

Supplemental material

Microfluidic condensation nanoparticle counter using water as condensing liquid for assessing individual exposure to airborne nanoparticles

Hong-Beom Kwon, Seong-Jae Yoo, Yong-Jun Kim*

School of Mechanical Engineering, Yonsei University, Seoul, 03722, Republic of Korea

* To whom correspondence should be addressed: yjk@yonsei.ac.kr

[The description of species transport modelling]

Species transport modelling was carried out in the following manner. The continuity, momentum and energy equations, which were necessary for the basic computational fluid analysis, were incorporated in the model. In addition, a species transport equation (eqn S2) was added to analyze the water vapor concentration and relative humidity profiles in our system. There were three species, nitrogen, oxygen, and water vapor, in our model. In the algorithm, the concentration of each species (J) was calculated in the form of mass fraction (Y_j), which can be expressed as

$$Y_j = \frac{\rho_j}{\rho_{tot}}, \quad j = 1, 2, 3, \quad (S1)$$

where ρ_j is the partial density and $\rho_{tot} = \sum \rho_j$. This variable was applied to the species transport equation,

$$\sigma \frac{\partial}{\partial t} (\rho_{tot} Y_j) + \nabla \cdot (\rho_{tot} \vec{v} Y_j) = -\nabla \cdot \vec{J}_j + S_j, \quad (S2)$$

where \vec{v} is the velocity of the fluid, and \vec{J}_j is the mass diffusion flux. Since the modelling was assumed to be steady state (i.e., $\sigma \frac{\partial}{\partial t} (\rho_{tot} Y_j) = 0$) and to have no source (i.e., $S_j = 0$), eqn (S2) was reduced to

$$\nabla \cdot (\rho_{tot} \vec{v} Y_j) = -\nabla \cdot \vec{J}_j. \quad (S3)$$

The mass diffusion flux (\vec{J}_j) occurs due to the gradients of concentration and temperature. Dilute approximation (Fick's law) was used to simulate mass diffusion via concentration gradient. In laminar flows, mass diffusion can be written as

$$\vec{J}_j = -\rho_{tot} D_{m,j} \nabla Y_j - D_{T,j} \frac{\nabla T}{T}, \quad (S4)$$

where $D_{m,j}$ and $D_{T,j}$ are the mass and thermal diffusion coefficients, respectively. Since the temperature difference between the conditioner and condenser was present, the thermophysical properties of the species including the diffusion coefficients were set to temperature-dependent variables. Lastly, the boundary conditions were set to be the designed values and the above equations were incorporated in the model (Fig. S1).

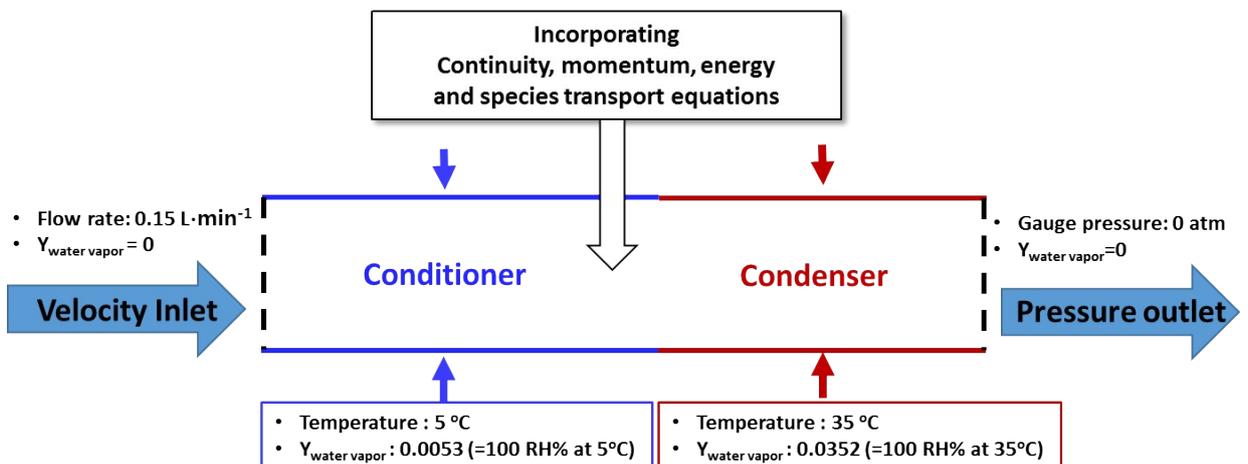


Fig S1. The details of the boundary conditions and used equations for solving the species transport.

