A Kinetic Model for Gas Mixtures Based on a Fokker–Planck Equation

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Abstract. We present a generalized nonlinear Fokker–Planck equation, which describes the dynamics of rarefied monatomic gas mixture flows. The devised kinetic model leads to correct transfer of energy and momentum between gas species and to consistent evolution of molecular stresses and heat fluxes with respect to the generalized Boltzmann equation. Thus, the correct diffusion coefficient together with the mixture viscosity and mixture heat conductivity coefficients are obtained. The strength of the presented model lies on the computational efficiency, which is due to the fact that the resulting stochastic processes are continuous in time. Therefore, unlike in Direct Simulation Monte Carlo (DSMC), here simulated particles do not collide with each other, but move along independent continuous stochastic paths. Another aspect of the new Fokker–Planck model equation is that here the effect of collisions is described via drift and diffusion type processes. Accordingly, a scheme can be derived for which the time step size limitation of the corresponding numerical simulation becomes independent of the Knudsen number. Consequently, this leads to more efficient simulations, especially in low or intermediate Knudsen numbers. Results are presented for helium-argon mixture in a one dimensional geometry. The calculated mixture viscosity is found to be in accordance with experimental data, which reveals the accuracy and relevance of the approach.

1. Introduction
Complexity of the Boltzmann collision operator together with the high dimensionality of its solution domain are the main motivations for devising simpler yet accurate approximations for rarefied gas flows. Among different approaches, Fokker–Planck equations provide computationally attractive kinetic models, which at the same time fulfill the basic properties of the Boltzmann equation, e.g. see [2]. Recently, a Fokker–Planck model for simple monatomic gas flows was proposed in [8], where accurate results were obtained up to intermediate Knudsen numbers. Extensions of the Fokker–Planck model to a nonlinear model equation in [5] resulted in the correct Prandtl number for monatomic molecules. The model was also generalized for simple diatomic gas flows with rotational and vibrational degrees of freedom [6].

In this study, the Fokker–Planck kinetic model is extended in order to include the kinetics of monatomic gas mixtures. The paper starts with the derivation of the model, where appropriate drift and diffusion coefficients are obtained. Then, an energy conserving numerical scheme based on the particle method is derived in §3. Afterwards, the results are presented for an argon-helium mixture in the hydrodynamic limit considering different mixture fractions. The paper is closed by some concluding remarks.
2. Kinetic Model
Consider a mixture of two gas species \( \alpha \) and \( \beta \) with molecular masses \( m^\alpha \) and \( m^\beta \). The statistical state of the mixture is determined by the molecular velocity distribution of each species. Here the probability density function (PDF) \( f(V;X,t) \) defined over the velocity sample space \( V \), position \( X \) and time \( t \), is employed. In the absence of an external force, the Fokker–Planck system of equations

\[
\frac{\partial f^\alpha}{\partial t} + V_i \frac{\partial f^\alpha}{\partial X_i} = - \frac{\partial}{\partial V_i} \left( A^\alpha_i f^\alpha \right) + \frac{\partial^2}{\partial V_i \partial V_j} \left( \frac{D^\alpha_{ij} f^\alpha}{2} \right)
\]

(1)

\[
\frac{\partial f^\beta}{\partial t} + V_i \frac{\partial f^\beta}{\partial X_i} = - \frac{\partial}{\partial V_i} \left( A^\beta_i f^\beta \right) + \frac{\partial^2}{\partial V_i \partial V_j} \left( \frac{D^\beta_{ij} f^\beta}{2} \right)
\]

(2)

describe the evolution of species PDFs, i.e. \( f^\alpha \) and \( f^\beta \) in time. Note that superscripts \( \alpha \) and \( \beta \) relate to gas species \( \alpha \) and \( \beta \), respectively. Also the index summation convention was used throughout this paper. The idea here is to choose the drift coefficients \( A^\alpha_i \) and \( A^\beta_i \) and the diffusion coefficients \( D^\alpha_{ij} \) and \( D^\beta_{ij} \) in a way that the above system become consistent with Boltzmann up to a certain order of velocity moments. First, we propose a linear model for \( A^\alpha_i \) and \( A^\beta_i \) and second, a cubic function will be studied.

