**Characterization of a multi-stage focusing nozzle for collection of spot samples for aerosol chemical analysis\_Dataset**

**Dataset # - RD-1074-2023-0**

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**Introductory Information**

Concentrated collection of aerosol particles on a substrate is essential for their chemical analysis using various microscopy and laser spectroscopic techniques. An impaction-based aerosol concentration system was developed for focused collection of particles using a multi-stage nozzle that consists of a succession of multiple smooth converging stages. Converging sections of the nozzle were designed to focus and concentrate a particle diameter range of 900 to 2500 nm into a relatively narrower particle beam to obtain particulate deposits with spot diameters of 0.5-1.56 mm. A slightly diverging section before the last contractions was included to allow for better focusing of particles at the lower end of the collectable diameter range. The characterization of this multi-stage nozzle and the impaction-based aerosol concentration system encompassing the nozzle was accomplished both numerically and experimentally. The numerical and experimental trends in collection efficiency and spot diameters agreed well qualitatively; however, the quantitative agreement between numerical and experimental results for wall losses was poor, particularly for larger particle diameters. The resulting concentrated particulate deposit, a spot sample, was analysed using Raman spectroscopy to probe effect of spot size on analytical sensitivity of measurement. The method’s sensitivity was compared against other conventional techniques, such as filtration and aerosol focused impaction, implementing condensational growth. Impaction encompassing the multi-stage focusing nozzle is the only method that can ensure high sensitivity at Reynolds numbers greater than 2000, that can be supported by small pumps which renders such method suitable for portable instrumentation.

**Experimental Methods**

**Focusing nozzle fabrication**

* The Multi-stage Focusing Nozzle (MSN) was 3D printed using plastic material of high clarity and resolution via Stereolithography (3DSystems, Rock Hill, SC, USA), which provided high precision and accuracy, with a tolerance of less than 0.05 mm. The printing was produced by a 3D model constructed in Solidworks (Dassault Systemes). A transparent, polycarbonate-like, plastic material was selected (Accura ClearVue; 3DSystems, Rock Hill, SC, USA), for detailed and smooth surface finish.
* The one-stage focusing nozzle (OSN) was fabricated through the material jetting 3D printing process (Stratasys Objet Eden 260 VS; Stratasys, Eden Prairie, MN, USA), providing an accuracy in the range of 25 to 80 μm, in a transparent, photopolymer material (VeroClearTM RGD810TM; Stratasys, Eden Prairie, MN, USA) for enhanced surface smoothness.
* The flat collection plate used for sample collection was made of tungsten and had a width of 1.56 mm and a length of 6 mm. The optimized distance between the jet and the collection plate selected, was 1.5 mm.

**Aerosol generation**

* Liquid solution of (NH4)2SO4 were aerosolized by a medical nebulizer (Salter 8900 Series Disposable Small Volume Jet Nebulizer; Salter Labs, Arvin, CA, USA). The aerosol sample was then dried through a diffusion dryer.
* The Aerodynamic Aerosol Classifier (AAC; Cambustion Ltd, Cambridge, United Kingdom) was used for generation of monodisperse aerosol streams. The air flow rate through the AAC was approximately 0.4 L min-1.
* A flow rate of 2 L min-1 at the inlet of the nozzle was attained when dilution air was mixed with the monodisperse aerosol flow that exited the classifier.
* A humidifier (MH-110-12F-4; Perma Pure LLC, NJ, USA) was located prior to the nozzle/impactor for eliminating particle bouncing on the collection surface.
* The Ultrafine Condensation Particle Counter (UCPC; model 3776, TSI Inc., Shoreview, MN, USA) was used downstream of the nozzle/impactor. UCPC was used for calculating the wall losses at the interior of the focusing nozzle and the collection efficiency of the impaction-based micro-concentrator. The UCPC’s internal vacuum pump (1.5 L min-1), along with an additional vacuum pump were used for maintaining the air flow rate at the nozzle inlet at approximately 2 L min-1.

**Sample collection for Raman analysis**

* The UCPC was connected at the inlet of the impactor, monitoring the number of particles ((NH4)2SO4) entering the impactor encompassing the nozzle, while a pump located downstream of the impactor regulated the flow through the impactor at 2 L min-1.

**Raman analysis of ‘spot sample’ obtained**

* A portable Raman spectrometer was used for the analysis (i-Raman®; B&W Tek, Newark, DE, USA).
* The excitation wavelength used in the spectrometer was 785 nm, with 420 mW of power.
* The working distance was approximately 9 mm, and the diameter of the laser beam was approximately 105 μm.
* The integration time selected for the spectra acquisition was 30 seconds.
* For the ammonium sulfate particles used for the characterization, the peak signal intensity is observed at a Raman shift of approximately 977 cm-1.
* Three replicates were obtained for each measurement by acquiring spectra from three different spots of the deposited sample.
* The average areas of the peaks were estimated for the extraction of calibration curves providing the association between the Raman signal intensity and the particulate mass accumulated on the collection plate.

**Citations- Publications based on the dataset**

Zervaki, O., P. Kulkarni, and D. Dionysiou. (2023). “Characterization of a Multi-Stage Focusing Nozzle for Collection of Spot Samples for Aerosol Chemical Analysis.” Journal of Aerosol Science, 174, pp 106235, [DOI:10.1016/j.jaerosci.2023.106235](https://doi.org/10.1016/j.jaerosci.2023.106235).

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