

1 **Mapping the performance of a versatile water-based**
2 **condensation particle counter (vWCPC) with COMSOL**
3 **simulation and experimental study**
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15 **Abstract.**

16 Accurate airborne aerosol instrumentation is required to determine the spatial distribution of ambient aerosol
17 particles, particularly when dealing with the complex vertical profiles and horizontal variations of atmospheric
18 aerosols. A versatile water-based condensation particle counter (vWCPC) has been developed to provide aerosol
19 concentration measurements under various environments with the advantage of reducing the health and safety
20 concerns associated with using butanol or other chemicals as the working fluid. However, the airborne deployment
21 of vWCPCs is relatively limited due to the lack of characterization of vWCPC performance at reduced pressures.
22 Given the complex combinations of operating parameters in vWCPCs, modeling studies have advantages in
23 mapping vWCPC performance.

24
25 In this work, we thoroughly investigated the performance of a laminar flow vWCPC using COMSOL
26 Multiphysics® simulation coupled with MATLAB. We compared it against a modified vWCPC (vWCPC Model
27 3789, TSI, Shoreview, MN, USA). Our simulation determined the performance of particle activation and droplet
28 growth in the vWCPC growth tube, including the supersaturation, $D_{p,ke1,0}$ (smallest size of particle that can be
29 activated), $D_{p,ke1,50}$ (particle size activated with 50% efficiency) profile, and final growth particle size D_d under
30 wide operating temperatures, inlet pressures P (30 – 101 kPa), and growth tube geometry (diameter D and
31 initiator length L_{ini}). The effect of inlet pressure and conditioner temperature on vWCPC 3789 performance was
32 also examined and compared with laboratory experiments. The COMSOL simulation result showed that
33 increasing the temperature difference (ΔT) between conditioner temperature T_{con} and initiator T_{ini} will reduce
34 $D_{p,ke1,0}$ and the cut-off size $D_{p,ke1,50}$ of the vWCPC. In addition, lowering the temperature midpoint ($T_{mid} =$
35 $\frac{T_{con}+T_{ini}}{2}$) increases the supersaturation and slightly decreases the $D_{p,ke1}$. The droplet size at the end of the growth
36 tube is not significantly dependent on raising or lowering the temperature midpoint but significantly decreases at
37 reduced inlet pressure, which indirectly alters the vWCPC empirical cut-off size. Our study shows that the current
38 simulated growth tube geometry ($D = 6.3$ mm and $L_{ini} = 30$ mm) is an optimized choice for current vWCPC flow
39 and temperature settings. The current simulation can more realistically represent the $D_{p,ke1}$ for 7 nm vWCPC and
40 also achieved a good agreement with the 2 nm setting. Using the new simulation approach, we provide an
41 optimized operation setting for the 7 nm setting. This study will guide further vWCPC performance optimization
42 for applications requiring precise particle detection and atmospheric aerosol monitoring.

43 **1 Introduction**

44 Aerosols, defined as any solid or liquid particles suspended in air, are one of the fundamental components of the
45 atmosphere and have a significant impact on air quality, climate change and human health (Seinfeld et al., 2016;
46 Anderson et al., 2020; Lighty et al., 2000; Pöschl, 2005; Prather et al., 2020; Li et al., 2017; Paasonen et al., 2013;
47 Darquenne, 2012). However, accurate and comprehensive monitoring of aerosol particles is challenging because
48 aerosol particle sizes and number concentrations vary widely both spatially and temporally (Davidson et al., 2005;
49 Yu and Luo, 2009; Krudysz et al., 2009). Airborne measurements and characterization, therefore, are often
50 required to capture the vertical profiles and horizontal variability of atmospheric aerosols.

51
52 In understanding the variability of atmospheric aerosol and determining the size distribution and number
53 concentration of aerosols, laminar-flow, butanol-based Condensation Particle Counters (CPCs) used in
54 conjunction with differential mobility analyzers (DMAs) can provide real-time measurements of airborne particles
55 and are widely used by effectively exploiting the working principle of condensation growth (Ahn et al., 1990,
56 Ahn et al., 1990; Hermann et al., 2007; Kangasluoma and Attoui, 2019; Mordas et al., 2008; Sem, 2002;
57 Wiedensohlet et al., 1997). However, conventional butanol CPCs face difficulties in characterizing particles below
58 3 nm in size. In addition, health and safety risks, such as the odor, flammability and toxicity of the butanol, are an
59 issue for many deployments in offices, homes, aircraft, and other inhabited locations. These limitations have led
60 directly to researchers designing advanced aerosol instruments that can be more widely used in both atmospheric
61 environments and laboratory studies.

62
63 In 2005, Hering and Stolzenburg (2005) developed a continuous-flow, water-based laminar condensation particle
64 counter (WCPC) (Hering et al., 2005; Hering and Stolzenburg, 2005), which uses distilled water as the working
65 fluid to avoid the health and safety concerns. It was also found to have comparable performance to butanol-based
66 CPCs in previous studies (Biswas et al., 2005; Franklin et al., 2010; Iida et al., 2008; Kupc et al., 2013; Liu et al.,
67 2006; Mordas et al., 2008). A modified version of the WCPC featuring an additional new moderator section has
68 been developed (Hering et al., 2014). With this new moderated approach, the initiator provides water vapor for
69 particle activation while the moderator provides distance and time for particle growth. This improved water CPC
70 achieves the same peak supersaturation and similar droplet growth while reducing the water vapor, particle loss,
71 and side effects of heating the flow in the earlier version of WCPC. Furthermore, a versatile WCPC was then
72 developed capable of particle detection near 1 nm without using a filtered sheath flow. The operating temperatures
73 can also be adjusted in accordance with the cut-point desired (Hering et al., 2017).

74

75 Since water-based CPCs have comparable performance to butanol-based CPCs while also offering the advantage
76 of avoiding health and safety risks, it is desirable to explore advanced water-based CPCs in a broader range of
77 environmental and energy applications. To improve the detection performance of the vWCPC, we need to identify
78 the effects of operational factors and geometry. However, the limited analysis of relevant temperature and
79 geometric parameters in the vWCPC makes it challenging to control condensational growth conditions. In
80 addition, the inlet pressure effect is another critical factor affecting the detection efficiency of vWCPCs. The
81 potential of using vWCPC for airborne deployment or other lower pressure monitoring has not been fully explored.
82 Mei et al. (2021) found that the counting efficiency of the vWCPC 3789 operated at the factory settings decreased
83 with decreasing the operating pressure, particularly at operating pressures below 700 hPa. However, determining
84 how to reduce the lower detection limit under various ambient pressures also needs to be investigated.

85

86 Due to the complex matrix of geometry, operating temperature, and inlet pressure parameters in vWCPCs,
87 modeling studies are advantageous in determining and optimizing the detection efficiency of vWCPCs. The
88 Graetz model was first used by Stolzenburg (1988) to examine the detection of ultrafine particles in CPCs. In
89 recent years, COMSOL Multiphysics® has been widely used to simulate coupled heat, mass, and momentum
90 transfer problems associated with complex geometries in CPCs. Moreover, COMSOL has advantages in
91 interfacing with post-processing software such as MATLAB™. A series of parametric analyses for butanol CPCs
92 were simulated using COMSOL to investigate the performance of particle activation and droplet growth (Hao et
93 al., 2021; Attoui, 2018; Kangasluoma et al., 2015; Barmounis et al., 2018; Thomas et al., 2018). Our previous
94 work (Hao et al., 2021) first demonstrated that the COMSOL results neglecting the temperature dependence of
95 vapor thermodynamic properties and axial diffusion, agree with the Graetz solution used by Stolzenburg (1988).
96 Considering temperature dependence of vapor thermodynamic properties and axial diffusion can generate more
97 accurate results that can guide the optimization of CPC designs. Previous research using COMSOL to examine
98 vWCPC performance has been limited. Bian et al. (2020) compared two-stage and three-stage operating
99 temperature methods for growth tubes and parameters such as flow rate and temperature difference to obtain the
100 ideal activation and final growth sizes. Mei et al. (2021) used COMSOL aiding to examine how inlet pressure
101 affects particle activation in the vWCPCs. However, the lack of thorough and systematic examination of vWCPC
102 performance using COMSOL leaves it unclear on how well the vWCPC will perform in multiple complex research
103 areas and applications, such as at reduced atmospheric pressure levels.

104

105 In this study, we thoroughly determined the saturation profile, activation efficiency, and droplet growth for
106 varying airborne operations through numerical simulation of laminar flow vWCPC in COMSOL and experimental
107 validation of a commercial vWCPC (TSI Model 3789). By mapping vWCPC performance in the modeling, the
108 effects of various operational factors, such as inlet pressures (30 - 101 kPa), growth tube diameter and initiator
109 length, and temperature gradients on particle activation and droplet growth, were investigated. In addition, detailed
110 modeling methods are outlined below. The detection efficiency was also examined in the experimental and
111 COMSOL modeling work. The results of this study will guide further optimization of the performance of vWCPCs
112 for accurate detection of particles and atmospheric aerosol measurement applications.

