Numerical Evaluation of Novel Kinetic Models for Binary Gas Mixture Flows

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Most flows of practical interest consist of mixture of gases. Therefore the capability to model a gas mixture flow is important. Kinetic models for multicomponent gases have been considered since the original Bhatnagar-Gross-Krook (BGK) model was formulated. BGK-derived models pose a number of difficulties, e.g. avoiding negative density and temperature(s). A distinct challenge of the BGK approximation lies in recovering correct transport coefficients in the continuum limit. Two new kinetic models for gas mixtures: a Shakhov-based model and an Ellipsoidal-Statistical (ES)-based model, were recently introduced. Both models are capable of modelling a binary mixture of monoatomic gases and account for separate species-mean velocity such that the species diffusion and velocity drift are accurately represented. The main advantage is the recovery of three correct transport coefficients in the hydrodynamic limit and as a result having a correct Prandtl number for the mixture. The goal of this paper is to numerically validate the two new kinetic models for a range of high-speed flows and demonstrate their capabilities and limitations. The models are first validated against known results for normal shocks, showing good agreement for species density and temperature profiles. Moreover, the importance of the Prandtl number correction is demonstrated with the evaluation of the heat flux. A parametric study demonstrates the variation in flow properties for different mass ratios between species and for different Mach numbers. Finally, the models are evaluated for the flow around a circular cylinder. A detailed comparison with Monte Carlo results demonstrates promising results from both kinetic models.

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I. INTRODUCTION

Many high-speed flows of engineering and scientific importance involve gas mixtures. Accounting for the species diffusion in such flows is essential when strong species gradients and temperature gradients occur. An example application where modelling the flow as a gas mixture is important includes gas separation in order to create multiple products or purify a single product^{1,2}. In high-speed flows, shock stand-off and position can be affected. Furthermore, the Navier-Stokes equations lose their validity in the rarefied flow regime and a more detailed level of flow modelling for applications like hypersonic rarefied gas flows, chemical reacting flows and plasmas is required. This can be provided by the Boltzmann equation³, since it is capable of modelling non-equilibrium flows, mixtures of monoatomic and diatomic gases and also flows with or without chemistry. However, the collision integral of the equation is highly complex and computationally unfeasible for most applications of interest. For that reason, Boltzmann relaxation models were introduced, but their capabilities are limited and still represent an area of active research. Current techniques include the statistical direct simulation Monte Carlo method (DSMC)⁴, which is a particle based method that is most widely used in modelling flows under rarefied conditions. Each DSMC simulator particle represents a large number of real molecules/atoms and are moved ballistically, while collision events are treated stochastically after the movement step. This makes the DSMC algorithm tractable across a wide range of Knudsen numbers. Alternatively, mainly the discrete velocity method, but also the Unified Gas-Kinetic Scheme (UGKS)⁵ and Discrete Unified Gas-Kinetic Scheme (DUGKS)⁶ schemes are deterministic numerical methods, which apply kinetic models. Zhang et al.⁷ presented a DUGKS method for a binary mixture based on the McCormack model. For microchannel flows, Lorenzani⁸ showed semi-analytical solutions for a linearized BGK mixture model. Without this linearization, such semi-analytical solutions cannot be obtained and in the present work the DVM approach is used instead. In comparison to the Monte Carlo method, typical characteristics of deterministic methods include larger memory overhead than DSMC. However, there are no statistical sampling errors allowing modelling of flows in regimes that represent a challenge for DSMC. Beyond the numerical scheme used to discretize the models, there is a need for further improvements of the kinetic models for gas mixtures.

There are two main categories of BGK models that deal with gas mixtures. Depending on the treatment of the collision term, models are classified as single-relaxation models, e.g.^{9–12} and multi-relaxation models, e.g.^{13–15}. A new consistent BGK mixture model was introduced recently¹⁶ for

both Maxwellian and arbitrary potential molecules. Bobylev et al.¹⁶ as well as Klingenberg and Pirner¹⁴ provide a detailed comparison of the mathematical properties of the two types of modelling. The multi-relaxation models allow treating self- and cross-collisions with different relaxation rates, while the collisions of the single-relaxation models are treated with the same relaxation rate. This suggests multi-relaxation models are advantageous for the modelling of multi-species gases, specifically when the species differ significantly from each other, e.g. high mass ratio. However, important advantages the single-relaxation models provide are the reduced complexity and higher computational efficiency. For this reason, in this work we focus our attention on studying single-relaxation models and evaluating their capabilities.

