Modified GHS model compared with the VHS collision model in DSMC computations

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The generalized hard sphere (GHS) collision model was introduced by Hash and Hassan [2]. It is a generalization of the Sutherland collision model proposed by Kuščer [4]. At low temperatures, where the attractive intermolecular forces are important, the GHS collision model produces a more accurate variation of viscosity with temperature than the standard variable hard sphere (VHS) collision model [1]. In spite of this, the GHS model remains virtually unused owing to its computational expense. A slight modification of the GHS model, described in [9], makes it no more than 15% more computationally expensive than the VHS model. In this 'modified GHS' model the total collision cross-section $\sigma(g)$ is set $\propto 1/g$ for collision speeds $g < g_0$ so that all values of $g < g_0$ are equally likely in collisions. If $g_0 = \sqrt{4RT_{min}}$, the modification makes a negligible difference to the viscosity law for $T > T_{min}$. This 'Maxwell cross-section' for low speed collisions is more physically reasonable than the original GHS cross-section. The latter gives an unrealistic collision rate that approaches infinity as $g \to 0$.

We compare the modified GHS and VHS models for a blunt body flow with stagnation temperature $T_o = 1300$ K. We calculate the supersonic flow of argon, with a freestream temperature of 100 K, around a flat plate normal to the freestream. The wall temperatures were 1300 K (front) and 500 K (rear), with diffuse reflection. The model parameters were chosen to give the two collision models identical viscosities at the freestream and stagnation temperatures. In the recirculation region behind the flat plate, where the temperature is ≈ 500 K, the local mean free path was about 12% greater for the GHS compared to the VHS model.

The pressure and heat transfer to the front wall (near the stagnation region) were found to be virtually identical for the two models. There was a slight difference in pressure on the rear wall, but again the heat transfer was virtually identical for the two models. The results imply that good results can be obtained with the VHS model provided the model parameters are selected to match the desired viscosity as closely as possible, over the temperature range in the flow.

1 Variable diameter hard sphere collision models

Although only two different collision models were used in the calculations, we discuss here three different collision models, each having a different viscosity law $\mu = \mu(T)$. Each collision model is a 'variable hard sphere', in that, although the total collision cross-section varies with collision speed, the scattering is as for hard-spheres, *i.e.* isotropic in the reference frame of the centre of mass of the collision pair. The viscosity law for each collision model is determined primarily by the total cross-section σ as a function of collision speed g. The three cross-sections are

1. Variable hard sphere (VHS) [1]:

$$\sigma = \sigma_r \left(g_r/g\right)^{2\upsilon}. \text{ (Constants } g_r,\ \sigma_r,\ \upsilon\text{).}$$

2. Sutherland hard sphere proposed by Kuščer [4]:

$$\sigma = \sigma_s \left[1 + \left(g_s/g\right)^2\right]. \text{ (Constants } g_s = \sqrt{12RT_s},\ \sigma_s\text{).}$$

3. Generalized hard sphere (GHS) proposed by Hash and Hassan [2], for example:

$$\sigma = \sigma_r \left[\phi \left(g_r/g\right)^{2\upsilon_1} + (1-\phi)\left(g/g_r\right)^{2\upsilon_2}\right]. \text{ (Constants } g_r, \sigma_r, \upsilon_1, \upsilon_2, \phi.\text{)}$$

The generalized hard sphere GHS is an extension of Kuščer's collision model which reproduces the well-known Sutherland viscosity. Kruščer's model is discussed below because it is simpler to explain the modification we have proposed (for this model and the GHS) in reference to Kruščer's model.