113

114 **2 Methods**

115 **2.1 Numerical simulation**

116 **2.1.1 COMSOL setup**

117 The finite element COMSOL simulation software (COMSOL Multiphysics 5.3a, COMSOL Inc, Stockholm,
118 Sweden) can handle a variety of fields including, but not limited to, electromagnetics, fluid dynamics, heat
119 transfer, chemical reactions, and structural mechanics. Here, a two-dimensional axisymmetric model is developed
120 to simulate fluid flow in a cylindrical tube. The heat, momentum, and mass transfer equations are solved for
121 incompressible parabolic flow. This COMSOL model follows the three-stage tube of the versatile water-based
122 CPC (TSI Inc, Shoreview, MN, USA) described by Hering et al. (2017), which consists of a fully developed
123 laminar flow tube that can be separated into a cool-wall conditioner region, a warm-wall initiator region, and a
124 cool-wall moderator region, where r is the radial coordinate of the tube diameter and z is the axial coordinate of
125 the tube length (**Fig. 1a**). At the inlet of the conditioner tube, sampled aerosols are fed and saturated with water
126 vapor before entering the initiator region. The manufacturer provides two default cut-off diameter settings: 2 and
127 7 nm configurations based on the characteristics introduced by Kangasluoma et al. (2017). This study used the 7
128 nm configuration as an example to demonstrate the simulation mapping effort. The methodology can also be used
129 for other targeted cut-off sizes. The tube diameter (D) is 6.3 mm, the conditioner length (L_{con}) is 73 mm, the
130 initiator length (L_{ini}) is 30 mm, and the moderator length (L_{mod}) is 73 mm. The default settings are (**Table 1**): the
131 conditioner temperature (T_{con}) is 30 °C, the initiator temperature (T_{ini}) is 59 °C, and the moderator temperature
132 (T_{mod}) is 10 °C. The aerosol flow rate (Q_v) is 0.3 L min⁻¹. The relative humidity (RH) of inlet flow is set at 20%,
133 and the water vapor is assumed to be saturated at the wall. The inlet pressure (P) is 101 kPa. To investigate how
134 the vWCPC performance depends on these parameters, we simulate a wide range of values for mapping the

135 vWCPC geometry, working temperature conditions, and inlet pressure, as discussed in Section 2.1.4 for the tasks
136 in this study.

137

138 In this COMSOL model, the coupled heat transfer and fluid flow are first solved by the conjugate heat transfer
139 module, and then the mass transfer of the water vapor is solved based on the obtained temperature and flow field.
140 Lastly, the particles are introduced from the inlet of the vWCPC and are considered diluted species that follow
141 the convective diffusion equation in the simulation, which is numerically solved to calculate the temperature,
142 supersaturation, and water vapor concentration profiles (**Fig. 1**). Regarding the initial and boundary value settings,
143 the inflow temperature is set to an ambient temperature of 25 °C, and wall temperature is set to the default factory
144 settings described above and changed as the experimental conditions changed for mapping performance. The
145 simulated temperature and concentration fields are then imported into MATLAB™ R2022b (The MathWorks,
146 Inc., Natick, MA, USA) and interpolated at any given point in the r - z plane. COMSOL Multiphysics 5.3a with
147 MATLAB allows us to adjust geometry, modify physics settings, perform parametric studies, control solvers, and
148 post-process the results.

149

150 **2.1.2 Theory of particle activation**

151 Particle activation is key to the evaluation of CPC performance. Particle activation within the vWCPC depends
152 on the degree of supersaturation, namely the saturation ratio (S) of water vapor, which is the ratio of the partial
153 pressure of the water vapor (p) to the saturation vapor pressure of the water vapor (p_s) for the given flow
154 temperature (T), calculated by

$$S = \frac{p}{p_s} \quad (1)$$

155 The spatial profile of S within the vWCPC allows us to calculate the Kelvin effect, the homogeneous nucleation,
156 and further condensational particle growth, as discussed in Section 2.1.3. The Kelvin effect is dependent upon
157 thermodynamic principles and described as the Kelvin equivalent size ($D_{p, \text{kel}}$), the minimum diameter of a particle
158 that can be activated for condensation growth. It is determined by water surface tension (σ), water molecular
159 volume (v_m), the Boltzmann constant (k), temperature (T) and the saturation ratio (S) calculated at each location
160 within the initiator,

$$D_{p, \text{kel}} = \frac{4\sigma v_m}{kT \ln(S)} \quad (2)$$

161 The Kelvin equivalent size is inversely proportional to the distribution of saturation ratio, where the greater the
162 saturation ratio, the smaller the size of the particles that can be activated. In other words, the smaller the particle,
163 the higher the degree of supersaturation required to activate growth. When particle size (D_p) is above $D_{p, \text{kel}}$, the
164 particle can be successfully activated and grown by water vapor condensation, while when D_p is below $D_{p, \text{kel}}$, the
165 particles cannot be activated. **Fig. 1b - 1e** show examples of saturation ratio, Kelvin equivalent size, water vapor
166 concentration, and temperature profiles within the simulated geometry at the default temperature condition of T_{con}
167 = 30 °C, $T_{\text{ini}} = 59$ °C, $T_{\text{mod}} = 10$ °C, respectively.

168
169 It is worth noting that $D_{p, \text{kel}}$ varies at different locations of the initiator due to the spatial variation of temperature,
170 surface tension and saturation ratio. We observed the potential particle activation in the moderator by simulation
171 results. However, only the Kelvin equivalent size in the initiator was considered in this work. Although the
172 particles were activated in the moderator, particle detection was unlikely due to droplet growth being the dominant
173 water vapor sink in the initiator. Thus, in reality, the actual supersaturation in the moderator may be different, and
174 the activation of smaller particles will be hindered by droplet growth (Hering et al., 2014; Hering et al., 2017).
175 Note that the $D_{p, \text{kel}}$ in the conditioner region is blank in color due to no particles being activated in this region (S
176 ≤ 1). Particles near the wall of the initiator, where there is a lower S , are more difficult to activate due to the
177 larger $D_{p, \text{kel}}$. This difference can be explained by the water mass and heat diffusivity differences. As the colder,
178 water-saturated flow passes through the growth tube, the mass transport of water vapor is faster than the heating
179 of the flow from the wall because the mass diffusivity of water vapor is higher than the thermal diffusivity of air,
180 producing a maximum supersaturation of water vapor at the centerline of the tube. As a result, the seed particles
181 entering near the centerline of the growth tube are activated in the warmer initiator. One comparison of the
182 saturation ratio and Kelvin equivalent size along the centerline ($r = 0$) is shown in **Fig. S1a and S1b**. We observed
183 the appearance of a double-peaked saturation ratio curve. Again, only the Kelvin equivalent size in the initiator
184 was considered in this work due to insufficient water vapor and droplet growth in the moderator. Note that the
185 solute effect is negligible under the water-based condensation particle growth and is not included in the following
186 simulation. As shown in **Fig. S2**, around 1% variation was observed in the final droplet size by adding the solute
187 effect into the droplet growth simulation.

188

189 The activation efficiency of particles with a size of D_p in vWCPC is derived using an approach similar to our
 190 previous work (Hao et al., 2021), which is calculated by the ratio of the number concentration of the activated
 191 particles over the total particle number concentration in the growth tube. The activation efficiency is calculated as

$$\eta_{\text{act}} = \frac{\int_0^{R_{\text{act}}} 2\pi r w N dr}{Q_v N_0} \quad (3)$$

192 where w is the velocity along the axial direction, N is the concentration of particles, both at the axial location of
 193 $z = Z_{\text{act}}$. R_{act} is the maximum radius of the contour corresponding to $D_{p,\text{kel}} = D_p$. N_0 is the particle concentration
 194 at the inlet of the conditioner. Q_v is the flow rate through the vWCPC. An example of activation efficiency as a
 195 function of particle diameter D_p can be found in **Fig. S1c**. Note that the calculation of the activation efficiency in
 196 Eq. (3) does not consider the diffusion loss of the particles in the conditioner. Since this model does not have
 197 sheath flow that minimizes the diffusion losses and constrains the aerosols to the high supersaturation region, the
 198 activation efficiency cannot reach 100%. On the activation curve, there are two points of interest: minimum
 199 activated size, $D_{p,\text{kel},0}$ (the smallest size of particle that can be activated in the initiator), and 50% cut-off
 200 size, $D_{p,\text{kel},50}$ (the size of a particle with 50% activation efficiency extracted from the activation efficiency curve).
 201 $D_{p,\text{kel},50}$ is essential to the performance of CPCs because it determines the general particle size range in which
 202 the CPC can confidently measure. $D_{p,\text{kel},50}$ can be used as the representative of particle activation efficiency
 203 performance. Furthermore, note that negligible homogeneous nucleation occurs in the growth tube of the initiator
 204 and moderator under all tested conditions in this study, which means the total nucleation rate is equal to or less
 205 than one particle per second (1 s^{-1}).
 206

207 2.1.3 Theory of droplet growth

208 Once the particles are activated, their condensational growth along their trajectories in the initiator region was
 209 simulated by numerically solving two coupled differential equations in MATLABTM. First, the evolution of
 210 droplet diameter (D_p) can be estimated by (Seinfeld and Pandis, 2008; Wang et al., 2017)

$$\frac{dD_p}{dt} = \frac{4D'_v M (C - C_d)}{\rho D_p} \quad (5)$$

211 where M and ρ represent the molecular weight and density of water, D'_v represents the modified diffusivity of the
 212 water vapor accounting for the non-continuum effect of the particles and is given by $D'_v = D_v \left[1 + \right.$

