Performance Evaluation of a Virtual Impactor with an Additional Pretreatment Structure for Particle Separation

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ABSTRACT

In this paper, a proposed method based on a microfluidic chip that can arrange the collected particles in radial positions according to their sizes before virtual impactor separation was introduced. The main objective of this paper was to design a novel micro-separator structure composed of two major parts: a virtual impactor, and a pretreatment that consists of a sheath flow and a backward-facing step flow configuration. In the separation process, the particles firstly were aggregated on the middle channel by the sheath flow, then ordered in radial position of backward-facing step flow, and finally separated in virtual impactor. To determine the effects of the pretreatment, both simulations and experiments were conducted. A parameter optimization was performed on the micro-separator where the cut-off size of the virtual impactor was 2.5 μm . The results demonstrated that when the flow ratio between inlet flow rate and the total flow rate was set to 50% and the expansion ratio (E_r) was 2. The cut-off size of the micro-separator was reduced by 20.77% from 2.436 μm to 1.93 μm , and the wall loss (WL) was acceptable compared with the result only using PM_{2.5} virtual impactor. The effect of pretreatment on PM₁ and PM₅ virtual impactor also saw an improvement of collection efficiency even when the additional pretreatment had varying Reynold numbers and nozzle sizes. Accordingly, the stk_{50} value was reduced by 44.39% from 0.669 to 0.372 by adding pretreatment before the virtual impactor.

Keywords: Microfluidics, Pretreatment, Particle arrangement, Virtual impactor, Collection efficiency

1 INTRODUCTION

Bioaerosols such as viruses, bacteria, and fungal spores pose a great threat to human lives and health, especially for patients with respiratory diseases (Blachere *et al.*, 2009; Tsuda *et al.*, 2013; Cui *et al.*, 2015). The dispersed bioaerosols can also lead to an outbreak of epidemics in some areas due to the quick spread of fungi and viruses (Nasrabadi *et al.*, 2017). Therefore, a high-efficiency separation device is the foundation for detecting different sizes of particles.

Nowadays, owing to the simple operation and principle, virtual impactor has attracted much interest in aerosol science and widely used to classify particles according to their sizes (Marple *et al.*, 1980; Zhang *et al.*, 2016). To improve the collection efficiency of the impactor, various parameters of inertial impactor have been studied. Such as Reynolds number (Marple *et al.*, 1974; Marple *et al.*, 1975), the jet-to-plate distance (Marple *et al.*, 1967; Grinshpun *et al.*, 2005), the particle density (Huang *et al.*, 2002), gravitational force (May *et al.*, 1975; Huang *et al.*, 2001) and etc. Besides, some novel structures have also been discovered to improve the collection efficiency curve. For example, Cheon *et al.* (2017) added an additional punched impaction plate between

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the nozzle outlet and the existing impactation plate to improve the collection efficiency and reduce the cut-off diameter by changing the particle trajectories. Lee *et al.* (2019) also proposed an inertial impactor with vertical annular nozzle to separate particles, as a result, it will increase the pressure slightly but increase collection efficiency significantly. However, there is also a significant problem called wall loss, it is caused by the trapped particles on the walls of the virtual impactor. To decrease the wall loss, a two-partitioned inlet which can supply both aerosol and clean air in particle separation process has been placed before the virtual impactor (Chen *et al.*, 2016; Zahir *et al.*, 2019; Lim *et al.*, 2020), it can also adjust the flowrate ratios of aerosol to clean air to seek an optimal proportion to reduce the cut-off diameter efficiently.

Meanwhile, the combination of impactor and microfluidic chip has been used extensively to realize the airborne microorganism separation. Such as, Kang *et al.* (2012) proposed a microscale cascade impactor system for bioaerosol sampling and separation. Liu *et al.* (2016) presented a high-efficiency collection system based on microfluidic chip to measure the airborne mineral dust. Most importantly, impactor based on microfluidic chip can also overcome the limitations of bioaerosols real-time detection directly. For instance, Kang *et al.* (2014) integrated inertial impactation and mini-fluorescent microscopy to realize the airborne pathogenic microorganism's real-time detection successfully. Kim *et al.* (2009) integrated the electrode pair and virtual impactor based on microfluidic chip together to accelerate the electrical particle and improve the collection efficiency. Xu *et al.* (2013) observed the fine particle behavior successfully in microfluidic chip when it passed a triangular cylinder in a laminar airflow. Wang *et al.* (2020) replaced the impactation plate by a low-pressure collection chamber which eliminates the re-entrainment and bounce effects of particles, and finally confirmed a satisfied collection efficiency. However, most of the abovementioned studies does not include the improvement of the collection efficiency curve.

