**ABSTRACT**

This paper proposes general conditions for the simulation of aerosol jet in the air based on the Eulerian approach. The effect of the particle diameter on the dispersion was investigated. The particle velocity profiles obtained were similar to the air velocity in one-phase jets for the dilute dispersions. Along the transversal axis of the jet, the particle velocity profile assumes the gaussian form as well as the particle concentration in the centerline of the jet. On the other hand, along the longitudinal axis, the particle velocity profile is inversely proportional to the distance of the ejection point and the particle concentration has a quasi-linear behavior. Besides, the particle diameter influences the mixture behavior as the Stokes number increases. This work concludes that the Eulerian-Eulerian method is especially useful to describe aerosol jet behavior.

**Keywords**: Dispersions, Aerosol jets, Computational fluid dynamics, Eulerian approach

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**RESUMO**

Este artigo propõe condições gerais para a simulação de jatos de aerossol no ar com base na abordagem euleriana. O efeito do diâmetro das partículas na dispersão foi investigado. Os perfis de velocidade das partículas obtidos foram semelhantes aos da velocidade do ar em jatos monofásicos para as dispersões diluídas. Ao longo do eixo transversal do jato, o perfil de velocidade das partículas assume a forma gaussiana, bem como a concentração de partículas na linha central do jato. Por outro lado, ao longo do eixo longitudinal, o perfil de velocidade das partículas é inversamente proporcional à distância do ponto de ejeção e a concentração de partículas tem um comportamento quasi linear.
Além disso, o diâmetro das partículas influencia o comportamento da mistura à medida que o número de Stokes aumenta. Este trabalho conclui que o método euleriano-euleriano é especialmente útil para descrever o comportamento do jato de aerosol.

**Keywords:** Dispersões, Jatos de aerosol, Fluidodinâmica computacional, Abordagem euleriana

## 1 INTRODUCTION

Aerosol jets are mass transfer phenomena related to particle dispersion found in a wide variety of fields such as medicine, agriculture, environment, and defense. Drug delivery in human airways in the form of aerosol particles is a conventional treatment for respiratory diseases (Augusto et al. 2016; Yousefi et al. 2017). Aerosol pollution of the atmospheric air is caused by pesticide application in agriculture (Davydov et al. 2018; Gil and Sinfot 2005), industries (Emetere et al. 2015), thermal power plants (Bhaskar et al. 2017), forests fire (Zhu et al. 2018), urban traffic (Wrobel 2000), volcanoes (Tam et al. 2016), and aircraft engines (Testa et al. 2013; Makridis and Lazaridis 2019). In relation to the current global crisis of the outbreak of SARS-CoV-2 contamination, a recent study indicates that viruses like SARS-CoV-2 may remain infectious for at least 3 hours in the form of aerosols (van Doremalen et al. 2020). Consequently, several studies are discussing aerosol physics in order to take the necessary safety measures (Setti et al. 2020, Asadi et al. 2020). Atomizers may be used to produce aerosol streams, which can be employed in the microscale digital manufacturing of nanomaterials such as graphene (Secor 2018) to produce supercapacitors, transistors, displays, and sensors (Jabari and Toyserkani 2015). The comprehension of aerosol jet dynamics is also important for the design of civilian and military pyrotechnics (Ellern 1968; Shaw et al. 2016), such as hand smoke grenades. However, for all these applications, aerosol measurements may need expensive instrumentation, and depending on the characteristics of the flow, it could be challenging to design the sampling process. Therefore, computational fluid dynamics (CFD) studies play an important and available alternative method to investigate the behavior of aerosols and other complex multiphase fluid systems (Nichele and Teixeira, 2015; Vianna Jr and Nichele 2010).

One useful approach to describe the particle movement in aerosols is based on the Lagrangian frame of reference (Maxey and Riley 1983) and was developed from previous works (Basset 1888; Boussinesq 1895; Buevich 1966; Corrsin and Lumley 1956; Oseen 1927). Using the Direct Numerical Simulation (DNS) for the carrier flow, the authors proposed the equation of motion of a small sphere in a nonuniform flow for \( Re \leq 1 \) evaluating several forces acting over it. This technique solves the time-dependent Navier-Stokes equation without any turbulence model. It implies that the whole range of time and spatial scales are resolved. However, as the high computational cost of this method limits its use for low Reynolds flows (Moin and Mahesh 1998), latter studies adapted the
problem to include turbulence models for the continuous phase (Wang and Squires 1996, Lain and Sommerfeld 2003). Furthermore, the description evolved to include different approaches for the particle-fluid coupling (Squires and Eaton 1990, Yamamoto et al. 2001).