213 $\frac{2D_v}{\alpha_c D_p} \left(\frac{2\pi M}{RT} \right)^{1/2} \Big]^{-1}$, where D_v is the diffusivity of the water vapor, and α_c is the mass accommodation coefficient of
 214 water and is assumed as 1. C_d represents the equilibrium water concentration at the surface of the growth droplets
 215 and is given by $C_d = C_s(T_d) \exp\left(\frac{4\sigma M}{\rho R T_d D_p}\right)$, where C_s is saturation water concentration, T_d is the droplet surface
 216 temperature, which is governed by

$$\frac{dT_d}{dt} = \frac{3}{c_p \rho D_p} \left(H_{\text{vap}} \rho \frac{dD_p}{dt} - 4k'_g \frac{(T_d - T)}{D_p} \right) \quad (6)$$

217 where c_p , ρ , and H_{vap} are the heat capacity, density, and heat of vaporization of water. k'_g represents the modified
 218 thermal conductivity of air accounting for the non-continuum effects in heat transfer and is calculated as $k'_g =$
 219 $k_g \left[1 + \frac{2k_g}{\alpha_T D_p \rho_g c_{p,g}} \left(\frac{2\pi M_g}{RT} \right)^{1/2} \right]^{-1}$, where M_g , ρ_g , $c_{p,g}$, and k_g are the molecular weight, density, heat capacity, and
 220 thermal conductivity of air. α_T is the thermal accommodation coefficient and was assumed to be 1 (Seinfeld and
 221 Pandis, 2008; Wang et al., 2017).

222
 223 In the simulation of droplet growth, the Brownian motion of the particles inside the conditioner before activation
 224 is neglected. Since there is also no electric field inside the conditioner, we assume that the particles move axially
 225 along the vWCPC with a velocity of w . Therefore, Eqs. (5) and (6) can be converted to a function of axial location
 226 using $w = dz/dt$, and the droplet size and droplet surface temperature at the end of the moderator ($z = L_{\text{ini}} +$
 227 L_{mod}) can be calculated. To determine the final droplet growth size at the outlet of the moderator, the
 228 condensational growth of 8 nm particles as seed particles was studied along the centerline ($r = 0$) of the growth
 229 tube in this work. An example of droplet growth size as a function of distance along the axis of the tube for the
 230 default temperature condition of $T_{\text{con}} = 30$ °C, $T_{\text{ini}} = 59$ °C, $T_{\text{mod}} = 10$ °C can be found in **Fig. S1d**. Note that in
 231 this simulation, we do not consider the increase in the equilibrium vapor pressure due to warming of the flow from
 232 condensational heat release, which would further reduce the droplet growth.

233

234 **2.1.4 Simulation plan**

235 **Table 1** summarizes the operating temperatures, inlet pressures, and geometric parameters for each simulation
 236 task characterizing the vWCPC in this study. In Task 1, we first conducted two matrix combinations of absolute
 237 conditioner and initiator operating temperatures, with an interval of 5 °C in each region, for a total of nine different
 238 combinations. Task 2 investigates how raising or lowering the temperature midpoints (T_{mid}), the average value

239 between the conditioner temperature and initiator temperature ($\frac{T_{con}+T_{ini}}{2}$) affects particle activation and droplet
240 growth. In addition, different inlet pressures are also included when comparing different temperature midpoints.
241 Task 3 examines the effect of inlet pressure at the default conditioner temperature of 30 °C and the customized
242 conditioner temperature of 27 °C. Tasks 4 and 5 further test how the vWCPC geometry, including tube diameter
243 D , and initiator length L_{ini} , affects the performance of the vWCPC. These simulations reveal optimal working
244 conditions and effects for the influence of each parameter.

245

246 **2.2 Experimental measurement**

247 The modified vWCPC 3789 (TSI Inc, Shoreview, MN, USA) was tested in this study. Given that the standard
248 commercially available vWCPC 3789 is not specifically designed for low-pressure applications, some
249 modifications were made to the instrument for this study. First, the vWCPC 3789 was tested to ensure its vacuum
250 tightness, and the exhaust line was filtered and returned back to the make-up flow line after a flow buffer. Second,
251 we added pressure transducers to the inlet and exhaust lines of the vWCPC 3789 to monitor the inline pressure
252 variation. Note that the aerosol flow rate through the condenser tube and optical particle detector was 0.3 L min⁻¹.
253 When we operated with 0.6 L min⁻¹ inlet aerosol flow, we blocked the make-up flow port. Details of operating
254 flow, temperatures and geometry are provided in Section 2.1.1. Further specifics can be found in our previous
255 study (Mei et al., 2021).

256

257 Two methods were used to generate the test aerosol: an atomizer coupled with a furnace; and a glowing wire
258 generator (GWG). Ammonium sulfate (AS) has been commonly used for CPC characterization and was the tested
259 material used in this study (Hering et al., 2014; Kangasluoma et al., 2017). It was dissolved into deionized water
260 for aerosol generation using atomization techniques. To increase the aerosol number concentration for particles
261 less than 30 nm, polydisperse AS aerosols were also passed through a tube furnace generator at the temperature
262 of 500 °C and flow rate of 1.5 lpm (Lindberg/Blue, Thermal Scientific, TX, USA) to shift the size distribution to
263 a smaller size. A lab-built GWG was also used to generate aerosol particles in size range between 2.5 – 16 nm.
264 More details about the generator can be found in Attoui (2022). Using the low-pressure testing setup shown in
265 **Fig. 2**, the counting efficiency of a vWCPC 3789 was measured between 51 and 91 kPa for AS particles of 3 – 20
266 nm (mobility diameter) and NiCr oxidants of 2.5 -16 nm. The aerosol concentrations in this test were maintained

267 in the range of $2 \times 10^4 - 4 \times 10^4 \text{ cm}^{-3}$. During the testing, the temperature variations in the conditioner and moderator
268 were less than $0.5 \text{ }^\circ\text{C}$, and the initiator temperature had a variation of $1 \text{ }^\circ\text{C}$.

269

270 **3 Results and discussion**

271 **3.1 Comparisons of temperature-dependent particle activation and droplet growth performance**

272 Selection of appropriate operating temperatures in CPCs is essential because the supersaturation is significantly
273 temperature dependent, which affects particle activation and further droplet growth. In addition, the temperature
274 difference between different regions in CPCs is an important factor in controlling supersaturation. For this reason,
275 the minimum activation size for butanol-based CPCs is significantly impacted by the temperature difference
276 between the saturator and condenser and the raising or lowering of the temperature midpoints, as has been
277 demonstrated by many previous studies (Hermann and Wiedensohler, 2001; Kangasluoma and Attoui, 2019;
278 Barmounis et al., 2018; Kuang et al., 2012). The results showed that in the butanol-based CPCs, the greater the
279 temperature difference between the saturator and condenser, the higher the degree of supersaturation, and the
280 smaller particle could be activated.

281

282 The numerical COMSOL model was used to compare operating temperature-dependent particle activation and
283 droplet growth performance in the vWCPC, including minimum activated size ($D_{p,ke1,0}$), 50% cut-off size
284 ($D_{p,ke1,50}$), and final growth particle size at the outlet of the moderator along the centerline ($r = 0$) (D_d), as shown
285 in **Fig. 3**. Previous studies confirmed that the centerline saturation rate is insensitive to the moderator wall
286 temperature (Hering et al., 2014; Bian et al., 2020). Thus, this study investigated moderator temperature (T_{mod})
287 at the constant of $10 \text{ }^\circ\text{C}$, conditioner temperature (T_{con}) at the range of $25 - 35 \text{ }^\circ\text{C}$, initiator temperature (T_{ini}) at
288 the range of $55 - 65 \text{ }^\circ\text{C}$. Note that conditions that can lead to a lower $D_{p,ke1,50}$ value and larger droplet growth size
289 are favored for improving the performance of the vWCPC.