[The dimension of the 3D-printed channel and integrating process of the chip]

Figure S2 (a) the structure and (b) dimensions of the 3D-printed channel. The channel consists of a reservoir and an aerosol path that are separated from each other by a wall. There is a water path which passes through the separating wall. Since this channel has a height of only 250 μm , it allows the water in the reservoir to be supplied to the conditioner and condenser without affecting the laminar flow pattern of the aerosol sample stream. Figure S3 shows the integrating process of the chip. After C-shaped electrodes were attached the side wall of the channel for electrical connection, the top, bottom substrates and channel were assembled using polymethyl methacrylate (PMMA) holders. Finally, a cooling module was mounted at the outer wall.

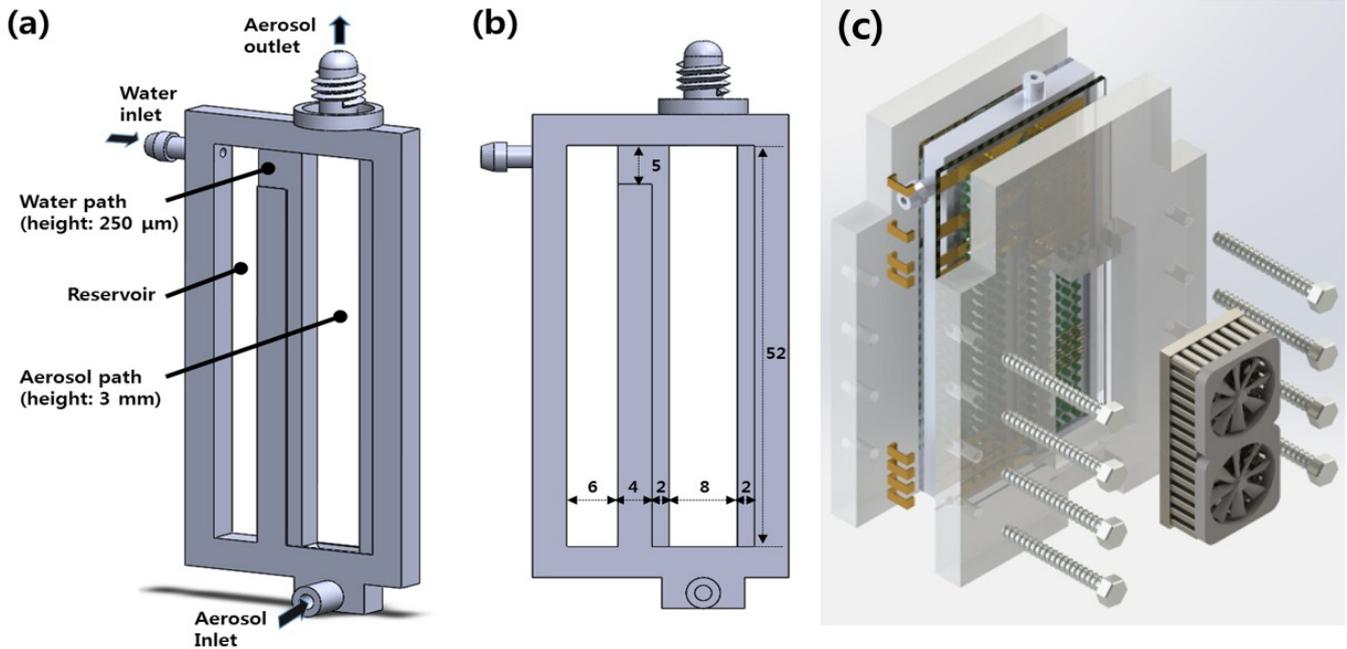


Fig S2. The structure of (a) the chip and (b) its dimensions in mm; the integrating process of the chip.