The first consistent single relaxation kinetic model was introduced by Andries, Aoki and Perthame (AAP)⁹. Three further developed models, e.g. Brull, Pavan and Schneider's BGK mixture¹⁰, Brull's ES-BGK mixture¹¹ and Groppi, Monica and Spiga's¹² models were established. A common characteristic for these models is that the simplified collision term of the Boltzmann equation contains one relaxation term, which captures interspecies collisions as well as self-collisions. This collision frequency is not dependent on velocity, but only on the viscosity and pressure of the mixture, as is common in BGK models. Furthermore, the models are shown to have good mathematical properties, including the reduction of the distribution function to a Maxwellian distribution in equilibrium and the conservation of mass, momentum and energy. One of the biggest challenges for inert monoatomic gas mixtures is the correct fit of transport coefficients in the continuum limit. Andries et al.'s model recovers the correct viscosity, Brull et al.'s BGK mixture model has the correct Fick and Newton's laws as does the Groppi et al.'s model. The ES-BGK mixture model by Brull recovers the correct viscosity and Fourier coefficient.

We have previously introduced two new kinetic models by building upon the Groppi et al.'s model and incorporating Shakhov-based and ES-based corrections¹⁷. The models inherit the described mathematical properties and the correct ordinary diffusion and viscosity coefficients of the Groppi et al.'s model. Similar to the Groppi et al.'s model, both models account for separate species-mean velocity such that the species diffusion and velocity drift are accurately represented. The modified equilibrium distribution functions in the Shakhov- and ES-based mixture models together with the updated definitions for the relaxation parameters and target species velocities and temperature address the correct fit of the thermal conductivity coefficient. The novelty of the two newly-introduced models lies in the capability to capture one extra transport property in the continuum limit in comparison to the existing kinetic mixture models, e.g.^{10–12}. This leads to a

correct Prandtl number for gas mixtures. To summarize, the key contribution of these two new models is the correct fit of three transport coefficients- Fick, Newton and Fourier laws and a correct Prandtl number. We have previously derived and demonstrated the mathematical properties of the models¹⁷. The Chapman-Enskog (CE) procedure was followed to derive the asymptotic hydrodynamic limit and provides expressions for viscosity, thermal conductivity and diffusion coefficients. Furthermore, the Shakhov-based mixture model was incorporated in the gas-kinetic scheme (GKS)^{18–20} to achieve numerical efficiency and compared against results from the discrete velocity method (DVM) in²¹.

In this paper a detailed numerical testing and validation of the Shakhov-based and ES-based kinetic models is conducted. Previously, from the single-relaxation models for gas mixtures, the AAP model⁹ has been numerically studied in different schemes, e.g.^{5,6,22}. However, as described earlier only one transport coefficient is recovered with this model. Even though improved schemes, e.g.^{10–12}, are available in the literature, they have not been tested numerically yet. The key contribution of the current work is the application of new kinetic models for gas mixtures with three correct transport coefficients in the continuum limit. Moreover, an assessment of a model with two correct transport coefficients: the Groppi et al. model¹², is also demonstrated, which enables a discussion of the change and quantification of the improvement brought by an additional correct transport coefficient. The Shakhov-based and ES-based mixture models are also compared with each other. Moreover, the two models are evaluated against the solution for a normal shock wave by the Boltzmann equation²³ and a solution for a circular cylinder provided by DSMC simulations. To summarize, the novelty of this paper lies in application of two new kinetic models, which are validated with well-established test cases and assessed in detail for varied flow conditions.

