Introduction to Kinetic Model Equations

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1 The BGK model

The correct description of rarefaction effects requires replacing hydrodynamic equations with the more general Boltzmann equation (Cercignani, 1988) which takes the form:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{r}} f + \frac{1}{m} \nabla_{\boldsymbol{v}} \cdot (\boldsymbol{F} f) = \mathcal{C}(f,f) \tag{1}$$

when written for a simple monatomic gas composed of atoms of mass m. In Eq. (1), the distribution function $f(\boldsymbol{r}, \boldsymbol{v}|t)$ gives the number of atoms with position $\boldsymbol{r}$ and velocity $\boldsymbol{v}$ at time t. The vector field $\mathbf{F}(\boldsymbol{r}, \boldsymbol{v}|t)$ describes the effects of an assigned external force field. The rate of change of f due to atomic interactions is given by the source term $\mathcal{C}(f,f)$ which is a non-linear functional of f, whose precise structure depends on the assumed atomic interaction forces. For instance, hard sphere interaction leads to the following form of the collision integral:

$$\mathcal{C}(f,f) = \frac{\sigma^2}{2} \int_{R^3} d\boldsymbol{v}_1 \int_{\mathcal{S}^2} d^2\hat{\boldsymbol{k}} \left[f(\boldsymbol{x}, \boldsymbol{v}_1^*|t) f(\boldsymbol{x}, \boldsymbol{v}^*|t) - f(\boldsymbol{x}, \boldsymbol{v}_1|t) f(\boldsymbol{x}, \boldsymbol{v}|t) \right] |\hat{\boldsymbol{k}} \cdot \boldsymbol{v}_r| \tag{2}$$

In Eq. (2), σ is the hard sphere diameter, $\boldsymbol{v}_r = \boldsymbol{v}_1 - \boldsymbol{v}$ is the relative velocity of two colliding atoms whereas $\hat{\boldsymbol{k}}$ is a vector, belonging to the unit sphere $\mathcal{S}^2$, used to specify the relative position of two atoms at the time of their impact. The collisional dynamics of two colliding atoms determines the pre-collisional velocities $\boldsymbol{v}^*$ and $\boldsymbol{v}_1^*$ which are changed into $\boldsymbol{v}$ and $\boldsymbol{v}_1$ by a binary collision. In this case $\boldsymbol{v}^*$ and $\boldsymbol{v}_1^*$ are obtained from $\boldsymbol{v}$, $\boldsymbol{v}_1$ and the impact vector $\hat{\boldsymbol{k}}$ by the simple relationships:

$$\boldsymbol{v}^* = \boldsymbol{v} + (\boldsymbol{v}_r \cdot \hat{\boldsymbol{k}})\hat{\boldsymbol{k}} \qquad \boldsymbol{v}_1^* = \boldsymbol{v}_1 - (\boldsymbol{v}_r \cdot \hat{\boldsymbol{k}})\hat{\boldsymbol{k}} \tag{3}$$

The complicated structure of the Boltzmann collision integral leads quite naturally to ask weather it is possible to replace $\mathcal{C}(f,f)$ with a collision term which has a simpler mathematical form and yet preserves the basic properties of the original expression. The simplest and most widely used kinetic model equation has been proposed in 1954 by Bhatnagar, Gross and Krook(Bhatnagar et al., 1954) and independently by Welander(Welander, 1954). In the BGK model $\mathcal{C}(f,f)$ is replaced by a relaxation term having the following form:

$$\left(\frac{\partial f}{\partial t} \right)_{BGKW} = \nu \left[\Phi(\boldsymbol{r}, \boldsymbol{v}|t) - f(\boldsymbol{r}, \boldsymbol{v}|t) \right] \tag{4}$$

In Eq.(4), ν is the collision frequency, whereas $\Phi(\boldsymbol{r}, \boldsymbol{v}|t)$ is a Maxwellian distribution function:

$$\Phi(\boldsymbol{r}, \boldsymbol{v}|t) = \frac{\tilde{n}(\boldsymbol{r}|t)}{\left[2\pi R \tilde{T}(\boldsymbol{r}|t) \right]^{3/2}} \exp\left\{ -\frac{1}{2} \frac{[\boldsymbol{v} - \tilde{\boldsymbol{u}}(\boldsymbol{r}|t)]^2}{2R\tilde{T}(\boldsymbol{r}|t)} \right\} \tag{5}$$

characterized by the density $\tilde{n}(\boldsymbol{r}|t)$, bulk velocity $\tilde{\boldsymbol{u}}(\boldsymbol{r}|t)$ and temperature $\tilde{T}(\boldsymbol{r}|t)$; the gas constant R is defined as the ratio $\frac{k_B}{m}$, being k_B the Boltzmann constant and m the molecular mass.

The form of the collision term given by Eq. (4) can somehow be justified by observing that $\mathcal{C}(f,f)$ can be rewritten as the difference of two terms:

$$\begin{aligned}
\mathcal{C}(f,f) &= \mathcal{G}(f,f) - \nu(\boldsymbol{r},\boldsymbol{v}|t) f(\boldsymbol{r},\boldsymbol{v}|t) && (6)\\
\mathcal{G}(f,f) &= \frac{\sigma^2}{2}\int_{R^3} d\boldsymbol{v}_1 \int_{\mathcal{S}^2} d^2\hat{\boldsymbol{k}} \left[f(\boldsymbol{x},\boldsymbol{v}_1^*|t) f(\boldsymbol{x},\boldsymbol{v}^*|t) |\hat{\boldsymbol{k}}\cdot\boldsymbol{v}_r| \right] && (7)\\
\nu(\boldsymbol{r},\boldsymbol{v}|t) &= \frac{\sigma^2}{2}\int_{R^3}\int_{\mathcal{S}^2} f(\boldsymbol{x},\boldsymbol{v}_1|t)|\hat{\boldsymbol{k}}\cdot\boldsymbol{v}_r|\, d\boldsymbol{v}_1\, d^2\hat{\boldsymbol{k}} && (8)
\end{aligned}$$

The *loss* term $\nu(\boldsymbol{r},\boldsymbol{v}|t)f(\boldsymbol{r},\boldsymbol{v}|t)$ has exactly the same form both in the original and in the BGKW model. The *gain* term $\mathcal{G}(f,f)$ in the Boltzmann equation describes the effects of the "arrival" of new molecules at the phase space point $(\boldsymbol{r},\boldsymbol{v})$ as a result of collisions. Since collisions tend to drive the gas toward a local equilibrium condition, described by a Maxwellian distribution function, the BGKW model assumes that collisions immediately thermalize molecules through the approximate gain term $\nu\Phi(\boldsymbol{r},\boldsymbol{v}|t)$. The model structure is made much simpler by assuming that the collision frequency ν does not depend on velocity $\boldsymbol{v}$, although it is allowed to let it depend on local macroscopic quantities.

If collision frequency does not depend on velocity, then the requirement of local mass, momentum and energy conservation leads to the relationships:

$$\begin{aligned}
\int \Phi(\boldsymbol{v})\, d\boldsymbol{v} &= \int f(\boldsymbol{v})\, d\boldsymbol{v} && (9)\\
\int \boldsymbol{v}\Phi(\boldsymbol{v})\, d\boldsymbol{v} &= \int \boldsymbol{v} f(\boldsymbol{v})\, d\boldsymbol{v} && (10)\\
\int \boldsymbol{v}^2\Phi(\boldsymbol{v})\, d\boldsymbol{v} &= \int \boldsymbol{v}^2 f(\boldsymbol{v})\, d\boldsymbol{v} && (11)\\
& && (12)
\end{aligned}$$

which determine the moments $\tilde{n}$, $\tilde{\boldsymbol{u}}$ and $\tilde{T}$ as:

$$\begin{aligned}
\tilde{n} &= n = \int f(\boldsymbol{v})\, d\boldsymbol{v} && (13)\\
\tilde{\boldsymbol{u}} &= \boldsymbol{u} = \frac{1}{n}\int \boldsymbol{v} f(\boldsymbol{v})\, d\boldsymbol{v} && (14)\\
\tilde{T} &= T = \frac{1}{3n}\int (\boldsymbol{v}-\boldsymbol{u})^2 f(\boldsymbol{v})\, d\boldsymbol{v} && (15)\\
& && (16)
\end{aligned}$$

In other words, the Maxwellian density, bulk velocity and temperature coincide with the corresponding moments of the distribution function f.

1.1 Basic Model Properties

In spite of the linear apparence of the BGKW collision term, its non-linearity is much stronger (exponential) than the quadratic Boltzmann collision integral. However, the derivation of many important model properties turns out to be much simpler.

The gas homogeneous relaxation toward the final equilibrium state is described by the equation:

$$\frac{\partial f}{\partial t} = \nu(n,T)\left[\Phi(\boldsymbol{r},\boldsymbol{v}|t) - f(\boldsymbol{r},\boldsymbol{v}|t)\right] \qquad (17)$$

Mass, momentum and energy conservations keep the moments n, $\boldsymbol{u}$ and T, constant during the evolution of f. Hence, their constant values n_0, $\boldsymbol{u}_0$ and T_0 are determined by the initial gas state $f_0 = f(\boldsymbol{v}|0)$. Being completely determined by n_0, $\boldsymbol{u}_0$ and T_0, both the Maxwellian Φ and the collision frequency ν, will be time independent, too. Hence, the solution of Eq. (17) can easily written as a linear combination of the initial and final state at each time t:

$$f(\boldsymbol{v}|t) = f_0(\boldsymbol{v})e^{-\nu_0 t} + (1 - e^{-\nu_0 t})\Phi(\boldsymbol{v}) \tag{18}$$

The possibility of determining a simple explicit expression for the homogeneous relaxation is quite useful in the application of fractional time step schemes to the numerical solution of BGKW model equation.

