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Variable soft sphere molecular model for inverse-power-law or Lennard-Jones potential

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The variable soft sphere (VSS) molecular model is introduced for both the viscosity and diffusion cross sections (coefficients) to be consistent with those of the inverse-power-law (IPL) or Lennard-Jones (LJ) potential. The VSS model has almost the same analytical and computational simplicity (computation time) as the variable hard sphere (VHS) model in the Monte Carlo simulation of rarefied gas flows. The null-collision Monte Carlo method is used to make comparative calculations for the molecular diffusion in a heat-bath gas and the normal shock wave structure in a simple gas. For the most severe test of the VSS model for the IPL potential, the softest practical model corresponding to the Maxwell molecule is chosen. The agreement in the molecular diffusion and shock wave structure between the VSS model and the IPL or LJ potential is remarkably good.

I. INTRODUCTION

In the Monte Carlo simulation of rarefied gas flows, a realistic but sufficiently simple molecular model is required and the variable hard sphere (VHS) model^{1,2} defined for the inverse-power-law (IPL) potential³ has been proposed. In a previous paper,⁴ however, it was indicated that the VHS model is not compatible with the diffusion coefficient of the IPL model and a serious discrepancy between the VHS and IPL models may appear when the molecular diffusion plays an important role in gas mixture flows.

In this paper, the variable soft sphere (VSS) molecular model is introduced for both the viscosity and diffusion cross sections (coefficients) to be consistent with those of the IPL or Lennard-Jones (LJ) potential.^{5,6} The null-collision test-particle⁷ and direct-simulation^{7,8} Monte Carlo methods are, respectively, used to make comparative calculations for the molecular diffusion in a heat-bath gas and the normal shock wave structure in a simple gas. For the most severe test of the VSS model for the IPL potential, the softest practical model corresponding to the Maxwell molecule is chosen.²

II. VSS MOLECULAR MODEL

A. Inverse-power-law potential

The VHS model is defined¹ to have a definite but variable (energy-dependent) diameter d and the hard sphere (isotropic) scattering law; i.e., the impact parameter b is given by

$$b = d \cos(\chi/2), \quad (1)$$

where χ is the deflection angle. The diameter d is determined from the IPL potential so that the viscosity cross section (coefficient) of the VHS model is consistent with that of the IPL potential. The VHS model has the definite total, viscosity, and diffusion cross sections defined by^{3,6}

$$\begin{aligned} \sigma_t &= 2\pi \int b db \\ &= \pi d^2, \end{aligned} \quad (2)$$

$$\begin{aligned} \sigma_\eta &= 2\pi \int (1 - \cos^2 \chi) b db \\ &= (2/3)\pi d^2, \end{aligned} \quad (3)$$

$$\begin{aligned} \sigma_D &= 2\pi \int (1 - \cos \chi) b db \\ &= \pi d^2, \end{aligned} \quad (4)$$

respectively. On the other hand, the IPL potential with the intermolecular force $F = \kappa/r^\nu$, κ and ν being the force constant and the exponent of the intermolecular distance r , respectively, has the definite viscosity and diffusion cross sections³

$$\sigma_\eta = 2\pi A_2(\nu) (\kappa/2)^{2/(\nu-1)} \epsilon^{-2/(\nu-1)}, \quad (5)$$

$$\sigma_D = 2\pi A_1(\nu) (\kappa/2)^{2/(\nu-1)} \epsilon^{-2/(\nu-1)}, \quad (6)$$

respectively, where ϵ is the relative collision energy and the definition of the integrals $A_1(\nu)$ and $A_2(\nu)$ and their values are given in Ref. 3, but the total cross section σ_t becomes infinite.

A comparison of Eq. (3) with Eq. (5) indicates that the energy-dependent diameter d is taken to be

$$\pi d^2 = c \epsilon^{-\omega} \quad (7)$$

with the energy exponent

$$\omega = 2/(\nu - 1) \quad (8)$$

and the cross-section constant $c = 3\pi A_2(\nu) (\kappa/2)^\omega$. In the practical application of the VHS model, ω (or ν) and c are, respectively, determined from the temperature exponent and absolute value of the experimental viscosity or diffusion coefficient at an appropriate temperature T by taking account of the fact that the viscosity coefficient η and (self) diffusion coefficient D of the first approximation of the Chapman-Enskog solution (for a simple gas) is given by

$$\eta_{\text{VHS}} = (15/8c) (\pi m)^{1/2} (kT)^{\omega+1/2} / \Gamma(4-\omega), \quad (9)$$

$$\eta_{\text{IPL}} = \frac{(5/8) (m/\pi)^{1/2} (2/\kappa)^\omega (kT)^{\omega+1/2}}{[A_2(\nu) \Gamma(4-\omega)]}, \quad (10)$$

$$D_{\text{VHS}} = [2(3-\omega)/5nm] \eta_{\text{VHS}}, \quad (11)$$

$$D_{\text{IPL}} = [3(3-\omega)/5nm] [A_2(\nu)/A_1(\nu)] \eta_{\text{IPL}}, \quad (12)$$