2.1. Linear Model
The relaxation of the mean species velocities \( U^\alpha,\beta \), species temperatures \( T^\alpha,\beta \) and densities \( \rho^\alpha,\beta \) can be calculated from the Boltzmann equation. Before we proceed note that for the rest of this study we only discuss the equations related to species \( \alpha \). The corresponding equations for the other species \( \beta \) can be obtained by switching the indices \( \alpha \) and \( \beta \) in all terms. Given the intermolecular force constant \( \chi^\alpha\beta \), the Boltzmann collision operator for Maxwell molecules leads to [7]

\[
\frac{dU^\alpha}{dt} = -A^\alpha\beta \rho^\beta \left( U^\alpha_i - U^\beta_i \right)
\]

(3)

and

\[
\frac{dT^\alpha}{dt} = -2 A^\alpha\beta \rho^\beta \left[ \frac{m^\alpha}{m^\beta} \sigma^\alpha\beta (T^\alpha - T^\beta) - \frac{m^\beta}{3k} (U^\alpha - U^\beta)^2 \right],
\]

(4)

where the constant \( A^\alpha\beta \) is given by

\[
A^\alpha\beta = \frac{8\sqrt{\pi}}{3} \Gamma\left(\frac{5}{2}\right) \mathcal{A}_1 \left( \frac{(m^\alpha + m^\beta)\chi^\alpha\beta}{m^\alpha m^\beta} \right).
\]

(5)

Here the Boltzmann constant is denoted by \( k \) and the mass ratio between two species is given by \( \sigma^\alpha\beta = m^\alpha/m^\beta \). Also note that \( \mathcal{A}_1 \approx 0.422 \) is the collision cross section for MaxWel type molecules [3]. In order to construct a consistent Fokker–Planck model for relaxation of mean velocities and temperature, the drift coefficient reads

\[
A^\alpha_i = - \frac{A^\alpha\beta \rho^\beta (V_i - U^\beta_i)}{\mathcal{A}} - \frac{A^\alpha\beta \rho^\beta (V_i - U^\beta_i)}{\mathcal{A}}.
\]

(6)
Further, based on the energy equation (4) the diffusion coefficient becomes

\[ D^{\alpha 2} = \frac{2}{1 + \sigma^{\alpha \beta}} \left( \frac{kT^{\alpha}}{m^{\alpha}} + \frac{kT^{\beta}}{m^{\beta}} + \frac{1}{3} \left| U^{\alpha} - U^{\beta} \right|^2 \right) \]

\[ \text{collisions between unlike molecules} \]

\[ + \frac{2A^{\alpha \alpha} \rho^{\alpha \beta} kT^{\alpha}}{m^{\alpha}} \]

\[ \text{collisions between same molecules} \]

\[ (7) \]

Using the above discussed closures for \( A^{\alpha i} \) and \( D^{\alpha} \), consistency between the Fokker–Planck system and the Boltzmann equation can be achieved for the relaxation of mean velocities and energies. Thus e.g. the diffusion property of a binary gas mixture can be calculated accurately using the Fokker–Planck model. However, still the viscosity and heat conductivity of the mixture calculated from the model may deviate from those obtained from Boltzmann. This is the main intention for the cubic model, which is discussed in the following sub-section.

2.2. Cubic Model

The idea of this part is to employ a cubic ansatz for the drift coefficient in order to match the evolution of the pressure tensor and the heat flux vector resulting from the Fokker-Planck model with those resulting from the Boltzmann equation. Therefore, similar to the monatomic model of [5], the following expression is adopted for the drift coefficient

\[ A^{\alpha i} = b^{\alpha i} + c^{\alpha ij} V^{\alpha j'} + \gamma^{\alpha i} \left( V^{\alpha j'} V^{\alpha j'} - \frac{3kT^{\alpha}}{m^{\alpha}} \right) + \Lambda^{\alpha} \left( V^{\alpha i} V^{\alpha j'} V^{\alpha j'} - 2q^{\alpha i} \right), \]

\[ (8) \]

