A Novel Slip Correction Factor for Spherical Aerosol Particles

Abouzar Moshfegh, Mehrzad Shams, Goodarz Ahmadi, and Reza Ebrahimi

Abstract—A 3D simulation study for an incompressible slip flow around a spherical aerosol particle was performed. The full Navier-Stokes equations were solved and the velocity jump at the gas-particle interface was treated numerically by imposition of the slip boundary condition. Analytical solution to the Stokesian slip flow past a spherical particle was used as a benchmark for code verification, and excellent agreement was achieved. The Simulation results showed that in addition to the Knudsen number, the Reynolds number affects the slip correction factor. Thus, the Cunningham-based slip corrections must be augmented by the inclusion of the effect of Reynolds number for application to Lagrangian tracking of fine particles. A new expression for the slip correction factor as a function of both Knudsen number and Reynolds number was developed.

Keywords—CFD, Cunningham correction, Slip correction factor, Spherical aerosol.

I. INTRODUCTION

AEROSOLS in the nature typically have the size range from a few nanometers to several micrometers. When the characteristic size of the particle decreases down to a value comparable to the mean free path of the molecules, the rarefaction effects become important and significantly affect the flow properties, wall shear stress and aerodynamic drag force. In this case, the continuum assumption fails and the Navier-Stokes equations with no-slip boundary conditions cannot be applied. In such situations, intermolecular collisions play a prominent role and the flow properties will be affected by the Knudsen number (Kn), which is a dimensionless measure of the relative magnitudes of the gas mean free path and flow characteristic length. Schaaf and Chambre [1] have proposed the following ranges to determine the degree of rarefaction flow regime based on the local Knudsen number. For $Kn < 0.01$, the continuum hypothesis holds and fluid is in local thermodynamic equilibrium. Thus, the Navier-Stokes equation in conjunction with no-slip

A. Moshfegh is with the Faculty of Mech. Eng., K.N.Toosi U of Tech., Pardis St., Vanak Sq., Tehran 19395-1999, Iran.

M. Shams is with the Faculty of Mech. Eng., K.N.Toosi U of Tech., Pardis St., Vanak Sq., Tehran 19395-1999, Iran (phone: +982184063214; fax: +982188677273; e-mail: shams@kntu.ac.ir).

G. Ahmadi is with the Department of Mech. and Aeronautical Eng., Clarkson U, Potsdam, NY 13699-5725, USA.

R. Ebrahimi is with the Faculty of Aerospace Eng., K.N.Toosi U of Tech., East-Vafadar St., Tehranpars Ave., Tehran 16765-3381, Iran.

boundary condition describes the flow behaviors. The rarefaction effects become noticeable when the Knudsen number is in the range of 0.01 and 0.1. This range is referred to as the slip flow regime, where the continuum hypothesis is still valid, but the local thermodynamic equilibrium of near-wall gas is violated. That is, the conventional no-slip boundary condition imposed at the gas-solid interface begins to break down but the linear stress-strain relationship is still valid [2]. In this range, the Navier-Stokes equations can be utilized, but the slip boundary condition is used to account for the non-equilibrium effects at the gas-solid interface. The range of $Kn > 10$ represents the free molecular regime where the collisions among the molecules are negligible and individual molecules colloid with the particle [3]. Finally, in the transitional regime ($0.1 < Kn < 10$) the size of particle is comparable to the gas mean free path, and continuum assumption breaks down but the flow cannot be regarded as free molecular regime. The ultra fine (nanometer) aerosols under normal condition typically experience a rarefied flow regime, and therefore the drag force acting on the particle reduces compared with what is predicted by the Stokes' law [4]. It has been customary to account for the drag reduction by introducing a correction factor to consider the rarefaction effects and velocity discontinuity at the gas-particle interface.