The models are implemented in the parallel multi-block discrete-velocity solver within the M Φ C (Multi-Physics Code) framework^{24,25} and applied to a range of test cases. A benchmark test case for validation of new models is the profile of a normal shock wave, since it is the simplest form of high speed non-equilibrium flow. It is well-inspected for binary mixtures of monoatomic gases, e.g experimentally^{26,27} and numerically^{5,6,28–30}, where all numerical papers validate their results against the results from the full Boltzmann equation²³. Here, the mixture models are first shown to reduce to single species models and are validated with known results³¹. Next, the normal shock profile of a gas mixture with a mass ratio between species is investigated. We present a comparison between the Groppi, Shakhov-based and ES-based corrections with results from the full Boltzmann equation²³. Third, by introducing a study of the total heat flux through the shock for

the gas mixture, the significance of the new kinetic models is emphasized. A parametric study, varying the mass ratio between species and the upstream Mach number is conducted to demonstrate the variation between species velocities and temperatures. The more complex flow around a circular cylinder is then considered and a parametric study shows the change in the flow-field when the temperature of the wall is varied and when the mass ratio between species is increased. The Shakhov-based and ES-based models are compared with results for neon-argon and neon-krypton mixtures, acquired with a DSMC solver. The DSMC simulations reported in the current work make use of the open-source dsmcFoam+ solver³². The numerical results demonstrate good agreement with validation data and are promising for engineering applications that include gas mixtures.

The rest of the paper is organized as follows. In the next section important characteristics for BGK-type single-relaxation kinetic models for gas mixture are detailed. Furthermore, the key points of the two newly introduced Shakhov-based and ES-based models for a binary monoatomic gas mixture are summarized, while a more detailed derivation and description can be found in¹⁷. The focus of this paper is the application of the two models and is split between the numerical results for a normal shock wave and the results for a circular cylinder. In section 3 the details for the numerical method, problems setup and non-dimensionalization are provided. Section 4 includes all normal shock profile results. The normal shock profile is validated with the solution of the full Boltzmann equation in three steps. The recovery of the single-species results is demonstrated, the shock profile for a gas mixture with mass ratio between species is shown and the total heat flux for the gas mixture is evaluated. Furthermore, section 4 proceeds with a parametric study for the mass ratio between species and the inflow Mach number. In section 5 the flow past a circular cylinder is demonstrated for different initial parameters and then validated with results obtained from DSMC. The last part of the paper includes concluding remarks and future work.

II. KINETIC MIXTURE MODELS

For a binary gas mixture the governing equation is defined per species $s = 1, 2$ (Eq. 1) and the simplified collision operator Q_s involves a target equilibrium distribution function G_s^{eq} and the non-equilibrium distribution function f_s . Single-relaxation models are defined by a common

collision rate ν for all collision types. The governing equation is in the form:

$$\frac{\partial f_s}{\partial t} + \underline{u} \cdot \frac{\partial f_s}{\partial \underline{x}} = Q_s \quad ; \quad Q_s = \nu (G_s^{eq} - f_s) \quad ; \quad s = 1, 2, \quad (1)$$

where the common collision rate is defined by the gas mixture properties: the pressure p and viscosity μ based on the mixture temperature T , such that $\nu = p/\mu$ and $\underline{u}$ is the particle velocity. In the numerical simulations the power-law viscosity is used and the molecular potential is defined by the value of ω in $\mu = \mu_{ref} \left(\frac{T}{T_{ref}} \right)^\omega$. A necessary condition for all models is that the collision term preserves mass, momentum and energy. For a chemically inert gas mixture mass conservation is per species, while momentum and energy can be exchanged between species and the sum of momentum and energy over all species is conserved. Therefore, the following constraints on the collision operator are imposed:

$$\begin{aligned} \iiint_{-\infty}^{\infty} Q_s d\underline{u} &= 0 \quad ; \quad s = 1, 2 \\ \sum_{s=1}^2 \iiint_{-\infty}^{\infty} m_s \underline{u} Q_s d\underline{u} &= 0 \\ \sum_{s=1}^2 \iiint_{-\infty}^{\infty} \frac{1}{2} m_s |\underline{u}|^2 Q_s d\underline{u} &= 0 \end{aligned} \quad (2)$$

where $d\underline{u} = du dv dw$. We denote with n_s , ρ_s , $\underline{u}_s$ and T_s the species macroscopic quantities: number density, density, mean velocity and temperature of a species s . The species macroscopic variables are obtained as moments of the non-equilibrium distribution function:

$$\begin{aligned} n_s &= \iiint_{-\infty}^{\infty} f_s d\underline{u} \\ n_s \underline{u}_s &= \iiint_{-\infty}^{\infty} \underline{u} f_s d\underline{u} \\ \frac{3}{2} n_s k T_s &= \frac{m_s}{2} \iiint_{-\infty}^{\infty} (\underline{u} - \underline{u}_s)^2 f_s d\underline{u} \end{aligned} \quad (3)$$

where k is the Boltzmann constant. From the species macroscopic variables, the overall gas mixture properties are obtained as shown in Eq. 4.

$$\sum_{s=1}^2 n_s = n \quad ; \quad \sum_{s=1}^2 \rho_s = \rho \quad ; \quad \sum_{s=1}^2 \rho_s \underline{u}_s = \rho \underline{u}_0 \quad ; \quad \sum_{s=1}^2 \rho_s (\underline{u}_s - \underline{u}_0)^2 = \sum_{s=1}^2 \rho_s |\underline{u}_s|^2 - \rho |\underline{u}_0|^2$$

$$\frac{3}{2}nkT = \sum_{s=1}^2 \frac{3}{2}n_s kT_s + \frac{1}{2} \sum_{s=1}^2 \rho_s (\underline{u}_s - \underline{u}_0)^2 \quad (4)$$

These properties are standard for all single-relaxation models and are used by the two new kinetic models. A main difference between kinetic models is introduced by the different definition of the target equilibrium distribution function G_s^{eq} . In the following sections the two new models and their key definitions are summarized, while the full description, derivation and Chapman-Enskog expansion of the two models were detailed previously¹⁷.

A. Shakhov-based Model

In the Shakhov-based mixture model the simplified collision operator Q_s involves the Shakhov-based³³ equilibrium distribution function G_s^{sh} and a common collision rate ν . The governing equation is in the form:

$$\frac{\partial f_s}{\partial t} + \underline{u} \cdot \frac{\partial f_s}{\partial \underline{x}} = Q_s \quad ; \quad Q_s = \nu (G_s^{sh} - f_s); \quad ; \quad s = 1, 2 \quad (5)$$

The distribution function G_s^{sh} is in the form:

$$G_s^{sh}(\underline{u}) = G_s(\underline{u}) \left\{ 1 + \frac{2(1-Pr)(\underline{u} - \underline{u}_s^{(g)}) \cdot \underline{q}_s^{corr}}{5p_s k \hat{T} / m_s} \left[\frac{m_s}{2k\hat{T}} (\underline{u} - \underline{u}_s^{(g)})^2 - \frac{5}{2} \right] \right\}, \quad (6)$$

where species pressure p_s is defined as $p_s = \rho_s k \hat{T} / m_s = n_s k \hat{T}$ ($\hat{T}$ is defined later in this section). The Prandtl number Pr is the target Prandtl number and for monoatomic gas that is $Pr = 2/3$. The function $G_s(\underline{u})$ is the equilibrium distribution function in the Groppi et al. model¹²:

$$G_s(\underline{u}) = n_s \left(\frac{m_s}{2\pi k \hat{T}} \right)^{3/2} \exp \left[- \frac{m_s}{2k\hat{T}} (\underline{u} - \underline{u}_s^{(g)})^2 \right] \quad (7)$$

The Shakhov-based model modifies the distribution function by introducing a heat flux correction as in the original single-species Shakhov model³³. For a mixture of gases the heat flux is an energy flux dependent on a coupling between the Fourier and the Duffour effects. The correction $\underline{q}_s^{corr}$ in the distribution function is only affected by the temperature gradient. As derived in Eq. (8), $\underline{q}_s^{corr}$ follows from the moment integration with respect to the species mean velocity. The heat flux correction obtained from the Chapman-Enskog expansion (with ε the small parameter related to Knudsen) becomes:

$$\begin{aligned} \underline{q}_s^{corr} &= \int_{-\infty}^{\infty} m_s (\underline{u} - \underline{u}_s) \frac{1}{2} ((\underline{u} - \underline{u}_s)^2) \left\{ G_s^{sh} - \frac{\varepsilon}{\nu} \left(\frac{\partial f_s^M}{\partial t} + \underline{u} \cdot \frac{\partial f_s^M}{\partial \underline{x}} \right) \right\} d\underline{u} \\ \underline{q}_s^{corr} &= - \frac{\varepsilon}{\nu} \frac{5}{2} \frac{k}{Pr} \frac{n_s k T}{m_s} \frac{\partial T}{\partial \underline{x}} + O(\varepsilon^2). \end{aligned} \quad (8)$$

