Materials and Methods

Materials

All solutions were prepared using > 18 MΩ-cm deionized water from an Evoqua water purification system. Peracetic acid (PAA) solution (32% w/w of PAA, 40-45% w/w of acetic acid, and <6% w/w of H2O2) was supplied by Sigma Aldrich (USA). A V-2000 photometer and PAA and Hydrogen Peroxide (HP) Vacu-vials® instrumental test kits (K-7913, K-5543) were purchased from Chemetrics. A DR1900 portable spectrophotometer and DPD total chlorine reagent powder pillows were purchased from HACH. 50-mL glass impingers were purchased from Ace Glass (NJ, USA). Plastic impingers were purchased from SKC (PA, USA). 25mm Acrodisc® syringe filters with 0.45µm PTFE membranes were purchased from Pall Corporation (USA). The 3D printed nozzle was printed using an Objet Eden 260vs with Veroclear™ and SUP 705 was used as support material. The support material was washed away before experimental use. Flow-limiting critical orifices (1 L/min) and Aerosol Adapter connectors were purchased from Millipore. A Bios DryCal Defender flowmeter was used to measure the orifice flow rate. Tygon® tubing was purchased from Sigma Aldrich.

Colorimetric determination of PAA concentration from stock solutions.

Figure 3, Supplemental Table S1

The concentrations of the PAA solution ($C_{Measured}$) were determined using the Chemetrics Vacu-vials® ampoule and HACH PAA test kits according to the manufacturer's instructions. The photometers were blanked according to the manufacturer's instructions. In the Chemetrics method, excess potassium iodide is added to the PAA solution where peracetic acid oxidizes the iodide to iodine. The iodine then oxidizes the DPD contained in an ampoule, forming a pink colored Würster dye. The HACH method is similar to Chemetrics; a DPD total chlorine powder pillow was mixed with the PAA solution in a cuvette, producing a pink color. The intensity of the pink color is directly proportional to the peracetic acid concentration. The V200 photometer for Chemetrics and DR1900 portable spectrophotometer for HACH measured the absorbance of the pink color and automatically converted that to $C_{Measured}$. The Chemetrics method was used for all studies in this paper and the HACH method was used to verify the Chemetrics results. Impinger samples must be worked-up and colorimetric measurements made as soon as possible to avoid PAA degradation and HP interference. The measurements were made within five minutes of dilution or impinger collection, which is before HP has time to significantly oxidize the iodide. The HP results were analyzed using the Chemetrics K-5543 HP Vacu-vials® Instrumental Kit instructions and HACH method 10290.

Various amounts of 32% PAA (V_{PAA}) ranging from 0.45 to 14.9-µL were placed into a 0.25-L ($V_{Dilution}$) volumetric flask and diluted to the mark with deionized water. To make lower concentrations, aliquots of the aforementioned solutions were placed into 50-mL volumetric flasks and diluted to the mark with deionized water. The experimentally determined concentration of the product ($C_{Experimental}$) of PAA was used to calculate the weight percent ($W_{\%}$) of PAA in solution, using the density of PAA solution (ρ_{PAA}) (eq. 1-2). $C_{Measured}$ was determined for each V_{PAA} three times and an average weight percent ($W_{Average\%}$) for all experimental concentrations was determined and used to calculate the theoretical concentration ($C_{Calculated}$) (eq. 3). The V2000 photometer has a maximum range of 5 mg/L and the DR 1900 photometer has a maximum range of 10 mg/L, thus sample solutions must be diluted below this concentration before measurements are made.

$$C_{Experimental} = \frac{C_{Measured} \times V_{Dilution}}{V_{PAA}} \quad (1)$$

$$W_{\%} = \frac{C_{Experimental}}{\rho_{PAA}} \times 100 \quad (2)$$

$$C_{Calculated} = \frac{V_{PAA} \times \rho_{PAA} \times W_{Average\%}}{V_{Dilution} \times 100} \quad (3)$$

Colorimetric determination of PAA vapor concentrations as collected by glass impinger.
Table 1, Table 3, Supplemental Table S2

A glass impinger was filled with 15-mL of deionized water. Tygon® tubing was used to connect the impinger to an Acrodisc® syringe filter with a 0.45µm PTFE membrane. 0.5-6.5-µL aliquots of PAA were pipetted onto the filter and air was pulled through the impinger at 1 L min^{-1} for 15 minutes. The impinger sample was diluted to 500-mL and the PAA concentration was measured by using the Chemetrics PAA test kit, according to the manufacturer's directions. Each measurement was taken in triplicate. It was determined that tube-to-filter length did not appreciably affect the recovery of PAA in the impinger solution. A 1-inch tube length was used in all experiments unless noted.
Impinger collection efficiency studies were conducted and the collection efficiency was greater than 96.6% so no backup impinger was used for these studies.

Colorimetric determination of PAA vapor concentrations collected by plastic impinger
Table 2, Table 4, Supplemental Table S3, Supplemental Table S4

Three plastic impingers were compared for the use of PAA collection. Two impingers were commercially available from SKC; one having a vertical inlet and horizontal outlet and one having both inlet and outlet ports vertical. The other plastic impinger had vertical inlet and outlet ports with a 3D printed nozzle to improve collection of PAA vapors. The commercially available perfluoroalkoxy alkane (PFA) plastic impingers have a non-tapered, flat tip where a typical glass impinger has a nozzle. The taper of the tip increases the linear velocity of air, which improves the collection efficiency of the impinger for aerosols, and reduces the bubble size, which improves the collection efficiency of the impinger for vapors. Nozzles and ports for the plastic impingers were designed and 3D printed in-house. The plastic impinger was assembled using the printed ports and nozzle piece and the purchased impinger body and lid. The plastic impinger procedure is the same as the glass procedure, above. There was poor collection efficiency when using the impinger with the horizontal port. No backup impinger was used for the 3D printed impinger studies because impinger collection efficiency was greater than 95.8%.