II. LITERATURE REVIEW

About a century ago, Cunningham [5] derived a correlation of the form $(1 + A \cdot Kn)$ to consider the slip effects on the drag force of acting on a spherical particle in the Stokesian flow regime. An experimental study for $Kn < 0.3$ was carried out in the same year by Millikan [6] who reported the linear dependency of Cunningham correction factor on the gas mean free path. More rarefied flow regimes were experimentally investigated by Knudsen and Weber [7] and the parameter A was expressed as a function of Knudsen number. That is,

$$C(Kn) = 1 + A \cdot Kn$$
$$A = \alpha + \beta \cdot \exp(-\gamma/Kn) \qquad (1)$$
$$Kn = \lambda/\ell$$

where λ is the gas mean free path, and ℓ is the flow reference length-scale which has been taken equal to the spherical particle radius in the following results. The constants α, β and γ are determined experimentally. Cunningham suggested a value of $A = 1.26$ [8] disregarding its dependence on Kn as indicated in the Eq. (1). Until recently,

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researchers have tried to propose slip correction factors based on the Eq. (1). Millikan [9] tested various particle surfaces using his conventional oil drop method in air with the mean free path of $0.094\,\mu m$, and different particle size, which generated a range of $0.5 < Kn < 134$. In another experiment by Millikan [10], a first-order correction technique was proposed to account for the rarefaction effects on an oil drop. He found that the Stokes law cannot predict accurately the terminal velocity when the oil drop size is reduced to nanometer ranges. Polystyrene spherical microparticles were used by Allen and Raabe [11] to measure their appropriate slip correction factors over the range of Knudsen numbers from 0.03 to 7.2. Five years later, Rader [12] re-analyzed the slip correction factor of the small particles in various gaseous mediums for the range of $0.2 < Kn < 0.95$, and provided accurate values for α, β and γ. Hutchins et al. [13] used modulated dynamic light scattering to find the slip correction factor of polystyrene and polyvinyl toluene spherical particles with the diameters between 1 and $2.12\,\mu m$. They measured the drag force acting on the spherical particles suspended in dry air to determine the diffusion coefficient of a single levitated particle from which the slip correction factor could be obtained. Recently, Kim et al. [4] have investigated the slip correction factor at reduced pressure and high Knudsen numbers using polystyrene latex (PSL) particles. Nano-differential mobility analyzer (NDMA) was used to determine the slip correction factor for $0.5 < Kn < 83$. The data obtained for three particle sizes were fitted well by the expression given in Eq. (1).

Table I includes the experimental slip correction factors in form of Eq. (1), which have been proposed and used by the researchers in the past several decades. All these expressions assume the correction factor to be as a function of Knudsen number based on the particles radius.

TABLE I
CUNNINGHAM-BASED SCFs ($1 + Kn.[\alpha + \beta \exp(-\gamma / Kn)]$) FOR AIR AT 101.3 KPA AND 23 °C WITH MEAN FREE PATH OF 67.3 NM.

No.	(α, β, γ)	Particle Material / Reference
1	(1.034, 0.536, -1.219)	glass / [7] [a]
2	(1.209, 0.406, -0.893)	oil drop / [9] [b]
3	(1.155, 0.471, -0.596)	oil drop / [14]
4	(1.142, 0.558, -0.999)	polystyrene latex (PSL) / [11]
5	(1.209, 0.441, -0.779)	oil drop / [12]
6	(1.231, 0.469, -1.178)	polystyrene latex (PSL) / [13]
7	(1.257, 0.400, -1.100)	- / [15]
8	(1.170, 0.525, -0.780)	- / [3]
9	(1.165, 0.483, -0.997)	polystyrene latex (PSL) / [4]

[a]They originally reported the slip correction factor as $1 + Kn\,[0.683 + 0.354 \exp(-1.845 / Kn)]$ using the mean free path of 100.65 nm at 101.3 kPa and 20.2 °C [4].

[b]The correlation was originally reported in the standard conditions and mean free path of 94.17 nm [4].

For an incompressible fluid, an analytic solution to the Stokesian slip flow past a stationary, impermeable and solid microsphere was derived by Barber and Emerson [16]. Inertia terms of the Navier-Stokes equations were neglected in their analysis. The existence of an additional drag force component

originating from the normal stress was confirmed. This additional drag component is unlike what appears in the continuum flow regime. In a related work, Barber and Emerson [17] also simulated the slip flow regime past a confined microsphere within a circular pipe using a two-dimensional finite-volume Navier-Stokes solver that accounts for the slip boundary condition. The confined sphere in the circular pipe was also studied numerically over a wide range of Knudsen numbers by Liu et al. [18]. This configuration is used in macro-scale spinning rotor gauges to measure the pressure, viscosity and molecular weights in low pressure gases ([19], [20]).