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where the subscripts VHS and IPL denote the VHS model and the IPL potential, respectively, m is the molecular mass, k is the Boltzmann constant, and n is the number density. It is seen from Eqs. (3)–(6) or Eqs. (9)–(12) that both the viscosity and diffusion cross sections (coefficients) of the VHS model are not compatible with those of the IPL potential, because $A_1(\nu)/A_2(\nu) \neq 3/2$ except for $\nu = \infty$ ($\omega = 0$). The mean free path defined by $\lambda = (8kT/\pi m)^{1/2}/\nu_c$ with the mean collision frequency $\nu_c = 4cn(kT)^{1/2-\omega} \times \Gamma(2-\omega)/(\pi m)^{1/2}$ of the VHS model can be converted into the viscosity² and diffusion⁴ mean free paths defined by the VHS model,

$$\lambda_\eta(\text{VHS}) = (8\eta/15)(3-\omega)(2-\omega)(2\pi mkT)^{-1/2}/n, \quad (13)$$

$$\lambda_D(\text{VHS}) = (4D/3)(2-\omega)(2\pi kT/m)^{-1/2}, \quad (14)$$

by eliminating the cross-section constant c by the use of the viscosity [Eq. (9)] and diffusion [Eq. (11)] coefficients, respectively.

The simplest extension of the VHS model for both the viscosity and diffusion cross sections (coefficients) to be consistent with those of the IPL potential is realized by the variable soft sphere (VSS) model with the impact parameter given by

$$b = d \cos^\alpha(\chi/2), \quad (15)$$

where d and α are the energy-dependent diameter and exponent of the cosine of deflection angle, respectively. This model is called the variable soft sphere model because the diameter d is variable and the deflection angle χ is smaller than the VHS deflection angle χ_{VHS} defined by $\cos(\chi_{\text{VHS}}/2) = \cos^\alpha(\chi/2)$ for $\alpha > 1$. The diameter d and exponent α are determined from the IPL potential so that both the viscosity and diffusion cross sections (coefficients) are consistent with those of the IPL potential. (The VHS model assumes $\alpha = 1$.) The VSS model has the definite total, viscosity, and diffusion cross sections

$$\sigma_t = \pi d^2, \quad (16)$$

$$\sigma_\eta = S_\eta(2/3)\pi d^2, \quad (17)$$

$$\sigma_D = S_D\pi d^2, \quad (18)$$

respectively, where S_η and S_D are the softness coefficients defined by

$$S_\eta = 6\alpha/[(\alpha+1)(\alpha+2)], \quad (19)$$

$$S_D = 2/(\alpha+1), \quad (20)$$

for the viscosity and diffusion cross sections, respectively. A comparison of Eqs. (17) and (18) with Eqs. (5) and (6) indicates that the diameter d is taken to be the same form as the VHS model,

$$\pi d^2 = c\epsilon^{-\omega} \quad (21)$$

with the same energy exponent $\omega = 2/(\nu-1)$ as the VHS model and the cross-section constant $c = 3\pi A_2(\nu)(\kappa/2)^\omega/S_\eta$ with the additional factor of S_η , and the exponent α is taken to be

$$\alpha = [A_1(\nu)/A_2(\nu) - 1/2]^{-1}. \quad (22)$$

The softness coefficients vary over the range

$0.95 < S_\eta < 1.03$ and $0.58 < S_D \leq 1.0$ for $\nu > 4.3$ or $\omega < 0.61$ (see Table I). The viscosity (η_{VSS}) and diffusion (D_{VSS}) coefficients of the first approximation of the Chapman–Enskog solution for the VSS model are related to those for the VHS model as

$$\eta_{\text{VSS}} = \eta_{\text{VHS}}/S_\eta, \quad (23)$$

$$D_{\text{VSS}} = D_{\text{VHS}}/S_D. \quad (24)$$

The viscosity [$\lambda_\eta(\text{VSS})$] and diffusion [$\lambda_D(\text{VSS})$] mean free paths defined by the VSS model in the same way as the VHS model are related to those defined by the VHS model as

$$\lambda_\eta(\text{VSS}) = S_\eta \lambda_\eta(\text{VHS}), \quad (25)$$

$$\lambda_D(\text{VSS}) = S_D \lambda_D(\text{VHS}). \quad (26)$$

In the Monte Carlo simulation, a value of $\cos \chi$ is required⁹ instead of the deflection angle χ itself. For the impact parameter b of the VSS model [Eq. (15)], $\cos \chi$ is evaluated as

$$\cos \chi = 2 \cdot R^{1/\alpha} - 1 \quad (27)$$

with a uniform random number R in the range (0,1), and therefore the VSS model has almost the same computational simplicity (computation time) as the VHS model. Because the VSS model requires the values of $A_1(\nu)$ and $A_2(\nu)$ for the evaluation of the exponent α [Eq. (22)], the integrals $A_1(\nu)$ and $A_2(\nu)$ are evaluated using an accurate quadrature scheme of the double exponential formula¹⁰ and the values of α , S_η , and S_D are presented in Table I for various values of ν (or ω) of the molecular species compiled in Ref. 3, where ν was derived from the experimental viscosity, diffusion, or thermal diffusion coefficient.