2 Viscosity laws $\mu = \mu(T)$

The parameters used in the two different collision models tested were

$$\text{VHS: } \omega = 0.827; \quad \text{GHS: } (\phi, \upsilon_1, \upsilon_2) = (0.27, 0.1, 1.1);\ T_r = 100 \text{ K};\ \sigma_r = 1.443 \times 10^{-18}\text{m}^2$$

The viscosity $\mu(T)$ for each model is compared in Fig. 1 with the experimental data for argon [3] over the temperature range 100 - 1300 K. This is the temperature range for which the simple power law differs most from the experimental data. The parameters for each model were chosen to make the model viscosity and experimental viscosity match at $T =$ 100 K (0.797×10^{-5} Pa s) and 1300 K (6.63×10^{-5} Pa s). The GHS viscosity is a better representation of the experimental data than the VHS model[1]. The VHS and GHS viscosities differ by 13% at 500 K, and the test flow considered below was chosen to produce a large rarefied region of flow at this temperature.

[1]The Sutherland viscosity is not shown in the figure. It is given by $\mu = \mu_r \left(\frac{1+T_s/T_r}{1+T_s/T}\right)\sqrt{\frac{T}{T_r}}$ and can also match the data over this temperature range better than the VHS model.

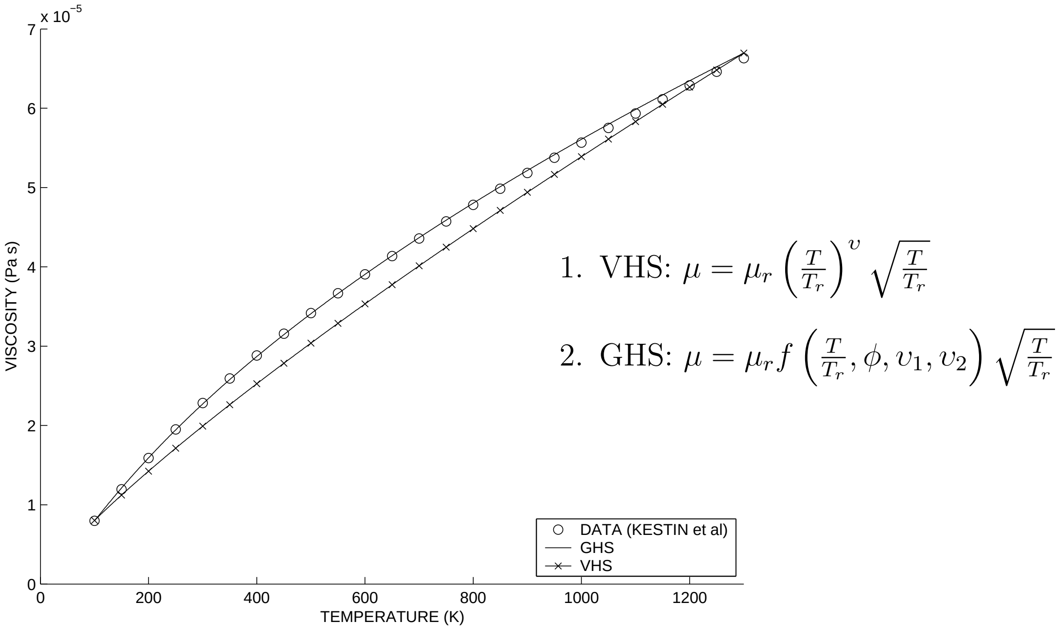


Figure 1: The viscosity of the two collision models, compared with the recommended data for argon [3]. Constants were chosen to make their viscosities agree at $T = 100$ K & 1300 K

One advantage of the better viscous modelling provided by the GHS model arises in hybrid DSMC/Navier-Stokes solvers, or any studies where DSMC is compared to a Navier-Stokes solver. The Navier-Stokes code will typically have a viscosity law chosen to fit experimental data reasonably well, and will rarely be a simple power law $\mu \propto T^{\omega}$. Although it would be easy enough to change the Navier-Stokes solver so that its viscosity matches the DSMC solver, it would be preferable (other things being equal) to use a more realistic viscosity in the DSMC calculations