Alternatively, the Eulerian-Eulerian approach has been extensively applied in the study of multiphase flows (Andersson et al. 2012). This approach is often used with RANS to model the continuous fluid turbulence, but the dispersed phase may need different models for the turbulence (Andersson et al. 2012). One of them is the kinetic theory of granular flow (Gidaspow 1994; Jenkins and Savage 1984; Lun et al. 1984), which was developed from the kinetic theory of gases and can be applied from very dilute to dense flows (Kong and Fox 2020). The general Eulerian-Eulerian equations were also adapted to investigate the aerosol transport in laminar and turbulent flows (Armand et al. 1998) leading to good agreement with experimental data. Moreover, in the Eulerian framework, models based on probability density functions (PDF) models are used to predict the statistical behavior of particles in a turbulent flow in a similar manner to the classical kinetic theories (Ramkrishna 2000, Reeks 2014, Février 2005, Silva et al. 2010). In another Eulerian approach, particle dispersions are modeled by a transport equation for the aerosol concentration (Hinds 1999), in which the diffusion term includes Brownian motion and turbulence modeling.

In aerosol systems, several internal processes can modify the size distribution of the aerosol. These internal processes are coagulation, agglomeration, fragmentation, nucleation, particle condensation, and particle evaporation (Crowe 2006). When the internal processes are relevant, populational balance equations, known as general dynamic equations (GDE) can be used to describe the particle phase. Information about the continuous phase is necessary for the solution of the GDE and it can be obtained by solving the Navier-Stokes equations (Friedlander 2000).

In the present study, we investigate the effect of the particle diameter on the behavior of a free aerosol jet. This investigation is limited to the cases in which the time scale for particle dispersion is smaller than all other internal processes such as coagulation, nucleation and particle evaporation. Moreover, the present study presents overall conditions for the Eulerian-Eulerian simulation of aerosol jets without focusing on the internal processes.

2 THEORETICAL FUNDAMENTALS
2.1 AEROSOLS

An aerosol is a suspension of solid or liquid particles in a gas, usually air. Aerosol particle sizes range from 0.001 to 100 µm (Crowe 2006). The particle concentration and the particle size strongly influence the aerosol behavior. Other parameters, such as the particle shape and the size distribution,
may also influence the dispersion (Kulkarni et al. 2011). Particle concentration can be expressed in terms of particle volume fraction, \( \alpha_p \), given by

\[
\alpha_p = \frac{1}{V_T} \sum n_i V_{pi}
\]

which represents the volume occupied by the particles in a unit volume. In Eq. (1), \( V_T \) is the total volume of the mixture, and \( n_i \) is the number of particles with a specific size \( i \) and volume \( V_{pi} \).

Generally, as the aerosol concentration decreases, the influence of the particles on the aerosol behavior decreases as well. Particle volume fraction is used to distinguish a dense suspension from a dilute one. The mixture is considerate dilute if \( \alpha_p \leq 10^{-3} \), and dense otherwise (Elghobashi 1994). In multiphase flows, the interaction between particles and fluid is a vital aspect of the dispersion. Based on the particle volume fraction, three regimes may classify the multiphase flow: one-way coupling, two-way coupling, and four-way coupling (Elghobashi 1994). For \( \alpha_p < 10^{-6} \), the mixture is one-way coupling, and the fluid influences the particle, but the particle does not influence the fluid. When \( 10^{-6} < \alpha_p < 10^{-3} \), the mixture is two-way coupling, and the fluid and the particle influence each other. For \( \alpha_p > 10^{-3} \), the four-way coupling regime, besides the particle-fluid influence, the collisions between particles are also relevant.

In the two-way coupling regime, the presence of particles may intensify or attenuate the turbulence of the main flow in a phenomenon denominated turbulence modulation (Elghobashi 1994). The particle inertia, the particle drag, and the effective viscosity of the particle phase have a direct effect on the turbulence dissipation of the carrier flow (Balachandar and Eaton 2010). Conversely, the main contribution to intensification of the turbulence of the carrier flow is the enhanced velocity fluctuation by wake dynamics and self-induced vortex shedding (Balachandar and Eaton 2010).