Since the Shakhov-based correction affects the distribution function and only high order moments, the expressions for $\underline{u}_s^{(g)}$ and $\hat{T}$ are unchanged in comparison to the original model by Groppi et al.¹².

$$\underline{u}_s^{(g)} = \left(1 - \frac{\eta}{\nu}\right) \underline{u}_s + \frac{\eta}{\nu} \underline{u}_0 \quad (9)$$

From energy conservation, the modified temperature follows:

$$\hat{T} = T - \frac{1}{3nk} \sum_{s=1}^2 \rho_s (\underline{u}_s^{(g)} - \underline{u}_0)^2 = T - \frac{1}{3nk} \left(1 - \frac{\eta}{\nu}\right)^2 \sum_{s=1}^2 \rho_s (\underline{u}_s - \underline{u}_0)^2 \quad (10)$$

Substituting the expression for the mixture temperature T with the species properties from the last expression of Eq. (4), leads to an expression for the modified temperature in the form:

$$\hat{T} = \frac{1}{nk} \sum_{s=1}^2 n_s k T_s + \frac{1}{3nk} \frac{\eta}{\nu} \left(2 - \frac{\eta}{\nu}\right) \sum_{s=1}^2 \rho_s (\underline{u}_s - \underline{u}_0)^2 \quad (11)$$

To preserve positive temperature fields the ratio of relaxation parameters η/ν needs inspection. The collision rate is defined by strictly positive quantities: viscosity μ and pressure p and therefore $\nu > 0$. The second relaxation coefficient η , defined below, has the same constraint $\eta > 0$, as imposed by the Groppi et al.³⁴. Therefore, the lower bound of the ratio is $\eta/\nu > 0$. In Eq. (11) for $T_s > 0$, the $\hat{T} > 0$ is guaranteed for $(2 - \frac{\eta}{\nu}) \geq 0$, leading to the upper bound $\frac{\eta}{\nu} \leq 2$. The limits of the ratio of relaxation coefficients are then $0 < \eta/\nu \leq 2$.

As shown above, the expressions for $\underline{u}_s^{(g)}$ and $\hat{T}$ depend on the macroscopic velocities and temperatures of the species and the gas mixture, but also on the relaxation parameters ν and η . The collision rate ν is related to p and μ as defined previously and η was introduced by Groppi et al.³⁴ as a constraint on the species velocity equalization:

$$\frac{1}{n_1} \iiint_{-\infty}^{\infty} \underline{u} Q_1 d\underline{u} - \frac{1}{n_2} \iiint_{-\infty}^{\infty} \underline{u} Q_2 d\underline{u} = -\eta (\underline{u}_1 - \underline{u}_2). \quad (12)$$

Clearly the ratio η/ν is an important part of the definition of the model and is bound by limits defined above. It is derived from the expressions of the viscosity and diffusion coefficients¹⁷ and results in:

$$\frac{\eta}{\nu} = \frac{5}{3} \frac{1}{(m_1 + m_2) A_{12}^*} \frac{\rho}{n}, \quad (13)$$

where A_{12}^* is a non-dimensional coefficient and for noble gas mixtures a good approximation is $A_{12}^* = 1.11$ ³⁵.

It is easy to check that the relaxation ratio is within the defined limits for the above expression

(Eq. (13)). A positive density leads to $\eta/\nu > 0$. The upper bound requires considering part of the expression:

$$\frac{1}{m_1 + m_2} \frac{\rho}{n} = \frac{1}{m_1 + m_2} \frac{n_1 m_1 + n_2 m_2}{n_1 + n_2} = \frac{n_1 m_1 + n_2 m_2}{n_1 m_1 + n_2 m_2 + n_1 m_2 + n_2 m_1} < 1, \quad (14)$$

which is always less than 1 and therefore $\frac{\eta}{\nu} < \frac{5}{3A_{12}^*}$, which in turn leads to $\frac{\eta}{\nu} < 2$ for all ρ, m_1, m_2 , etc. This means that the temperature field is always positive for every possible species mass or density.