In the space homogeneous case, the BGKW model also allows a simple proof of the $\mathcal{H}$-theorem(Cercignani, 1988). As in the case of the full Boltzmann equation, the entropy functional is defined as $\mathcal{H}(t) = \int f(\boldsymbol{v}) \log[f(\boldsymbol{v}|t)]\, d\boldsymbol{v}$. The following equality is easily obtained:

$$\frac{d\mathcal{H}}{dt} = \nu \int (\Phi - f) \log(f)\, d\boldsymbol{v} \tag{19}$$

Since $\log(\Phi)$ is a linear combination of the collision invariants, the r.h.s. of Eq. (19) can be also written as

$$\frac{d\mathcal{H}}{dt} = \nu \int (\Phi - f) \log(f/\Phi)\, d\boldsymbol{v} + \nu \int (\Phi - f) \log(\Phi)\, d\boldsymbol{v} \tag{20}$$

being the last integral equal to zero. The remaining term gives

$$\frac{d\mathcal{H}}{dt} \leq 0 \tag{21}$$

since $(\Phi - f)\log(f/\Phi) \leq 0$, the equality applying only if $f = \Phi$.

1.2 Hydrodynamic limit of the BGKW Model

Investigating the hydrodynamic limit of the BGKW model is extremely important to judge about the model properties and capabilities as well as to determine the proper form of the collision collision frequency ν.

The classical Chapman-Enskog (Ferziger and Kaper, 1972) expansion provides the simplest way to establish a connection between nu and the transport properties predicted by Eq. (4). It is convenient to rescale the space variable $\boldsymbol{r}$ to the flow macroscopic reference scale L and time to the *slow* time scale $L/\sqrt{RT_{ref}}$, being $\sqrt{RT_{ref}}$ a reference thermal speed value. Since ν is of the order of $\frac{1}{\tau_{ref}}$, being τ_{ref} a reference value of the mean free time, the rescaled Eq. (4) reads

$$\epsilon \left(\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{r}} f \right) = \nu \left[\Phi(\boldsymbol{r}, \boldsymbol{v}|t) - f(\boldsymbol{r}, \boldsymbol{v}|t) \right] \tag{22}$$

where the (assumed) small parameter $\epsilon = \frac{\sqrt{RT_{ref}}\tau_{ref}}{L}$ has the meaning of a reference Knudsen number. In the limit of small ϵ, collisions dominate the flow evolutions; it is then assumed that kinetic (i.e. non hydrodynamic modes) rapidly decay and that the distribution function is determined by the macroscopic quantities

$$\boldsymbol{\beta} = \begin{pmatrix} \rho(\boldsymbol{r}|t) \\ \boldsymbol{u}(\boldsymbol{r}|t) \\ T(\boldsymbol{r}|t) \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{n} \\ \frac{1}{3nR} \end{pmatrix} \int \begin{pmatrix} m \\ m\boldsymbol{v} \\ m(\boldsymbol{v}-\boldsymbol{u})^2 \end{pmatrix} f(\boldsymbol{r},\boldsymbol{v}|t)\, d\boldsymbol{v} \tag{23}$$

and their spatial gradients. Accordingly, it is assumed that

$$f(\boldsymbol{v}|\boldsymbol{\beta}, \nabla_{\boldsymbol{r}}\boldsymbol{\beta}, \nabla_{\boldsymbol{r}}\nabla_{\boldsymbol{r}}\boldsymbol{\beta}, \dots) \tag{24}$$

The macroscopic fields ρ, $\boldsymbol{u}$, and T appear in the mass, momentum and kinetic energy conservation equations:

$$\frac{D\rho}{Dt} = -\rho\nabla \circ \boldsymbol{u} \tag{25}$$

$$\rho\frac{D\boldsymbol{u}}{Dt} = -\nabla \circ \hat{\boldsymbol{P}} \tag{26}$$

$$C_v\rho\frac{DT}{dt} = -\nabla \circ \boldsymbol{q} + \boldsymbol{P} : \nabla\boldsymbol{v} \tag{27}$$

where $C_v = \frac{3R}{2}$ is the gas specific heat per unit mass, whereas the kinetic stress tensor $\boldsymbol{P}$ and the kinetic heat flux vector q are defined as

$$\begin{pmatrix} \boldsymbol{P} \\ \boldsymbol{q} \end{pmatrix} = \int \begin{pmatrix} m(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u})) \\ \frac{m}{2}(\boldsymbol{v}-\boldsymbol{u})^2(\boldsymbol{v}-\boldsymbol{u}) \end{pmatrix} f(\boldsymbol{r},\boldsymbol{v}|t)\, d\boldsymbol{v} \tag{28}$$

Taking into account Eq. (24), the conservation equations written above can be formally written as

$$\frac{\partial\boldsymbol{\beta}}{\partial t} = \boldsymbol{\Phi}(\boldsymbol{\beta}, \nabla_{\boldsymbol{r}}\boldsymbol{\beta}, \nabla_{\boldsymbol{r}}\nabla_{\boldsymbol{r}}\boldsymbol{\beta}, \dots) \tag{29}$$

The dependence of f on macroscopic fields can be determined from the expansion

$$f = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \dots \tag{30}$$

which also induces a similar expansion of the streaming term. Hence, Eq. (22) can be formally written as

$$\epsilon\left[\left(\frac{Df}{Dt}\right)^{(0)} + \epsilon\left(\frac{Df}{Dt}\right)^{(1)} + \dots\right] = \nu\left(\Phi - f^{(0)} - \epsilon f^{(1)} - \epsilon^2 f^{(2)} + \dots\right) \tag{31}$$

The zero and first order terms are then readily obtained by equating terms of corresponding order in ϵ:

$$f^{(0)} = \Phi(\boldsymbol{r},\boldsymbol{v}|t) \tag{32}$$

$$f^{(1)} = -\frac{1}{\nu}\left(\frac{Df}{Dt}\right)^{(0)} \tag{33}$$

where the term $\left(\frac{Df}{Dt}\right)^{(0)}$ is obtained from the expression

$$\frac{\partial f^{(0)}}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{r}} f^{(0)} \tag{34}$$

by eliminating time derivatives of ρ, $\boldsymbol{u}$ and T in favor of spatial derivatives using the zero order (Euler) form of Eqs. (26-27). The final expression reads(Ferziger and Kaper, 1972):

$$f^{(1)} = -f^{(0)}\frac{1}{\nu}\left[\left(\frac{\boldsymbol{c}^2}{2RT}-\frac{5}{2}\right)\boldsymbol{c}\circ\nabla_{\boldsymbol{r}}\log T + \frac{1}{RT}\boldsymbol{c}\boldsymbol{c}:\nabla_{\boldsymbol{r}}\boldsymbol{u} - \frac{1}{3}\frac{\boldsymbol{c}^2}{RT}\nabla_{\boldsymbol{r}}\circ\boldsymbol{u}\right] \tag{35}$$

Inserting expression (35) into Eqs.(28) provides Navier-Stokes and Fourier law closures for stress tensor and heat flux, respectively. More precisely the following expressions are obtained:

$$\hat{\boldsymbol{P}^{(1)}} = m\int \boldsymbol{c}\boldsymbol{c}f^{(1)}\,d\boldsymbol{c} = -2\frac{p}{\nu}\hat{\boldsymbol{S}} \tag{36}$$

$$\hat{\boldsymbol{q}^{(1)}} = -\frac{5}{2}R\frac{p}{\nu}\nabla_{\boldsymbol{r}}T \tag{37}$$

where $\hat{\boldsymbol{S}}$ is the traceless symmetric component of $\nabla\boldsymbol{u}$. As is clear from the equations above, the BGKW model predicts the following expressions for the shear viscosity coefficient μ and thermal conductivity λ:

$$\mu = \frac{p}{\nu}, \quad \lambda = \frac{5}{2}R\frac{p}{\nu} \tag{38}$$

In principle, Eqs.(38) provide an easy recipe to fit the single model adjustable quantity, $\nu(\rho, T)$ to the properties of a specific gas. However, it can be readily verified that the BGKW model predicts a unit value of the Prandtl number $Pr = \frac{C_p\mu}{\lambda}$, whereas the correct value is slightly temperature dependent and close to $2/3$ for a monatomic gas. Therefore, the velocity independent collision frequency ν can be tuned to obtain either the correct gas viscosity or the correct gas thermal conductivity but not both.

Before describing and discussing the model modifications and extensions, which aim at eliminating drawbacks and extend its applications to more complex fluids, it is worth considering a few test problem where the flow properties obtained by the model described above are compared with the solutions of the full Boltzmann equation.