290

291 Firstly, in order to compare the effect of the conditioner temperature T_{con} , we varied T_{con} from $25 \text{ }^\circ\text{C}$ to $35 \text{ }^\circ\text{C}$
292 while maintaining the same initiator temperature T_{ini} and moderator temperature T_{mod} . The results show that
293 $D_{p,ke1,0}$ increased significantly by 5.21, 3.32, and 2.27 nm at the initiator temperature T_{ini} of 55, 60, and $65 \text{ }^\circ\text{C}$,
294 respectively, and $D_{p,ke1,50}$ increased significantly by 6.65, 4.16, and 2.75 nm at the initiator temperature T_{ini} of 55,
295 60, and $65 \text{ }^\circ\text{C}$, respectively. The final droplet size D_d decreased by approximately $1 \text{ } \mu\text{m}$ at all the initiator

296 temperature T_{ini} of 55, 60, 65 °C. The lower conditioner temperature provided higher saturation ratios in the
297 initiator and more water vapor for particle growth, which is also consistent with the previous growth tube
298 simulation (Bian et al., 2020; Mei et al., 2021). Secondly, the initiator temperature T_{ini} was increased from 55 °C
299 to 65 °C while maintaining the same conditioner temperature T_{con} and moderator temperature T_{mod} , $D_{\text{p,ke1,0}}$ was
300 decreased by 1.90, 3.74, and 4.87 nm at the conditioner temperature T_{con} of 25, 30, and 35 °C, respectively,
301 $D_{\text{p,ke1,50}}$ was decreased significantly by 2.32, 3.74, and 6.21 nm at the conditioner temperature T_{con} of 25, 30, and
302 35 °C, respectively, and D_{d} was increased by 2.9 μm at all the conditioner temperature T_{con} of 25, 30, and 35 °C.
303

304 By comparing all combinations, we can find that the activated size becomes smaller as the temperature difference
305 between T_{con} and T_{ini} increases, indicating that the temperature differences between the conditioner and initiator
306 dominate the particle activation. After comparing the temperature differences, we conclude that the higher the
307 temperature between these two regions, the better the particle activation. However, in the actual operation of the
308 CPC, one also needs to ensure that the self-nucleation in the growth tube is minimized ($<1 \text{ s}^{-1}$) so that the CPC
309 does not report false particle counting. The homogeneous nucleation rate is less than 10^{-8} s^{-1} at all tested conditions,
310 meaning that the temperatures can be further adjusted to optimize particle activation and droplet growth.
311 Moreover, D_{d} is the greatest, with a maximum size of 12.20 μm , at the temperature setting of 25–65–10 °C among
312 all these temperature conditions. We also found that the effect of the initiator temperature on droplet growth was
313 greater than that of the conditioner temperature. Thus, the following section examines the effect of temperature
314 midpoint on the vWCPC performance.
315

316 **3.2 Effect of temperature midpoint on particle activation and droplet growth performance**

317 In addition to temperature difference, lowering the temperature midpoint was also found to cause higher
318 supersaturation. However, there is limited research on how the performance of the vWCPC changes under various
319 temperature midpoints and especially under different inlet pressures, which will be important for applications such
320 as atmospheric airborne deployment and environmental monitoring at elevated locations. Here, we compared the
321 particle activation and droplet growth performance for three different temperature midpoints (40 °C, 43 °C, and
322 46 °C) of conditioner temperature (from 24 °C to 30 °C) and initiator temperature (56 °C to 62 °C) at a wide range
323 of inlet pressures from 30 kPa to 101 kPa, as shown in **Fig. 4**. The temperature difference ΔT between the
324 conditioner and the initiator was kept constant at 32 °C. The moderator temperature remained constant at 10 °C
325 in all simulations.

326

327 Results show that the minimum activated size $D_{p,ke1,0}$ decreases from 5.15 nm to 4.96 nm, and the 50% cut-off
328 size $D_{p,ke1,50}$ decreases from 5.88 nm to 5.65 nm as the temperature midpoint decreases from 46 °C to 40 °C, as
329 shown in **Fig. 4a and 4b**. Thus, a slight control of the minimum activation size can be achieved by lowering the
330 temperature midpoint. Higher supersaturation can explain this slight decrease in the initiator, which also agrees
331 with the previous growth tube WCPC simulation (Bian et al., 2020). On the other hand, a slight increase of 0.07,
332 0.1, and 0.14 nm occurs in $D_{p,ke1,0}$, and negligible change in $D_{p,ke1,50}$ by reducing the inlet pressure from 101 to
333 30 kPa under three temperature midpoints of 40 °C, 43 °C, and 46 °C. This slight increase is due to a low peak
334 supersaturation caused by the decrease in inlet pressure. Since water vapor transport is faster than heat transport,
335 the decrease in pressure affects the location of the peak supersaturation, whereas the degree of the supersaturation
336 does not change significantly.

337

338 In **Fig. 4c**, we show that the droplet growth is not significantly dependent on raising or lowering the temperature
339 midpoint. By lowering the temperature midpoint by 6 °C, D_d becomes smaller by approximately 14%. When
340 studying the effect of inlet pressure on the D_d , unlike $D_{p,ke1,0}$ and $D_{p,ke1,50}$, D_d decreases substantially from 101
341 to 30 kPa, by approximately 45%. Limited by the optical chamber design of the commercial vWCPC, the droplets
342 smaller than 8 μm may not gain sufficient pulse signal to get counted. Thus, when operating under lower inlet
343 pressure, the apparent cut-off size of vWCPC may increase and needs to be further determined. The reduced
344 pressure strongly affects the final droplet growth size, likely due to the faster water vapor and heat transport at
345 reduced pressure. The thermal and mass diffusivity is inversely proportional to the pressure in the growth tube,
346 resulting in insufficient time for droplet growth. In addition, we found that with the lower inlet pressure, the final
347 droplet size reduced more notably. For example, D_d decreased from 10.6 to 10.4 μm (by 0.2 μm) as pressure
348 reduced from 101 to 91 kPa, while D_d decreased from 7.2 to 6.1 μm (by 1.1 μm) as pressure reduced from 41 to
349 30 kPa. The difference can be explained by the competition between heat and water vapor transport. The mass
350 transport of water vapor is faster than the heat flow from the wall because the mass diffusivity of water vapor is
351 higher than the thermal diffusivity of air. Therefore, by reducing the inlet pressure, water vapor transport becomes
352 even faster than heat transfer due to the water vapor diffusivity and air thermal diffusivity being inversely
353 proportional to the pressure, further shortening the time for particle growth at high supersaturation. This
354 observation demonstrates for the first time how the final droplet size is affected by raising or lowering temperature
355 midpoints at standard and various reduced inlet pressure conditions in the vWCPC.

356

357 **3.3 Effect of inlet operation pressure on particle activation and droplet growth performance**

358 With the advantages of safe, eco-friendly and readily available distilled water as working fluid in the vWCPC,
359 applying the vWCPC in various inlet pressures will expand broader applications such as atmospheric airborne
360 aerosol measurements. Here, we examined the effect of inlet pressure on minimum activated size, $D_{p,ke1,0}$, 50%
361 cut-off size, $D_{p,ke1,50}$, and final growth particle size at the outlet of the moderator along the centerline ($r = 0$), D_d
362 from 30 to 101 kPa for two different temperature settings: the conditioner, initiator, and moderator temperatures
363 were 30, 59, and 10 °C and 27, 59, and 10 °C in **Fig. 5**.

364

365 **Figs. 5a** and **5b** show $D_{p,ke1,0}$ and $D_{p,ke1,50}$ as a function of inlet pressure, relatively greater (2 - 3%) $D_{p,ke1,0}$ was
366 observed at reduced inlet pressures at both conditioner temperatures of 27 °C and 30 °C. This increase is because
367 the supersaturation value at reduced pressure is lower than the saturation profile under standard conditions. We
368 also found that the saturation profile peaked earlier, closer to the entrance of the initiator in the low-pressure
369 condition. In addition, greater $D_{p,ke1,50}$ is observed at reduced inlet pressures due to the reduction of the saturation
370 peak at both conditioner temperatures of 27 °C and 30 °C. Again, the difference at reduced inlet pressure can be
371 explained by the competition from heat transfer and water vapor transport, as discussed in Section 3.2. For this
372 reason, greater $D_{p,ke1,50}$ was observed at reduced inlet pressures. This reduction of saturation peaks is also
373 associated with the growing droplet size decreasing with the decrease in the operating pressure. Again, lowering
374 the conditioner temperature while maintaining the same temperature difference between the initiator and the
375 moderator provided higher saturation ratios in the initiator over all pressure ranges.

376

377 **Fig. 5c** shows the final droplet size as a function of inlet pressure. When the conditioner temperature is 27 or 30
378 °C, a lower final droplet size (~ 40 % reduction in the droplet size) was observed at a reduced inlet pressure of 30
379 kPa, indicating insufficient droplet growth happens at low-pressure conditions, which is consistent with the
380 previous study that insufficient droplet growth becomes more significant under low-pressure operation (Mei et
381 al., 2021).

382

383 Furthermore, in addition to showing consistent results with the previous study (Mei et al., 2021), our simulations
384 enhance guidance for aircraft applications under extreme conditions, which can be achieved by simulating low
385 atmospheric pressure at 30 kPa. As shown in Section 3.5, by comparing with experimental results, our simulations

386 can provide more accurate estimates of particle activation and droplet growth to guide vWCPC for low-pressure
387 applications.

388

389 **3.4 Effect of tube diameter and initiator length on particle activation and droplet growth performance**

390 The geometry in CPCs also impacts the CPC activation performance and particle growth due to the changed
391 supersaturation and temperature profile in the tube, as discussed in previous studies (Hao et al., 2021; Hering et
392 al., 2014). Here, we examined how the tube diameter D and the length of initiator L_{ini} in the vWCPC may affect
393 the minimum activated size, $D_{p,ke1,0}$, 50% cut-off size, $D_{p,ke1,50}$, and final growth particle size at the outlet of the
394 moderator along the centerline ($r = 0$), D_d under default temperature $T_{con} - T_{ini} - T_{mod}$ of 30–59–10 °C, standard
395 inlet pressure and reduced pressure of 51 kPa using the numerical COMSOL model. Again, one needs to note that
396 conditions that can lead to a lower $D_{p,ke1,0}$ and $D_{p,ke1,50}$ value and larger droplet growth size are favored for
397 improving the performance of the vWCPC.