Figure 1 shows a comparison of the deflection angle χ versus the reduced impact parameter $\beta = b(2\epsilon/\kappa)^{\omega/2}$ for the Maxwell molecule, $\nu = 5$ or $\omega = 0.5$, between the VSS and VHS models and the IPL potential, where β for the VHS and VSS models is given by $\beta = [3A_2(\nu)]^{1/2}\cos(\chi/2)$ and $\beta = [3A_2(\nu)/S_\eta]^{1/2}\cos^\alpha(\chi/2)$, respectively. It is noted that the deflection angle for the VSS model clings to that for the IPL potential.

B. Lennard-Jones potential

The VSS model can generally be defined for any intermolecular potential with the definite viscosity and diffusion cross sections, from which the energy-dependent diameter d and exponent α are determined. Here, the VSS model is defined for a realistic potential function of the LJ (6–12) potential

$$\phi(r) = 4\epsilon_{\text{LJ}} [(d_{\text{LJ}}/r)^{12} - (d_{\text{LJ}}/r)^6], \quad (28)$$

where ϵ_{LJ} is the depth of the potential well and d_{LJ} is the value of the intermolecular distance for which $\phi(r) = 0$. The numerical values of the reduced viscosity ($\sigma_\eta^* = \sigma_\eta/\sigma_{\text{LJ}}$) and diffusion ($\sigma_D^* = \sigma_D/\sigma_{\text{LJ}}$) cross sections of the LJ potential were obtained¹¹ over the wide range of the reduced relative energy $\epsilon^* = \epsilon/\epsilon_{\text{LJ}}$ using an accurate quadrature scheme and are presented in Fig. 2, where $\sigma_{\text{LJ}} = \pi d_{\text{LJ}}^2$ is the constant LJ cross section; the fitted equations for the reduced viscosity and diffusion cross sections are available in Ref. 5. Equating σ_η and σ_D of the VSS model [Eqs. (17) and (18)]

TABLE I. Values of integrals $A_1(\nu)$ and $A_2(\nu)$, exponent α of the cosine of deflection angle, and softness coefficients S_η and S_D for various values of the IPL force exponent ν or the VSS energy exponent ω of the molecular species compiled in Ref. 3 (first edition *; third edition).