The Stokes number, \( St = t_p/t_e \), is an essential parameter in fluid-particle flows associated with the effect of changes in the fluid velocity changes on the particles. This parameter relates the particle response time, \( t_p \), defined as

\[
t_p = \frac{\rho d_{pi}^2}{18\mu}
\]

and the characteristic time of the flow field, \( \tau_e \), given by

\[
\tau_e = \frac{L}{u^*}
\]
where \( r_{pi} \) is the particle density, \( d_{pi} \) is the particle diameter, and \( L \) and \( u^* \) are, respectively, the characteristic length and the characteristic velocity of the flow field. When \( \text{St} \ll 1 \), the particles have sufficient time to respond to changes of velocity in the flow. In consequence, the particle velocity and the fluid velocity will be the same. In contrast, when \( \text{St} \gg 1 \), the particle velocity is not affected by changes in the fluid velocity (Crowe 2006).

Particle size is also essential to determine the set of equations applicable to the flow regime. Navier-Stokes equations are only applicable in the continuum flow regime. The Knudsen number, \( \text{Kn} \ (\equiv 2\lambda/d_p) \) is the parameter that determines the flow regime, which depends on the gas molecular free path \( \lambda \). \( \text{Kn} \ll 1 \) indicates continuum flow, while \( \text{Kn} \gg 1 \) indicates free molecular flow. For the free molecular flow regime, the governing equations are obtained by the gas kinetic theory (Friedlander 2000).

2.2 MULTIPHASE MODELS

The Eulerian-Eulerian model (or two-fluid model) treats the dispersed multiphase flow as a two fully interpenetrating quasi-fluids. In the Eulerian treatment, the particle’s properties (such as velocity, concentration, and temperature) are stored in computational nodes. Therefore, one advantage of the Eulerian-Eulerian model is that the increase in the number of particles does not influence the computational cost as much as in the Lagrangian-Eulerian model (Loth 2000). For this reason, this model was chosen by the authors.

A key assumption of the Eulerian-Eulerian model is that the particle properties can be approximated as a continuum at the grid scale (Michaelides et al. 2016). The premise can be supported by different criteria. One of the most rigorous states that the grid spacing should be much larger than the particle-particle spacing. If the property of interest is the mean property, the criterion for the continuum assumption is more relaxed. The mean concentration of particles in a cell can be interpreted as the probability of a particle in a cell in a given time. Therefore, the only criterion is that the particle size should be much smaller than the grid size (Michaelides et al. 2016).

In this framework, the continuity equation for each incompressible phase without change of phase is expressed by

\[
\frac{\partial \alpha_k}{\partial t} + \nabla \cdot (\alpha_k U_k) = 0
\]
where \( k \) is a phase indicator (\( p \) for particle or \( g \) for gas) and \( U_k \) is the mean velocity of the phase (Ishii and Hibiki 2011). The momentum conservation with an interfacial momentum transfer term, \( M_k \), (Enwald et al. 1996) is expressed by the two momentum equations for incompressible fluids

\[
\frac{\partial \alpha_g U_g + \nabla \cdot (\alpha_g \mathbf{U} \mathbf{U})}{\partial t} = -\frac{\alpha_g \nabla P}{\rho_g} + \frac{1}{\rho_g} \nabla \cdot (\sigma^p_{eff} + \alpha_g \mathbf{g}) + \frac{M_g}{\rho_g} \tag{5}
\]

\[
\frac{\partial \alpha_p U_p + \nabla \cdot (\alpha_p \mathbf{U} \mathbf{U})}{\partial t} = -\frac{\alpha_p \nabla P}{\rho_p} - \frac{\nabla P_p}{\rho_p} + \frac{\nabla \cdot \sigma^p_{eff} + \alpha_p \mathbf{g}}{\rho_p} + \frac{M_p}{\rho_p} \tag{6}
\]

where \( \rho_k \) is the density of each phase, \( P \) is the pressure and \( \sigma^p_{eff} \) is the effective stress of the gas phase given by

\[
\sigma^p_{eff} = \mu^p_{eff} (\nabla \mathbf{U}_p + (\nabla \mathbf{U}_p)^T) - (2 \mu^p_{eff} / 3) (\nabla \cdot \mathbf{U}_p) \delta - \frac{2}{3} \rho_k \delta \tag{7}
\]

where \( \mu^p_{eff} \) is the sum of the fluid dynamic viscosity and the turbulent viscosity, \( \delta \) is the Kronecker delta, and \( \kappa \) is the turbulence kinetic energy per unit mass. Both the turbulent viscosity and the turbulence kinetic energy per unit mass are given by the \( \kappa-\varepsilon \) turbulence model (Wilcox 2006).