398

399 We examined four values of D from 4 to 8 mm, and five values of L_{ini} from 10 to 50 mm, shown in **Fig. 6** and
400 **Fig. 7**, respectively. The results indicate that a smaller D can slightly decrease in $D_{p,ke1,0}$ approximately 0.03 nm,
401 while no noticeable changes on $D_{p,ke1,50}$ at the standard pressure (**Figs. 6a and 6b**). By reducing the tube diameter,
402 the flow speed in the tube increases under the same flow rate, reducing the residence time of the condensed water
403 vapor. This reduction in residence time suppresses homogeneous nucleation in the initiator. Unlike our previous
404 study on CPCs (Hao et al., 2021), the homogeneous nucleation rate is minimal in vWCPC and has no impact on
405 the temperature difference compared to butanol-based CPCs. For this reason, this suppressed homogeneous
406 nucleation has limited effects on $D_{p,ke1,0}$ and $D_{p,ke1,50}$. However, the increase of the flow speed will significantly
407 limit the time for droplet growth, as will be discussed later. At the reduced pressure of 51 kPa, a smaller D can
408 slightly decrease in $D_{p,ke1,0}$ approximately 0.08 nm, and a slight decrease of approximately 0.03 nm on $D_{p,ke1,50}$
409 (**Figs. 6a and 6b**). Overall, the reduction in pressure plays a more critical role in negatively impacting CPC
410 performance for relatively large tube diameters. Note that buoyancy effects (Roberts and Nenes, 2005) may be
411 critical for large temperature differences if the tube diameter is too large, which is not discussed in the study.

412

413 On the other hand, we found that reducing L_{ini} leads to limited effects on $D_{p,ke1,0}$ and $D_{p,ke1,50}$, except for the
414 shortest initiator length of 10 mm at the standard pressure (**Figs. 7a and 7b**). The effect of these relatively long

415 initiator lengths is limited because the degree of supersaturation is determined by the absolute temperature of the
416 tube flow. The temperature difference did not change in the standard pressure and reduced pressure, leaving both
417 $D_{p,ke1,0}$ and $D_{p,ke1,50}$ unchanged. However, at the initiator length of 10 mm, $D_{p,ke1,0}$ and $D_{p,ke1,50}$ increase
418 significantly due to insufficient water vapor diffusion before passing through the next moderator region, resulting
419 in a lower peak supersaturation along the centerline than for longer initiators operating at the same temperature
420 (Hering et al., 2014). At reduced pressure, $D_{p,ke1,0}$ and $D_{p,ke1,50}$ have no noticeable changes at all tested initiator
421 lengths, however, this is due to the sufficient diffusion of water vapor, from which the water transport is faster
422 than at the standard pressure. Again, if the initiator is longer, the difference in peak supersaturation will be
423 negligible, while the peak temperature along the centerline and the amount of added water vapor will be higher.
424 Thus, for relatively short initiators, such as 20 mm used in the simulation, one can provide all the necessary water
425 vapor to create the same peak supersaturation as for the longer initiators. However, the droplet growth size will
426 be smaller (**Fig. 7c**), mainly due to the shorter growth time discussed later.

427

428 With regard to the performance of particle growth, an increased D and an increased L_{ini} are beneficial for
429 improving the performance of particle growth in vWCPC at both standard and reduced pressure (**Figs. 6c and 7c**).
430 An increased D implies a decrease in the flow velocity through the high saturation region, greatly increasing the
431 time for particle growth and contributing to the sufficient growth of the particles. **Fig. 6c** shows that the final
432 droplet sizes increase significantly from 6.72 μm to 13.88 μm when D is increased from 4 mm to 8 mm at the
433 standard pressure and increase from 4.92 to 10.78 μm at the reduced pressure of 51 kPa. The final droplet size is
434 found to be 2 – 3 μm smaller than the standard pressure at the reduced pressure. Similarly, a longer L_{ini} also leads
435 to a larger droplet growth size. The final droplet size increases from 8.66 μm to 11.26 μm when L_{ini} is increased
436 from 10 mm to 50 mm at the standard pressure and from 7.40 to 8.29 μm at the reduced pressure of 51 kPa (**Fig.**
437 **7c**). This increase is likely due to the longer growth time of the longer initiator. Also, we found that the final
438 droplet size increases much faster at shorter initiator lengths than at lengths above 20 mm, which tells us that the
439 droplet size is more susceptible to the effects of initiator length below 20 mm. This difference also means that
440 having a longer length does not further enhance the final size of the particle growth.

441

442 In addition to the performance of particle activation, it is crucial to evaluate the droplet growth performance of
443 complex geometries in the vWCPC. The time that allows the activated particle to grow in the initiator and

444 moderator is an important droplet growth kinetics assumption, representing the vWCPC performance of droplet
445 growth. We use t_g to represent allowed particle growth time, approximated with Eq. (7).

$$t_g \sim D^2 L^* / Q_v \quad (7)$$

446 where L^* indicates the length of the initiator and moderator beyond the point of activation. This equation can
447 explain that the residence time is impacted more by the change in tube diameter than the initiator length. The
448 allowed particle growth time as a function of final growth particle size at the outlet of the moderator along the
449 centerline ($r = 0$), D_d is shown in **Fig. S3**. The longer the allowed particle growth time, the larger the droplet
450 growth size. Based on this droplet growth time shown, the vWCPC geometry of D and L_{ini} are not independent
451 variables if we consider the droplet growth for further particle detection.

452

453 **3.5 Experimental measurement validation of detection efficiency**

454 Experimental validation is essential for simulation work in terms of the accuracy of the simulation model and the
455 correctness of the underlying trends. Furthermore, validation and good agreement will provide well-guided
456 approaches for future applications. Therefore, we compare the experimental and simulation results of the counting
457 efficiency and detection efficiency of vWCPC set in two default configurations (2 nm and 7 nm) at different
458 conditioner and initiator temperature settings and different low-pressure conditions in **Fig. 8**.

459

460 As the experimental results in a previous study (Mei et al., 2021) are shown in **Fig. 8a**, the counting efficiency of
461 vWCPC 3789 varied with different working pressures (51, 71 and 91 kPa) when the conditioner temperature is
462 27 °C, the initiator temperature is 59 °C, and the moderator temperature is 10 °C. The y-axis error bar indicates
463 the standard deviation of the counting efficiency averaged over ~ 5 min of sampling time at a 1 Hz sampling rate.
464 The results indicate that the counting efficiency slightly decreases with the decrease in the operating pressure of
465 51, 71 and 91 kPa, which shows the same trend in **Fig. 8b**. In addition, the cut-off size in both experimental and
466 simulation results are in the range of 5 - 7 nm, which is also an acceptable range within error when compared to
467 commercial vWCPC detection efficiency.

468

469 **Fig. 8c** and **8d** compare the counting efficiency and detection efficiency versus particle size from experimental
470 and simulation results under initiator temperatures of 75 and 90°C and pressure of 91 and 51 kPa for the 2 nm
471 configuration. As expected, the detection efficiency of both experimental and simulated results is lower at the
472 temperature $T_{con} - T_{ini} - T_{mod}$ of 7-75-10 °C at a lower pressure (at 51 kPa). When the temperature $T_{con} - T_{ini} - T_{mod}$

473 is 7-90-10 °C, the higher detection efficiency is seen, and the effect of inlet pressure becomes insignificant.
474 However, it is not feasible to maintain 90 °C when operating under lower pressure, such as 51 kPa. Thus, the
475 default 2 nm setting in vWCPC can only be operated near sea level. One should note that although we do not
476 present many simulations for the 2 nm configuration, what we learned from the modeling results with the 7 nm
477 setting will guide future simulations with the 2 nm setting.

478

479 By comparing with counting efficiency curves, the present simulations can more realistically represent the $D_{p, \text{kel}}$
480 for 7 nm vWCPC, which also achieved a good agreement with the 2 nm setting. Thus, from the merits of the
481 results of this work, we can find that this work not only provides guidance for 7 nm, but this trend can also help
482 guide one for other desired cut-off sizes.

483

484 **4 Conclusions**

485 This study evaluated the particle activation and droplet growth performance of a commercial versatile water CPC
486 using COMSOL in combination with MATLAB data processing. In addition, validation experiments on the
487 detection efficiency of the modified vWCPC (TSI 3789) agreed with the simulation work. Increasing the
488 temperature difference between T_{con} and T_{ini} and lowering the temperature midpoint can enhance particle
489 activation at both standard and reduced ambient pressure conditions. However, the lack of droplet growth becomes
490 more significant under low-pressure operations, which might affect the apparent counting efficiency of the
491 vWCPC due to the limited measurable size range of the optical chamber. Additionally, reducing the diameter of
492 the growth tube slightly improved particle activation but significantly reduced the droplet growth, while increasing
493 the initiator length had a limited effect on improving the performance of the vWCPC at both standard and reduced
494 pressure.