In the research works cited above, all investigators tried to correlate the rarefaction effects on the particle drag force only to the Knudsen number, and the effect of Reynolds number (Re) on the slip correction factor was not directly reported. That is they were mainly concerned with the creeping flow regime and the limit of Stokes drag. For example, the slip flow simulation past the sphere carried out by Barber and Emerson [17] was limited to low (creeping flow) Reynolds numbers. In many gas-solid two-phase flows encountered in the industry, environment and biomedical applications, the gas-particle relative Reynolds number may become finite, for which an accurate expression for the slip correction is not available. In addition, the earlier reported experiments did not cover the Knudsen numbers associated with the slip flow regime ($0.01 < Kn < 0.1$); therefore, the proposed correlations may not be accurately for predicting the rarefaction effects in this range. Thus, the slip flow regime merits more rigorous studies for developing more accurate correlations. Many researchers ([21]-[26]) have used the Cunningham-based slip correction factors for their Lagrangian simulations of gas-solid two-phase flows. Therefore, availability of a more accurate expression would be helpful in the related areas.

In the present work, the incompressible slip flow regime past an unconfined, stationary, impermeable, solid and spherical particle is simulated. The main goal of the study is to provide a better understanding of dynamic effects originating from the slip regime for a typical aerosol particle. In particular, a more accurate slip correction factor as a function of both Reynolds and Knudsen numbers is proposed. A comparison of the new slip correction with those proposed by other researchers is also performed.

III. PROBLEM FORMULATION

For the steady and incompressible flow of a Newtonian, isotropic and monatomic gas which is in local thermodynamic equilibrium, the Navier-Stokes equations governing in continuum physical space can be written as

$$\frac{\partial (u_k)}{\partial x_k} = 0 \tag{2}$$

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$$\rho \frac{\partial (u_k u_i)}{\partial x_k} = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial}{\partial x_k} [(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i})$$
$$-\frac{2}{3} \delta_{ik} (\frac{\partial u_j}{\partial x_j})] \tag{3}$$

where x represents the position in coordinates system, **u** is the velocity, p is the pressure, ρ is the fluid density, μ is the fluid dynamic viscosity and δ_{ik} is the Kronecker delta function.

To account for the effects of local non-equilibrium in the slip flow regime, the conventional no-slip boundary condition must be replaced appropriately. As postulated first by Navier in 1827 [27], the tangential slip velocity is proportional to the tangential wall shear. That is,

$$u_t\big|_{wall} \approx \alpha \tau_t\big|_{wall} \tag{4}$$

Here, α is a constant. Later, Maxwell in 1879 [27] showed from the kinetic theory of gases that $\alpha \approx \lambda/\mu$. For gases, the mean free path (λ) is the average distance traveled by molecules between collisions. For a perfect gas, the mean free path is given as

$$\lambda = \frac{kT}{\sqrt{2}\pi p d_m^2} \tag{5}$$

where k is the Boltzmann constant, T is the gas temperature, and d_m is the collision diameter of the molecules. To account for the portion of molecules reflected diffusely from the solid surface in the slip velocity formulation, Schaaf and Chambre [1] suggested that the constant α in Eq. (4) must be multiplied by a factor of $((2-\sigma)/\sigma)$ where σ is the tangential momentum accommodation coefficient (TMAC). Consequently, the slip velocity can be written as

$$u_t\big|_{wall} \approx \left(\frac{2-\sigma}{\sigma}\right) \frac{\lambda}{\mu} \tau_t\big|_{wall} \tag{6}$$
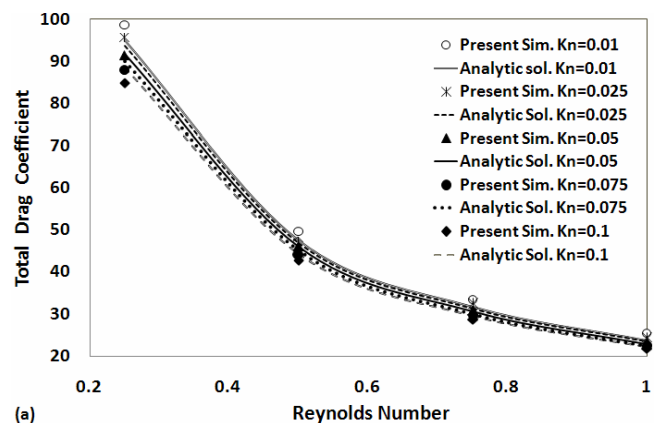
Equation (6) relates the tangential slip velocity to the tangential shear stress via the TMAC, gas mean free path and gas dynamic viscosity. Regarding the Eq. (1), the flow length-scale, ℓ, is typically evaluated as the ratio of a flow thermodynamic property (such as temperature or density) to its spatial gradient. Alternatively, ℓ may be estimated as a length scale of the flow geometry. For the incompressible and isothermal flow simulated here, we used the particle radius ($d/2$) as the reference length-scale of the flow, which is consistent with the definition used in aerosol communities. Using the definition of Knudsen number (Eq. (1)), the relation