Gases	ν	ω	$A_1(\nu)$	$A_2(\nu)$	α	S_η	S_D
NH ₃	4.3	0.606	0.4633	0.5090	2.4377	0.9587	0.5818
SO ₂	4.6	0.556	0.4418	0.4719	2.2924	0.9733	0.6075
HCl	4.8	0.526	0.4308	0.4525	2.2122	0.9810	0.6226
Cl ₂	4.9	0.513	0.4262	0.4440	2.1743	0.9845	0.6301
HCl*	4.97	0.504	0.4232	0.4385	2.1500	0.9868	0.6349
Maxwell, C ₂ H ₂ , Cl ₂ *	5.0	0.500	0.4219	0.4362	2.1403	0.9877	0.6369
NH ₃ *	5.16	0.481	0.4160	0.4250	2.0885	0.9924	0.6476
Kr-Xe*	5.2	0.476	0.4146	0.4224	2.0767	0.9934	0.6500
N ₂ O	5.5	0.444	0.4060	0.4054	1.9941	1.0005	0.6680
CO ₂ , Ar-Xe*, CO ₂ *	5.6	0.435	0.4036	0.4005	1.9695	1.0025	0.6735
Ar-Kr*	5.7	0.426	0.4014	0.3960	1.9469	1.0043	0.6787
-----	6.0	0.400	0.3959	0.3840	1.8833	1.0092	0.6937
N ₂ O*	6.15	0.388	0.3937	0.3788	1.8541	1.0113	0.7007
H ₂ -Rn*	6.3	0.377	0.3917	0.3741	1.8280	1.0132	0.7072
CH ₄ *	6.36	0.373	0.3910	0.3723	1.8174	1.0139	0.7099
H ₂ -CO ₂ , He-CO ₂	6.9	0.339	0.3861	0.3589	1.7368	1.0190	0.7308
CH ₄ , Ne-Xe*	7.0	0.333	0.3854	0.3568	1.7237	1.0197	0.7343
Ne-CO ₂	7.05	0.331	0.3851	0.3558	1.7172	1.0201	0.7361
N ₂ -Ar*, H ₂ -CO ₂ *	7.2	0.323	0.3843	0.3529	1.6979	1.0211	0.7413
H ₂ -O ₂ *, He-Rn*	7.3	0.317	0.3838	0.3511	1.6860	1.0218	0.7446
Ar*	7.35	0.315	0.3836	0.3502	1.6796	1.0221	0.7464
Ar	7.5	0.308	0.3830	0.3477	1.6624	1.0229	0.7512
O ₂ -CO ₂	7.54	0.306	0.3828	0.3471	1.6588	1.0231	0.7522
Ne-Kr*, O ₂ *	7.6	0.303	0.3826	0.3462	1.6525	1.0234	0.7540
CH ₄ -O ₂	7.83	0.293	0.3819	0.3429	1.6294	1.0244	0.7606
NO, Ne-Ar*	7.9	0.290	0.3818	0.3420	1.6224	1.0247	0.7627
-----	8.0	0.286	0.3815	0.3407	1.6135	1.0251	0.7652
NO*	8.1	0.282	0.3814	0.3394	1.6032	1.0255	0.7683
H ₂ -O ₂	8.13	0.281	0.3813	0.3391	1.6014	1.0256	0.7688
H ₂ -N ₂ *, D ₂ -N ₂ *	8.2	0.278	0.3812	0.3383	1.5954	1.0258	0.7706
He-Xe*	8.3	0.274	0.3811	0.3371	1.5860	1.0262	0.7734
Air, O ₂	8.4	0.270	0.3810	0.3360	1.5775	1.0265	0.7760
Air*	8.46	0.268	0.3809	0.3354	1.5732	1.0266	0.7773
H ₂ -D ₂ *	8.6	0.263	0.3808	0.3340	1.5622	1.0270	0.7806
He-Kr*	8.7	0.260	0.3808	0.3331	1.5547	1.0272	0.7829
CO*	8.75	0.258	0.3808	0.3326	1.5506	1.0273	0.7841
N ₂ *	8.8	0.256	0.3808	0.3321	1.5464	1.0274	0.7854
N ₂ -CO ₂	8.91	0.253	0.3808	0.3312	1.5390	1.0277	0.7877
He-Ar*	9.0	0.250	0.3808	0.3304	1.5325	1.0278	0.7897
-----	9.33	0.240	0.3810	0.3278	1.5099	1.0284	0.7968
N ₂	9.4	0.238	0.3810	0.3273	1.5059	1.0285	0.7981
CO	9.5	0.235	0.3811	0.3266	1.4995	1.0286	0.8001
He-N ₂ *, He-Ar	9.9	0.225	0.3816	0.3241	1.4762	1.0290	0.8077
-----	10.0	0.222	0.3817	0.3235	1.4708	1.0291	0.8095
CO-O ₂	10.52	0.210	0.3825	0.3208	1.4444	1.0293	0.8182
D ₂ *	11.0	0.200	0.3834	0.3187	1.4225	1.0294	0.8256
D ₂	11.1	0.198	0.3836	0.3183	1.4181	1.0294	0.8271
H ₂ *	11.3	0.194	0.3841	0.3176	1.4097	1.0294	0.8300
H ₂ -Ne*, He-Ne*	11.4	0.192	0.3843	0.3172	1.4054	1.0294	0.8315
He-N ₂	11.45	0.191	0.3844	0.3171	1.4040	1.0294	0.8319
He*	11.8	0.185	0.3852	0.3159	1.3901	1.0294	0.8368
-----	12.0	0.182	0.3856	0.3153	1.3832	1.0293	0.8392
H ₂	12.9	0.168	0.3878	0.3130	1.3532	1.0290	0.8499
-----	13.0	0.167	0.3880	0.3128	1.3506	1.0289	0.8508
Ne	13.4	0.161	0.3890	0.3120	1.3391	1.0287	0.8550
He, Ne*	13.7	0.157	0.3898	0.3115	1.3309	1.0285	0.8580
-----	14.0	0.154	0.3905	0.3110	1.3234	1.0283	0.8608
Ne*	14.5	0.148	0.3918	0.3103	1.3112	1.0280	0.8653
He*	14.6	0.147	0.3921	0.3101	1.3082	1.0279	0.8665
-----	15.0	0.143	0.3931	0.3096	1.2992	1.0276	0.8699
-----	21.0	0.100	0.4069	0.3066	1.2090	1.0233	0.9054
-----	25.0	0.083	0.4144	0.3066	1.1743	1.0208	0.9199
Hard sphere	∞	0.000	0.5000	0.3333	1.0000	1.0000	1.0000

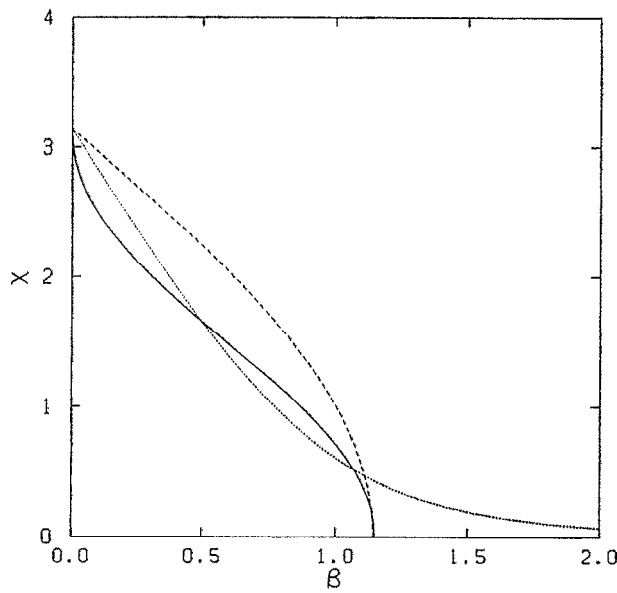


FIG. 1. Comparison of deflection angle versus reduced impact parameter for $\nu = 5$ ($\omega = 0.5$) between the VSS (—) and VHS (---) models and the IPL potential (· · ·).

to those of the LJ potential determines the exponent α and the diameter d or reduced total cross section $\sigma_t^* = \pi d^2 / \sigma_{LJ}$ as

$$\alpha = (\sigma_D^* / \sigma_\eta^* - 1/2)^{-1}, \quad (29)$$

$$\sigma_t^* = (3/2 S_\eta) \sigma_\eta^*. \quad (30)$$

The variation of α and σ_t^* vs ϵ^* is shown in Fig. 3.