Although the turbulence model has its limitations, the model is adequate for simplified simulations (Ribeiro et al. 2018). In Eq. (6), \( \sigma^p_{eff} \) is given by

\[
\sigma^p_{eff} = \mu^p_{eff} (\nabla \mathbf{U}_p + (\nabla \mathbf{U}_p)^T) - (2 \mu^p_{eff} / 3) (\nabla \cdot \mathbf{U}_p) \delta - \frac{2}{3} \rho_p \delta \tag{8}
\]

where \( \mu^p_{eff} \) is the effective dynamic viscosity of the particle phase, \( \xi_p \) is particle bulk viscosity and \( P_p \) is the particle pressure. These three terms are described by the Kinetic Theory of Granular Flow (KTGF) (Gidaspow 1994). The interfacial momentum transfer arises especially from drag force, lift force, virtual mass force, and Basset force. Brownian forces are also important for aerosol flows. However, they are more relevant than gravitational and inertial forces only when \( d_p < 0.5 \mu m \) (Li and Ahmadi, 1992) and, therefore, they were not considered in this study. Virtual mass force and Basset force may be neglected when \( \rho_p / \rho_p < 10^{-3} \). The lift force can also be neglected once it does not affect the particle trajectory outside the viscous sub-layer (Crowe 2006; Namazian et al. 2015). The drag
force over the particle phase, $F_D$, represents the fluid resistance to the movement of a submerged particle (Loth, 2000), and is expressed by (Enwald et al. 1996)

$$F_D = \frac{3}{4} C_D \frac{\alpha_p \rho_s}{d_p} \left| U_p - U_g \right| (U_p - U_g)$$

(9)

where $C_D$ is the drag coefficient which can be obtained by (Schiller and Naumann 1933)

$$C_D = \begin{cases} 
(24 / \text{Re}_p)(1 + 0.15 \text{Re}_p^{0.687}), & \text{Re}_p < 10^3 \\
0.44, & \text{Re}_p > 10^3
\end{cases}$$

(10)

where Re$_p$ is the particle Reynolds number given by

$$\text{Re}_p = \frac{\rho_s (U_p - U_g) d_p}{\mu_s}$$

(11)

and the parameter $C_C$ is the Cunningham slip corrector (Allen and Raabe, 1985), computed by

$$C_C = 1 + \text{Kn}[1.142 + 0.558\exp(-0.999/\text{Kn})]$$

(12)

which is relevant when Kn >> 1 and reduces the drag force. In this work, the Cunningham slip corrector was only considered for the case $d_P = 1 \mu m$.

3 METHODS OF SIMULATION

The computational experiments analyzed an upward aerosol jet from the ground into quiescent air. The CFD simulations of the aerosol jets were carried out using the OpenFOAM software version 5 (Weller et. al 1998, Greenshields 2017). All simulations were held in a Cray XK7 supercomputer. The aerosol flow equations – Eqs. (6) to (8) – were solved using the twoPhaseEulerFoam solver. This solver was developed for an isothermal two-phase incompressible flow with a continuous phase and a dispersed one. Complex phenomena such as agglomeration, coagulation and nucleation are not considered by the solver as well as mass and heat transfer between the phases.

The time, diffusion, and convective terms of the Navier-Stokes equation were discretized with second-order schemes. Pressure-velocity coupling is addressed via the PIMPLE algorithm.
(Greenshields 2017), a hybrid method between SIMPLE (Patankar et al., 1972) and PISO (Issa 1981) algorithms. The OpenFOAM native mesh generator blockMesh was used to build a 2D structured mesh, with 2 m × 2 m length. The mesh was divided into two types of regions according to Figure 1.