of tangential slip velocity on the particle surface (Eq. (6)) becomes

$$u_t\big|_{wall} \approx \left(\frac{2-\sigma}{\sigma}\right) Kn \frac{d}{2\mu} \tau_t\big|_{wall} \tag{7}$$

IV. NUMERICAL SOLUTION

A multiblock structured and body-fitted grid was considered for analyzing the flow over a single spherical particle with the diameter of d. The finite-volume method (FVM) through the pressure-based segregated algorithm was employed to discretize the 3D, incompressible, steady, laminar and Navier-Stokes equations (Eqs. (2-7)). Modified Quadratic Upstream Interpolation for Convective Kinematics (QUICK) scheme, which can be implemented on the multidimensional, nonuniform and unstructured grids ([28]-[33]), was adopted to discretize the convective and diffusive fluxes in the momentum equations. Pressure-Velocity coupling is treated by the SIMPLE-Consistent (SIMPLEC) algorithm on a colocated grid. A second-order pressure interpolation method is also used to calculate the pressure at cell faces from the neighboring nodes. Gradient reconstruction is done by Green-Gauss node-based formulation. The linearized system of equations is solved using a point implicit (Gauss-Seidel) linear equation solver in conjunction with an aggregative algebraic multigrid (AAMG) method [34]. Flexible multigrid cycle is prepared for the three momentum equations, while the V-cycle is considered for continuity equation. To achieve a stable solution through the iterations, under-relaxation factors are devised for pressure, velocity and tangential slip velocity. The capability of foregoing set of schemes to simulate the slip flow regimes has been examined as reported by some researchers ([35]-[37]).
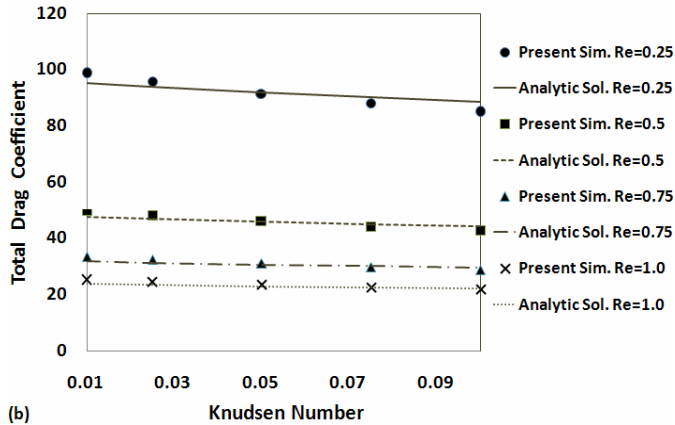

(a)

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Fig. 1 Comparison of total drag coefficient calculated by analytic solution with that computed by present simulation at $\sigma = 1$: (a) total drag coefficient vs. the relative Reynolds number; (b) total drag coefficient vs. the Knudsen number

The analytic expression for the total drag coefficient derived in the Stokesian slip flow regime by Barber and Emerson [16] is used to ensure the validity of the CFD (Computational Fluid Dynamics) procedure that considers the velocity jump (rarefaction effect) at the gas-particle surface interface. The result of comparison is demonstrated in Fig. 1 from two completely disparate aspects. Fig. 1 (a) and (b) show this comparison respectively versus the Re and *Kn* numbers variations.