495

496 This simulation realistically represents the $D_{p, \text{kel}}$ for 7 nm vWCPC and shows that the current growth tube
497 geometry is an optimized choice for aerosol measurements. This study will guide further vWCPC performance
498 optimization for applications requiring precise particle detection and atmospheric aerosol monitoring.
499 Furthermore, the developed simulation capability provides a vital tool for the aerosol community to understand
500 the effects of temperature, pressure, and geometry on vWCPC behavior. The knowledge gained will guide the
501 field deployment of vWCPC on the ground level and airborne measurements. However, limitations of this
502 modeling approach likely lie in the computational capacity and the difference from actual flow and temperature

503 profile distribution in the growth tube (due to non-ideal temperature control and system configuration). Thus,
504 several future experimental studies will be carried out to investigate the performance of the vWCPC.

505

506 **Data availability**

507 The vWCPC data in the study are available upon request to Fan Mei (fan.mei@pnnl.gov).

508

509 **Author contributions**

510 WH, FM, and YW designed the research. FM carried out the measurements. WH led the simulation and data
511 analyses. WH led the writing, with significant input from FM and YW as well as further input from all other
512 authors. SH, SS, BS, and JT provided suggestions on the revision.

513

514 **Competing interests**

515 Susanne Hering has a commercial interest in the success of the vWCPC instrument.

516

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519

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Figures and Tables of

Mapping the performance of a versatile water-based condensation particle counter (vWCPC) with COMSOL simulation and experimental study

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Table of Nomenclature

c : Molecular concentration of the water vapor [mol m^{-3}]

C_d : Equilibrium water concentration at the surface of the growth droplets [mol m^{-3}]

C_s : Saturation water concentration [mol m^{-3}]

c_p : Heat capacity of the water [$\text{J K}^{-1} \text{kg}^{-1}$]

$c_{p,g}$: Heat capacity of air [$\text{J K}^{-1} \text{kg}^{-1}$]

D_v : Diffusivity of the water vapor [$\text{m}^2 \text{s}^{-1}$]

D'_v : Modified diffusivity of the water vapor [$\text{m}^2 \text{s}^{-1}$]

D : Diameter of the growth tube in vWCPC [m]

D_p : Particle size [m]

D_d : Final growth droplet size in vWCPC [m]

$D_{p, \text{kel}}$: Size of particle that can be activated according to the Kelvin equation [m]

$D_{p, \text{kel}, 0}$: Smallest size of particle that can be activated in the vWCPC [m]

$D_{p, \text{kel}, 50}$: Size of particle that has a 50% activation efficiency [m]

H_{vap} : Heat of vaporization of water [J kg^{-1}]

k : Boltzmann constant, 1.38×10^{-23} [J K^{-1}]

k_g : Thermal conductivity of air [$\text{W m}^{-1} \text{K}^{-1}$]

k'_g : Modified thermal conductivity of air [$\text{W m}^{-1} \text{K}^{-1}$]

L_{con} : Length of the conditioner [m]

L_{ini} : Length of the initiator [m]

L_{mod} : Length of the moderator [m]

L^* : Length of the initiator and moderator beyond the point of activation [m]

m : Molecular mass of water [kg]

M : Molecular weight of water [kg mol^{-1}]

M_g : Molecular weight of air [kg mol^{-1}]

n : Molecular concentration of the water vapor [molecules m^{-3}]

N : Concentration of the particles at the axial location of $z = Z_{\text{act}}$ [particles m^{-3}]

N_0 : Concentration of particles at the inlet of the conditioner [particles m^{-3}]

p : Partial pressure of the water vapor [Pa]

p_s : Saturation vapor pressure of the water vapor [Pa]

P : Inlet pressure in vWCPC [Pa]

Q_v : Flow rate through the vWCPC [$\text{m}^3 \text{s}^{-1}$]

r : Radial coordinate of the tube diameter of the vWCPC [m or as otherwise explicitly designated]

R : Gas constant [$\text{J mol}^{-1} \text{K}^{-1}$]

R_{act} : Maximum radius of the contour corresponding to $D_{p, \text{kel}} = D_p$ [m]

S : Saturation ratio [1]

t : Allowed particle growth time [s]

T : Flow temperature in the CPC [K]

T_{con} : Conditioner temperature [K]

T_{ini} : Initiator temperature [K]

T_{mid} : Temperature midpoint corresponding to $\frac{T_{\text{con}}+T_{\text{ini}}}{2}$ [K]

T_{mod} : Moderator temperature [K]

T_{d} : Droplet surface temperature [K]

v_{m} : Molecular volume of the water vapor [m^3]

w : Velocity along the axial direction in the vWCPC [m s^{-1}]

z : Axial coordinate of the tube length of the vWCPC [m or as otherwise explicitly designated]

Z_{act} : Axial location corresponding to $r = R_{\text{act}}$ [m]

α_{c} : Mass accommodation coefficient of water [1]

α_{T} : Thermal accommodation coefficient of air [1]

η_{act} : Activation efficiency [1]

ρ : Density of water [kg m^{-3}]

ρ_{g} : Density of air [kg m^{-3}]

σ : Surface tension of water [N m^{-1}]

ΔT : Temperature difference between conditioner temperature and initiator temperature [K]

Table 1. Parameters of vWCPC for different simulation tasks. Note that the default settings of VWPCPC are: the conditioner temperature (T_{con}) is 30 °C, the initiator temperature (T_{ini}) is 59 °C, and the moderator temperature (T_{mod}) is 10 °C. The aerosol flow rate (Q_v) is 0.3 L min⁻¹. The relative humidity (RH) of inlet flow is set at 20%, and the water vapor is assumed to be saturated at the wall. The inlet pressure (P) is 101 kPa (1 atm).

Task	T_{con} (°C) - T_{ini} (°C)	T_{mod} (°C)	T_{mid} (°C)	P (kPa)	D (mm)	L_{ini} (mm)
1	(25, 30, 35) - (55, 60, 65)	10	-	101	6.3	30
2	24 - 56, 27 - 59, 30 - 62	10	40, 43, 46	30 - 101	6.3	30
3	27 - 59, 30 - 59	10	-	30 - 101	6.3	30
4	30 - 59	10	-	51, 101	4, 5, 6.3, 8	30
5	30 - 59	10	-	51, 101	6.3	10, 20, 30, 40, 50

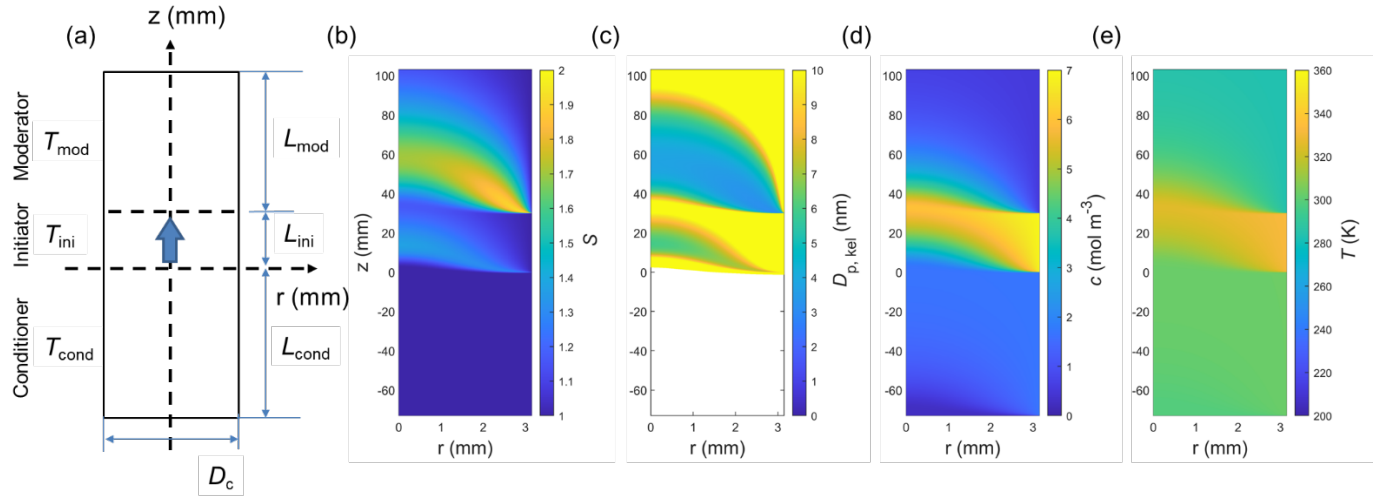


Figure 1. Geometry of vWCPC used in COMSOL simulation and spatial distribution of saturation ratio and Kelvin equivalent size under 30–59–10 °C temperature setting. (a) Geometry of the vWCPC used in COMSOL simulation, (b) Spatial distribution of saturation ratio (S , color contour plot), (c) Spatial distribution of Kelvin equivalent size ($D_{p, kel}$, color contour plot), (d) Spatial distribution of water vapor concentration (c , color contour plot), and (e) Spatial distribution of temperature (T , color contour plot). Note that the color of $D_{p, kel}$ in the conditioner region is blank because no particles are activated in this region.