1.3 BGKW Model Applications

The properties of the BGKW kinetic model with velocity independent collision frequency are discussed below on the basis of the following simple test problems:

1. Normal shock profiles in a hard sphere gas
2. 1-D heat flow in a rarefied hard sphere gas confined between parallel plates.
3. Low Mach number 2D flow in a driven square cavity

1.3.1 Normal shock profiles in a hard sphere gas

The propagation of a planar shock wave is studied in the wave front reference frame. The resulting stationary flow field is assumed to be governed by the one-dimensional steady BGKW equation

$$v_x\frac{\partial f}{\partial x} = \nu(\Phi - f) \tag{39}$$

x being the spatial coordinate which spans the direction normal to the (planar) wave front. The model collision frequency is computed as

$$\nu(\rho, T) = \frac{p}{\mu_{HS}(T)}, \quad \mu_{HS}(T) = \frac{5}{16\pi\sigma^2} m\sqrt{\pi R T} \tag{40}$$

being $p = \rho R T$ the pressure and $\mu_{HS}(T)$ the first approximation(Ferziger and Kaper, 1972) of the viscosity of a gas of hard spheres of mass m and diameter σ. It is further assumed that, far from the wave front, the distribution function $f(x, \boldsymbol{v})$ satisfies the boundary conditions

$$\lim_{x \to \mp\infty} f(x, \boldsymbol{v}) = \Phi^{\mp}(\boldsymbol{v}) = \frac{n^{\mp}}{(2\pi R T^{\mp})^{3/2}} \exp\left[-\frac{(v_x - V^{\mp})^2 + v_y^2 + v_z^2}{2 R T^{\mp}} \right] \tag{41}$$

where $n^{\mp}$, $V^{\mp}$ and $T^{\mp}$ are the upstream and downstream values of number density, velocity and temperature, respectively. The parameters of the equilibrium states specified by Eq. (41) are connected by the Rankine-Hugoniot relationships

$$\frac{V^-}{V^+} = \frac{n^+}{n^-} = \frac{4(M^-)^2}{(M^-)^2 + 3} \qquad \frac{T^+}{T^-} = \frac{[5(M^-)^2 - 1]\,[(M^-)^2 + 3]}{16(M^-)^2} \tag{42}$$

In Eqs. (42) M^- denotes the upstream infinity Mach number defined as

$$M^- = \frac{V^-}{(\gamma R T^-)^{1/2}} \tag{43}$$

being $\gamma = 5/3$ the specific heat ratio of a monatomic gas.
Shock profiles obtained from the numerical solution of Eq. (39) are compared to the full Boltzmann results, obtained from DSMC simulations, in Figures 1 and 2. As expected, the faster thermalization intrinsic in the BGKW approximation produces steeper density profiles. The advance of the temperature profile rise is also smaller, although a longer upstream tail is present in the $M^- = 5.0$. Moreover the slight temperature overshoot present in BE solution, seems to be absent in the BGKW solution.

1.3.2 1-D heat flow in a rarefied hard sphere gas

The limitations on the accuracy of BGKW model predictions imposed by the incorrect value of the Prandtl number clearly appear in the study of the one-dimensional flow of a monatomic gas confined in the gap between two infinite parallel plates located at points $x = \pm L/2$ of a reference frame in which the x coordinate spans the direction normal to the plates, kept at constant and uniform temperatures T_{w1} and T_{w2}, respectively. Without loss of generality, it is assumed that the "cold" plate position is $x = -L/2$ and its temperature is T_{w1} whereas the "hot" plate position is $x = +L/2$ and its temperature is $T_{w2} > T_{w1}$. The gas motion is assumed to be governed by Eq. (39) in which the collision frequency is obtained by Eqs. (40). The boundary conditions at the wall are assigned adopting a simple Maxwell's gas surface interaction model which mixes diffuse and specular re-emission with

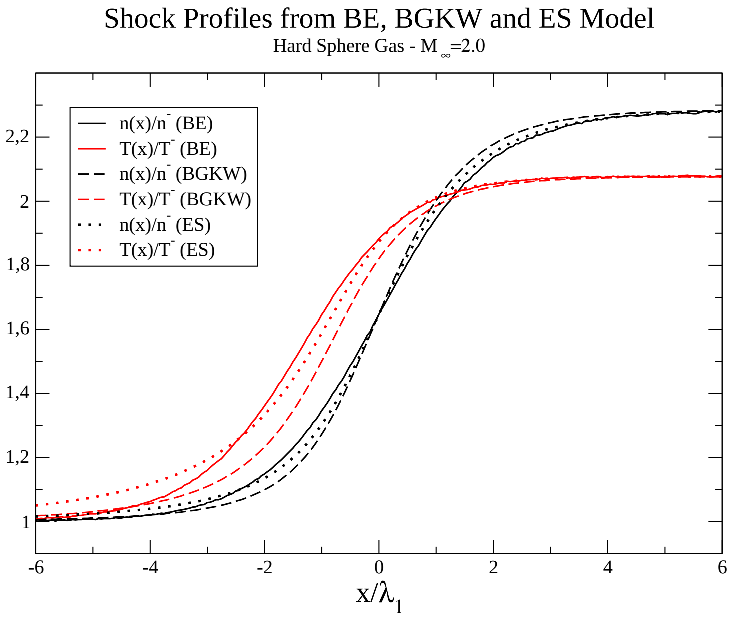

Figure 1: Normal shock profiles in a hard sphere gas, $M^- = 2.0$. Black: normalized density $n(x)/n^-$; green: normalized temperature $T(x)/T^-$; red: normalized mean velocity (x-component) $u_x(x)/\sqrt{RT^-}$. Solid lines: DSMC; symbols: direct solution of the Boltzmann equation; dashed lines: BGKW model

weights α and $1-\alpha$, respectively. Accordingly:

$$f(-\frac{L}{2}, \boldsymbol{v}) = \alpha \frac{n_{w1}}{(2\pi R T_{w1})^{3/2}} \exp\left[-\frac{\boldsymbol{v}^2}{2RT_{w1}}\right] + (1-\alpha) f(-\frac{L}{2}, \boldsymbol{v}^*), \quad v_x < 0 \tag{44}$$

$$f(\frac{L}{2}, \boldsymbol{v}) = \alpha \frac{n_{w2}}{(2\pi R T_{w2})^{3/2}} \exp\left[-\frac{\boldsymbol{v}^2}{2RT_{w2}}\right] + (1-\alpha) f(\frac{L}{2}, \boldsymbol{v}^*), \quad v_x > 0 \tag{45}$$

$$\boldsymbol{v}^* = (-v_x, v_y, v_z) \tag{46}$$

Mass conservation at boundaries determines the densities of wall Maxwellians as

$$n_{w1} = \sqrt{\frac{2\pi}{RT_{w1}}} \left| \int_{vx<0} v_x f(-\frac{L}{2}, \boldsymbol{v})\, d\boldsymbol{v} \right|, \quad n_{w2} = \sqrt{\frac{2\pi}{RT_{w2}}} \left| \int_{vx>0} v_x f(\frac{L}{2}, \boldsymbol{v})\, d\boldsymbol{v} \right| \tag{47}$$

It is esily found that the solutions of the problem depend on the three parameters α, T_{w2}/T_{w1} and Kn. The Knudsen number Kn is defined as λ_0/L, being $\lambda_0 = \frac{1}{\sqrt{2}n_0\pi\sigma^2}$ a reference value for the mean free path obtained from the mean density $n_0 = \frac{1}{L}\int_{-L/2}^{L/2} n(x)\, dx$.

Density, temperature and heat flux profiles obtained by numerical solutions of Eq. (39) are compared to DSMC simulations of the hard sphere dilute gas in Figure 3 in the case $\alpha = 0.826$, $T_{w2}/T_{w1} = 1.14$, $Kn = 0.7582$. It is worth observing gas rarefaction produces the typical temperature jumps at walls where the gas temperature differs from the wall temperature. The agreement between the the DSMC and BGKW density and temperature profiles is quite good. However, as expected, a discrepancy is found on the heat fluxes predicted by the two models because the BGKW collison frequency has been obtained

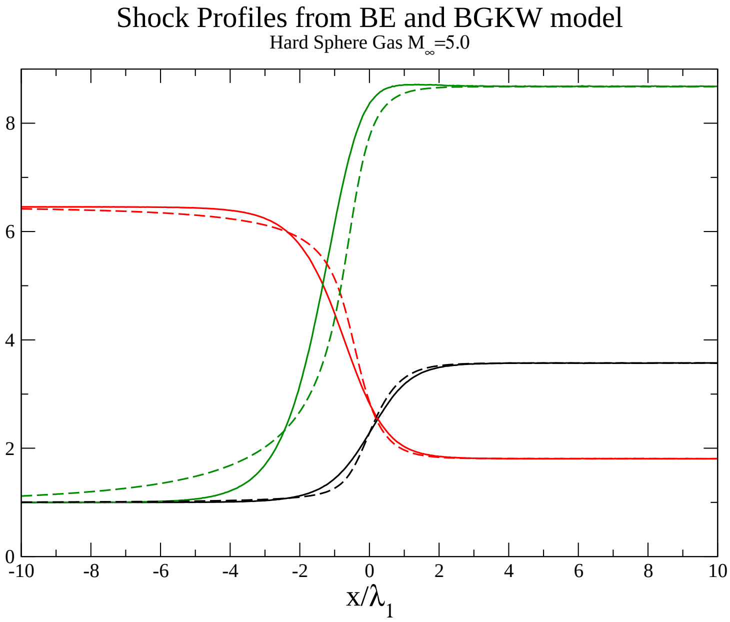

Figure 2: Normal shock profiles in a hard sphere gas, $M^- = 5.0$. Black: normalized density $n(x)/n^-$; green: normalized temperature $T(x)/T^-$; red: normalized mean velocity (x-component) $u_x(x)/\sqrt{RT^-}$. Solid lines: DSMC; dashed lines: BGKW model

from viscosity. A more complete data set is given in Table **??** which reports values of the ratio of the computed heat flux q_x to the heat flux value in free molecular flow conditions ($Kn \to \infty$), q_x^{FM}, as function of the Knudsen number Kn for $\alpha = 0.826$, $T_{w2}/T_{w1} = 1.14$. As is clear, tuning collision frequency on viscosity leads to incorrect predictions of heat fluxes but the accuracy can be recovered by obtaining ν from the *correct* thermal conductivity λ_{HS} of the hard sphere gas. Of course, such choice would spoil any shear stress prediction.