V. RESULTS AND DISCUSSION

In this work, it is assumed that the particle is traveling within the dry air at standard ambient temperature and pressure (SATP), respectively, equal to 298.15 K and 101.3 kPa. Under such conditions, the air mean free path becomes 69.2 nm, and density and air dynamic viscosity are respectively equal to 1.1686 kg/m3 and 1.832e-5 N-s/m2. We assumed a value of unity for the TMAC to study the SCF at the most probable limiting extent of the TMAC values in micro materials appearing in the industry and nature. To account for the slip effects on the particle drag force in the rarefied regimes, Cunningham slip correction factor (C_c) is defined as a function of Knudsen number in the Stokesian regime that equals the ratio of Stokes' drag force to the particle drag force in the rarefied regime (F_{slip}). That is,

$$C_c = \frac{3\pi\mu U d}{F_{slip}} = fcn(Kn) > 1.0 \quad for \quad Re \ll 1 \quad (8)$$

where the numerator denotes the analytical drag force experienced by the particle in the continuum Stokes ($Re \ll 1$) flow, and F_{slip} is the drag force in the slip flow regime. This relation assumes that the particle drag force (F_{slip}) is decreased by the rarefaction effects as a function of Knudsen number.

In this section, it will be shown that the Cunningham slip correction factor is accurate only for Re numbers very close to zero where the inertial forces are negligible. But for slightly larger Reynolds numbers ($0 \ll Re < 1$), the Cunningham-based correlations are not sufficiently accurate. To better recognize the philosophy of the slip correction factor, we separate the slip dynamic effects on the particle to two exactly opposite phenomena. One is the flow dynamic effects which pertain to the nature of continuum regime that we call it "continuum effects", and the other is all differences exist between the continuum and slip regimes which can be referred as "pure rarefaction effects". The latter effect incorporates the flow rarefaction effects which deviate the flow behaviors from what is observed in the non-slip continuum regime. Since this factor (Eq. (8)) has been defined as a function of *Kn* number, it should represent the "pure rarefaction effects". But it is shown that this conventional definition of slip correction not only represents the "pure rarefaction effects" but also contains some inertial effects coming from the "continuum effects". The slip correction factor (Eq. (8)) in that F_{slip} is replaced by numerical data is illustrated in Fig. 2.
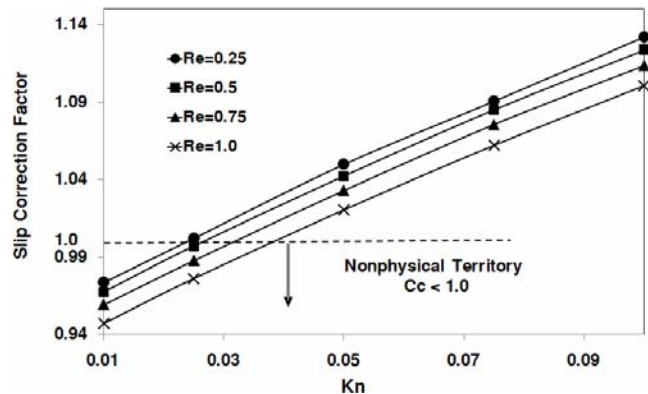

Fig. 2 Slip correction factor calculated from Eq. (8) using the numerical results

A visual detection in the diagrammed behavior reveals that the slip correction factor calculated using the Eq. (8) is less than unity in some areas. It is a rudimentary fact that rarefied regimes always reduce the particle drag force. Disability of Stokes' drag formula to account for all inertia effects of the flow combines with the "pure rarefaction effects" misrepresented by the Eq. (8), and then ignores the fluid slip in the nonphysical territory identified in Fig. 2. By a simple extrapolation on this figure, it is evident that for very low Reynolds numbers (too close to the zero) the computed slip correction shows a completely physical behavior ($C_c \geq 1.0$), and no point will locate inside the nonphysical territory. The increment of Reynolds number mitigates the accuracy of Stokes' formula to predict the real drag force (or real "continuum effects"). This brings about some artificial (or unreal) "pure rarefaction effect" posing itself through the term ($3\pi\mu U d$) and the Eq. (8), and hence some parts of these graphs become subunit.