In this study, a novel separator structure based on microfluidic chip consists of two major parts: a virtual impactor, and a pretreatment that consists of a sheath flow and a backward-facing step flow configuration was proposed. To improve the collection efficiency curve and decrease wall loss rate, both simulations and experiments were performed to seek for optimum parameters. During the particle separation process, the distribution of the collected particles can realize an order pattern (the collected particles sequence according to their size in radial position) from a disordered pattern (all the particles were randomly distributed when they were collected) by the combination of a sheath flow and a backward-facing step flow. Then, the performance of the micro-separator was evaluated by detecting the monodispersed polystyrene latex (PSL) particles. It was expected that the new pretreatment structure can be applied to improve the performance of the existing virtual impactor, and enhance the measurement accuracy for the detection object assessment.

2 MATERIALS AND METHOD

2.1 Micro-separator

The detailed structure of the proposed micro-separator is schematically shown in Fig. 1(a), in which the micro-separator consists of pretreatment structure and virtual impactor, the pretreatment structure contains two parts including sheath flow area and backward-facing step flow area. In the working process, the aerosol sample with different particle sizes was firstly aggregated in the middle of the microchannel due to the sheath flow (Chen *et al.*, 2016). Then, different aerosols were dispersed in a backward-facing step flow radial position according to their size. Therefore, the particle sequencing can be realized by the combination of sheath flow and backward-facing step flow. Finally, all particles were separated by the following virtual impactor. The results were validated by numerical analysis and compared to the experimental results. The geometric parameters of the proposed micro-separator are shown in Table 1. In this section, the thickness of the microchannel was determined to be 160 μm to prevent a strong Dean Vortex effect because the maximum sample flow rate is 96.5 mL min^{-1} . The parameters of the backward-facing step flow were obtained by numerical simulation. The jet-to-plate distance was determined by the width of the injection nozzle (W_4), and the S/W_4 ratio is within 1.2 to 1.8 (Loo *et al.*, 1988). In this study, the width of the injection nozzle was set to 290 μm , so the jet-to-plate distance was 435 μm . The photograph of the micro-separator is shown in Fig. 1(b). In addition, to analyze the

Fig. 1. (a) Schematic of the proposed micro-separator. The micro-separator consists of two parts including pretreatment and virtual impactor, and the pretreatment was separated into sheath flow and back-forward facing step flow. (b) The photograph of the micro-separator.

Table 1. The geometric parameters of the proposed micro-separator.

Description	Value (μm)
The width of inlet (W_1/W_2)	500
The thickness of the microchannel	160
The width of the channel between the sheath flow outlet and the Backward-facing step flow inlet (W_3)	500
The distance between the sheath flow outlet and the Backward-facing step flow inlet (S)	5000
The width/length of the injection nozzle (W_4)	290
The length of the backward-facing step flow (L)	5000
The width of the minor/major flow (W_5/W_6)	435

performances of the collection efficiency and the WL of the proposed micro-separator, additional enrichment microfluidic chips, as shown in Fig. S1, were placed after the outlets of the micro-separator to collect the separated particles. In this process, the retention of the particles in the micro-separator was recorded as WL , and the particles collected in the enrichment microfluidic chip was used to calculate the collection efficiency of the micro-separator. The enrichment microfluidic chip comprised an inlet, a collection area, and an outlet.

2.2 Pretreatment

In the first part of pretreatment, the sheath flow was set symmetrically to squeeze the sample flow into the middle of the convergence channel, as shown in Fig. 2(a). The sheath flow also has a great impact on reducing the WL and the influences caused by the random distribution of the initial position due to the particle aggregation effect (Chen *et al.*, 2016). In the second part of pretreatment, the backward-facing step flow was designed after sheath flow. The working mechanism of the backward-facing step flow can be explained as follows: the trajectories of particles past the backward-facing step flow vary from the streamline due to particle inertia which is mainly determined by the particle size. Particles with different sizes that past the backward-facing step flow were shown in Fig. 2(b), it was observed that, due to the strong inertia force and radial drag force, particle trajectories will diverge in terms of their sizes in radial position, therefore, small particles have greater tendency to follow the airflow, while the trajectories of larger ones will not change due to the sufficient particle inertia (Klemz *et al.*, 2017). As a result, particles collected by micro-separator will be separated in radial position. Here, particles with different sizes experienced different focusing patterns and exhibited different trajectories.