where \( V^{\alpha j'} = V - U^{\alpha} \) is the fluctuating velocity of species \( \alpha \). Here the model constants \( b^{\alpha i}, c^{\alpha ij} \) and \( \gamma^{\alpha i} \) should be chosen such to enforce consistency between the model and Boltzmann. The constant \( \Lambda^{\alpha} \) is responsible to keep the drift coefficient stable [5]. The constant term \( b^{\alpha i} \) can be found from the linear model to be

\[ b^{\alpha i} = -A^{\alpha \beta} \rho^{\beta} \left( U^{\alpha i} - U^{\beta i} \right), \]

\[ (9) \]

while the constants \( c^{\alpha ij} \) and \( \gamma^{\alpha i} \) should be found from relaxations of the pressure tensor and the heat flux vector. Consider \( p^{\alpha \beta}_{ij} \) and \( q^{\alpha \beta i} \) as pressure tensor and heat flux of gas species, thus the relaxation equation for the pressure tensor takes form

\[ \frac{dp^{\alpha \beta}_{ij}}{dt} = p^{\alpha i}_{ij} \rho^{\beta} \left( -2m_0^{\alpha} A^{\alpha \beta} - 3m_0^{\beta} B^{\alpha \beta} \right) + p^{\beta i}_{ij} \rho^{\alpha} \left( 2m_0^{\alpha} A^{\alpha \beta} - 3m_0^{\beta} B^{\alpha \beta} \right) \]

\[ + \frac{3k(T^{\alpha} + T^{\beta})}{m^{\alpha} + m^{\beta}} \rho^{\alpha} \rho^{\beta} B^{\alpha \beta} \delta_{ij} \]

\[ + m_0^{\beta} \rho^{\alpha} \rho^{\beta} \left( U^{\alpha} - U^{\beta} \right)^2 B^{\alpha \beta} \delta_{ij} + (U^{\alpha i} - U^{\beta i})(U^{\alpha j} - U^{\beta j})(-3B^{\alpha \beta} + 2A^{\alpha \beta}) \]

\[ - 3p^{\alpha}_{ij} \rho^{\alpha} A^{\alpha} \rho^{\beta} B^{\alpha \beta} \delta_{ij} + \frac{3\rho^{\alpha} kT^{\alpha}}{m^{\alpha}} \rho^{\beta} B^{\alpha \beta} \delta_{ij} \]

\[ (10) \]
and for the heat fluxes, the relaxation becomes

\[
\frac{dq_{ij}^\alpha}{dt} = -q_{ij}^\alpha \rho^\beta \left( (3m_0^\alpha + m_0^\beta) A^{\alpha\beta} + 4m_0^\alpha m_0^\beta B^{\alpha\beta} \right) + 4q_{i0}^\beta \rho^\alpha m_0^{\beta2} \left( A^{\alpha\beta} - B^{\alpha\beta} \right) + 4m_0^\beta \left( A^{\alpha\beta} - B^{\alpha\beta} \right) \left( U_j^\alpha - U_j^\beta \right) \left( \rho^\alpha p_{ij}^\alpha + \rho^\beta p_{ij}^\beta \right) - \left( A^{\alpha\beta}(m_0^\alpha - m_0^\beta) - m_0^\beta B^{\alpha\beta} \right) \left( U_j^\alpha - U_j^\beta \right) \rho^\beta p_{ij}^\alpha + 2\rho^\alpha \rho^\beta m_0^{\beta2} \left( A^{\alpha\beta} - B^{\alpha\beta} \right) \left( U_i^\alpha - U_i^\beta \right) \left( \left| U^\alpha - U^\beta \right|^2 + 3k \left( \frac{T_0^\alpha}{m_0^\alpha} + \frac{T_0^\beta}{m_0^\beta} \right) \right) - \frac{1}{2} \rho^\alpha \rho^\beta \left( A^{\alpha\beta}(4m_0^\beta - 1) - 6m_0^\beta B^{\alpha\beta} \right) \left( U_i^\alpha - U_i^\beta \right) \frac{3kT_0^\alpha}{m_0^\beta},
\]