1.4 Driven Cavity Flow

The two test problems described above show that the simpler mathematical structure of the BGKW model is not without consequences on the accuracy of rarefied flow pre-

Kn	Boltzmann Equation^1	BGKW (ν from μ)^2	BGKW (ν from λ)^1
0.7582	0.7558	0.6759	0.7566
0.2994	0.5807	0.4774	0.5756
0.1942	0.4843	0.3811	0.4786
0.1395	0.4094	0.3117	0.4041
0.0658	0.2538	0.1813	0.2512

Table 1: Heat flux ratio q_x/q_x^{FM} as a function of Kn; $\alpha = 0.826$, $T_{w2}/T_{w1} = 1.14$; 1 - (Ohwada, 1996); 2 - (Graur and Polikarpov, 2009).

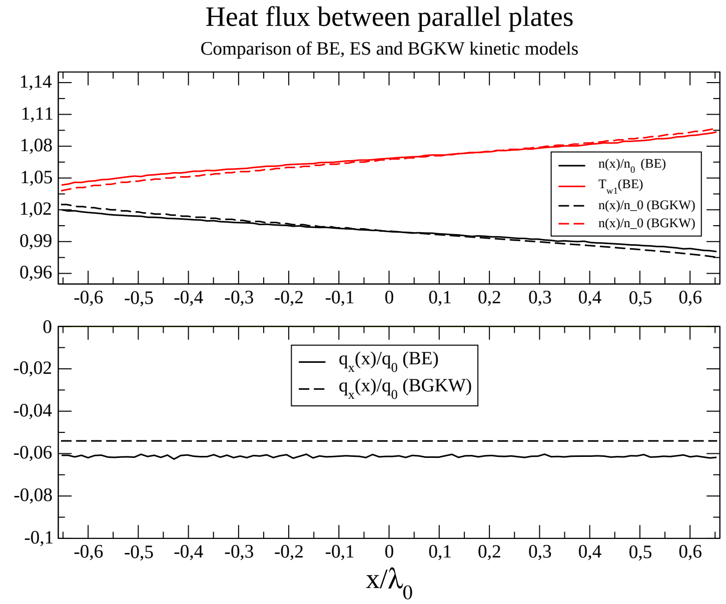

Figure 3: Heat flux between parallel plates. Hard sphere gas, $\alpha = 0.826$, $T_{w2}/T_{w1} = 1.14$, $Kn = 0.7582$.

dictions. However, there are situations where the application of typical numerical tools used to obtain solutions of the full Boltzmann equation becomes difficult. For instance, in standard implementations of DSMC schemes it is difficult to reduce statistical noise to describe accurately the tiny deviations from equilibrium met in low Mach number micro-flows. In such situations, the adoption of kinetic models allows adopting deterministic schemes which can easily capture small deviation from equilibrium. The following example shows that sensible tuning of the BGKW model collision frequency produces a fairly accurate description of two-dimensional rarefied gas flows.
A monatomic gas is confined in the two-dimensional square cavity

$$\mathcal{C} = \{(x, y) : 0 < x < L, 0 < y < L\}$$

The flow is driven by a uniform translation of the top with velocity $V_w \hat{\boldsymbol{e}}_x$, being $\hat{\boldsymbol{e}}_x$ a unit vector parallel to x direction. The gas flow is governed by the two-dimensional steady BGKW equation

$$v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} = \nu(\Phi - f) \tag{48}$$

where the collision frequency is obtained from the *viscosity* of the hard sphere gas, as discussed above. It is further assumed that all the walls are kept at uniform and constant temperature T_w and that the gas atoms which strike the walls are re-emitted according to the Maxwell's scattering kernel with complete accommodation

$$f(\overline{\boldsymbol{x}}, \boldsymbol{v}) = \frac{n_w(\overline{\boldsymbol{x}})}{(2\pi R T_w)^{3/2}} \exp\left\{-\frac{[\boldsymbol{v} - \boldsymbol{V}_w(\overline{\boldsymbol{x}})]^2}{2RT_w}\right\}, \quad (\boldsymbol{v} - \boldsymbol{V}_w) \circ \hat{\boldsymbol{n}} > 0 \tag{49}$$

where $\overline{\boldsymbol{x}}$ is a point of the boundary, $\hat{\boldsymbol{n}}(\overline{\boldsymbol{x}})$ the inward normal at $\overline{\boldsymbol{x}}$, $\mathbf{V}_w(\overline{\boldsymbol{x}})$ is the wall velocity, different from zero only on the top wall, T_w the wall temperature and $n_w(\overline{\boldsymbol{x}})$ the wall density which is determined by impinging mass flux through the following relationship

$$n_w(\overline{\boldsymbol{x}}) = \left(\frac{2\pi}{RT_w}\right)^{1/2} \int_{(\boldsymbol{v}-\boldsymbol{V}_w)\circ\hat{\boldsymbol{n}}<0} |(\boldsymbol{v}-\boldsymbol{V}_w)\circ\hat{\boldsymbol{n}}| f \, d\boldsymbol{v} \tag{50}$$

which ensures zero net mass flux at boundary points.
It is assumed that the initial gas state, at time $t = 0$, is described by the uniform equilibrium Maxwellian

$$f(\boldsymbol{x}, \boldsymbol{v}|0) = \Phi_0(\boldsymbol{v}) = \frac{n_0}{(2\pi RT_0)^{3/2}} \exp\left(-\frac{\boldsymbol{v}^2}{2RT_0}\right) \tag{51}$$

being n_0 and $T_0 = T_w$ the initial values of the uniform density and temperature, respectively. The non-dimensional form of the governing equation is easily obtained by adopting the reference mean free time $\tau_0 = 1/\nu_0$ and mean free path $\lambda_0 = \sqrt{2RT_0}\tau_0$ as time and length units, respectively. It is also immediately seen that the problem solutions depend on the dimensionless wall velocity $V_w/\sqrt{2RT_0}$ and the rarefaction parameter $\delta = L/\lambda_0$ which is the reciprocal value of the Knudsen number $\mathrm{Kn} = \lambda_0/L$.
Eq. (48) can be easily solved by a variety a finite difference schemes(**?**). The BGKW velocity field is compared to the full Boltzmann equation results in Figure 4. It should be noted that the top wall velocity ratio $V_w/\sqrt{2RT_0}$ has been set equal to 10^{-2} and that the full Boltzmann equation has been solved by a semi-deterministic method which adopts a Monte Carlo quadrature scheme to compute the Boltzmann collision integral given in Eq. (2). As Figure 4 shows, the agreement of BGKW and BE flow fields is pretty good. Moreover, BGKW computing time is a small fraction of the computing time of Boltzmann equation solutions. Hence, kinetic models are of some interest for micro-flows modeling.

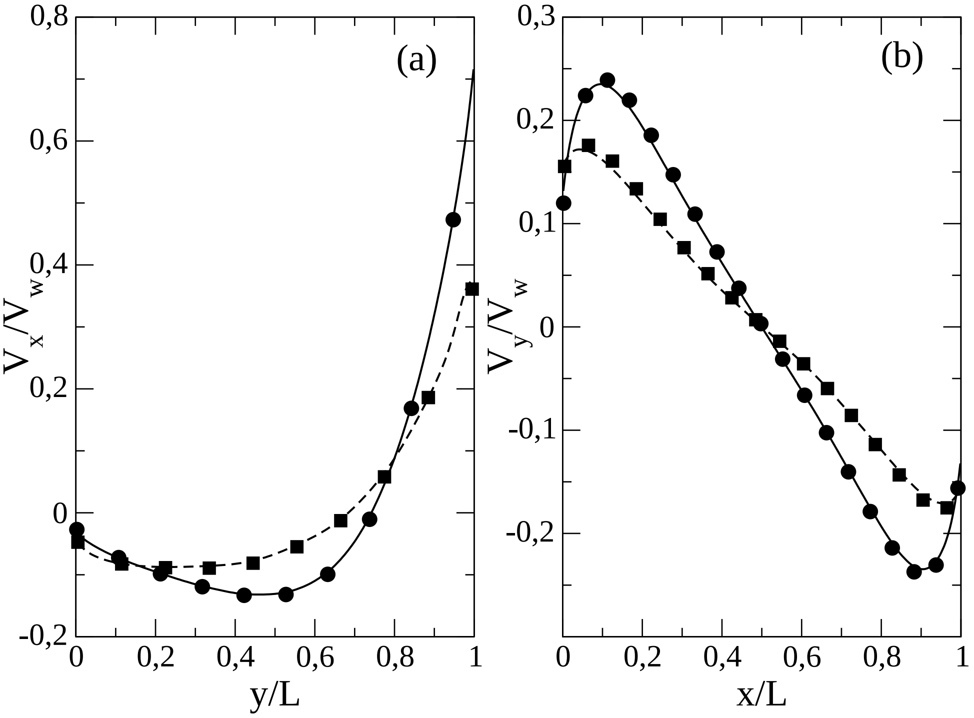

Figure 4: Profiles of the dimensionless **(a)** horizontal mean velocity along the vertical line crossing the center of the cavity, and **(b)** vertical mean velocity component along the horizontal line crossing the center of the main vortex. Solid and dashed lines: numerical solutions obtained by solving the full Boltzmann equation with a semi-regular method(Frezzotti et al., 2010) for $\delta = 10$ and $\delta = 0.1$, respectively. Circles and squares: numerical solutions reported in Ref. (Varoutis et al., 2008) for $\delta = 10$ and $\delta = 0.1$, respectively.

2 BGKW model extensions

Several attempts have been made to improve the BGKW model and, in particular, to obtain kinetic models that, while keeping its simplicity, do have the correct hydrodynamic limit. As far as the linearized form of the kinetic equation is concerned, there exist a systematic procedureCercignani (1988) to construct a sequence of linear models which contains the linearized BGKW model as first element and it has the linearized Boltzmann operator as final limit. For some linearized models a non-linear counterpart can be found.