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To ensure the speculated root of this behavior, we use a more rational definition of slip correction factor, which can be found in the literatures [12], as follows

$$Slip\ Correction\ Factor\,(SCF) = \frac{F_{cont.}}{F_{Slip}} \qquad (9)$$

where $F_{cont.}$ is the particle drag force in the continuum no-slip regime. The experimental data are more realistic and sensible than the numerical ones to evaluate $F_{cont.}$. Therefore, we use the curve fit formula proposed by [38] as given below

$$F_{cont.} = \left[\frac{24}{Re} + \frac{6}{1+\sqrt{Re}} + 0.4\right]\left(\frac{1}{2}\rho U^2 A\right) \qquad (10)$$

Fig. 3 shows the numerical slip correction factors evaluated using the Eq. (9) in the Stokesian regime. As was noted before, there is no available experimental data for F_{slip} in this range. Here, the numerical simulation data for the drag force in the slip flow regime are used.
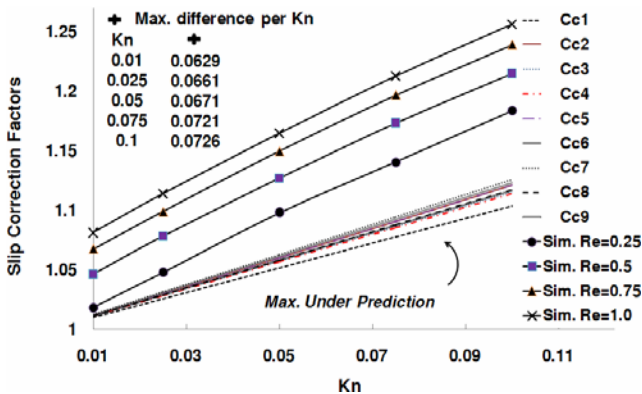

Fig. 3 Comparison of Cunningham-based correlations (Table I) and slip corrections (Eq. (9)) resulted from the present simulation.

Fig. 3 shows that the resultant slip correction factor is always greater than unity and increases roughly linearly with Kn. It is also seen that the slip corrections varies significantly depending on Reynolds number. The observed dependence on Re, suggests that the correlation for slip correction should include a dependence on Re. As was recognized by some researchers ([38]-[40]), the fluid inertia or Reynolds number has an important role to mitigate and/or intensify the rarefaction effects in the slip flow regimes. Fig. 3 clearly shows that higher values of Re lead to higher rarefaction effects and consequently higher fluid slip on the particle surface that yields higher values of SCF.

Maximum difference between numerical slip correction factors at each Knudsen number is also appended to the diagram. A comparison between the Cunningham-based correlations (Table I) and the slip correction factor computed through the present simulation using the Eq. (9) is also carried out in Fig. 3. Our computed slip correction factors are all under-predicted by the Cunningham-based corrections (Table I). These correlations were proposed for very close Reynolds numbers to zero, and they neglect the Re prominence on the slip correction, so this brings about considerable under-prediction by Cunningham-based correlations in the range $0 \ll Re < 1$. As one closes to the $Re = 0$, this difference gets smaller that logically proofs the higher accuracy of Eq. (9) at the limiting case of creeping (very low Reynolds number) flows.

Barber and Emerson [41] studied the effects of Kn and Re numbers on the hydrodynamic development length in circular and parallel plate ducts. Similar to Fig. 3, their results showed that both Reynolds and Knudsen numbers affect the slip flow physical parameters in a similar manner (in some flow cases). The increment of these numbers (Kn, Re) intensifies the gas slip as recorded in Fig. 3. Zuppardi [40] quantified the effects of rarefaction in high velocity slip flow regimes, and reported that both slip velocity and temperature jump are increased when the free stream velocity (or the flow Reynolds number) increases.

Regarding such behaviors, the Cunningham-based slip corrections (Table I) do not seem to be appropriate to describe completely the rarefaction effects only through the Knudsen number. One main goal in this study is to modify the slip correction factor based on the Cunningham's mathematical definition ($F_{cont.}$ divided by F_{slip}). In particular, we plan to incorporate the dependence of slip correction on the Reynolds number in the correlation. Therefore, a correction as a function of both relative Re and Kn numbers has to be prepared. Curve-fit statistics were analyzed quantitatively and it was found that the original form of Cunningham correction (Eq. (1)) is just appropriate to correlate the Kn variations in the slip regime when the Re is considered to be fixed. The original form can be multiplied by an additional term to introduce the Re into the correction. Several additional functions of Reynolds number were tested and it was recognized that the basic proposed form of Cunningham correction (Eq.1) is not the best choice for 3D curve-fitting process involving both Kn and Re numbers. Exponential curve fitting (Eq. (1)) is commonly used when the rate of variations accelerates suddenly, so the Cunningham-based correlations are appropriate to correlate the rarefaction effects over a wide range of Knudsen numbers, but this is not the case in the slip flow regime. Moreover, if we could find an appropriate additional expression as a function of Re, the final slip correction would be too large in terms, and could not be utilized easily by the users during the particle tracking procedure. Here, we propose a novel and concise expression (Eq. (11)) which was the best among the 480 tested 3D functions.

