Chemical and Toxicological Properties of Aerosol Emissions Subject to Atmospheric Processing

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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.

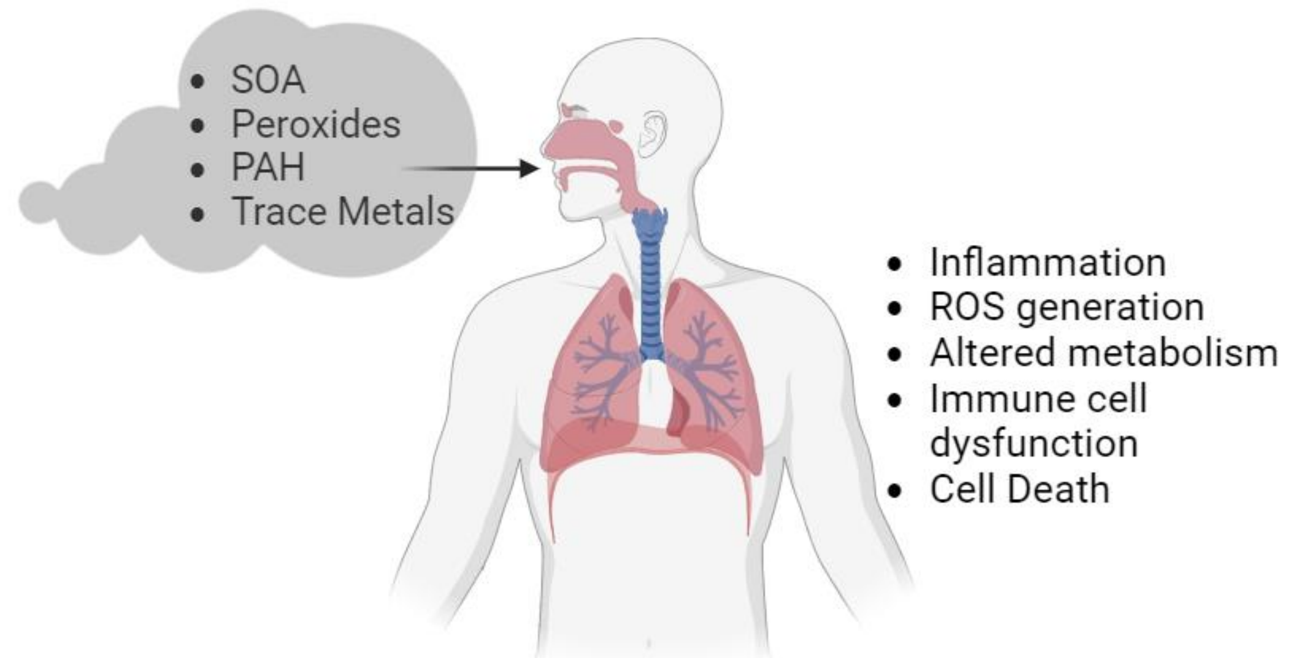

Figure 1: The Toxic effects of aerosols during ageing. Image was created on BioRender