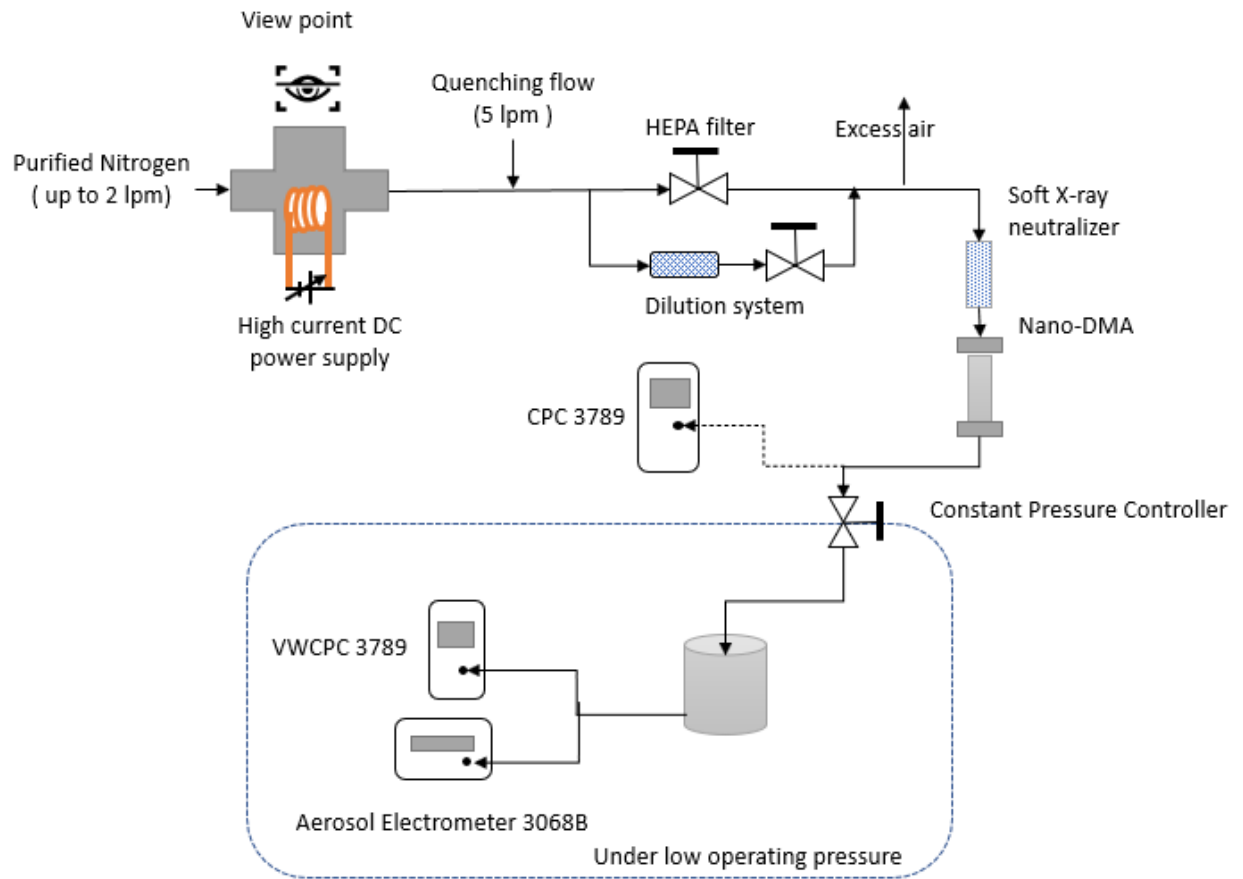


Figure. 2. Schematic diagram of the vWCPC 3789 and flow system under the low-pressure testing.

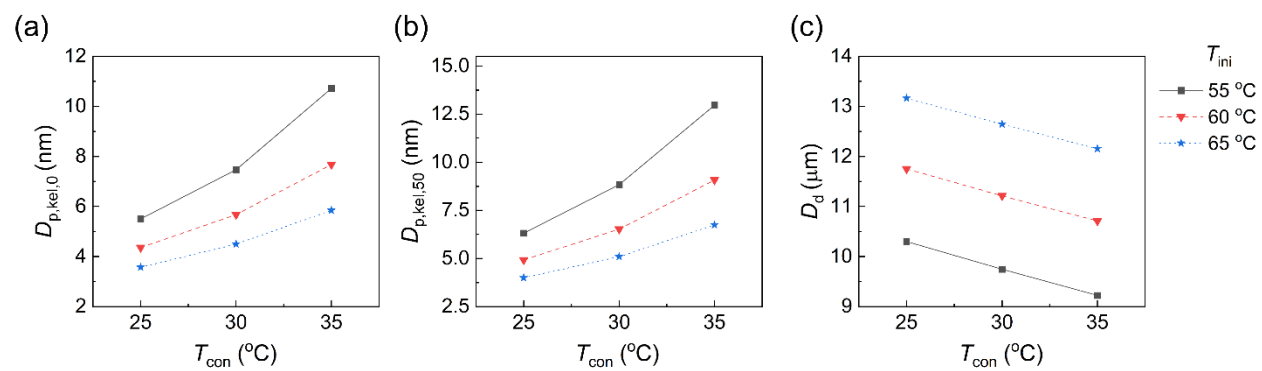


Figure 3. Effect of conditioner (T_{con}) and initiator temperature (T_{ini}) on (a) minimum activated size, $D_{p,kei,0}$, (b) 50% cut-off size, $D_{p,kei,50}$, and (c) final growth particle size at the outlet of the moderator along the centerline ($r = 0$), D_d . The condensational growth of 15 nm particles was tested as seed particles.

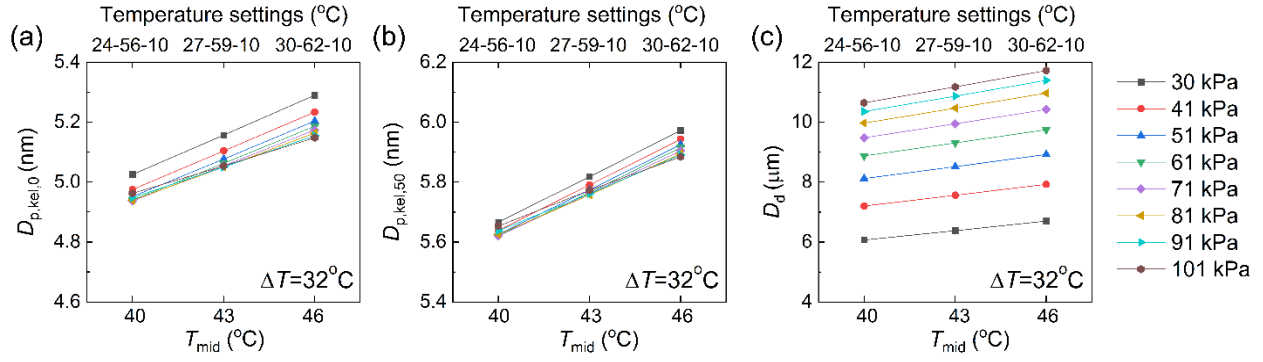


Figure 4. Effect of temperature midpoints at 40 °C, 43 °C, and 46 °C at $T_{con}-T_{ini}-T_{mod}$ of 24–56–10 °C, 27–59–10 °C and 30–62–10 °C with a constant temperature difference of 32 °C on (a) minimum activated size, $D_{p,kei,0}$, (b) 50% cut-off size, $D_{p,kei,50}$, and (c) final growth particle size at the outlet of the moderator along the centerline ($r = 0$), D_d . The condensational growth of 8 nm particles was tested as seed particles.

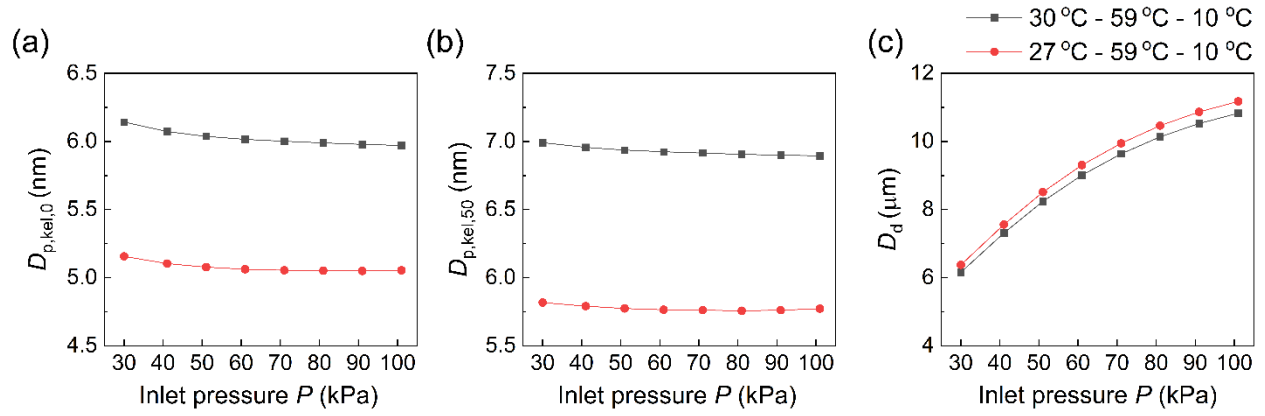


Figure 5. Effect of inlet operation pressure at $T_{\text{con}}-T_{\text{ini}}-T_{\text{mod}}$ of 27-59-10 °C and 30-59-10 °C on (a) minimum activated size, $D_{p,ke1,0}$, (b) 50% cut-off size, $D_{p,ke1,50}$, and (c) final growth particle size at the outlet of the moderator along the centerline ($r = 0$), D_d . The condensational growth of 8 nm particles was tested as seed particles.

