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Modified Generalized Hard Sphere Collision Model for Direct Simulation Monte Carlo Calculations

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Nomenclature

a	=	$\hat{g}^*/\hat{T}^{1/2}$
f_γ	=	distribution of γ
g	=	relative speed
$(\hat{g}_{\min}, \hat{V}_{\min})$	=	point of minimum $\hat{V}$ for generalized hard sphere (GHS) model
$(\hat{g}^*, \hat{V}^*)$	=	modified GHS (MGHS) transition point
m	=	molecular mass
N_{pairs}	=	number of possible collision pairs to test
n	=	number density
R	=	specific gas constant
T	=	temperature
V	=	$\sigma g \propto$ collision probability
$V_{\max}$	=	maximum value of V
υ	=	variable hard sphere model parameter
υ_1, υ_2	=	GHS model parameters
α	=	MGHS model parameter
γ	=	non-dimensional collision speed $= g/(4RT)^{1/2}$
Δt	=	simulation time step
μ	=	coefficient of viscosity
ν	=	molecular collision frequency
ρ	=	mass density
σ	=	total collision cross section
σ_μ	=	viscosity cross section
τ_{nom}	=	nominal collision time
ϕ	=	GHS model parameter
Ω	=	weighted average σ_μ

Subscript

r	=	reference value

Superscript

$\wedge$	=	normalized value; $\hat{x} = x/x_r$

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Introduction

In THE direct simulation Monte Carlo (DSMC) technique for modeling rarefied gas flows,[1] collision cross sections are usually determined using phenomenological molecular models. The most common DSMC molecular model is the variable hard sphere (VHS) model, described by Bird,[1] where $\sigma \propto g^{-2\upsilon}$. The VHS model has the same variation of σ_μ with g as the inverse power repulsive intermolecular potential, but with hard sphere scattering. Consequently, the VHS model gives a power law viscosity relation $\mu \propto T^{\upsilon+1/2}$, which is inaccurate for most gases over extended temperature ranges with $T \lesssim 1000$ K.

The generalized hard sphere (GHS) model, introduced by Hassan and Hash,[2] is an extension of the VHS model to include terms that model both repulsive and attractive potentials. For the GHS model, σ may be written as

$$\sigma = \sum_i^N \sigma_i \left(\frac{g_r}{g}\right)^{2\upsilon_i}$$

where $g_r = (4RT_r)^{1/2}$ and T_r is an arbitrary reference temperature. Although any number of terms N may be used, the present analysis is limited to $N = 2$. When $\sigma_r = \sigma_1 + \sigma_2$ and $\sigma_1 = \phi\sigma_r$ are used, the GHS cross section is described by

$$\hat{\sigma} = \phi\hat{g}^{-2\upsilon_1} + (1-\phi)\hat{g}^{-2\upsilon_2}$$

Values of the constants σ_r, ϕ, υ_1, and υ_2 are determined using viscosity data.

The GHS model can represent the viscosity behavior of gases more accurately than the VHS model over temperature ranges with $T \lesssim 1000$ K, where attractive intermolecular forces have a significant influence. Despite this advantage, it appears that the GHS model is not used because of its poor computational efficiency. Only one DSMC study using the GHS model appears in the refereed literature (Hash et al.[3]), and the model proposed by Kuščer,[4] which may be considered as a special case of the GHS model, has been used only by Boyd,[5] who noted that σ for this model approached infinity as $g \to 0$, but did not make any specific comments regarding computational efficiency. Here we introduce a modification to the GHS model that significantly improves the computational efficiency, with minimal but advantageous effects on the viscosity behavior of argon.

Viscosity and Collision Frequency for the GHS Model

The Chapman–Enskog viscosity for a given viscosity cross section $\sigma_\mu(g)$ is

$$\mu = \frac{5m}{8}\frac{(\pi RT)^{\frac{1}{2}}}{\Omega(\hat{T})} \qquad \text{where} \qquad \Omega(\hat{T}) = \int_0^\infty \gamma^7 \sigma_\mu \exp(-\gamma^2)\,\mathrm{d}\gamma$$

For hard sphere scattering, $\sigma_\mu = 2\sigma/3$. It can be shown that $\Omega(\hat{T})$ for the GHS model is

$$\Omega(\hat{T}) = (\sigma_r/3)\left[\phi\hat{T}^{-\upsilon_1}\Gamma(4-\upsilon_1) + (1-\phi)\hat{T}^{-\upsilon_2}\Gamma(4-\upsilon_2)\right]$$