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

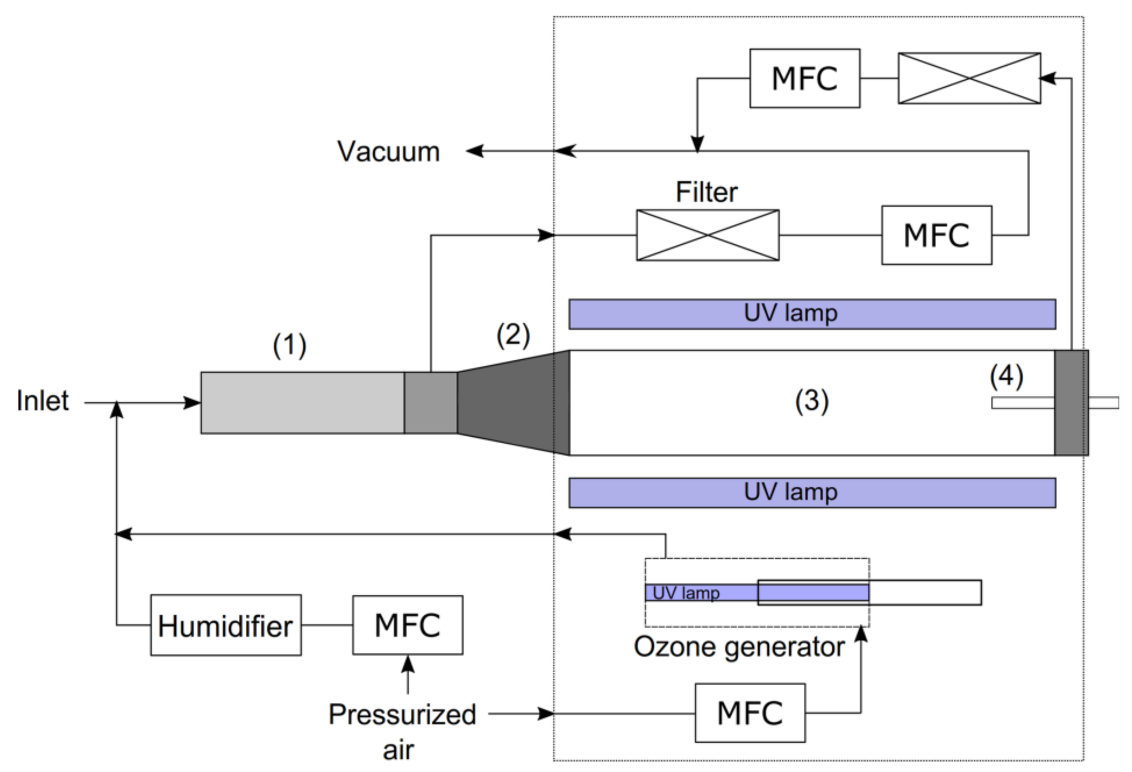

Figure 2: Design of a TSAR (TUT secondary aerosol reactor). Composed of (1) the residence time chamber, (2) the expansion tube, (3) the oxidation reactor and (4) the adjustable outlet. (3) and (4) are contained in a single housing.[3]

5. Methodology

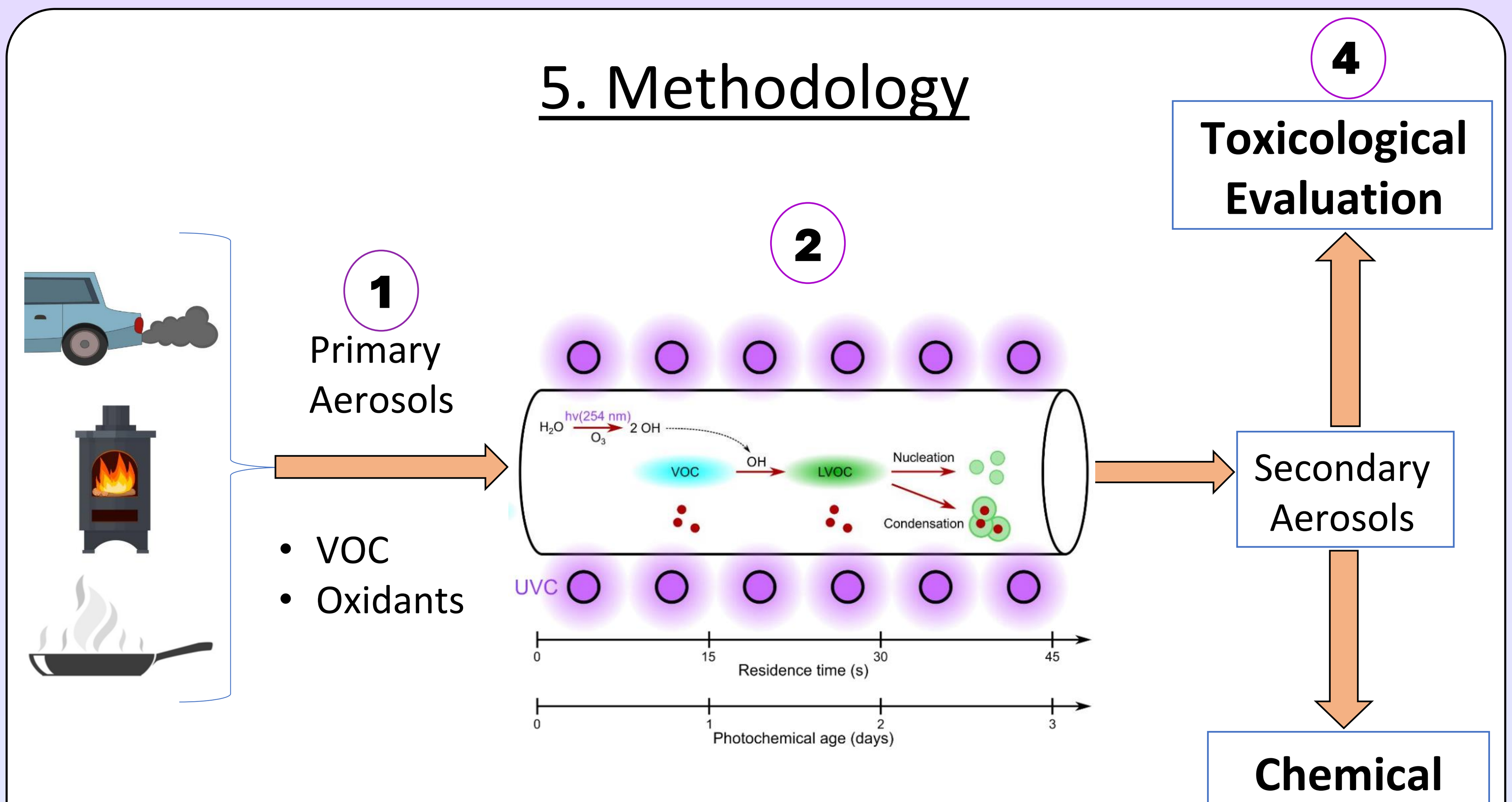

Figure 3: Flow diagram of research stages including diagram of operating principle of the OFR.[4] Each stage is referenced below.

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