2.1 The Ellipsoidal Statistical Model

In 1963 Holway(Holway, 1963) and, independently, Cercignani proposed the Ellipsoidal Statistical model (ES-model) which keeps the overall structure of the BGKW model, but approximates the *gain* term in Eq. (1) as the product of the collision frequency ν and an anisotropic Gaussian. More precisely, the ES-model kinetic equation has the form:

$$\begin{aligned} \frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{r}} f &= \nu \left[G(\boldsymbol{r}, \boldsymbol{v}|t) - f(\boldsymbol{r}, \boldsymbol{v}|t) \right] && (52) \\ G(\boldsymbol{r}, \boldsymbol{v}|t) &= \frac{n(\boldsymbol{r}|t)}{\sqrt{(2\pi)^3 \det \hat{\boldsymbol{A}}}} \exp\left(-\frac{1}{2} \hat{\boldsymbol{A}}^{-1} : \boldsymbol{cc} \right) && (53) \end{aligned}$$

In Eq. (57) $\boldsymbol{c} = \boldsymbol{v} - \boldsymbol{u}(\boldsymbol{r}|t)$ is the peculiar velocity, whereas the tensor $\hat{\boldsymbol{A}}$ is defined as:

$$\hat{\boldsymbol{A}} = (1-\beta) RT \boldsymbol{I} + \beta \frac{1}{\rho} \hat{\boldsymbol{P}} \qquad (54)$$

being $\beta = \frac{1}{1-P_r}$. It can be shown that the collision term of the ES-model conserves mass, momentum and energy and leads to a hydrodynamic limit with a specified Prandtl number equal to P_r, provided the relationship between collision frequency and viscosity is modified as:

$$\nu = P_r \frac{p}{\mu} \qquad (55)$$

Unfortunately, ES-model more complicated structure makes the study of some of its properties more difficult. For instance, the proof of the $\mathcal{H}$-theorem for ES-model is far from being trivial and it has been given only a few years ago(Andries et al., 2000). On the other hand, numerical solutions of Eq. (57) can be easily obtained by the same deterministic schemes developed for the BGKW model or by particle schemes(Andries et al., 2002b). Although the model provides the correct hydrodynamic limit, it is not guaranteed that it will yield accurate results in the transition regime. Therefore, an investigation of the model properties through the study of simple test problems is advisable. Normal shock profiles can be easily obtained by using Eq. (57) in place of Eq. (4)Ferziger and Kaper (1972). Figure 5 compares BGKW, ES-model and full Boltzmann density and temperature profiles in a stationary shock wave in a hard sphere gas with upstream infinity Mach number $M^- = 2.0$. It is interesting to observe that the slope of the density profile in the central region of the shock is closer to the Boltzmann equation results. The overall agreement with the temperature profile is also generally better than the BGKW model,

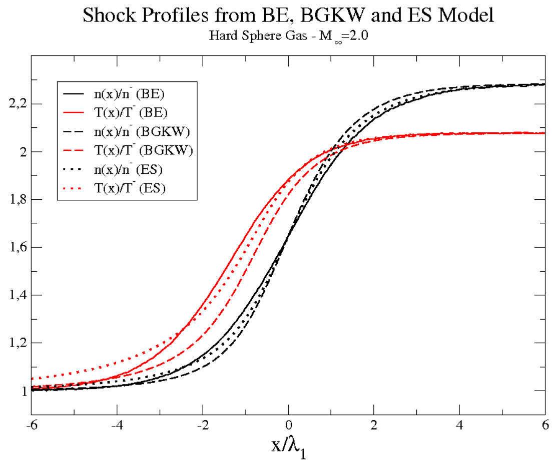

Figure 5: Normal shock profiles in a hard sphere gas, $M^{-} = 2.0$.

however the ES-model exhibits a more pronounced temperature tail which extends upstream.

As shown in Table 2.1, the improvements brought by the ES-model are also evident in the heat flux problem described in the previous section and recently studied in Ref.(Graur and Polikarpov, 2009) on ground of different kinetic models. Es-model applications to hypersonic flows have been described in Ref.Andries et al. (2002b) which also contains the description of a particle scheme for its numerical solution.

2.2 Shakhov Model

As is clear from the expression of the gain term in Eq. (57), the strategy to extend BGKW model capabilities is to replace a Maxwellian with function containing a larger number of adjustable parameters. The Gaussian function is by no means the unique possible choice. In order to obtain a model with the correct Prandtl number, Shakhov(Shakhov, 1968)

Kn	q_x/q_x^{FM} (a)	q_x/q_x^{FM} (b)
0.7582	0.7558	0.7488
0.2994	0.5807	0.5684
0.1942	0.4843	0.4719
0.1395	0.4094	0.3980
0.0658	0.2538	0.2466

Table 2: Heat flux ratio q_x/q_x^{FM} as a function of Kn; $\alpha = 0.826$, $T_{w2}/T_{w1} = 1.14$; (a) Boltzmann Equation(Ohwada, 1996); (b) ES-model (ν from μ, $P_r = 2/3$)(Graur and Polikarpov, 2009)

proposed the following model (S-model):

$$\begin{aligned}\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{r}} f &= \nu \left[S(\boldsymbol{r}, \boldsymbol{v}|t) - f(\boldsymbol{r}, \boldsymbol{v}|t) \right] &(56)\\ S(\boldsymbol{r}, \boldsymbol{v}|t) &= \Phi(\boldsymbol{r}, \boldsymbol{v}|t) \left[1 + \frac{1 - P_r}{5pRT} \boldsymbol{c} \circ \boldsymbol{q} \left(\frac{\boldsymbol{c}^2}{RT} - 5 \right) \right] &(57)\end{aligned}$$

S-model gain term is the product of the local Maxwellian times a third degree polynomial of peculiar velocity components. Although it generally performs better than BGKW medel, it should be observed that a proof of the (H)-theorem is still lacking for S-model. Moreover, the polynomial which multiplies Φ may become negative in some regions of the velocity space. Since negative values usually occur in high velocity regions, negative values of the gain term do not harm in modeling low speed flows where the model has been successfully applied(Graur and Polikarpov, 2009).

2.3 Models with velocity dependent ν

Kinetic models with the correct Prandtl number can also be obtained by allowing the collision frequency ν to depend on molecular velocity $\boldsymbol{v}$, as it does in the Boltzmann equation where the collision frequency is a functional of f, which for hard sphere interaction, takes the form shown in Eq. (2)

$$\nu(\boldsymbol{r}, \boldsymbol{v}) = \frac{\sigma^2}{2} \int_{R^3} d\boldsymbol{v}_1 \int_{\mathcal{S}^2} d^2\hat{\boldsymbol{k}}\, f(\boldsymbol{x}, \boldsymbol{v}_1|t) |\hat{\boldsymbol{k}} \cdot \boldsymbol{v}_r| = n(\boldsymbol{r})\, \pi \sigma^2 \overline{\boldsymbol{v}_r} \tag{58}$$

As shown in Ref. (Mieussens and Struchtrup, 2004), when the collision frequency ν in Eq. (4) depends on velocity, then the Prandtl number is given by the following expression:

$$P_r = \frac{5}{2} R \frac{\mu}{\lambda} = \frac{\int \frac{\eta^6}{\nu(\eta)} \exp\left(-\eta^2\right) d\eta}{\int \frac{\eta^4 (\eta^2 - \frac{5}{2})^2}{\nu(\eta)} \exp\left(-\eta^2\right) d\eta} \tag{59}$$

where $\eta = c/\sqrt{2RT}$. The model greater generality is obtained at the cost of some complications. Actually, the macroscopic fields $\tilde{n}(\boldsymbol{r}|t)$, $\tilde{\boldsymbol{u}}(\boldsymbol{r}|t)$, $\tilde{T}(\boldsymbol{r}|t)$ no longer coincide with local density, bulk velocity and temperature. The comprehensive study in Ref. (Mieussens and Struchtrup, 2004) also show that frequency dependent model do allow some improvements if a sensible choice for $\nu(\boldsymbol{c})$ is made. However, the choice is problem dependent as expected on ground of expression (58)

3 Kinetic models for mixtures

The aim of this section is to briefly sketch the methods and models which lead to the extension of the kinetic models described above to gaseous mixtures. For simplicity, the case of a binary mixture of monatomic species in absence of external fields will be considered.
The mixture is described by a system of two coupled Boltzmann equation in the form:

$$\frac{\partial f_i}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{r}} f_i = \sum_{j=1}^{2} \mathcal{C}_{ij}(f_i, f_j) \tag{60}$$