The viscosity (η for a simple gas) and binary diffusion (D) coefficients of the first approximation of the Chapman-Enskog solution are given by⁶

$$\eta = (5/16) (\pi m k T)^{1/2} / \sigma_{LJ} \Omega_\eta^*, \quad (31)$$

$$D = (3/16 n) (2 \pi k T / \mu)^{1/2} / \sigma_{LJ} \Omega_D^*, \quad (32)$$

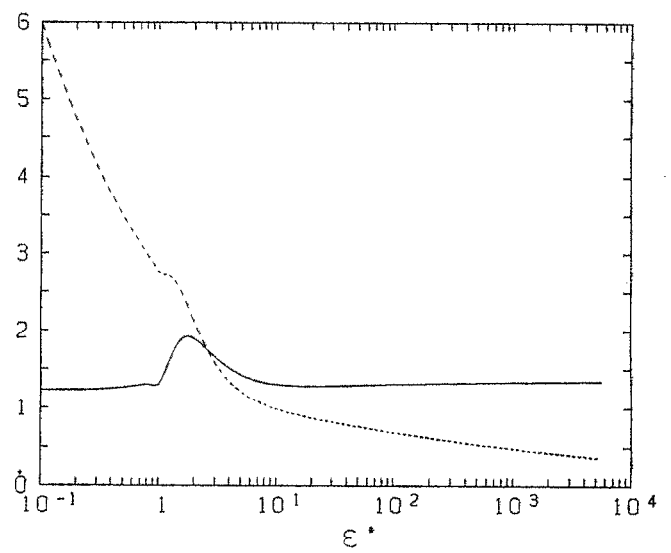


FIG. 3. Exponent α (—) of the cosine of deflection angle and reduced total cross section σ_t^* (---) of the VSS model defined for the LJ potential versus reduced relative energy ϵ^* .

where μ is the reduced mass and Ω_η^* and Ω_D^* are the integrals defined by

$$\Omega_\eta^* = \left(\frac{1}{4 T^{*4}} \right) \int \epsilon^{*3} \sigma_\eta^* \exp \left(- \frac{\epsilon^*}{T^*} \right) d\epsilon^*, \quad (33)$$

$$\Omega_D^* = \left(\frac{1}{2 T^{*3}} \right) \int \epsilon^{*2} \sigma_D^* \exp \left(- \frac{\epsilon^*}{T^*} \right) d\epsilon^*, \quad (34)$$

in which $T^* = kT / \epsilon_{LJ}$ is the reduced temperature. The mean free path defined by $\lambda = (8kT / \pi m)^{1/2} / \nu_c$ with the mean collision frequency ν_c of the VSS model leads to

$$\lambda = (\sqrt{2} n \sigma_{LJ} \nu_c^*)^{-1} \quad (35)$$

with the reduced collision frequency $\nu_c^* = [4(kT / \pi m)^{1/2} n \sigma_{LJ}]^{-1} \nu_c$ given by

$$\nu_c^* = \left(\frac{1}{T^{*2}} \right) \int \epsilon^* \sigma_t^* \exp \left(- \frac{\epsilon^*}{T^*} \right) d\epsilon^*. \quad (36)$$

Eliminating σ_{LJ} in Eq. (35) by the use of the viscosity coefficient η [Eq. (31)] yields the viscosity mean free path defined by the VSS model

$$\lambda_\eta = (16/5 n) (2 \pi m k T)^{-1/2} \eta \Omega_\eta^* / \nu_c^*. \quad (37)$$

III. COMPARISON BETWEEN VSS AND VHS MODELS AND IPL OR LJ POTENTIAL

A. Molecular diffusion in a heat-bath gas

Comparative calculations between the VSS and VHS (VSS with $\alpha = 1$) models and the IPL or LJ potential are made for the diffusion of trace molecules,⁴ which are mutually noninteracting, in a heat-bath gas. At initial time $t = 0$, the positions and velocities of trace molecules are taken as the origin of position vector $\mathbf{r} = 0$ and the isotropic same velocity $v = (3kT_0 / m)^{1/2}$, respectively, where m and T_0 are the mass and initial temperature of trace molecules, respectively. The heat-bath gas of the molecular mass M and num-