For Ar, $\sigma_r = 6.425 \times 10^{-19}$ m^2 can be obtained by using $\mu_r = 2.283 \times 10^{-5}$ Pa·s at $T_r = 300$ K (Ref. 6) and $(\phi, \upsilon_1, \upsilon_2) = (0.61, 2/13, 14/13)$. These parameters give a reasonable fit to the Ar viscosity data recommended by Kestin et al.[6] (Fig. 1). In Fig. 1, the reference quantities[6] are as follows: $\mu_r = 2.283 \times 10^{-5}$ Pa·s at $T_r = 300$ K. The GHS parameters are $\sigma_r = 6.425 \times 10^{-19}$ m^2 and $(\phi, \upsilon_1, \upsilon_2) = (0.61, 2/13, 14/13)$. The MGHS parameters are $\alpha = 0$ and $(\hat{g}^*, \hat{V}^*) = (\hat{g}_{\min}, \hat{V}_{\min})$ (Fig. 2). The power law relation

Table 1 Summary of collision rates and computational efficiency

Model	T, K	Tests performed per τ_{nom} per simulator	Collisions performed per τ_{nom} per simulator	Acceptance rate, %	Theoretical collisions per τ_{nom} per simulator	CPU time relative to VHS CPU time
GHS	100	1022	2.009	0.197	1.997	83.5
GHS	300	247.4	1.547	0.625	1.547	24.3
GHS	3000	17.76	1.200	6.76	1.182	2.29
MGHS	100	1.804	1.551	86.0	1.556	1.14
MGHS	300	2.232	1.430	64.0	1.435	1.15
MGHS	3000	2.487	1.160	46.7	1.180	1.02
VHS	——	2.390	1.201	50.3	1.190	1

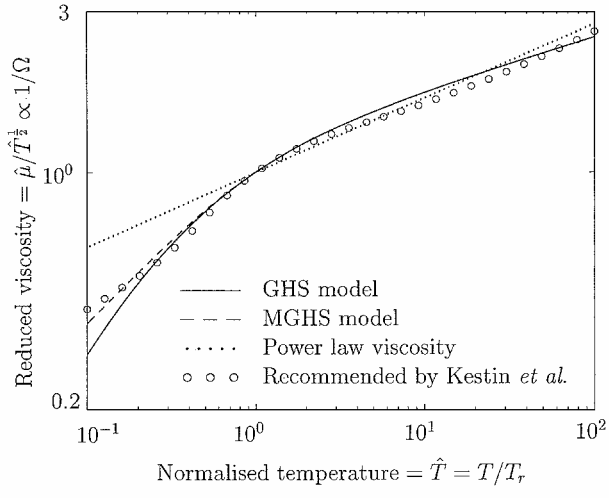

Fig. 1 Reduced viscosity $\hat{\mu}/\hat{T}^{1/2} = (\mu/\mu_r)/(T/T_r)^{1/2} \propto 1/\Omega$ vs $\hat{T}$.

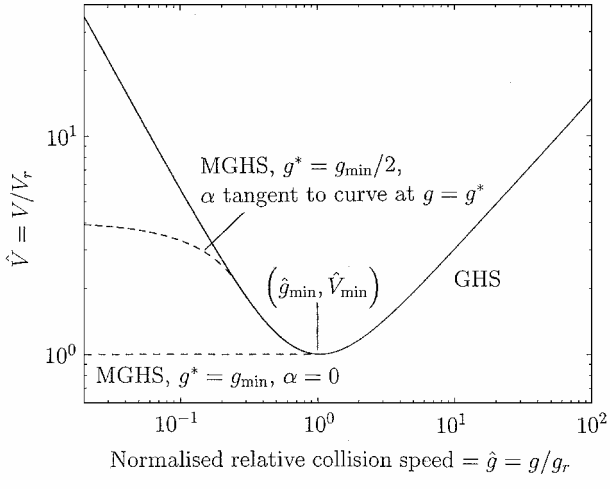

Fig. 2 $\hat{V} = V/V_r = \sigma g/(\sigma_r g_r)$ vs $\hat{g} = g/g_r$ for GHS and MGHS models; see Fig. 1.

is $\mu = \mu_r (T/T_r)^{1/2+\upsilon}$, where $\upsilon = 0.22$. Note that the GHS viscosity is unrealistically low for $T \lesssim 100$ K. This arises from a large cross section and consequent high collision rate.

The probability of collision between two particles with relative speed g is proportional to $\sigma g = V$. Figure 2 shows $\hat{V} = V/V_r = \sigma g/(\sigma_r g_r)$ vs $\hat{g}$ for the Ar parameters. It is apparent that $\hat{V} \to \infty$ as $\hat{g} \to 0$. The number of possible collision pairs tested N_{pairs} is proportional to the maximum value of V found in the simulation, denoted V_{max}. The probability of collision is given by the ratio V/V_{max}. Because V_{max} becomes extremely large when possible collision pairs having $\hat{g} \ll \hat{g}_{min}$ are found, N_{pairs} becomes extremely large, and each possible collision pair has a small probability of actually participating in a collision. This has an adverse effect on computational efficiency, particularly when T is low.