The collision integrals $\mathcal{C}_{ij}(f_i, f_j)$ satisfy the following relationships:

$$\begin{aligned}
\int \mathcal{C}_{ii}(f_i, f_j)\psi_i(\boldsymbol{v})\, d\boldsymbol{v} &= 0, \quad \psi_i(\boldsymbol{v}) = m_i, m_i\boldsymbol{v}, \frac{1}{2}m_i\boldsymbol{v}^2, i = 1, 2 && (61)\\
\int \mathcal{C}_{ij}(f_i, f_j)\, d\boldsymbol{v} &= 0, \quad i \neq j && (62)\\
m_i \int \mathcal{C}_{ij}(f_i, f_j)\boldsymbol{v}\, d\boldsymbol{v} &+ m_j \int \mathcal{C}_{ji}(f_i, f_j)\boldsymbol{v}\, d\boldsymbol{v} = 0, \quad i \neq j && (63)\\
m_i \int \mathcal{C}_{ij}(f_i, f_j)\boldsymbol{v}^2\, d\boldsymbol{v} &+ m_j \int \mathcal{C}_{ji}(f_i, f_j)\boldsymbol{v}^2\, d\boldsymbol{v} = 0, \quad i \neq j && (64)
\end{aligned}$$

expressing conservation of mass momentum and energy in self-interaction of individual species, conservation of mass in cross-interactions and conservation of total momentum and energy in cross-interaction.
Following the arguments leading to the BGKW model, it is quite natural to replace each collision term in the Boltzmann equations (60) with a relaxation term:

$$\begin{aligned}
\frac{\partial f_i}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{r}} f_i &= \sum_{j=1}^{2} \nu_{ij} \left(\Phi_{ij} - f_i\right) && (65)\\
\Phi_{ij}(\boldsymbol{r}, \boldsymbol{v}|t) &= \frac{n_{ij}(\boldsymbol{r}|t)}{\left[2\pi R_i T_{ij}(\boldsymbol{r}|t)\right]^{3/2}} \exp\left\{-\frac{\left[\boldsymbol{v} - \boldsymbol{u}_{ij}(\boldsymbol{r}|t)\right]^2}{2R_i T_{ij}(\boldsymbol{r}|t)}\right\} && (66)
\end{aligned}$$

It is immediately realized that the *twenty four* model disposable parameters/fields ν_{ij}, n_{ij}, T_{ij} and $\boldsymbol{u}_{ij}$ cannot be determined by the the sixteen equations 61 and the request that the total number of cross-collisions is (obviously) the same for both components:

$$n_i \nu_{ji} = n_j \nu_{ij} \tag{67}$$

There is no unique way to define the quantities ν_{ij}, n_{ij}, T_{ij} and $\boldsymbol{u}_{ij}$. Hamel(Hamel, 1965), for instance, adds to Eqs. (61,67) the request that the expressions for momentum and energy transfers in cross-collisions is the same as in a mixture of Maxwell's molecules(Cercignani, 1988). The resulting expressions read(Hamel, 1965):

$$\begin{aligned}
n_{ii}(\boldsymbol{r}|t) &= n_{ij}(\boldsymbol{r}|t) = n_i(\boldsymbol{r}|t) = \int f_i(\boldsymbol{r},\boldsymbol{v}|t)\,d\boldsymbol{v} && (68)\\
\boldsymbol{u}_{ii}(\boldsymbol{r}|t) &= \boldsymbol{u}_i(\boldsymbol{r}|t) = \frac{1}{n}\int \boldsymbol{v} f_i(\boldsymbol{r},\boldsymbol{v}|t)\,d\boldsymbol{v} && (69)\\
\boldsymbol{u}_{ij}(\boldsymbol{r}|t) &= \boldsymbol{u}_i(\boldsymbol{r}|t) + \alpha_{ij}(\boldsymbol{u}_i(\boldsymbol{r}|t) - \boldsymbol{u}_j(\boldsymbol{r}|t)) && (70)\\
T_{ii}(\boldsymbol{r}|t) &= T_i(\boldsymbol{r}|t) = \frac{1}{3nR_i}\int (\boldsymbol{v}-\boldsymbol{u}_i)^2 f_i(\boldsymbol{r},\boldsymbol{v}|t)\,d\boldsymbol{v} && (71)\\
T_{ii}(\boldsymbol{r}|t) &= T_i(\boldsymbol{r}|t) + \beta_{ij}[T_j(\boldsymbol{r}|t) - T_i(\boldsymbol{r}|t)] + \gamma_{ij}[\boldsymbol{u}_i(\boldsymbol{r}|t) - \boldsymbol{u}_j(\boldsymbol{r}|t)]^2 && (72)
\end{aligned}$$

being α_{ij}, β_{ij} and γ_{ij} constants depending on molecular masses and interaction potentials strenght. In the case of Maxwell's molecules collision frequencies can be written as $\nu_{ij} = n_j\kappa_{ij}$, being κ_{ij} interaction potential constants that can be determined to match individual components an mixture viscosities.

It is to be observed that a more systematic procedure to obtain kinetic models for mixtures is possible for linearized kinetic models(Mc Cormack, 1973).

It should also be observed that BGKW-like kinetic model for mixtures in the form of Eqs. (65) generally do not reduce to one-component model when one considers a fictitious mixture of mechanically identical components(Garzó et al., 1989). Consistent kinetic models which correct such inconsistency have been proposed in Refs.(Garzó et al., 1989; Andries et al., 2002a).

4 Kinetic models for polyatomic gases

The problem of bringing the effects of internal molecular structure into kinetic equations is not trivial for several reasons. Hence, the present notes does not even attempt to give a complete account of kinetic theory of dilute polyatomic gases which is properly described in a few textbooks. It will simply be noted that the difficulty of describing collisional processes between molecules with internal degrees of freedom (rotational, vibrational, electronic) reduces the "distance" between a description based on the full Boltzmann equation and kinetic model. As a matter of fact, the former is sometimes based on quite phenomenological collision models. The content of the following notes is therefore limited to the short presentation of the widely used Bognakke-Larsen collision model and of one of the possible extensions of the BGKW kinetic model. The predictions of the two polyatomic gas models will be compared on a simple one-dimensional flow resulting from the intense evaporation from a planar surface.

The problem treatment presented here is limited to the temperature range where vibrational excitation can be neglected. Moreover, since the gap between quantized rotational energy levels is supposed to be much smaller than κT_{ref} (T_{ref} is a reference characteristic flow temperature value), vapor molecules are supposed to behave as classical rigid rotators of *average* diameter a and mass m with $j = 2$ (linear molecule) or $j = 3$ (non-linear molecule) rotational degrees of freedom. It is assumed that the gas motion is governed by the following one-dimensional Boltzmann equationCercignani (1988); Kuščer (1989):

$$\xi_x \frac{\partial f}{\partial x}(\boldsymbol{v}, \mathcal{E}|x) = \int \left[f(\boldsymbol{v}_1', \mathcal{E}_1'|x) f(\boldsymbol{v}', \mathcal{E}'|x) - f(\boldsymbol{v}_1, \mathcal{E}_1|x) f(\boldsymbol{v}, \mathcal{E}|x) \right] Q \mathcal{E}_1^{\mu} \, d^3\xi_1 \, d\mathcal{E}_1 \tag{73}$$

being $f(\boldsymbol{v}, \mathcal{E}|x)$ the distribution function of molecular velocity $\boldsymbol{v}$ and *rotational* energy $\mathcal{E}$ at location x. *It is to be noted that rotational degrees of freedom are taken into account only through the rotational energy $\mathcal{E}$, not through the whole set of angular coordinates and momenta.* In Eq.(73), Q is defined as

$$Q = \int_{\mathcal{S}} d^2\hat{e}' \int_0^{E-\mathcal{E}'} \mathcal{E}'^{\mu} \, d\mathcal{E}' \int_0^{E-\mathcal{E}_1'} \mathcal{E}_1'^{\mu} \, d\mathcal{E}_1' \frac{\xi_r'^2}{\xi_r} \sigma(E; \hat{\boldsymbol{e}}' \circ \hat{\boldsymbol{e}}; \mathcal{E}', \mathcal{E}_1' \to \mathcal{E}, \mathcal{E}_1) \tag{74}$$

being $\sigma(E; \hat{\boldsymbol{e}}' \circ \hat{\boldsymbol{e}}; \mathcal{E}', \mathcal{E}_1' \to \mathcal{E}, \mathcal{E}_1)$ the differential cross-section associated with a binary collision which produces a pair of molecules in the final states $(\boldsymbol{v}, \mathcal{E})$, $(\boldsymbol{v}_1, \mathcal{E}_1)$ from a pair of molecules in the initial states $(\boldsymbol{v}', \mathcal{E}')$, $(\boldsymbol{v}_1', \mathcal{E}_1')$. The argument E denotes the conserved total energy in the center of mass reference frame:

$$E = \frac{1}{4} m \xi_r^2 + \mathcal{E} + \mathcal{E}_1 = \frac{1}{4} m \xi_r'^2 + \mathcal{E}' + \mathcal{E}_1' \tag{75}$$

The unit vectors $\hat{\boldsymbol{e}}' = \frac{\boldsymbol{v}_r'}{\xi_r'}$ and $\hat{\boldsymbol{e}} = \frac{\boldsymbol{v}_r}{\xi_r}$ have the directions of the relative velocities $\boldsymbol{v}_r' = \boldsymbol{v}_1' - \boldsymbol{v}'$ and $\boldsymbol{v}_r = \boldsymbol{v}_1 - \boldsymbol{v}$ before and after a collision, respectively. The exponent μ in Eq.(73) takes the values 0 for $j = 2$ and $\frac{1}{2}$ for $j = 3$.

4.1 The collision model

The collision dynamics and cross-section have been obtained from a phenomenological model proposed by Borgnakke and LarsenBorgnakke and Larsen (1975). The model overcomes some of the restrictions and complications of previous mechanical models of translational-rotational coupling (rough spheres, loaded spheres, spherocylinders)Chapman and Cowling (1990) since it can be easily adapted to reproduce experimental translational-rotational relaxation rates with good accuracyWysong and Wadsworth (1998). Moreover, the collision algorithm derived from the model is very well suited to particle schemes used to obtain numerical solutions of the Boltzmann equationBird (1994). In the particular form of the Borgnakke-Larsen model adopted here, collision dynamics is organized as follows:

- The collision probability of two molecules in the pre-collision states $(\boldsymbol{v}', \mathcal{E}')$, $(\boldsymbol{v}'_1, \mathcal{E}'_1)$ is proportional to $\sigma_{hs}\xi'_r$, where $\sigma_{hs} = \pi a^2$ is the integral cross-section of hard sphere molecules and $\xi'_r = \|\boldsymbol{v}'_1 - \boldsymbol{v}'\|$ is the relative velocity modulus.