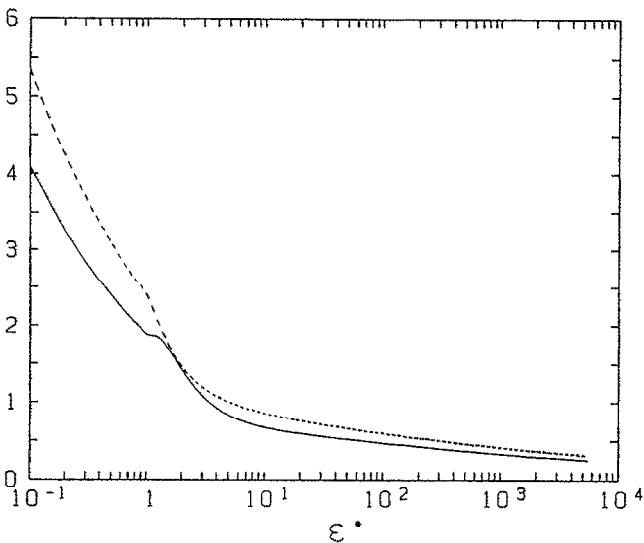


FIG. 2. Reduced viscosity σ_η^* (—) and diffusion σ_D^* (---) cross sections of the LJ potential versus reduced relative energy ϵ^* .

ber density n is assumed to remain as the equilibrium Maxwellian velocity distribution at the reservoir temperature T_R . In the present null-collision scheme for the IPL or LJ potential, the deflection angle χ is actually calculated at every collision with an accurate quadrature scheme,¹² and the molecular collisions for the deflection angle $|\chi|$ less than a small cutoff angle χ_{\min} are ignored so that the effective total cross section σ , used in the Monte Carlo simulation is finite. Because the difference between $\chi_{\min} = 0.1^\circ$ and 1° is confirmed to be negligible, the results for the smaller cutoff angle $\chi_{\min} = 0.1^\circ$ are presented. The total number of trace molecules is taken as 10^5 .

For comparison between the IPL potential and the VSS and VHS ($\alpha = 1$) models defined for the IPL potential, the length scale is taken as the viscosity mean free path defined by the VSS model [Eq. (25)] at the temperature T_R ,

$$\lambda_\eta = S_\eta (8\eta/15) (3 - \omega) (2 - \omega) (2\pi mk T_R)^{-1/2} / n, \quad (38)$$

and the time scale is taken as the viscosity mean collision time defined by $t_\eta = \lambda_\eta / \langle c \rangle$ with the mean thermal speed $\langle c \rangle = (8kT_R/\pi m)^{1/2}$. The evolution of the radial mean-square displacement $\langle r^2 \rangle / \lambda_\eta^2$ of trace molecules versus time t/t_η is compared in Fig. 4 for the mass ratio $m/M = 1$ and the initial temperature ratio $T_0/T_R = 10$ between the VSS and VHS models and the IPL potential. The agreement with the diffusion for the IPL potential is good for the VSS model but poor for the VHS model in the VSS viscosity scale; the gradient of $\langle r^2 \rangle / \lambda_\eta^2$ vs t/t_η for the IPL potential or the VSS model approaches the theoretical value of $6D/\lambda_\eta \langle c \rangle = (3\pi/2)/S_D$, where D is the binary diffusion coefficient of the first approximation of the Chapman-Enskog solution.³ Therefore the VSS model may be preferable to the VHS model especially when the molecular diffusion

plays an important role in gas mixture flows. It is noted that the (overall) velocity distribution functions of the VSS and VHS models relax via similar shapes, which are, however, rather different from that for the IPL potential.

For comparison between the LJ potential and the VSS and VHS ($\alpha = 1$) models defined for the LJ potential, the length scale is taken as the viscosity mean free path defined by the VSS model [Eq. (37)] at the temperature T_R ,

$$\lambda_\eta = (16/5n) (2\pi mk T_R)^{-1/2} \eta \Omega_\eta^* / v_c^*, \quad (39)$$

and the time scale is taken as the viscosity mean collision time $t_\eta = \lambda_\eta / \langle c \rangle$. The evolution of the radial mean-square displacement $\langle r^2 \rangle / \lambda_\eta^2$ of trace molecules versus time t/t_η is compared in Fig. 5 for the mass ratio $m/M = 1$, the initial temperature ratio $T_0/T_R = 10$, and the reduced temperature $T^* = kT_R/\epsilon_{LJ} = 1$ between the VSS and VHS models and the LJ potential. The agreement with the diffusion for the LJ potential is good for the VSS model but poor for the VHS model in the VSS viscosity scale, consistent with the case of the IPL potential; the gradient of $\langle r^2 \rangle / \lambda_\eta^2$ vs t/t_η for the LJ potential or the VSS model approaches the theoretical value of $6D/\lambda_\eta \langle c \rangle = (9\pi/16) (m/\mu) v_c^* / \Omega_D^*$, where the reduced mass is given by $\mu = mM/(m + M)$. As in the case of the IPL potential, the (overall) velocity distribution functions of the VSS and VHS models are similar but rather different from that for the LJ potential.