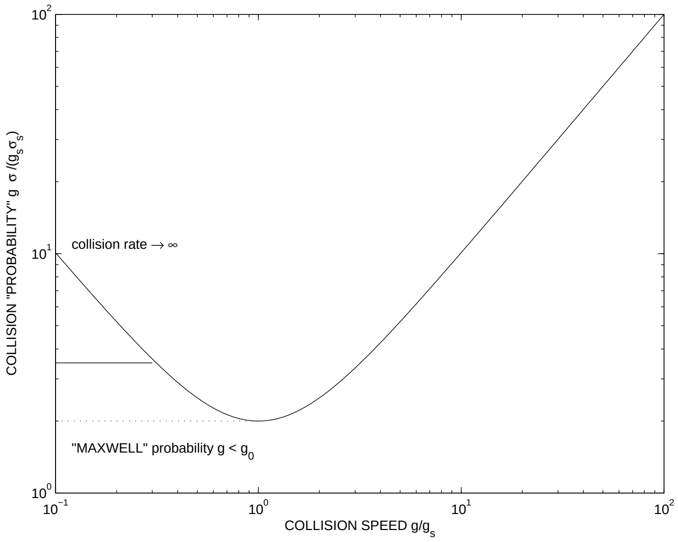
2.1 Computational efficiency

We surmise that there are two reasons why Kuščer's Sutherland hard sphere or Hash and Hassan's generalized hard sphere are not used.

1. Both new models are inefficient in CPU time compared with the VHS model. The CPU time may be as much as 20 times greater.

2. The standard collision-based DSMC chemistry models [1] are based on the VHS cross-section. New models (new cross-sections) would require a significant investment in developing new collision-based chemistry models.

The second reason can be addressed by using the 'macroscopic' chemistry method [5, 7, 8] for which the chemical modelling is decoupled from the specific details of the collision cross-section (and hence viscosity law). The first reason is the most serious and can be addressed by a slight modification [9], to the collision cross-section, discussed below.



SHS model:
$\sigma = \sigma_s \left[1 + g_s^2/g^2\right]$, with $g_s = \sqrt{12RT_s}$

Collisions $\propto g\sigma = g\sigma_s \left(1 + g_s^2/g^2\right)$

- Infinite collision rate as $g \to 0$
- low g - NEGLIGIBLE contribution for $T > g^2/4R$
- Modify σ for $g < g_0$: Maxwell cross-section $g < g_0$ - finite collision rate

Figure 2: Collision probability for SHS and modified SHS model.

2.2 Collision probability

The reason for the low computational efficiency of the GHS cross-section can best be explained by considering Kuščer's model, which suffers from the same problem, for the same reason. The collision probability is proportional to $g\sigma$ and this product $\to \infty$ as $g \to 0$. Even if, as in the standard DSMC codes of Bird [1], there is a minimum value of g which is allowed for in collisions, the corresponding value of $g_{min}\sigma\left(g_{min}\right)$ can be very large. This maximum value of $g\sigma$ sets the collision rate, with the result that a very large number of potential collision pairs are considered at each time step. Most of these collision pairs do not result in a collision and many of those that do are very low speed collisions.

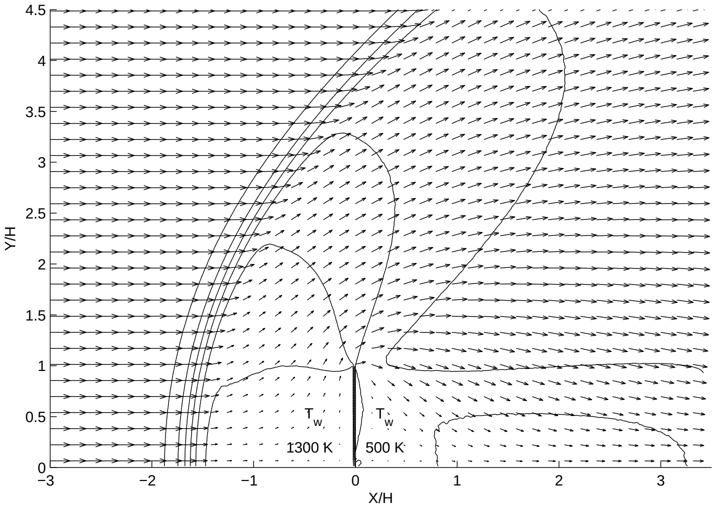
The following questions arise: Why are we spending so much effort looking for low speed collisions which transfer negligible amounts of momentum and energy? Can the low-speed collisions make any significant difference to the viscous behaviour of the simulation?