B. ES-based Model

In the second proposed kinetic model, a modification is added to create an anisotropic equilibrium (target) distribution function, following the approach used for the ES model for a single-species monoatomic gas flow^{36,37}. The collision operator is modified to include the relaxation characteristic for the ES model. The governing relaxation equation is in the form:

$$\frac{\partial f_s}{\partial t} + \underline{u} \cdot \frac{\partial f_s}{\partial \underline{x}} = Q_s \quad ; \quad Q_s = \frac{\nu}{1 - \nu_{ES}} (G_s^{ES} - f_s); \quad ; \quad s = 1, 2 \quad (15)$$

The new distribution function has the form:

$$G_s^{ES}(\underline{u}) = \frac{n_s}{\sqrt{\det(2\pi\overset{\leftrightarrow}{\Lambda}_s)}} \exp \left[-\frac{1}{2} (\underline{u} - \underline{u}_s^{(g)}) \cdot \overset{\leftrightarrow}{\Lambda}_s^{-1} \cdot (\underline{u} - \underline{u}_s^{(g)}) \right]$$

The tensor $\overset{\leftrightarrow}{\Lambda}_s$ is introduced by the temperature $\hat{T}$ and the ES relaxation parameter ν_{ES} :

$$\overset{\leftrightarrow}{\Lambda}_s = \nu_{ES} \overset{\leftrightarrow}{\Theta}_s + (1 - \nu_{ES}) \left(\frac{k\hat{T}}{m_s} \right) \overset{\leftrightarrow}{I} \quad ; \quad \overset{\leftrightarrow}{\Theta}_s = \frac{1}{n_s} \int_{-\infty}^{\infty} (\underline{u} - \underline{u}_s^{(g)}) \otimes (\underline{u} - \underline{u}_s^{(g)}) f_s d\underline{u} \quad (16)$$

The collision operator Q_s is modified by dividing it with $(1 - \nu_{ES})$ which introduces changes in the species target velocity and temperature. A comparison of the target temperature $\hat{T}$ with the equilibrium gas mixture temperature T shows that the additional terms come from the relaxation change of the ES model with ν_{ES} and from the introduced drift velocity:

$$\begin{aligned} \underline{u}_s^{(g)} &= \left(1 - \frac{\eta}{\nu} (1 - \nu_{ES}) \right) \underline{u}_s + \frac{\eta}{\nu} (1 - \nu_{ES}) \underline{u}_0 \\ \hat{T} &= T - \frac{1}{3nk} \left[\left(1 - \frac{\eta}{\nu} (1 - \nu_{ES}) \right)^2 \sum_{s=1}^2 \rho_s (\underline{u}_s - \underline{u}_0)^2 \right]. \end{aligned} \quad (17)$$

To guarantee positive temperature the following constraint is placed on the ratio η/ν : $0 < \eta/\nu \leq 2/(1 - \nu_{ES})$. The ratio is derived similarly to the η/ν ratio in the Shakhov-based model and has

the same dependency as in Eq.(13)¹⁷. In comparison to the Groppi and Shakhov-based models the upper boundary for the η relaxation parameter is more restricted due to the introduction of v_{ES} . A typical value for the Prandtl number of a pure monoatomic gas is $Pr = 2/3$, which is the maximum value of the Prandtl number for a gas mixture. It corresponds to a $v_{ES} = -1/2$ for the ES-based model. A similar study of the relaxation ratio confirms it is always positive or $\eta/\nu > 0$ for all variables in Eq. (13). For $v_{ES} = -1/2$, the upper bound is limited to $\eta/\nu \leq 4/3$, which means a necessary condition is:

$$\frac{5}{3} \frac{1}{(m_1 + m_2)A_{12}^*} \frac{\rho}{n} \leq \frac{4}{3} \rightarrow \frac{1}{m_1 + m_2} \frac{\rho}{n} \leq 0.888, \quad (18)$$

which limits the possible species densities and masses. Note that this condition is for a strict guarantee of positivity, while in practical applications positivity of $\hat{T}$ occurs for a wider range of ratios η/ν . For the test cases considered with the ES-based model within this paper, the values of $\hat{T}$ were always found to be positive.