B. Structure of the normal shock wave

Comparative calculations between the VSS and VHS (VSS with $\alpha = 1$) models and the IPL or LJ potential are also made for the normal shock wave structure in a simple gas. A discontinuity surface that is perpendicular to the flow direction and separates the upstream and downstream equi-

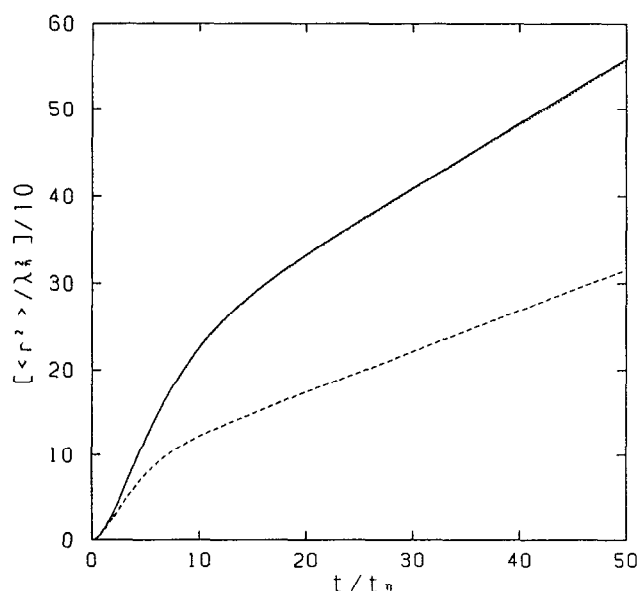


FIG. 4. Comparison of radial mean-square displacement of trace molecules in a heat-bath gas for $\nu = 5$ ($\omega = 0.5$) between the VSS (—) and VHS (---) models and the IPL potential (- · -) in the VSS viscosity scale.

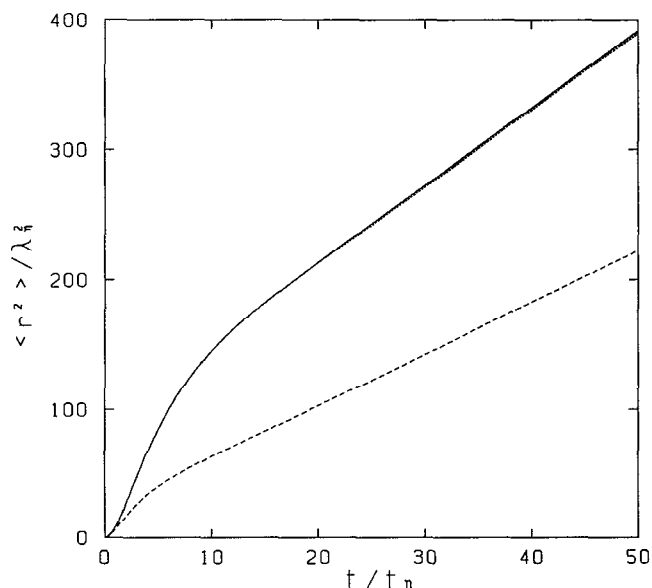


FIG. 5. Comparison of radial mean-square displacement of trace molecules in a heat-bath gas between the VSS (—) and VHS (---) models and the LJ potential (- · -) in the VSS viscosity scale.

librium states combined by the Rankine–Hugoniot relation is taken at the origin of the streamwise coordinate x . A large number of molecules are (uniformly) distributed in the computation domain with the upstream and downstream boundaries according to the upstream ($x < 0$) and downstream ($x > 0$) equilibrium Maxwellian velocity distributions. Influx molecules across the upstream and downstream boundaries are assigned by the boundary conditions of the upstream and downstream equilibrium Maxwellian distributions, respectively. At initial time, the discontinuity surface is removed. After the steady-state structure of a normal shock wave is established, the flow profiles and velocity distribution functions across the shock wave are calculated and averaged until the statistical fluctuations become sufficiently small. Because the difference between the cutoff angle $\chi_{\min} = 0.1^\circ$ and 1° for the IPL or LJ potential is confirmed to be negligible, the results for the smaller cutoff angle $\chi_{\min} = 0.1^\circ$ are presented.

For comparison between the IPL potential and the VSS and VHS ($\alpha = 1$) models defined for the IPL potential, the length scale is taken as the upstream viscosity mean free path λ_1 defined by the VSS model [Eq. (25)],

$$\lambda_1 = S_\eta (8\eta_1/15)(3 - \omega)(2 - \omega)(2\pi mkT_1)^{-1/2}/n_1, \quad (40)$$

where η_1 , T_1 , and n_1 are the upstream viscosity coefficient, temperature, and number density, respectively. The upstream Mach number is taken as $M_1 = 10$, for which the upstream and downstream boundaries of the computation domain are taken at $x/\lambda_1 = -100$ and 100 , respectively, and the size of a collision (data) cell is taken as $\Delta x/\lambda_1 = 1$. The total number of molecules is taken as about 4×10^5 , for which the mean molecular number per cell is about 2×10^3 . The number density (n) and temperature (T) profiles, $(n - n_1)/(n_2 - n_1)$ and $(T - T_1)/(T_2 - T_1)$, n_2 and T_2 being the downstream number density and temperature, respectively, are compared in Fig. 6 between the VSS and VHS models and the IPL potential. The difference between the profiles for the VSS and VHS models and the IPL potential is indistinguishable, although the velocity distribution functions of the VSS and VHS models are rather different from that for the IPL potential. The fact that the shock wave structure in a simple gas is little influenced by the scattering law is consistent with previous results.² The shock wave structure in a gas mixture, however, may be influenced by the molecular diffusion, and work on a comparative calculation for the shock wave structure in a binary gas mixture is in progress.

