Prediction of Terminal Speed Ratios in Spherical-Source Expansions

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Theme

THE direct simulation Monte Carlo method[1] has been used to calculate the terminal speed ratio, $S_{\parallel}^{\infty}$, for the spherical source expansion of He, Ne, and a hard sphere gas. Monte Carlo results have been used to examine the validity of the sudden freeze model in predicting $S_{\parallel}^{\infty}$. The parameter $P = |(1/\nu)/(\mathrm{d}\ell n\, n/\mathrm{d}t)|$ was used to characterize the location of the freeze surface. A range of values of the parameters P^{∞} between 0.2-3.3 can correlate all the results. Departures from a constant value of P^{∞} are attributed to the non-Maxwellian nature of the distribution function and have been correlated with the parameter $R^{\infty} = S_{\mathrm{kin}}^{\infty}/S_{\mathrm{hw}}^{\infty} = (T_{\mathrm{hw}}^{\infty}/T_{\mathrm{kin}}^{\infty})^{1/2}$, where subscripts kin and hw imply kinetic and half-width, respectively. Half-width temperature is defined by fitting a gaussian function through the points where the distribution function has half the maximum value. Parameter R^{∞} can be correlated with the logarithmic slope of the viscosity cross section, $s = \partial\, \ell n\, \Omega^{(2,2)^*}/\partial\, \ell n\, T$.

Contents

To correlate the data, the location of the freeze surface is characterized by use of the parameter P which is defined as the absolute value of the ratio of the logarithmic time derivative of the density following the streamline to the collision frequency.[2] Use of an isentropic relationship for the logarithmic time derivative of the density and an equilibrium relationship for the collision frequency leads to the required relationship between $S_{\parallel}^{\infty}$ and the parameter P^{∞}:

$$S_{\parallel}^{\infty} = \{[P^{\infty}/(4/3)(1.2)^{5/4}(5\pi/18)^{1/2}] \times [\Omega^{(2,2)^*}(T_{\parallel}^{\infty})/Kn^*\Omega^{(2,2)^*}(T_0)]\}^{2/5} \quad (1)$$

For the special case of the classical power law potentials, $\Omega^{(2,2)^*} \sim T^{-s}$, Eq. (1) can be simplified to give

$$S_{\parallel}^{\infty} = b(Kn^*)^{-2/(5-4s)} \quad (2)$$

where $b = (P^{\infty}/(4/3)(1.2)^{5/4}(5\pi/18)^{1/2}\, 2.5^{s})$ and Kn^* is the Knudsen number based on the stagnation conditions and the sonic radius. It should be noted that the value of the exponent $2/(5\text{-}4\ s)$ is in agreement with the prediction of Hamel and Willis.[3]

The direct simulation Monte Carlo method of Bird was used in Ref. 4 to calculate $S_{\parallel}^{\infty}$, for a range of values of initial Knudsen number, for the expansion of He, Ne, and a hard sphere gas. For the expansion of He and Ne, quantum cross sections corresponding to an appropriate Lennard-Jones potential were used. Monte Carlo results reported in Ref. 4 have been used here and analyzed for the location of freeze surface using Eq. (1).

For the expansion of the hard sphere gas, it was found that $S_{\parallel}^{\infty}$ showed the correct dependence on the initial Knudsen number, $S_{\parallel}^{\infty} \sim Kn^{*\,-.4}$, and satisfied Eq. (1) with $P_{\mathrm{hs}}^{\infty} = 3.22$ or $b_{\mathrm{hs}} = 1.32$. For the expansion of He and Ne, however, the parameter P^{∞} was found to be variable and a function of the initial Knudsen number suggesting the inadequacy of the sudden freeze criterion in predicting the terminal speed ratios. It is useful to relate these variations to some other known property of the flow. It is shown here (Fig. 1) that these variations are attributable to the non-Maxwellian nature of the distribution function of the parallel direction and have been correlated with the parameter R^{∞} characterizing the shape of the distribution function.

Physical basis for the existence of such a correlation can be seen more clearly by first establishing a second correlation between R^{∞} and s. A simple explanation for the correlation between R^{∞} and s is provided as follows. In an expansion process where the cross section is increasing with temperature, the expansion process is not able to cope with the changes in cross section so that a certain fraction of molecules is frozen earlier. These molecules have higher temperature and are responsible for the generation of the high-velocity tails of the distribution function. This explanation implies that the distribution function for the expansion of a hard sphere gas will always remain Maxwellian. This is confirmed by the Monte Carlo simulation results.[4] It can be further argued that if R^{∞} is a function of the slope s at the freeze temperature, then for a specific gas R^{∞} should correlate with the final freeze temperature and be independent of the initial expansion

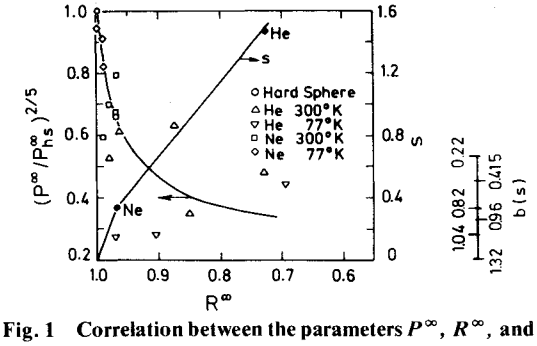

Fig. 1 Correlation between the parameters P^{∞}, R^{∞}, and s.