C. Indifferentiability principle

Note that for the same properties of the two species the binary-mixture model satisfies the indifferentiability principle and recovers the single-species Shakhov-model and ES-model respectively. This property is discussed previously¹⁷ and in this paper we demonstrate it numerically. We will show that the single-species models are recovered and we will validate the results by a comparison with the solution for a single-species normal shock wave.

III. NUMERICAL METHOD

The two models are validated and tested for the profile of a normal shock wave and the flow around a circular cylinder. The problem and solver setup are defined in this section, together with the non-dimensional values.

A. Discrete Velocity Method

The results of the kinetic models are obtained using the discrete-velocity method³⁸. The method is chosen for its simplicity and accuracy. Possible molecular velocities are uniformly spaced in a

defined velocity domain. The domain varies according to the initial conditions and is highly dependent on the Mach number. The number of molecular velocities in the domain vary with Mach number and mass ratio between species. For the profile of the normal shock wave 100 uniformly spaced discrete velocities are used, unless stated otherwise (e.g. for mass ratios of 10 and more), while the number of discrete velocities increases drastically for the two-dimensional cylinder case and is specified in the cylinder section for each case.

The distribution function and the fluxes are evaluated for each of the velocities in every cell. The moments of the distribution functions (macroscopic variables) are found by applying the trapezoidal rule. A finite-volume scheme and a second order Total Variation Diminishing (TVD) time marching method^{39,40} are used to numerically discretize the models' governing equation. Note that in contrast to a continuum solver, which stores only the macroscopic variables in each cell, the two kinetic solvers, based on the DVM, require much more computational time and memory.

B. Problems Setup

All shock profile simulations are set with the same uniform spatial domain, where $x \in [-75L_{ref}, 75L_{ref}]$, which is discretized by 1200 cells in the x-direction. Note the domain is selected to avoid the disturbances, downstream of the shock during the simulation, to reflect on the downstream boundary and affect the shock structure.

The setup of the problem is: a flow with initial conditions undergoes strong non-equilibrium changes through a normal shock wave to arrive at a different equilibrium state. The state to state change is initialized with the Rankine-Hugoniot conditions for the macroscopic variables and Maxwellian distributions are set at the two different initial equilibrium states.

For the two-dimensional problem a high-speed flow past a cylinder is presented. The flow is initialized with initial Mach number, species concentration, mass ratio between species, rarefaction level and fixed wall temperature. Note the rarefaction level is defined by a Knudsen number, based on the radius of the cylinder, where the radius has length $1L_{ref}$, where L_{ref} depends on the reference time and reference velocity as shown in the following subsections. Note that this is standard for kinetic modelling and it differs from the Knudsen number definition based on the mean free path as in molecular modelling⁴¹. These differences are taken into account when comparison between the kinetic models and the Monte Carlo method is conducted. The Knudsen number is equalized between the two modelling approaches and it is quoted based on the kinetic definition.

The used geometry is a quarter of a cylinder with a symmetry condition on the stagnation streamline. The spatial grid consists of 36 blocks and 27864 cells for the Shakhov- and ES-based models. The DSMC setup is described in the corresponding section. For two- and three-dimensional cases code parallelization is necessary and for the presented cylinder case the code is parallelized in both space and velocity phase space.

Validation for the normal shock is performed by comparing with results from the full Boltzmann equation available in the literature. The validation and comparison of the flow past a cylinder is through a comparison with solutions acquired through DSMC with the number of particles and samples specified for each condition.