Fig. 2. (a) The trajectories of particles in the sheath flow. In this figure, N represents the number of particles that flow into the particle inlet. (b) The trajectories of particles in the backward-facing step flow.

Additionally, the separation efficiency was influenced by the expansion ratio (E_r), which was defined as Eq. (1),

$$E_r = H_2/H_1 \quad (1)$$

In this study, H_1 is the half-width of the particle inlet, H_2 is the distance between centerline and boundary of the backward-facing step flow.

2.3 Virtual Impactor

In this section, the virtual impactor is an aerodynamic device that classifies particles in terms of their size. The working principle of the virtual impactor is simple, when particles flow into the virtual impactor, and the majority particles larger than the cut-off size are collected in the minor channel, the majority particles smaller than the cut-off size are passed through (The cut-off size is the aerodynamic diameter with a collection efficiency of 50%) (Kim *et al.*, 2009). In the virtual impactor design, their aerodynamic diameter was defined as (Lee *et al.*, 2019):

$$d_a = d_p \sqrt{\frac{\rho_p C_c(d_p)}{\chi \rho_a C_c(d_a)}} \quad (2)$$

where d_p is particle size, ρ_p is the particle density, χ is the dynamic shape factor, ρ_a is the standard particle density (i.e., 1000 kg m^{-3}), and $C_c(d_p)$ is the Cunningham slip correction factor (Kang *et al.*, 2014), which can be expressed by Eq (3):

$$C_c = 1 + 0.5Kn_p[2.34 + 1.05\exp(-0.195Kn_p)] \quad (3)$$

where Kn_p is particle Knudsen number, which is defined as $2\lambda/d_p$, where λ is the mean free path of the air molecule. The Stokes number (Kang *et al.*, 2014) was defined as the following Eq. (4).

$$stk = \frac{\rho_p d_p^2 C_c V}{9\mu W} \quad (4)$$

where V is the air velocity at the inlet, μ is the air viscosity, W is the hydraulic diameter of the nozzle. Then, the cut-off size (d_{50}) can be obtained by Eq. (5).

$$d_{50} = \sqrt{\frac{9\mu W stk_{50}}{\rho_p C_c V}} \quad (5)$$

where stk_{50} represents the Stokes number that corresponds to 50% particle collection efficiency.

2.4 Numerical Analysis

The effects of pretreatment on particle separation were evaluated by using computational fluid dynamics (CFD) simulation. In this study, COMSOL Multiphysics was utilized for fluid flow simulation.

The simulation conditions were set to a steady, two-dimensional simulation model under laminar and incompressible flow, which can quickly provide insights into the physical phenomena of the designed micro-separator. The particle density was set at 1050 kg m^{-3} . In this design, the cut-off sizes of PM_{10} , $\text{PM}_{2.5}$, and PM_5 were obtained with the same virtual impactor by changing the flow rate. According to the simulation results, the flow rates of the major and minor flow in PM_{10} , $\text{PM}_{2.5}$, and PM_5 were set as: 45 mL min^{-1} and 6.5 mL min^{-1} , 9 mL min^{-1} , and 1 mL min^{-1} , 1.8 mL min^{-1} and 0.3 mL min^{-1} , respectively, according, the flow rate ratios between the major flow and minor flow are about 7, 9 and 6, respectively. Then, the micro-separator was also simulated by changing these flow rates to verify the pretreatment effects, and the flow rate of the particle inlet was set to half of the total flow rate. The boundary condition of sheath flow inlet was set as pressure-inlet, and the other boundary conditions were set as no-slip wall. Smaller grid sizes can provide more accurate simulation results, but the greater the number of the grids, the longer the simulation time takes. Therefore, it is important to select suitable grids number to simulate, in this study, about 20000 grids were used. During the simulation, the particle samples with sizes of 0.2, 0.5, 0.7, 0.8, 0.9, 1, 1.1, 1.5, 1.8, 2, 2.5, 3, 3.5, 4, 4.5, 5, 5.5, 6.0, 7.0, 8.0, 9.0 and $10 \mu\text{m}$ were chosen, and 500 particles with uniform size and density were arranged at regular intervals from the center of particle inlet to the edge. Then, calculate the flow field, and the discrete phase model (DPM) with the Lagrangian approach was applied to simulate particle trajectories. The parametric studies were performed to optimize the pretreatment structure by varying the ratio of the inlet flow rate and total flow rate and changing the E_r of the backward-facing step flow. Finally, the particles collected in the major and minor flow were counted respectively, and the collection efficiency of a given particle size is calculated using the following equation:

$$E(\%) = \frac{N_{\text{Minor}}}{N_{\text{Major}} + N_{\text{Minor}}} \times 100\% \quad (6)$$

where $E(\%)$, N_{Major} , and N_{Minor} are the collection efficiency (%), the numbers of the given particle size collected in the major flow, and minor flow, respectively. Then, the WL of a given particle size can be calculated from Eq. (7):

$$WL = \left(1 - \frac{N_{\text{Major}} + N_{\text{Minor}}}{N_{\text{Total}}} \right) \times 100\% \quad (7)$$

where N_{Total} is the total number of the given particle size in the micro-separator and the enrichment microfluidic chip.

2.5 Experimental

Fig. 3 shows a schematic diagram of the experimental setup for the performance evaluation of the virtual impactor and the corresponding micro-separator. PSL spheres with diameters of 0.2, 0.5, 0.8, 1.0, 1.5, 2.0, 2.5, 3.0, and $4.0 \mu\text{m}$ were used, the density of PSL particle is 1050 kg m^{-3} . Firstly, the air was injected by the compressor through the HEPA filter into the aerosol generator (24 Jet Collision, BGI Collision) under the 3 atm for atomizing bioaerosols. Subsequently, the PSL particles flow through a diffusion dryer to remove the moisture contained in the particles, and a ^{210}Po neutralizer was placed after the diffusion dryer to remove the electrical charge of the particles. Thirdly, the sample flow into the microfluidic chip from the particle inlet at a fixed flow rate which was controlled by rotameter ($1\text{--}10 \text{ mL min}^{-1}$, $6\text{--}60 \text{ mL min}^{-1}$, measurement uncertainty is less than 0.66%), the inlets of sheath flow were connected with the HEPA filter, the excess flow was vented to the atmosphere. Particles that passed through the micro-separator were collected by enrichment microfluidic chip. Moreover, the whole flow in the microfluidic chip was controlled by three vacuum pumps which were placed after enrichment microfluidic chip. Finally, the polydimethylsiloxane (PDMS) of micro-separator and enrichment microfluidic chip were removed in the laboratory, only the microfluidic chip substrates were left and put in the scanning electron microscope (SEM, Hitachi, S-3400N) after the gold sputtering treated. Then, the images of the whole microfluidic channel were taken by SEM, and the size distribution of PSL particles was calculated based on Image Processing and Recognition.

Fig. 3. Schematic of the experimental setup.

3 RESULTS AND DISCUSSION

3.1 The Optimal Parameters of Sheath Flow and Backward-facing Step Flow

In this section, the flow ratio was defined as the flow rate of particle inlet to the total flow rate of the microfluidic chip, and E_r were optimized based on the micro-separator, in which the cut-off size of the virtual impactor is $2.5\ \mu\text{m}$.