3 Modified Cross-Section

The computational efficiency of the collision models can be improved by a simple modification of the cross-section for low speed collisions. For collision speeds below a certain value g_0 (to be specified) we replace the cross-section by the 'Maxwell cross-section' which make all values of $g < g_0$ equally probable.

$$\text{Modified cross-section: } \sigma = \begin{cases} \sigma_0 g_0/g & \text{for } g \le g_0 \\ \sigma_s\left(1 + g_s^2/g^2\right) & \text{for } g > g_0 \end{cases} \tag{1}$$

where $\sigma_0 = \sigma_s\left(1 + g_0^2/g_s^2\right)$. The modified collision probability corresponding to this cross-section is shown Fig. 2, for two different values of g_0. It can be shown [6, 9] that this



Argon; $M_\infty = 6$, $\gamma = 5/3$
$T_\infty = 100$ K, $V_\infty = 1117.9$ m/s,
$n_\infty = 1.2 \times 10^{21}$
$\lambda \equiv \frac{2\mu_\infty}{mn_\infty}\sqrt{\frac{\pi}{8RT_\infty}} = 8.73 \times 10^{-4}$ m
$H = 1.52 \times 10^{-2}$ m
$\mathrm{Kn}_\infty = \frac{\lambda}{H} = .057$
Rarefaction parameter
$M_\infty \mathrm{Kn}_\infty = 0.345$
Grid 250×200 cells & 2×2 sub-cells
$\frac{\Delta x}{\lambda} = 0.46$, $\frac{\Delta x}{\lambda_s} = 0.75$
Wall temperature
$T_w = 1300$ K and 500 K

Figure 3: Flow conditions, flow velocity & pressure contours.

modification only makes a significant difference[2] to the viscosity law, for temperatures less than $\approx \frac{g_0^2}{4R}$. For the modified GHS model we imposed equal collision probability for $g < \sqrt{4RT_\infty} = 173$ m/s, and $T_\infty = 100$ K was the freestream temperature in the simulations.

4 Test Flow. Blunt body. Argon, 100 K $< T <$ 1300 K

We used the code supplied in [1], which can calculate the 2D flow around a flat plate normal to the freestream. The (modified) GHS collision model was added as an option. The freestream Mach number was 6 and temperature varied from 100 K (freestream) to 1300 K (stagnation point). The rear wall of the plate was fixed at a wall temperature of 500 K (with diffuse reflection). The Knudsen number (based on the nominal mean free path[3]) was $Kn_\infty = 0.057$. The time step was the same in all cells, and was set by the highest collision rate in any cell. It was adjusted at each step to ensure that the 'collision fraction' $2N_{\text{collisions}}/N_{\text{in cell}}$ was less than 0.75. This meant that no simulator particle has a probability greater than 75% of being selected for a collision in one time step, and in most cells the chance of collision was much less than 50%.

Stagnation flow - no difference

Fig. 4 shows the pressure and heat transfer on the front wall, calculated with the VHS and modified GHS collision models[4]. There is virtually no difference between the two models, which is not surprising as the viscosities of the two models are very close for temperatures approaching the stagnation temperature 1300 K. The apparent anomaly in the pressure

[2]The difference that the modified cross-section does make means that the modified viscosity law is even closer to experimental data for low temperatures. In other words, the infinite collision probability (as $g \to 0$)