As shown in Figure 1, the grid is more refined near the bottom along the y-axis. The total expansion ratio (largest cell/smallest cell) in y-axis is 2. Along the x-axis, in Region 1, the grid is more refined near the center and the total expansion ratio is 10, and in Region 2, this ratio is 1. The bottom and lateral sides of the domain are walls and the top of the domain is the atmosphere.

The aerosol is ejected from the bottom of Region 2 as shown in Figure 1. The inlet width is 0.012 m, which is the horizontal length of Region 2. For the grid convergence analysis, the total number of cells of the coarsest grid was approximately doubled, generating a new grid. The procedure was repeated until the generation of 4 grids as reported in Table 1. Then, the time-average velocities of the grids along the x and y-axis were compared until the convergence of the curves.

![Mesh generation scheme procedure](image)

**Figure 1.** Mesh generation scheme procedure (more details in Table 1).

| Region of cells | Number of cells | Δx_{1,min} (mm) | Δx_{1,max} (mm) | N_{x1} | Δy_{1,min} (mm) | Δy_{1,max} (mm) | N_{y1} | Δx_{2} (mm) | N_{x2} | Δy_{1,min} (mm) | Δy_{2,max} (mm) |
|-----------------|-----------------|-----------------|-----------------|-------|-----------------|-----------------|-------|--------------|-------|-----------------|-----------------|
| Mesh 1          | 410 000         | 200             | 12.6            | 1000  | 1.34            | 2.77            | 10    | 1.2          | 1000  | 1.34            | 2.77            |
| Mesh 2          | 820 120         | 283             | 8.97            | 1414  | 0.98            | 1.96            | 14    | 0.86         | 1414  | 0.98            | 1.96            |

Table 1. Details of the Regions 1 and 2 of the four meshes tested. N_{x1}, N_{y1}, N_{x2}, and N_{y2} are the number of grid divisions along x and y-axis in the Regions 1 and 2. Δx_{1}, Δy_{1}, Δx_{1}, and Δy_{2} are the mesh element width (x-axis) and height (y-axis) in the Regions 1 and 2.
The effect of the variation of the diameter was analyzed ($d_p = 1, 5$ and 10 μm). In the simulations, the continuous phase was air with $\rho_g = 1.2$ kg/m$^3$ and $m_g = 18.4 \cdot 10^{-5}$ Pa·s, and the exit orifice diameter $D = 0.012$ m. The particle was considered spherical with $\rho_p = 1200$ kg/m$^3$. The term $a_p = 10^{-5}$, and the jet was discharged with velocity $U_0 = 5$ m/s. For the convergence tests, $d_p = 1$ μm.

All the discharge velocities have a turbulence intensity, $I$, of 5%. This parameter is given by the ratio of the fluctuation velocity to the mean velocity. This experiment is similar to a hand smoke grenade launch.

4 RESULTS AND DISCUSSION

Time-average velocity and time-average concentration were evaluated 3 seconds after the beginning of the aerosol ejection. Preliminary experiments showed that in 3 seconds a steady flow was formed. The $y$-axis curves represent the centerline of the jet, and the $x$-axis curves are taken at the height of 1 meter.

Meshes 1, 2, 3, and 4 were tested for time-average velocity along the $y$-axis and along the $x$-axis to reach a grid convergence solution. The result shows that the difference between the time-average velocities decreases as the grid is refined. In this work, the Mesh 3 was chosen due to computational efficiency. The results obtained for Mesh 3 and Mesh 4 are very close. The velocity difference is less than 5% in almost all the jet extension, and the computational cost is 40% lesser.

The experiment adopts $I = 5\%$ in the discharge velocity aiming to observe a turbulent behavior. Figure 2 shows the mean particle concentration distribution for $d_p = 1$ μm. One can observe in this figure how the particle path accompanies the fluid recirculation. The symmetry breaking evidenced from the deviation to the left of the particle path is provoked by the turbulence randomness. The shape of the jet can also be visualized by the time-average particle concentration for $d_p = 1$ μm in Figure 2.
4.1 ANALYSIS OF PARTICLE DIAMETER DEPENDENCY

Figures 3 and 4 show the time-average particle velocity profile along the x-axis and y-axis, respectively, for particle diameters of 1 μm, 5 μm and, 10 μm. Besides that, the time-average air velocity for the 10 μm particle diameter case and for the one-phase case are included in the charts.
Figure 4. Time-average particle velocity profile along the y-axis at $x = 0$ after 3 s of the ejection for $d_p = 1$, 5, and 10 μm and time-average air velocity when $d_p = 10$ μm. Simulation parameters: $\alpha_p = 10^{-5}$, $\rho_p = 1200$ kg/m$^3$, $D = 12$ mm, and $U_0 = 5$ m/s with $I = 5\%$.