- An individual collision is inelastic with probability z or elastic with probability $1 - z$. An inelastic collision gives rise to an exchange between translational and rotational energies, as explained below. In an elastic collision pre- and post-collision rotational energies do not change, i.e. $\mathcal{E} = \mathcal{E}'$, $\mathcal{E}_1 = \mathcal{E}'_1$. Conservation of total energy then implies $\xi_r = \xi'_r$ and, according to hard sphere impact dynamics, post-collision relative velocity is written as $\boldsymbol{v}_r = \xi_r \hat{\boldsymbol{e}}$, being $\hat{\boldsymbol{e}}$ a random vector uniformly distributed on the unit sphere $\mathcal{S}$.

- In an inelastic collision total energy E is randomly partitioned between translational and rotational motion by sampling the translational energy fraction E_{tr}/E from a given probability density function $\mathcal{P}_1(E_{tr}/E|j)$. The available total rotational energy $E_{rot} = \mathcal{E} + \mathcal{E}_1 = E - E_{tr}$ is then randomly distributed between the collision partners by sampling the fraction $\mathcal{E}/E_{rot}$ from a given probability density function $\mathcal{P}_2(\mathcal{E}/E_{rot}|j)$. The relative velocity after a collision is again written as $\boldsymbol{v}_r = \xi_r \hat{\boldsymbol{e}}$, where $\hat{\boldsymbol{e}}$ is a random unit vector and $\xi_r = \sqrt{\frac{4E_{tr}}{m}}$

The specific form of the probability densities $\mathcal{P}_1(\mathcal{E}/E_{rot}|j)$ and $\mathcal{P}_2(E_{tr}/E|j)$ depends both on the number of internal degrees of freedom and on the assumed intermolecular interactionBird (1994). In the case of hard sphere interaction and $j = 2$ they take a particularly simple formKuščer (1989); Bird (1994)

$$\mathcal{P}_1(E_{tr}/E|2) = 6\frac{E_{tr}}{E}\left(1 - \frac{E_{tr}}{E}\right) \tag{76}$$

$$\mathcal{P}_2(\mathcal{E}/E_{rot}|2) = 1 \tag{77}$$

As shown by Eq.(76), post-collision translational energy has a parabolic distribution; the available E_{rot} amount is then randomly divided between $\mathcal{E}$ and $\mathcal{E}_1$, according to Eq.(77). Taking into account the assumed scattering isotropy and Eqs.(76,77), the collision cross-section takes the form:

$$\sigma(E; \hat{\boldsymbol{e}}' \circ \hat{\boldsymbol{e}}; \mathcal{E}', \mathcal{E}'_1 \to \mathcal{E}, \mathcal{E}_1) = \frac{\sigma_{hs}}{4\pi E^2}\theta(\epsilon, \epsilon_1, \epsilon', \epsilon'_1) \tag{78}$$

$$\theta(\epsilon, \epsilon_1, \epsilon', \epsilon'_1) = (1 - z)\delta(\epsilon - \epsilon')\delta(\epsilon_1 - \epsilon'_1) + 6z(1 - \epsilon - \epsilon_1) \tag{79}$$

being $\epsilon = \mathcal{E}/E$.

The strength of translational-rotational coupling is determined by the mixing parameter z which can be made to depend on the local flowfield temperature to fit experimental relaxation ratesWysong and Wadsworth (1998) A kinetic model which closely patterns BGKW model has been proposed by Holway in 1966Holway (1966). As usual, relaxation terms replace the full Boltzmann collision integral:

$$\frac{\partial f}{\partial t} + \xi_x \frac{\partial f}{\partial x} = \nu_{el}(n, T_t)\,(\Phi_{el} - f) + \nu_{in}(n, T_t)\,(\Phi_{in} - f) \tag{80}$$

where the “frozen” local equilibrium and local equilibrium Maxwellian distribution functions, $\Phi_{el}(\boldsymbol{v}, \mathcal{E})$ and $\Phi_{in}(\boldsymbol{v}, \mathcal{E})$, are defined as follows:

$$\begin{aligned} \Phi_{el}(\boldsymbol{v}, \mathcal{E}) &= \frac{n(\mathcal{E}|x,t)}{[2\pi R T_t(x,t)]^{3/2}} \exp\left\{ -\frac{[\boldsymbol{v} - \boldsymbol{u}(x,t)]^2}{2RT_t(x,t)} \right\} && (81) \\ \Phi_{in}(\boldsymbol{v}, \mathcal{E}) &= \frac{N(x,t)}{[2\pi R T(x,t)]^{3/2}} \exp\left\{ -\frac{[\boldsymbol{v} - \boldsymbol{u}(x,t)]^2}{2RT(x,t)} \right\} \times \\ & \quad \frac{\mathcal{E}^{j/2-1}}{\Gamma(j/2)[\kappa T(x,t)]^{j/2}} \exp\left[-\frac{\mathcal{E}}{\kappa T(x,t)} \right] && (82) \end{aligned}$$

In Eq.(80) a BGK-likeBhatnagar et al. (1954) expression replaces the complicated collision integral of Eq.(73). The first term describes elastic collisions, whereas the second one models inelastic collisions. The macroscopic fields associated with $\Phi_{el}(\boldsymbol{v}, \mathcal{E})$ and $\Phi_{in}(\boldsymbol{v}, \mathcal{E})$ are defined as:

$$\begin{aligned} n(\mathcal{E}|x,t) &= \int f(\boldsymbol{v}, \mathcal{E}|x,t)\, d^3\xi && (83) \\ N(x,t) &= \int f(\boldsymbol{v}, \mathcal{E}|x,t)\, d^3\xi\, d\mathcal{E} = \int n(\mathcal{E}|x,t)\, d\mathcal{E} && (84) \\ \boldsymbol{u}(x,t) &= \frac{1}{N(x,t)} \int \boldsymbol{v} f(\boldsymbol{v}, \mathcal{E}|x,t)\, d^3\xi\, d\mathcal{E} = u_x(x,t)\hat{\boldsymbol{x}} + u_y(x,t)\hat{\boldsymbol{y}} && (85) \\ T_t(x,t) &= \frac{1}{3RN(x,t)} \int [\boldsymbol{v} - \boldsymbol{u}(x,t)]^2 f(\boldsymbol{v}, \mathcal{E}|x,t)\, d^3\xi\, d\mathcal{E} && (86) \\ T_r(x,t) &= \frac{2}{j\kappa N(x,t)} \int \mathcal{E} f(\boldsymbol{v}, \mathcal{E}|x,t)\, d^3\xi\, d\mathcal{E} && (87) \\ T(x,t) &= \frac{3T_t(x,t) + jT_r(x,t)}{3+j} && (88) \end{aligned}$$

The quantity $n(\mathcal{E}|x,t)$ is the number density of molecules having internal energy $\mathcal{E}$, $N(x,t)$ is the total number density, $\boldsymbol{u}(x,t)$ is the mean velocity of the gas, whereas $T_t(x,t)$, $T_r(x,t)$ and $T(x,t)$ are the translational, internal and overall temperature, respectively. The elastic and inelastic collision frequencies, $\nu_{el}(n, T_t)$ and $\nu_{in}(n, T_t)$ have been computed from the shear viscosity μ of the hard sphere gas as:

$$\begin{aligned} \nu_{el}(N, T_t) &= (1-z)\nu_{tot}(N, T_t) && (89) \\ \nu_{in}(N, T_t) &= z\nu_{tot}(N, T_t) && (90) \\ \nu_{tot}(N, T_t) &= \frac{N\kappa T_t}{\mu(T_t)} && (91) \end{aligned}$$

The numerical solution of Eq.(80) can be greatly simplified by a transformation first considered by ChuChu (1965). Let us define the reduced distribution functions $F(\xi_x|x,t)$, $G(\xi_x|x,t)$, $H(\xi_x|x,t)$ and $K(\xi_x|x,t)$ as:

$$\begin{pmatrix} F(\xi_x|x,t) \\ G(\xi_x|x,t) \\ H(\xi_x|x,t) \\ K(\xi_x|x,t) \end{pmatrix} = \int \begin{pmatrix} 1 \\ \xi_y \\ (\xi_y^2+\xi_z^2) \\ \mathcal{E} \end{pmatrix} f(\boldsymbol{v},\mathcal{E}|x,t)\, d\xi_y\, d\xi_z\, d\mathcal{E} \tag{92}$$

It can be easily verified that the reduced distribution functions defined above obey the following system of kinetic equations:

$$\frac{\partial}{\partial t}\begin{pmatrix} F \\ G \\ H \\ K \end{pmatrix} + \xi_x \frac{\partial}{\partial x}\begin{pmatrix} F \\ G \\ H \\ K \end{pmatrix} = \nu_{el}\begin{pmatrix} \hat{F}_{el}-F \\ \hat{G}_{el}-G \\ \hat{H}_{el}-H \\ \hat{K}_{el}-K \end{pmatrix} + \nu_{in}\begin{pmatrix} \hat{F}_{in}-F \\ \hat{G}_{in}-G \\ \hat{H}_{in}-H \\ \hat{K}_{in}-K \end{pmatrix} \tag{93}$$

where

$$\begin{pmatrix} \hat{F}_{el}(\xi_x|x,t) \\ \hat{G}_{el}(\xi_x|x,t) \\ \hat{H}_{el}(\xi_x|x,t) \\ \hat{K}_{el}(\xi_x|x,t) \end{pmatrix} = \begin{pmatrix} 1 \\ u_y(x,t) \\ u_y^2(x,t)+2RT_t(x,t) \\ \frac{j\kappa T_r}{2} \end{pmatrix} \frac{N(x,t)}{\sqrt{2\pi RT_t}} \exp\left\{-\frac{(\xi_x-u_x)^2}{2RT_t}\right\} \tag{94}$$

$$\begin{pmatrix} \hat{F}_{in}(\xi_x|x,t) \\ \hat{G}_{in}(\xi_x|x,t) \\ \hat{H}_{in}(\xi_x|x,t) \\ \hat{K}_{in}(\xi_x|x,t) \end{pmatrix} = \begin{pmatrix} 1 \\ u_y(x,t) \\ u_y^2(x,t)+2RT(x,t) \\ \frac{j\kappa T(x,t)}{2} \end{pmatrix} \frac{N(x,t)}{\sqrt{2\pi RT}} \exp\left\{-\frac{(\xi_x-u_x)^2}{2RT}\right\} \tag{95}$$