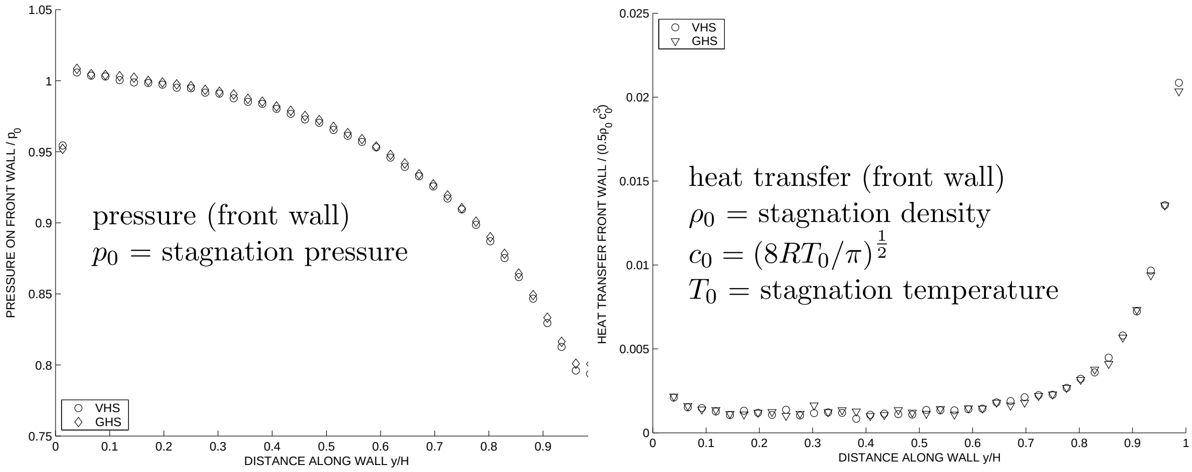
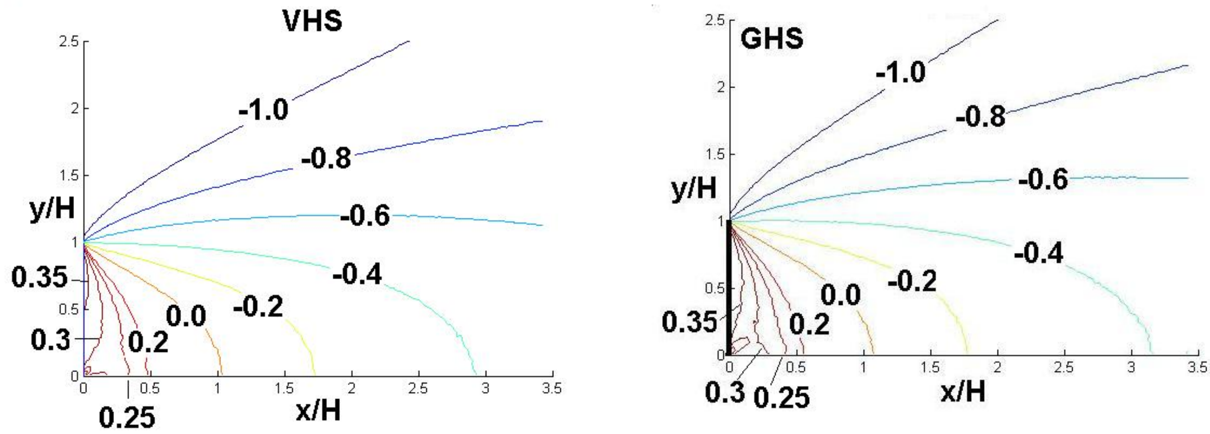


Figure 4: Pressure and heat transfer, front wall, modified GHS and VHS. Average sample size $= 2.6 \times 10^6$ particles.



local (nominal) Knudsen number

$Kn = 2\mu/(\rho\bar{c}H)$

Figure 5: Rarefaction in the re-circulation region: contours of $\log_{10} Kn$.

near the axis of symmetry may indicate a problem with treating an axis of symmetry as a specularly reflecting wall.

5 Rear surface & recirculation region

In the re-circulation region behind the wall, the degree of rarefaction as measured by the local (nominal) Knudsen number was found to to be about 12% greater for the GHS model than the VHS model (see Fig. 5). Note that the $\log_{10} Kn = 0.35$ contour (local $Kn = 0.46$)

of the original GHS model is physically unrealistic [9].