In the sheath flow area, the sheath flow angle was 45° (Chen *et al.*, 2016). Particle trajectories were aggregated by the squeeze phenomenon caused by the sheath flow at the final state. As shown in Fig. 4(a), with increasing the flow ratio, decreased small particle collection efficiency was observed in the minor flow channel. The particle aggregation is beneficial to reduce the cut-off size, however, it has an obvious negative influence that the small particles (smaller than the cut-off size) collection efficiency is high when the flow ratio is small, which could significantly affect the target detection precision. Therefore, taking the small particle collection efficiency (lower than 16%) into consideration, the flow ratio equals 50%. Besides, the Major and Minor ratio which was defined as the flow rate of the major flow rate to the minor flow rate has been also analyzed. At a fixed total flow rate ($93.5\ \text{mL min}^{-1}$), there are four Major and Minor ratios that have been studied, as shown in Fig. 4(b), the cut-off size reduced when the ratio decreases from 10 to 4, however, the collection efficiency of relatively small particles increases with the decrease of the ratio. Then, as presented in Fig. 4(c), the variation in cut-off sizes can be obtained by changing H_2 based on the proposed micro-separator. The result shows that the cut-off size decreases with the H_2 increasing firstly, and it changes slightly when H_2 is larger than $0.5\ \text{mm}$. Therefore, H_2 was set to $0.5\ \text{mm}$, accordingly, the E_r was 2.

3.2 The Collection Efficiency and WL of the Micro-separator

In this section, the traditional PM_{10} and $\text{PM}_{2.5}$ virtual impactor and the corresponding micro-separators were also generated based on different flow rate settings. The collection efficiency curves of the traditional virtual impactor and the corresponding micro-separator obtained from the experiments were shown in Fig. 5. According to the PM_{10} impactor results in Fig. 5(a), the cut-off size was $0.989\ \mu\text{m}$ without the combination of sheath flow and backward-facing step flow, and it was reduced to $0.759\ \mu\text{m}$ by adding an extra pretreatment. Likewise, as shown in Fig. 5(b), the cut-off size of the $\text{PM}_{2.5}$ impactor was reduced from $2.436\ \mu\text{m}$ to $1.93\ \mu\text{m}$ through by applying the pretreatment. Since PSL particles larger than $4\ \mu\text{m}$ were difficult to be atomized, therefore, PM_{10} impactor with or without pretreatment was compared by using the simulation method, as shown in Fig. 5(c), the cut-off size was reduced from $4.807\ \mu\text{m}$ to $2.981\ \mu\text{m}$. Furthermore, the sharpness (σ) of the experimental curve was evaluated by the following Eq. (8) (Hinds *et al.*, 1999).

Fig. 4. Variation in cut-off size of the proposed micro-separator obtained by numerical results: (a) The effect of the flow ratio, (b) The influence of the Major and Minor Ratio, (c) The optimization of the backward-facing step flow.

$$\sigma = \sqrt{\frac{d_{84}}{d_{16}}} \quad (8)$$

where σ is the geometric standard deviation. d_{84} and d_{16} are the particle size with a collection efficiency of 84% and 16%, respectively. The GSDs of micro-separator in three different conditions were 1.24, 1.189, 1.263. The sharpness of the collection efficiency curve is higher than the curve without the pretreatment, the reason is that the particle stream will be squeezed in the middle of the microchannel when the clean air was injected from the sheath flow, then the particles with relatively small size will tend to close the edge of microchannel in backward-facing step flow, therefore, the particles with different sizes will be ordered firstly in the pretreatment structure before the virtual impactor separation, the collection efficiency will be improved compared to the disordered particles. Besides, the WL of the proposed micro-separator with different flow ratio were calculated by using Eq. (7). As shown in Fig. 5(d), the WL is less than 20%, which is acceptable (Marple *et al.*, 1991; Hyun *et al.*, 2018). Thus, the additional pretreatment was confirmed to improve the collection efficiency curve.

To investigate the cut-off size reduction mechanism of the virtual impactor with an additional pretreatment, the flow streamlines and particle trajectories in the impactor were simulated and observed in Fig. 6. In the case of virtual impactor without the pretreatment, as shown in Fig. 6(a), the flow streamlines were evenly distributed. Meanwhile, as shown in Fig. 6(b), all the particles were randomly distributed, a part of particles with enough inertia force flow into the minor flow and the others can change direction by 90° after being accelerated through the nozzle. In the case of the micro-separator, the flow streamlines were focused on the centerline firstly, then it will disperse at both sides of the channel, as shown in Fig. 6(c). The Stokes number and the inertia

Fig. 5. The collection efficiency curves of the virtual impactor and the proposed micro-separator. (a) The collection efficiency curves of the traditional PM_{10} virtual impactor and the corresponding micro-separator obtained from the experimental data; (b) The collection efficiency curves of the traditional $\text{PM}_{2.5}$ virtual impactor and the corresponding micro-separator obtained from the experimental data; (c) The simulations of the traditional PM_5 virtual impactor and the corresponding micro-separator obtained from the numerical results; (d) The WL rate of the proposed micro-separator. In this figure, the WL rate of the PM_{10} and $\text{PM}_{2.5}$ with pretreatment were experimental results, the PM_5 with pretreatment were numerical results.