The collision frequency ν is given by $\nu = n\langle \sigma g \rangle$, where $\langle \sigma g \rangle$ represents the mean value of σg over all possible collision pairs. The equilibrium distribution of γ is $f_\gamma = (4/\pi^{1/2})\gamma^2 \exp(-\gamma^2)$, from which the collision frequency for the GHS model

$$\nu_{GHS} = 2nV_r(\hat{T}/\pi)^{\frac{1}{2}}\left[\phi\hat{T}^{-\upsilon_1}\Gamma(2-\upsilon_1) + (1-\phi)\hat{T}^{-\upsilon_2}\Gamma(2-\upsilon_2)\right] \tag{1}$$

may be obtained. If either υ_1 or $\upsilon_2 > \frac{1}{2}$, as in the present case, then $\nu_{GHS} \to \infty$ as $\hat{T} \to 0$.

Modified GHS Model

If the GHS model is modified such that $\hat{V}$ is limited at low $\hat{g}$, the computational efficiency of the model will be improved. Let the curve of $\hat{V}$ vs $\hat{g}$ for the GHS model be modified below a transition point $(\hat{g}^*, \hat{V}^*)$ on the curve with $\hat{g}^* \le \hat{g}_{min}$. The modification is linear, such that a finite value of $\hat{V}$ is obtained when $\hat{g} = 0$. The gradient $\alpha = d\hat{V}/d\hat{g}$ of the linear portion is set equal to the tangent slope at the transition point, given by

$$\alpha = \phi(1-2\upsilon_1)\hat{g}^{-2\upsilon_1} + (1-\phi)(1-2\upsilon_2)\hat{g}^{-2\upsilon_2} \tag{2}$$

Alternatively, for simplicity, $\alpha = 0$ could be used.

For $\hat{g} < \hat{g}^*$, $\hat{V} = \alpha(\hat{g} - \hat{g}^*) + \hat{V}^*$, and the modified GHS (MGHS) cross section is given by

$$\hat{\sigma} = \begin{cases} \alpha + (1/\hat{g})(\hat{V}^* - \alpha\hat{g}^*) & \text{when} \quad \hat{g} \le \hat{g}^* \\ \phi\hat{g}^{-2\upsilon_1} + (1-\phi)\hat{g}^{-2\upsilon_2} & \text{when} \quad \hat{g} > \hat{g}^* \end{cases}$$

Two possibilities are shown in Fig. 2: $g^* = g_{min}$ with $\alpha = 0$ and $g^* = g_{min}/2$ with α set to the gradient as given in Eq. (2). The following equations are derived for general α, $\hat{g}^*$, and $\hat{V}^*$, but computational efficiency is examined for the first possibility only.

It may be shown, after considerable calculus and algebraic manipulation, that

$$\Omega(\hat{T}) = (2\sigma_r/3)(A + B)$$

where

$$A(\hat{T}) = \alpha[I_7(0) - I_7(a)] + \hat{T}^{-\frac{1}{2}}(\hat{V}^* - \alpha\hat{g}^*)[I_6(0) - I_6(a)] \tag{3}$$

$$2B(\hat{T}) = \phi\hat{T}^{-\upsilon_1}\Gamma\left(4-\upsilon_1, a^2\right) + (1-\phi)\hat{T}^{-\upsilon_2}\Gamma\left(4-\upsilon_2, a^2\right)$$

$$I_n(a) = \int_a^\infty \gamma^n \exp(-\gamma^2)\, d\gamma$$

where n is an integer and

$$\Gamma(j, \beta) = \int_\beta^\infty x^{j-1} \exp(-x)\, dx$$

$\Gamma(j, \beta)$ is the incomplete gamma function. Algebraic expressions for the I_n terms that appear in Eq. (3) are given in Ref. 1. The MGHS viscosity is plotted in Fig. 1. At $T = 100$ K, $\mu_{MGHS}/\mu_{GHS} \approx 1.025$. This ratio decreases rapidly at higher T. At very low T, the MGHS model gives a viscosity closer to the recommendations of

Kestin et al.[6] than the GHS model. This suggests that the assumption of a finite collision probability at $g = 0$ is more realistic than the infinite value given by the GHS model.