where \( B^{\alpha\beta} = (\sqrt{m_0^\alpha/\sqrt{m_0^\beta}}) A^{\alpha\beta} \) and \( \sqrt{m_0^\alpha/\sqrt{m_0^\beta}} \approx 0.436 \) as shown in [3]. Here the reduced masses are denoted by \( m_0^\alpha = m_0^\alpha/(m_0^\alpha + m_0^\beta) \) and \( m_0^\beta = m_0^\beta/(m_0^\alpha + m_0^\beta) \) and \( \delta_{ij} \) is the Kronecker delta. In order to facilitate the references to equations (10) and (11), the abbreviations \( P_{ij}^\alpha \) referring the right hand side (r.h.s.) of (10) and \( P_i^\alpha \) referring the r.h.s. of (11) are used. The model coefficients \( c_i^\alpha \) and \( \gamma_i^\alpha \) have to be evaluated from the following moment relations

\[
-\rho^\alpha \int_{\mathbb{R}^3} \left( A_i^\alpha V_j^{\alpha'} + A_j^\beta V_i^{\alpha'} + D^{\alpha2} \delta_{ij} \right) f^{\alpha} dV = P_{ij}^\alpha \quad (12)
\]

and

\[
-\frac{\rho^\alpha}{2} \int_{\mathbb{R}^3} \left( A_i^\alpha V_j^{\alpha'} V_j^{\alpha'} + 2A_j^\beta V_i^{\alpha'} V_i^{\alpha'} \right) f^{\alpha} dV = P_i^\alpha. \quad (13)
\]

Note that the density \( \rho^\alpha \) can be calculated from the conservation of mass. At this point, the system of equations (1) and (2) becomes closed, where the transport properties of the mixture are enforced to be the same as those resulting from Boltzmann.

### 3. Numerical Scheme

Although the system of equations (1) and (2) provide a closed model for simulations of binary gas mixtures, the high dimensionality of the corresponding solution domain makes its direct solution very expensive. To cope with that the system of partial differential equations (1) and (2) is transformed into Itô type stochastic differential equations (SDEs) [4]. Let the velocity and position of representative particles be \( \mathbf{M}(t) \) and \( \mathbf{x}(t) \), respectively. Therefore the state of species \( \alpha \) should evolve according to

\[
dM_i^\alpha = A_i^\alpha dt + D^\alpha dW_i, \quad (14)
\]

where the increments \( dW_i \) are independent Gaussian numbers with zero mean and variance equal to \( dt \). Consequently the position of the particles follows

\[
dx_i^\alpha = M_i^\alpha dt. \quad (15)
\]

Note that the system of SDEs (14) and (15) is equivalent to the system of PDEs (1) and (2). Since the above SDEs are continuous in time, it is possible to devise very efficient particle based solution algorithms [8]. For that reason a Monte-Carlo particle scheme is adopted. However, unlike in DSMC [1], here the simulated particles do not collide with each other but follow the stochastic trajectories along \( \mathbf{x}(t) \). Therefore the collisional scales do not need to be resolved.
For simplicity we assume that \( U_i^\alpha = 0 \) and \( U_i^\beta = 0 \) in the following. Let us decompose the r.h.s. of (14) into a linear isotropic part \( L_i \) and a remainder \( N_i \)

\[
dM_i^\alpha = -A^{\alpha\beta} \rho^\beta M_i^\alpha dt - A^{\alpha\alpha} \rho^\alpha M_i^\alpha dt + D^\alpha dW_i + N_i dt
\]

(16)

Considering only the operator \( L_i \), the time integration can be performed analytically (for frozen coefficients) [8, 4]. Using the corresponding analytical solution together with an appropriate time integration for the nonlinear part, \( M_i^\alpha \) at the new time \( t^{n+1} = t^n + \Delta t \) can be computed as

\[
M_i^{\alpha,n+1} = e^{-\nu \Delta t} M_i^{\alpha,n} + \sqrt{S^\alpha} \xi_i + N_i \Delta t e^{-\nu \Delta t},
\]

(17)

where the frequency \( \nu = A^{\alpha\beta} \rho^\beta + A^{\alpha\alpha} \rho^\alpha \) and the diffusion factor \( S^\alpha = D^\alpha (1 - e^{-2 \nu \Delta t}) / (2 \nu) \) are employed. Note that here \( \xi_i \) are independent normal variables with zero mean and unity variance. It can easily be shown that in the limit of \( \nu \to \infty \) or \( \Delta t \to \infty \) a solution with the Gaussian distribution is obtained. However, because of the error resulting from the approximate time integration of the nonlinear term \( N_i \), the energy of the system does not evolve correctly. Therefore the solution needs to be scaled by a correction factor \( f \), i.e.