force are accordingly different due to different cut-off size, the particles will diffuse according to the resultant force of radial drag force and inertia force, so the particle disperses system with the fixed trend will be formed. Due to these flows, the particles can be ordered in the middle area before the virtual impactor, as shown in Fig. 6(d), the collection efficiency was enhanced effectively by coupling the sheath flow and backward-facing step flow.

In summary, the sheath flow and the backward-facing step flow complement each other. The sheath flow has significant effects on the reduction of cut-off size by aggregating the particles in the middle of the micro-channel. Meanwhile, the setting of backward-facing step flow provides a radial drag force which is beneficial for solving the problem that small particles with high collection efficiency caused by sheath flow. By applying this pretreatment, the particle sequence was ordered according to their sizes, the cut-off size was reduced and a satisfying collection efficiency curve was also obtained.

Fig. 7 shows the simulation results of the different virtual impactor with or without the pretreatment. The Stokes number is indicated in the x-axis of the graph. The width of the nozzle, aerosol flow rate, and the corresponding nozzle Reynolds number of various virtual impactor models used in the numerical parametric study are presented in Table 2. Because the collection efficiency relates to Stokes number, the fitting curve of the virtual impactor with or without the additional pretreatment can be obtained from each case. From the fitting curve comparison, Stk_{50} is 0.669 when only using the traditional virtual impactor; Stk_{50} is 0.372 when the additional

Fig. 6. Comparison between virtual impactors with and without the additional coupling structure: (a) and (b) are streamline and particle trajectory of the traditional virtual impactor, respectively. (c) and (d) are streamline and particle trajectory of micro-separator, respectively.

Fig. 7. The comparison of the collection efficiency curves of the virtual impactor and the proposed micro-separator obtained from the numerical data.

Table 2. Nozzle sizes and aerosol flow rates assumed for the numerical parametric study.

The width of nozzle (mm)	Cut-off size (μm)	Inlet flow rate (mL min^{-1})	Total flow (mL min^{-1})	Nozzle Reynolds Number
0.29	1	45	88	465.17
	2.5	7.5	14.7	77.7
	5	2	3.9	21.19
0.35	1	47.5	99.5	465.35
	2.5	11	21.75	101.68
	5	2.95	5.5	25.77
0.52	1	115.75	227.5	797.56
	2.5	20.5	41	143.69
	5	6.5	12.25	42.88

pretreatment was added, showing a decrease of 44.39%. According to Eq. (8), the sharpness of the collection efficiency curve was estimated to be 1.384 without the additional pretreatment, while the sharpness was 1.577 with the additional pretreatment, showing an increase of 13.6%.

4 CONCLUSION

In this study, a novel method enabling particles to be arranged firstly according to the sizes before the virtual impactor separation was proposed to improve the collection efficiency curve of the traditional virtual impactor. Accordingly, a novel micro-separator was designed which consists of sheath flow, backward-facing flow, and traditional virtual impactor. As a result, the flow ratio and H_2 were optimized to 50% and 0.5 mm, respectively. The cut-off size of the proposed micro-separator was smaller than the traditional virtual impactor, and it reduces from 0.989 to 0.759 μm for PM_{10} virtual impactor, 2.436 to 1.93 μm for $\text{PM}_{2.5}$ virtual impactor, and 4.807 to 2.981 μm for PM_{5} virtual impactor. Again, the fitting curves could be observed from the collection efficiency data, resulting in $Stk_{50} = 0.669$ in traditional virtual impactor and $Stk_{50} = 0.372$ with the additional pretreatment, a decrease of approximately 44.39% was achieved. In conclusion, the development of the proposed micro-separator can be applied to increase the particle collection efficiency and enhance the measurement accuracy for target assessment.

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CONFLICTS OF INTEREST

The authors declare no conflict of interest.

SUPPLEMENTARY MATERIAL

Supplementary data associated with this article can be found in the online version at <https://doi.org/10.4209/aaqr.2020.05.0269>

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