of this poster

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This is designed as a "#BetterPoster", an idea by Mike Morrison to improve UX in Science Communication: youtu.be/SYk29tnxASs (QR code to the right)