Figure 3 clearly shows the gaussian behavior of the velocity profile. Figure 4 shows that the time-average velocity in the y-axis is inversely proportional to the distance to the ejection point. Another important observation is that both figures show very close behavior in all of the curves. However, the presence of particles in the flow results in slightly lower velocity, comparing with the one-phase jet. The decrease in the dispersion velocity is a consequence of the energy dissipation due to the interaction between particles and air molecules. When $d_p = 10$ μm, the particle velocity is slightly different from the others. The main cause of this behavior is the high value of the Stokes number. As the Stokes number rises, the particle response time rises, and the fluid movement less influences the particle path. Another way to explain the difference observed in the curves is through the diameter. For the same particle concentration, as the particle diameter drops, the superficial contact area between the particle and the fluid rises, resulting in a more prominent influence of the fluid in the particle.

Figures 5 and 6 show the time-average particle concentration profile along the x-axis and y-axis, respectively. In the x-axis chart, the curves are similar. What stands out is the gaussian shape of the curve in a narrow 0.2 m space around the centerline of the jet. Independently of the diameter, the concentration drops to 10% of the initial one, 0.1 m away from the center of the jet. Figure 6 shows that the particle concentration is inversely proportional to the distance to the source point. Moreover, initially, the particle concentration in the flows of bigger particles flows drops faster than the smaller ones. This fact can be justified by the Stokes number. As the flow stabilizes, the particle concentration
profile gets smoother. The bigger particles have more inertia than the smaller ones, so, after 1.1 m, the curves are inverted.

Figure 5. Time-average particle concentration profile along the x-axis at $y = 1$ m for $d_p = 1, 5, \text{ and } 10 \mu$m. Simulation parameters: $\alpha_p = 10^{-5}$, $\rho_p = 1200 \text{ kg/m}^3$, $D = 12 \text{ mm}$, and $U_0 = 5 \text{ m/s}$ with $I = 5\%$.

Figure 6. Time-average particle concentration profile along the y-axis at $x = 0$ for $d_p = 1, 5, \text{ and } 10 \mu$m. Simulation data: $\alpha_p = 10^{-5}$, $\rho_p = 1200 \text{ kg/m}^3$, $D = 12 \text{ mm}$, and $U_0 = 5 \text{ m/s}$ with $I = 5\%$. 
5 CONCLUSION

This article briefly reviewed the aerosol theories. The governing equations of the flow in a Eulerian-Eulerian approach were discussed as well as the CFD techniques. The study consisted of understanding the particle velocity and particle concentration profiles of an upward aerosol dispersion. Furthermore, the effects of varying the particle diameter were analyzed.

The particle velocity profile in the aerosol dispersion is similar to the air velocity in the one-phase jet. Along the x-axis, the particle velocity profile assumes the gaussian form. On the other hand, along the y-axis, the particle velocity profile is inversely proportional to the distance of the ejection point. The same behavior is seen in the relation of the particle concentration along the y-axis. In the x-axis, the particle concentration in the centerline of the jet has a gaussian shape. Outside the gaussian area, horizontal lines at 10% of the initial concentration, and a short distance from the center may describe well the particle concentration pattern. In the simulation conditions, the particle does not have sufficient inertia to escape from the recirculating fluid.

The particle diameter influences the dispersion behavior as the Stokes number increases. Larger Stokes number implies that the particle velocity is less affected by changes in the fluid velocity. Therefore, their path starts to differ. It should be noticed that the range of particle diameter test is limited so for larger particles the effect is expected to be more pronounced.

Overall conditions for the Eulerian-Eulerian simulation of aerosol jets were presented and consistent results were obtained based on the theory. To summarize, the Eulerian-Eulerian method is an alternative for describing aerosol jet behavior. For future projects, we suggest the investigation of other parameters of the aerosol flow in order do propose practical correlations for engineering applications.

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