4.2 A simple application

We consider the steady one-dimensional flow of a polyatomic vapor evaporating from an infinite planar surface (interface) kept at constant and uniform temperature T_w. The surface, located at $x = 0$, separates the condensed phase, which occupies the half-space $x < 0$, from the vapor phase flowing in the half-space $x > 0$. The coordinate x spans the direction normal to the surface in a reference frame at rest with respect to the interface. The gas motion has been computed bu solving both Eq. (73) and Eq. (80). Molecular exchange processes between the vapor and condensed phase across the interface have been described by the following boundary condition for f at $x = 0$:

$$v_x f(\boldsymbol{v},\epsilon|0,t) = v_x f_e(\boldsymbol{v},\epsilon) + \int_{v_{1x}<0} K(\boldsymbol{v},\epsilon|\boldsymbol{v}_1,\epsilon_1)|v_{1x}|f(\boldsymbol{v}_1,\epsilon_1|0,t)\, d\boldsymbol{v}_1\, d\epsilon_1, \quad v_x > 0 \tag{96}$$

The distribution function of evaporating molecules, f_e, is assumed to be a half-range Maxwellian:

$$\begin{aligned} f_e(\boldsymbol{v},\epsilon) &= \sigma_e \frac{N_w}{(2\pi RT_w)^{3/2}} \exp\left(-\frac{\boldsymbol{v}^2}{2RT_w}\right) \\ &\quad \times \frac{\epsilon^{j/2-1}}{\Gamma(j/2)(\kappa T_w)^{j/2}} \exp\left(-\frac{\epsilon}{\kappa T_w}\right), \quad v_x > 0 \end{aligned} \tag{97}$$

The velocities of vapor molecules re-emitted into the gas phase after interacting with the interface are obtained by the following scattering kernel K which describes a pure diffusive re-emissionCercignani (1988):

$$\begin{aligned} K(\boldsymbol{v},\epsilon|\boldsymbol{v}_1,\epsilon_1) &= (1-\sigma_e)\frac{1}{2\pi(RT_w)^2}\exp\left(-\frac{\boldsymbol{v}^2}{2RT_w}\right) \\ &\quad\times\frac{\epsilon^{j/2-1}}{\Gamma(j/2)(\kappa T_w)^{j/2}}\exp\left(-\frac{\epsilon}{\kappa T_w}\right) \end{aligned} \tag{98}$$

In Eqs.(97,98) N_w denotes the saturated vapor density at temperature T_w, σ_e is the evaporation coefficient, κ is the Boltzmann constant, R denotes the ratio κ/m and Γ is the complete Gamma function. It is further assumed that the far downstream vapor state is described by an equilibrium Maxwellian distribution function:

$$\begin{aligned} f_\infty(\boldsymbol{v},\epsilon) &= \frac{N_\infty}{(2\pi RT_\infty)^{3/2}}\exp\left[-\frac{(\boldsymbol{v}-\boldsymbol{u}_\infty)^2}{2RT_\infty}\right] \\ &\quad\times\frac{\epsilon^{j/2-1}}{\Gamma(j/2)(\kappa T_\infty)^{j/2}}\exp\left(-\frac{\epsilon}{\kappa T_\infty}\right) \end{aligned} \tag{99}$$

As shown in Figures 6 and 7 the full Boltzmann equation corresponding to Borgnakke-Larsen model and Holway's kinetic model produce very close results.

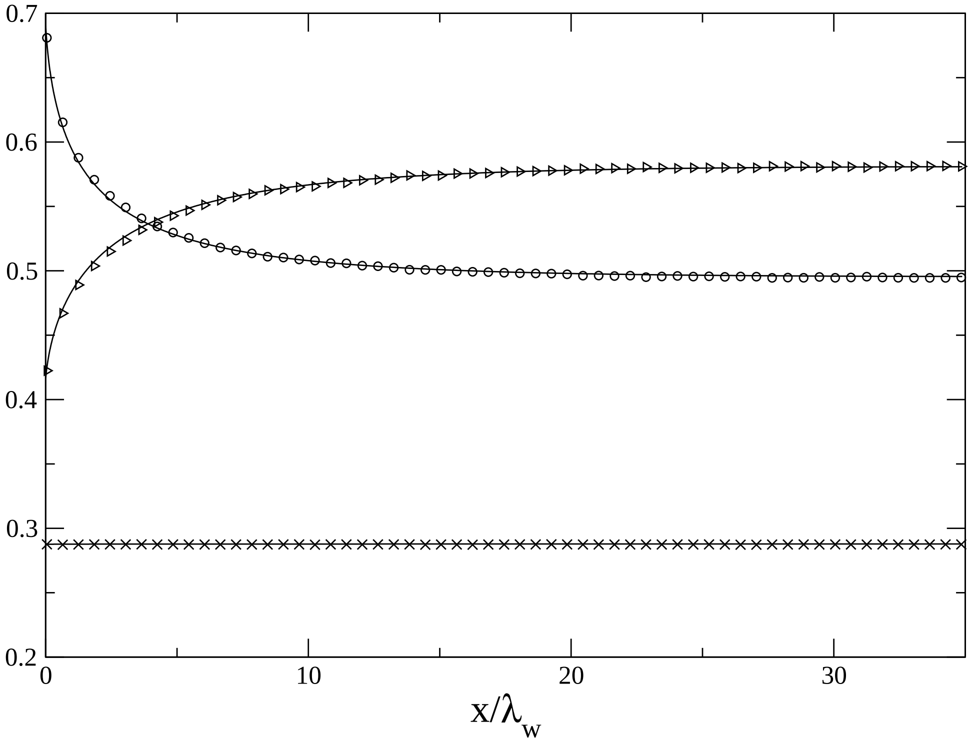

Figure 6: Density, velocity and mass flux profiles in evaporation flow of a polyatomic gas with $j = 3$ rotational degrees of freedom; z=0.3 $M_\infty = 0.534$. Numerical data from solution of Holway's kinetic model are represented by solid lines. DSMC results represented by symbols: $\circ$, $N(x)/N_w$; $\triangleright$, $u_x(x)/\sqrt{RT_w}$; $\times$, $J(x) = N(x)u_x(x)/N_w\sqrt{RT_w}$

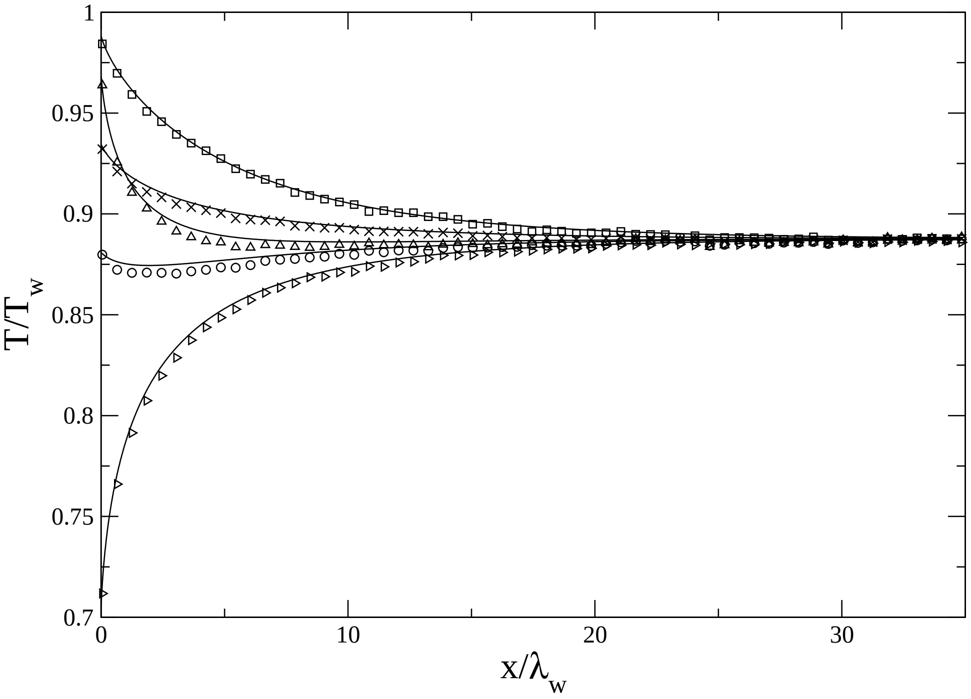

Figure 7: Temperature profiles in evaporation flow of a polyatomic gas with $j = 3$ rotational degrees of freedom; z=0.3, $M_\infty = 0.534$. Numerical data from solution of Holway's kinetic model are represented by solid lines. DSMC results represented by symbols: $\circ$, $T_t(x)/T_w$; $\triangleright$, $T_\|(x)/T_w$; $\triangle$, $T_\perp(x)/T_w$;$\Box$, $T_r(x)/T_w$; $\times$, $T(x)/T_w$.

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