For comparison between the LJ potential and the VSS and VHS ($\alpha = 1$) models defined for the LJ potential, the length scale is taken as the upstream viscosity mean free path λ_1 defined by the VSS model [Eq. (37)],

$$\lambda_1 = (16/5n_1)(2\pi mkT_1)^{-1/2}\eta\Omega_\eta^*/\nu_c^*, \quad (41)$$

where η , Ω_η^* , and ν_c^* are taken as the upstream values. Because the calculation for the LJ potential has been made¹² for the upstream Mach number $M_1 = 7.183$ and temperature $T_1 = 16$ K and the potential well depth $\epsilon_{LJ}/k = 124$ K for argon ($T^* = kT_1/\epsilon_{LJ} = 0.129$), the calculations for the

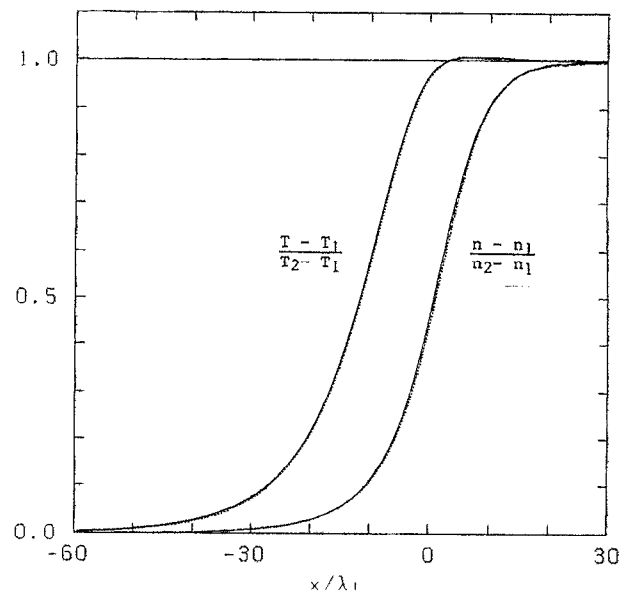


FIG. 6. Comparison of number density n and temperature T profiles across a shock wave of Mach number 10 for $\nu = 5$ ($\omega = 0.5$) between the VSS (—) and VHS (---) models and the IPL potential (- · -) in the VSS viscosity scale.

VSS and VHS models are made for the same shock wave condition.

The number density and temperature profiles are compared in Fig. 7 between the VSS and VHS models and the LJ potential. The agreement between the VSS and VHS models and the LJ potential is good and the shock wave structure in a simple gas is little influenced by the scattering law, consis-

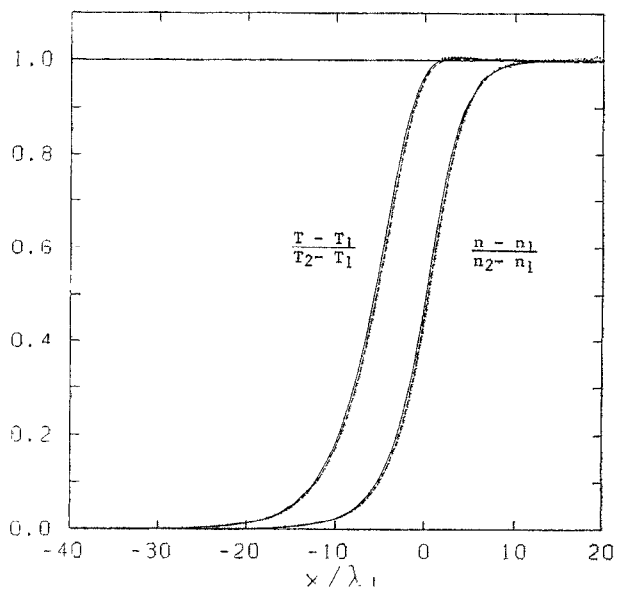


FIG. 7. Comparison of number density n and temperature T profiles across a shock wave of Mach number 7.183 for the reduced temperature $T^* = 0.129$ between the VSS (—) and VHS (---) models and the LJ potential (- · -) in the VSS viscosity scale.

tent with the case of the IPL potential. As in the case of the IPL potential, however, the velocity distribution functions of the VSS and VHS models are rather different from that for the LJ potential.

IV. CONCLUDING REMARKS

The VSS model is the simplest extension of the VHS model for both the viscosity and diffusion cross sections (coefficients) to be consistent with those for any (realistic) intermolecular potential¹³ and has almost the same analytical and computational simplicity (computation time) as the VHS model. In the present paper, the VSS model is defined for the IPL or LJ potential and applied to comparative calculations for the molecular diffusion in a heat-bath gas and the normal shock wave structure in a simple gas. It is shown that the agreement in the molecular diffusion and the shock wave structure between the VSS model and the IPL or LJ potential is remarkably good, while the VHS model is insufficient for the molecular diffusion. Therefore the VSS model may be preferable to the VHS model in the Monte Carlo simulation of gas mixture flows where the molecular diffusion plays an important role.

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