[3] The nominal mean free path is here defined as $\lambda_\infty \equiv 2\mu_\infty/(\rho\bar{c}_\infty)$, where $\bar{c}_\infty = \sqrt{8RT_\infty/\pi}$.

[4] All calculations for the GHS model used the modification previously described: the collision probability for $g < \sqrt{4RT_\infty}$ was constant

covers almost all the rear wall for the modified GHS calculations, but less than half the rear wall for the VHS calculations.

The pressure and heat transfer on the rear wall are shown in Fig. 6. The sample size of

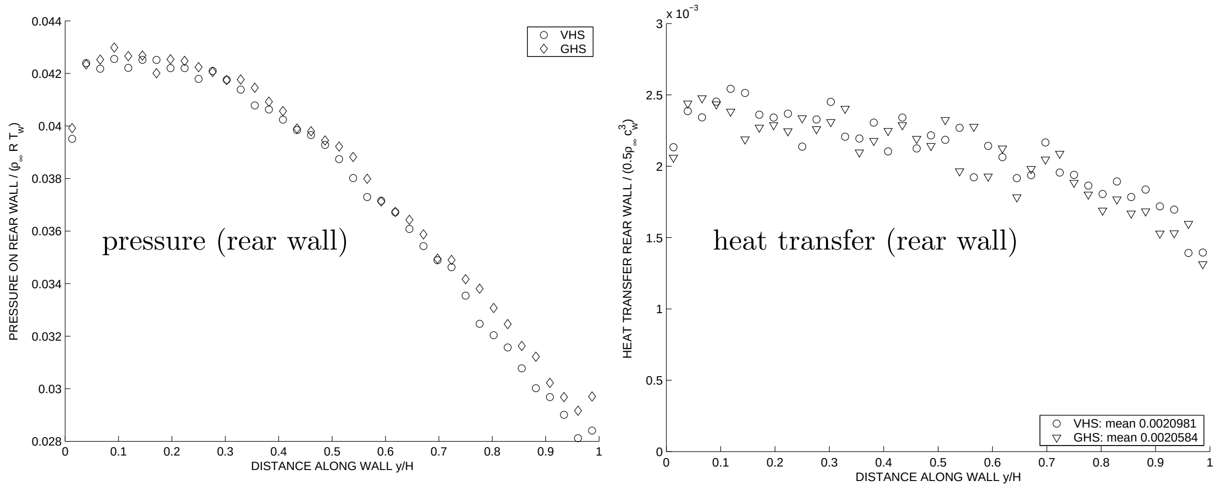


Figure 6: Pressure and heat transfer to rear wall, for the modified GHS and VHS collision models. Average sample size for surface coefficients was 1.7×10^4 particles. The mean value of heat transfer for each model, is shown in the figure legend at the right. Note the anomaly in the pressure and heat transfer near the near the axis of symmetry.

molecules hitting the rear surface is considerably less than for the front wall, and hence the scatter in the results is larger. Nevertheless, it appears there is a slight difference between the pressures for the two models at the edge of the plate ($y/H = 1$). The heat transfer values are too scattered to draw firm conclusions, but it appears that the difference (for the two collision models) in rarefaction makes negligible difference to the heat transfer to the rear surface. The average values of heat transfer coefficients over the entire rear wall for each model, are virtually identical at $\dot{q}'_{\rm av}/\left(\frac{1}{2}\rho_\infty c_\infty^2\right) = 2.08 \times 10^{-3} \pm 1\%$.

6 Conclusions

- For original GHS model, collision rate $\rightarrow \infty$ for $g \rightarrow 0$.
- Physically unreasonable and very expensive in CPU time.
- Low speed collisions make negligible contribution to high temperature viscosity.
- Modify the cross-section for $g < \sqrt{4RT_\infty}$, to give the modified GHS model.
- Difficult to find an 'aerospace flow' where the viscosity departure from power law (VHS) is significant.
- Important to match the viscosity to the flow being considered.
- With viscosity matched at T_∞ and T_0, effects on wall pressures and heat transfer were negligible.

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