\[
M_i^{\alpha,n+1} = f \left( e^{-\nu \Delta t} M_i^{\alpha,n} + \sqrt{S^\alpha} \xi_i + N_i \Delta t e^{-\nu \Delta t} \right).
\]

(18)

In order to find the factor \( f \), the energy of the ensemble of the whole mixture should remain unchanged after the time interval \( \Delta t \). Therefore, one obtains

\[
f = \sqrt{\frac{e^{-2 \nu \Delta t} kT^\alpha / m^\alpha + S^\alpha}{e^{-2 \nu \Delta t} kT^\alpha / m^\alpha + S^\alpha + \Delta t^2 e^{-2 \nu \Delta t} \text{Var}(N) / 3}},
\]

(19)

where \( \text{Var}(N) \) denotes the variance of the nonlinear term \( N_i \).

The position of a particle should evolve consistently with equation (15). An appropriate numerical scheme to update the positions of the particles was proposed in [8], and is also used for this study.

4. Results

For validation of the model, an Ar-He mixture was studied in the hydrodynamic limit. The problem is a planar supersonic Couette channel flow and the flow is driven by motion of two parallel walls with respect to each other. The distance between the walls is \( L = 1 \text{ m} \), which are considered to be diffusive and isothermal with temperature \( T_w = 273 \text{ K} \) and move with the velocities \( U_{up} = 500 \text{ m/s} \) and \( U_{down} = -500 \text{ m/s} \). For the simulations approximately 10000 particles have been used for each species, whereas the time weighted averaging was adopted for reducing statistical errors. The cross stream direction was discretized into 100 cells and flow in the direction parallel to the walls was assumed to be periodic. Therefore in streamwise direction the periodic boundary condition was employed. After reaching steady-state, the viscosity of the mixture was calculated from the shear stress and velocity gradient of the fluid. Three different molar fractions of helium were considered, i.e. \( \eta = 0\% \), \( \eta = 19.9\% \) and \( \eta = 37.7\% \). The number density of argon molecules was set to \( 1.4 \times 10^{20} \text{ m}^{-3} \) and for helium it was calculated from the mixture fraction. Thus the Knudsen number for all cases were around 0.01. The viscosity coefficient of the mixture was found to be \( 2.22 \times 10^{-5} \) and \( 2.24 \times 10^{-5} \) for \( \eta = 0\% \) and \( \eta = 19.9\% \), respectively, which are in a very good agreement with experimental results of \( 2.227 \times 10^{-5} \) and \( 2.270 \times 10^{-5} \) [3]. It can be seen that the model correctly predicts the viscosity increase of the mixture for a moderate helium-fraction. Different profiles for the mixture velocity and temperature are shown in figures 1-2.
Figure 1: Supersonic Couette flow: depicted is mean velocity of the Ar-He mixture for different molar fractions, i.e. $\eta = 0\%$, $\eta = 19.9\%$ and $\eta = 37.1\%$ along the cross stream direction $x$.

Figure 2: Supersonic Couette flow: depicted is temperature of the Ar-He mixture for different molar fractions, i.e. $\eta = 0\%$, $\eta = 19.9\%$ and $\eta = 37.1\%$ along the cross stream direction $x$. 
5. Conclusion
In this study a kinetic model based on a Fokker–Planck approximation of the Boltzmann equation was proposed for simulations of rarefied gas mixtures. The model was constructed such that the evolution of moments up to heat fluxes becomes identical with that by Boltzmann. An accurate Monte–Carlo particle based numerical method was then devised, which conserves the total energy of the mixture. It was shown that the scheme does not need to resolve the collisional scales and therefore the computational cost of the method is independent of the Knudsen number. Results were shown for simple supersonic Couette flow of Ar-He mixtures in the hydrodynamic limit. The agreement with experiments was found to be good. More challenging test cases will be studied in the future.

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