[Experimental setup]

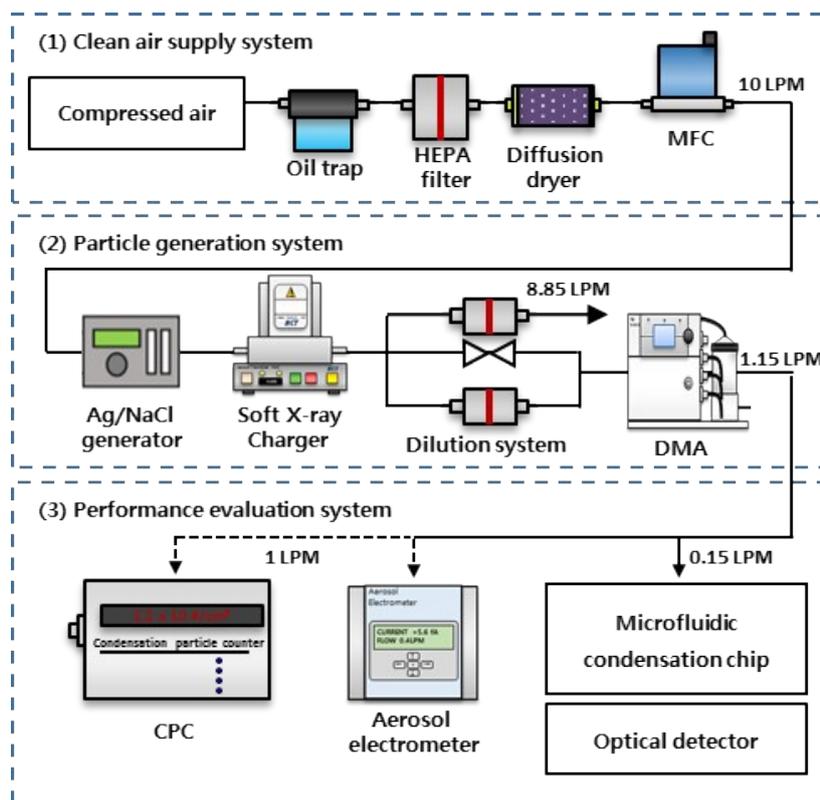


Fig S3. Experimental setup for the performance evaluation of our system.

Performance test of our system was characterized using the setup shown in Fig. S3. Compressed air was used as a carrier gas. Various contaminants in the air, including oil droplets, unwanted particles and moisture were removed using an oil trap, high efficiency particulate air (HEPA) filter and diffusion dryer. The clean air was then supplied at precise flow rates using mass flow controllers (MFCs). Ag and NaCl NPs were used as test aerosol and were generated using an evaporation/condensation technique. Their size and concentration ranges were 7-100 nm and 10^6 - 10^7 N \cdot cm $^{-3}$, respectively. The generated NPs were made have Boltzmann equilibrium charge distribution in a soft X-ray charger (XRC-05, HCT Inc., KR), and electrostatically classified to a specific diameter in a differential mobility analyzer (DMA; model 3081, TSI Inc., USA). The volumetric flow rates of the sample and sheath streams of the DMA were 1.15 LPM and 11.5 LPM, respectively. After diluted in the dilution bridge, the monodisperse, concentration-controlled NPs were then introduced into our system (0.15 LPM) and reference instrument (1 LPM). The counting efficiency and detectable concentration range of our system were characterized using an aerosol electrometer (AE; model 3068B, TSI Inc., USA), and the performance of our system was tested by comparing it with a commercially-available CPC (model 3772, TSI Inc., USA). The lengths of tubes leading to both the systems were carefully adjusted to guarantee the same concentrations.

[The reason why the counting probability exceeds 100% at some points]

The reason why counting probability is larger than 100 % at some points can be found in the experimental setup. As shown in Fig. S3, after Ag and NaCl particles were generated, they passed through a soft X-ray charger. Most of NPs were singly charged (+1) due to their limited surface area. The charged NPs were then classified to a specific diameter in a differential

mobility analyser. Accordingly, the classified NPs, which were transported to our system and reference aerosol electrometer, were singly charged.

The aerosol electrometer measured the current carried by the charged NPs (I_p), and converted it to the reference number concentration (C_R) using following equation,

$$I_p = C_r \cdot ne \cdot Q_r \quad , \quad (S5)$$

where n is the charge number (+1) on a single particle, e is the elementary charge (1.6×10^{-19} C), and Q_r is the volumetric flow rate entering the aerosol electrometer.

According to the specification of the aerosol electrometer (model 3068B, TSI Inc., USA), the detection limit of the current (I_p) is relatively high (1 fA = $375 \text{ N}\cdot\text{cm}^{-3}$ at 1 LPM) and the maximum error of the flow rate (Q_r) is 3 %, meaning that the fluctuation of the reference concentration (C_r) is inevitable. Therefore, given that our system counts all of the introduced NPs, the counting probability can exceed 100 % due to the fluctuation of the reference concentration.