$$SCF = A\left(Re^B\right).\ln(Kn+C) \qquad (11)$$
$$for\ \ 0 < Re < 1\ \&\ 0.01 < Kn < 0.1$$

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The calculated coefficients and the curve fit statistics are given in the Table II. The mean values of computed coefficients, standard deviation (SD) or uncertainty of fitted coefficients, the values of R-square (RS), adjusted R-square (ARS), standard deviation of the fitting (SDF) and average absolute residual (AAR) have been also reported.

TABLE II
COEFFICIENTS AND STATISTICS OF CURVE-FITTED SLIP CORRECTION FACTOR
(EQ. (11))

Coefficient	Mean Value	Uncertainty (SD)		
				$RS = 0.998$
A	2.905	0.193E-1		$ARS = 0.998$
B	0.436E-1	0.980E-3		$SDF = 0.257$E-2
C	1.442	0.397E-2		$AAR = 0.190$E-2

The 3D fitted curve on the computed slip correction factors based on the Eq. (9) is illustrated in Fig. 4. Scatter data points placed on the solid lines represent the computed data, and the dash lines constructing the 3D curve denote the fitted (predicted) data by the Eq. (11). Maximum error through the curve-fitting process amounts to less than 0.42% that shows an acceptable fit. To demonstrate the uncertainty limits of the fitted curve, confidence bounds are depicted in Fig. 5 as a function of Re and Kn numbers. Maximum confidence bound at each Kn number is also reported in the diagram.
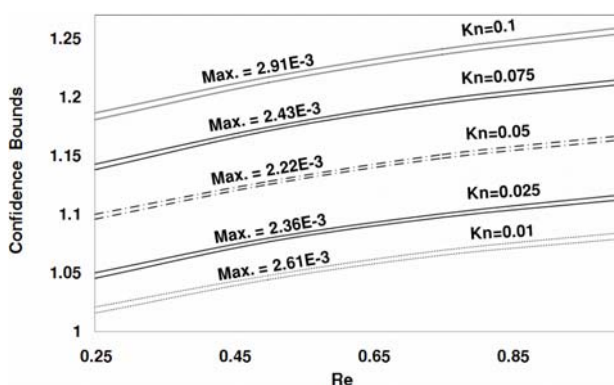

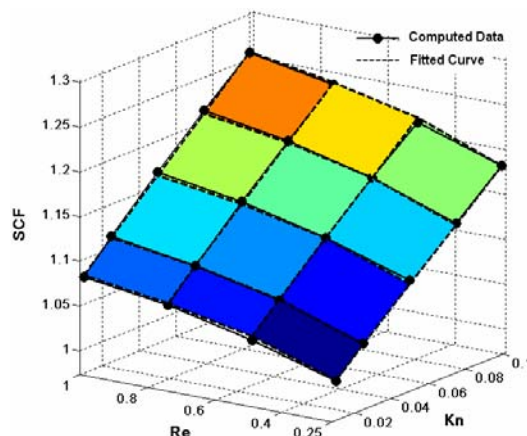Fig. 4 The 3D fitted curve for new proposed slip correction factor (SCF) plotted by Eq. (11)

Fig. 5 Confidence bounds of 3D fitted curve (Fig. 3) considering both Re and Kn numbers variations.

VI. CONCLUSION

Cunningham-Based slip correction factors are accurate only for very close Re numbers to zero. But for Re numbers a little greater than zero, the Cunningham-based correlations are inaccurate to be used for simulation purposes. Conventional definition of slip correction factor leads to a nonphysical prediction of slip flow rarefaction effects, and produces subunit values of C_c in the range $0 << \text{Re} < 1$. A more rational definition of slip correction factor, which replaces the Stokes' drag with experimental drag force, overcomes the problem. Prominent differences between the slip corrections at different Re numbers necessitate the incorporation of Re into the SCF in addition to the Kn number.

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