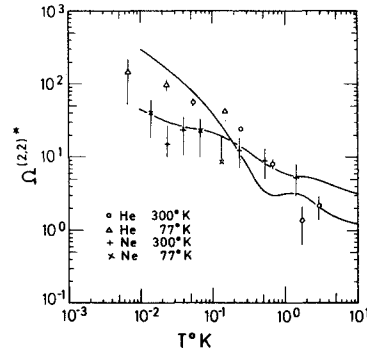

Fig. 2 Inferred absolute magnitude of $\Omega^{(2,2)^*}$.

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Table 1 Expansion properties for power-law potentials

Potential model	s	$2/(5\text{-}4s)$	$R^\infty = S^\infty_{kin}/S^\infty_{hw}$	P^∞	$b(s)$
Hard sphere	0.0	0.4	1.0	3.22	1.32
Repulsive 12	0.166	0.46	0.99	2.15	1.04
Repulsive 8	0.25	0.50	0.985	1.81	0.96
Repulsive 6	0.333	0.545	0.980	1.47	0.82
Maxwell molecules	0.50	0.667	0.942	0.66	0.415
Repulsive 3	0.666	0.857	0.905	0.49	0.22

temperature. Calculated as well as the experimental[5] values for the expansion of 300 and 77K helium and neon confirm this. Thus a correlation between P^∞ and R^∞ also implies a correlation between P^∞ and s. Or in other words this implies that $S^\infty_\P$ depends on the magnitude of $\Omega^{(2,2)^*}$ and its logarithmic slope s.

The present correlation can be used to calculate the temperature dependence of $\Omega^{(2,2)^*}$ from the observed values of $S^\infty_\P$ and R^∞. Figure 2 shows such an inversion for He and Ne. The points in Fig. 2 indicate magnitudes obtained by using Eq. (1) where the value of P^∞ is obtained from the correlation between P^∞ and R^∞. Error bands correspond to 2% scatter (one sigma) in the value of R^∞. The points are compared with the exact $\Omega^{(2,2)^*}$ indicated by the solid curves. The inferred values are accurate to within 50% and this establishes the essential accuracy of the present procedure. It can be observed that the inferred cross sections exhibit some averaging of the viscosity cross section and that any fast changes are not reproduced by the expansion process. The averaging is inherent in any such freeze model which approximates the approach to the freeze occurring over a range of temperatures with a single temperature. A similar approximation has also been made here with respect to the contribution to the tails of the distribution function, as it has been assumed that the entire contribution corresponds to the final freeze temperature. Both these factors are responsible for the averaging exhibited by the inferred cross sections.

The correlation can also be used to calculate $S^\infty_\P$ when $\Omega^{(2,2)^*}$ is known. For classical power law potentials, the value of b for a given value of s [Eq. (2)] is shown as the ordinate in Fig. 1. Various parameters characterizing the expansion for different values of s are shown in Table 1. Comparison of these results with the previous results and its implications are discussed in the full paper. For the case when $\Omega^{(2,2)^*}$ has arbitrary temperature dependence, the situation is more complicated. It is necessary to make a "reasonable" averaging before calculating $S^\infty_\P$. Accuracy of the procedure depends on the temperature dependence. An estimate of the accuracy can be obtained from the scatter in correlation presented in Fig. 1. If one allows for the maximum uncertainly of 6% in the value of R^∞ (three sigma) and shifts the calculated points horizontally in the appropriate direction to reduce the scatter, the remaining departures can be attributed to the parameter $(P^\infty/P^\infty_{hs})^{2/5}$. In the region where $R^\infty > 0.95$ and $s < 0.5$, all the shifted points lie on the smoothed curve so that good accuracy is expected for this region. In the region where $R^\infty < 0.95$ and $s > 0.5$, shifted points show a scatter of 0.1 or about 10% accuracy in $S^\infty_\P$. Thus the major source of uncertainty, in addition to the uncertainty due to the unknown nature of the averaging, comes from a region where $\Omega^{(2,2)^*}$ exhibits very fast increase with the temperature. Such a fast increase is expected only for systems exhibiting quantum effects, like He or possibly H_2. In such situations it will be best to avoid the sudden freeze model and base the prediction on more elaborate Monte Carlo calculations.

It is worth speculating that in an analogous fashion, departures from the Maxwellian shape of the distribution function are expected to play an important role for the expansion of a polyatomic gas or a mixture of monatomic gases and the knowledge of such departures can be expected to provide a more detailed understanding of the expansion process.

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