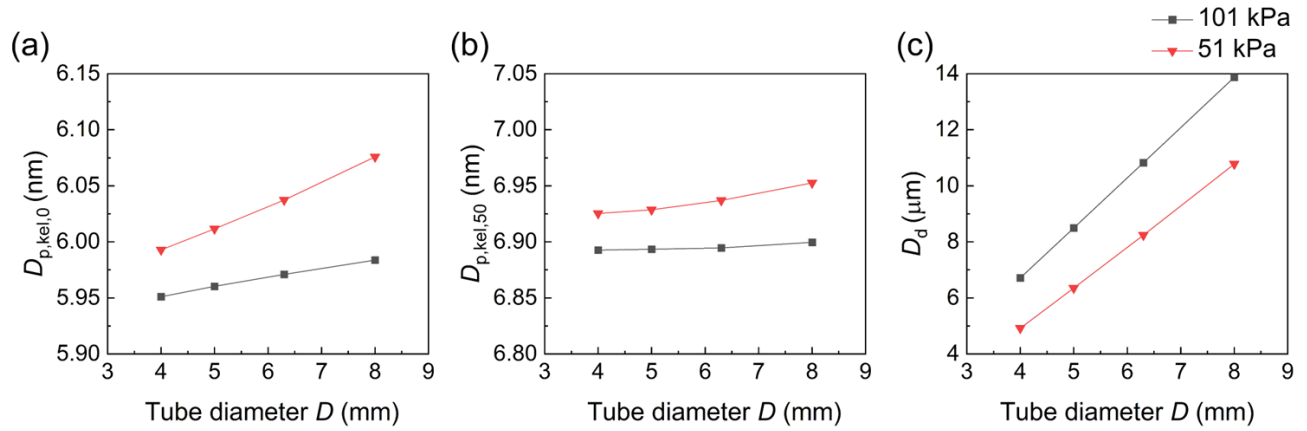


Figure 6. Effect of tube diameter (D) at 51 kPa and 101 kPa on (a) minimum activated size, $D_{p,ke1,0}$, (b) 50% cut-off size, $D_{p,ke1,50}$, and (c) final growth particle size at the outlet of the moderator along the centerline ($r=0$), D_d . The condensational growth of 8 nm particles was tested as seed particles.

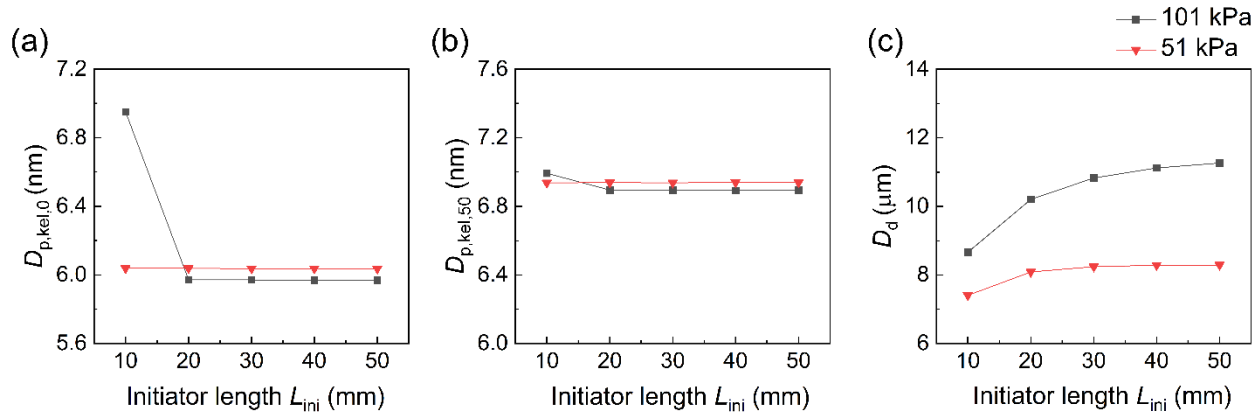


Figure 7. Effect of initiator length (L_{ini}) at 51 kPa and 101 kPa on (a) minimum activated size, $D_{p,ke1,0}$, (b) 50% cut-off size, $D_{p,ke1,50}$, and (c) final growth particle size at the outlet of the moderator along the centerline ($r = 0$), D_d . The condensational growth of 8 nm particles was tested as seed particles.

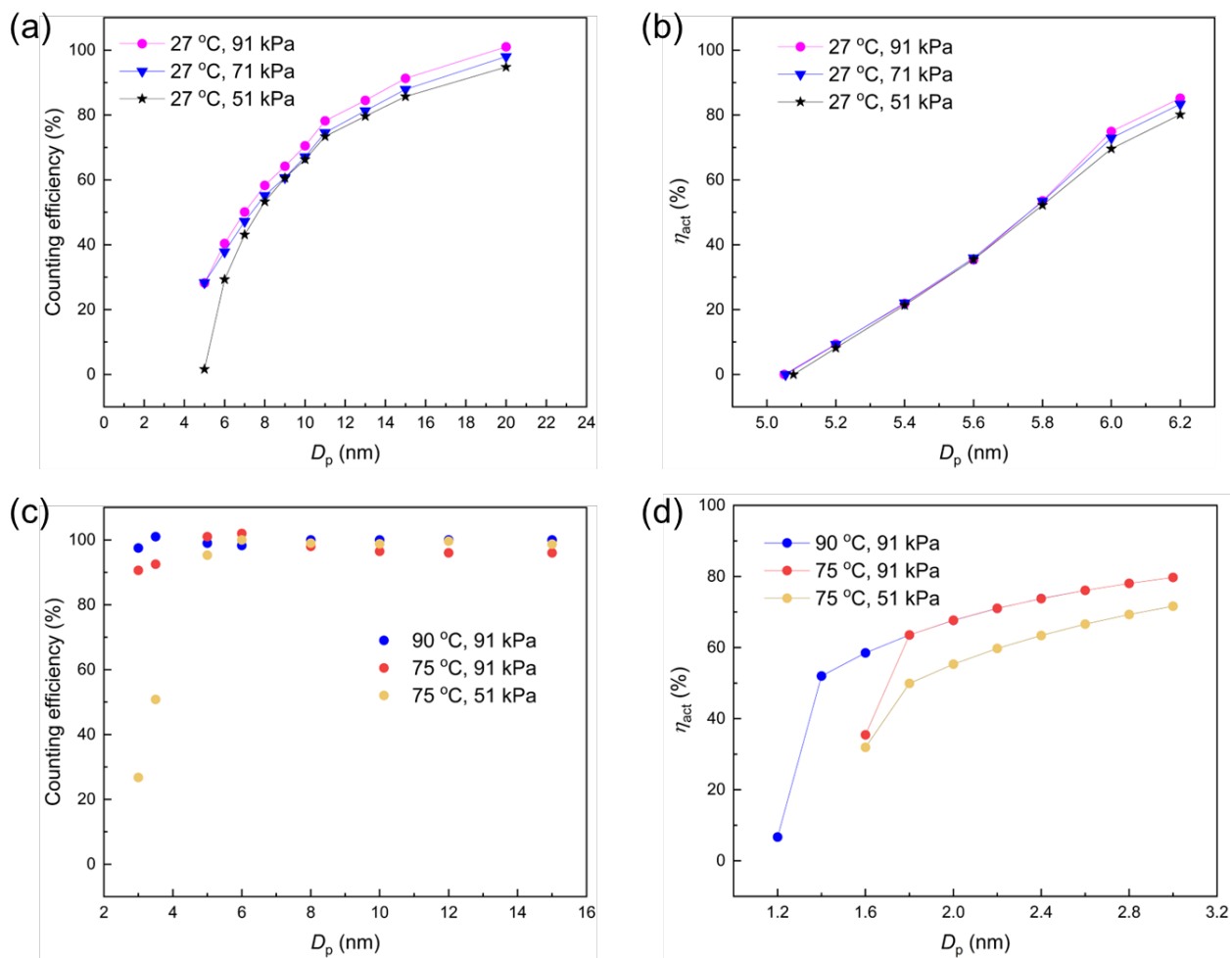


Figure 8. vWCPC operation validation: (a) the counting efficiency of experimental results as a function of particle size under the conditioner temperature of 27 °C and pressure of 91, 71, and 51 kPa for the 7 nm configuration, (b) the detection efficiency of simulation results as a function of particle size under the conditioner temperature of 27 °C and pressure of 91, 71, and 51 kPa for the 7 nm configuration, (c) the detection efficiency of experimental results as a function of particle size under initiator temperatures of 75 and 90°C and pressure of 91 and 51 kPa for the 2 nm configuration, and (d) the detection efficiency of simulation results as a function of particle size under initiator temperatures of 75 and 90°C and pressure of 91 and 51 kPa for the 2 nm configuration.