The collision frequency of the MGHS model $\nu_{\mathrm{MGHS}} = n\langle \sigma g \rangle$ is given by

$$\nu_{\mathrm{MGHS}} = 4nV_r(\hat{T}/\pi)^{\frac{1}{2}}(C + D) \tag{4}$$

where C and D are similar in form to A and B, respectively, and are given by

$$C(\hat{T}) = \alpha[I_3(0) - I_3(a)] + \hat{T}^{-\frac{1}{2}}(\hat{V}^* - \alpha\hat{g}^*)[I_2(0) - I_2(a)]$$

$$2D(\hat{T}) = \phi\hat{T}^{-\upsilon_1}\Gamma\left(2 - \upsilon_1, a^2\right) + (1 - \phi)\hat{T}^{-\upsilon_2}\Gamma\left(2 - \upsilon_2, a^2\right)$$

From Eqs. (1) and (4), it can be shown that ν_{MGHS} is considerably lower than ν_{GHS} for $\hat{T} \lesssim 1$. For example, at $\hat{T} = (1, 0.5, 0.1, 0.05)$, $\nu_{\mathrm{MGHS}}/\nu_{\mathrm{GHS}} \approx (0.92, 0.83, 0.49, 0.35)$.

Computational Efficiency

The computational efficiency of the GHS and MGHS models under conditions of thermal equilibrium was determined by simulations for a set of 1000 monatomic simulator molecules for a time of $100\tau_{\mathrm{nom}}$, where $\tau_{\mathrm{nom}} = \pi\mu_{\mathrm{GHS}}/(4\rho RT)$. The simulation time step Δt was $0.4\tau_{\mathrm{nom}}$. Temperatures of 100, 300, and 3000 K were simulated. At each time step, the number of collision pairs tested and the actual number of collisions performed were recorded. Simulations were also performed using the VHS model, with $\upsilon = 0.22$ and the viscosity matched to μ_{GHS}. The number of collisions per simulator particle per time τ_{nom} is independent of T for the VHS model, and a single VHS simulation was, therefore, sufficient.

The mean results from the second-half of each simulation are summarized in Table 1. The results are subject to statistical scatter, but demonstrate the poor computational efficiency of the GHS model, even at high temperatures. This inefficiency is caused primarily by the high number of pairs tested at each time step due to very high values of $V_{\max}$, but also by the higher collision frequency. The MGHS model requires no more than 15% more CPU time than the VHS model.

Conclusions

The GHS model can be modified to limit the collision probability at low collision speeds. This improves the computational efficiency both because the number of possible collision partners that must be tested is dramatically reduced and because the collision rate is lower. No more than 15% extra computational time is required, compared with the VHS model. For argon at $T \approx 100$ K, the theoretical viscosity is changed by less than 2.5%, and this difference decreases rapidly as T increases. The modified viscosity is in better agreement with recommended viscosity values. This modified generalized hard sphere model can be used in DSMC simulations, where, to obtain realistic viscosity behavior at low T, it is necessary to model the effect of the attractive portion of the intermolecular potential.

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Impingement Heat Transfer over a Rotating Disk: Integral Method

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Nomenclature

A	=	dimensionless parameter ($= ad_j/V_j$)
a	=	radial velocity gradient at the outer edge of the boundary layer
c_p	=	specific heat at constant pressure
d	=	disk diameter
d_j, h_j	=	jet nozzle diameter and nozzle-to-disk distance
k	=	thermal conductivity
Nu_d	=	local Nusselt number ($= q_w d/[k(T_w - T_\infty)]$)
Pr	=	Prandtl number ($= \mu c_p/k$)
q_w	=	heat flux at the wall
Re_j	=	jet Reynolds number ($= V_j d_j/\nu$)
Re_ω	=	rotational Reynolds number ($= \omega d^2/\nu$)
r, φ, z	=	radial, tangential, and axial cylindrical coordinates
T	=	temperature
V_j	=	axial velocity at infinity or at the nozzle outlet
v_r, v_φ, v_z	=	radial, tangential, and axial velocity components in cylindrical coordinates
δ	=	boundary-layer thickness
δ_T^{**}	=	enthalpy thickness $\left(= \int_0^1 \frac{v_r}{\omega r}\frac{T - T_\infty}{T_w - T_\infty}\,\mathrm{d}\xi\right)$
κ	=	nondimensional parameter ($= a/\omega$)
μ, ν	=	dynamic and kinematic viscosity
ρ	=	density
τ_{wr}	=	radial shear stress $[= \mu(\mathrm{d}v_r/\mathrm{d}z)_{z=0}]$
$\tau_{w\varphi}$	=	tangential shear stress $[= \mu(\mathrm{d}v_\varphi/\mathrm{d}z)_{z=0}]$
χ	=	Reynolds analogy parameter $\{= q_w\omega r/[\tau_{w\varphi}c_p(T_\infty - T_w)]\}$
ω	=	angular speed of rotation

Subscripts

j	=	parameters of the impinging jet
w	=	wall
0	=	free disk
∞	=	outer edge of the boundary layer

Introduction

UNDERSTANDING of peculiarities of real jets is frequently based on the solutions of simplified problems. For an

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