C. Dimensional Reduction

In the one-dimensional formulation, the distribution functions are dimensionally reduced to functions defined in one-dimensional velocity space to reduce computational cost⁴². Since the mean velocities v_0, w_0 in the y and z -directions are zero, the species distribution function f_s reduces to translational g_s and thermal h_s energy component, as demonstrated in Eq. (19). The macroscopic variables are then found by taking moments of the reduced distribution functions.

$$\begin{aligned} g_s &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_s \, dv \, dw \\ h_s &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (v^2 + w^2) f_s \, dv \, dw \end{aligned} \quad (19)$$

Therefore the solver uses four velocity distribution functions: two for each species to define the flowfield. Note the dimensional reduction for the cylinder follows the same procedure but for two-dimensional reduced functions. This leads also to four velocity distribution functions.

D. Dimensionless Form

The macroscopic variables are non-dimensionalized and the reference values are described in this subsection. The lighter species and its mass m_1 are taken as reference at free-stream conditions. All velocities are non-dimensionalized with the most probable speed u_r of the light species. Elements of the anisotropic tensor for the ES-based model λ_r^s are scaled per species to preserve the scaling for the distribution functions as in the Shakhov-based model - f_r, g_r, h_r .

Note the non-dimensionalization presented is for the one-dimensional flow formulation. The constant $\beta = m_2/m_1$ is the mass ratio in the expressions for the distribution functions of the heavy gas.

$$u_r = \sqrt{2kT_r/m_1} \quad (20)$$

$$\rho_r = n_r m_1$$

$$\lambda_r^s = R_s T_r = \frac{kT_r}{m_s}$$

$$f_r = \frac{n_r}{u_r^3} = \frac{n_r}{(2kT_r/m_1)^{3/2}}$$

$$g_r = \frac{n_r}{u_r} = \frac{n_r}{\sqrt{2kT_r/m_1}}$$

$$h_r = n_r u_r = n_r \sqrt{2kT_r/m_1}$$

$$\beta = m_2/m_1$$

$$q_r = \frac{1}{2} n_r m_1 u_r^3 = n_r kT_r \sqrt{\frac{2kT_r}{m_1}}$$

$$L_{ref} = \frac{u_{ref}}{t_{ref}} = \frac{u_{ref}}{\tau_{ref}} = \frac{u_{ref} \mu_{ref}}{p_{ref}}$$

In the kinetic model, the reference length L_{ref} is defined by reference time and velocity, where the $t_{ref} = \tau_{ref}$ - the collision time, expressed from the mixture pressure and viscosity at reference conditions. The reference viscosity is taken for a variable cross-section hard sphere model (VHS), which depends on the molecular potential ω and the mean free path for a VHS model, as described in⁴¹ and by Eq. (21).

$$\mu_{ref} = \frac{15}{2} \lambda_{ref} \rho \sqrt{\frac{2\pi kT}{m_{mix}}} \frac{1}{(7-2\omega)(5-2\omega)}, \quad (21)$$

where the mass of the mixture $m_{mix} = \rho/n$. Note that for a hard sphere model, the molecular potential is $\omega = 0.5$, which reduces the expression for the viscosity to:

$$\mu_{ref} = \frac{5}{16} \lambda_{ref} \rho \sqrt{\frac{2\pi kT}{m_{mix}}} \quad (22)$$

This allows for comparison with a variety of models, where the mean free path λ_{ref} is taken as a reference length. Note that in the following section the hard sphere model and Eq.(22) are used for a comparison with the Boltzmann solution²³ and the variable hard sphere model and Eq.(21) are used for the validation with DSMC. The resultant reference length is:

$$L_{ref} = \frac{\sqrt{\frac{2kT}{m_1}} \frac{15}{2} \lambda_{ref} \rho \sqrt{\frac{2\pi kT}{m_{mix}}} \frac{1}{(7-2\omega)(5-2\omega)}}{nkT} = \frac{15\sqrt{\pi}}{(7-2\omega)(5-2\omega)} \lambda_{ref} \sqrt{\frac{m_{mix}}{m_1}} \quad (23)$$

$$L_{ref} = \frac{15\sqrt{\pi}}{(7-2\omega)(5-2\omega)} \lambda_{ref} \sqrt{\frac{n_1 m_1 + n_2 m_2}{m_1 (n_1 + n_2)}}$$

The ratio of the two reference lengths L_{ref} for the kinetic models and λ_{ref} for the validation models is the required scaling factor with all variables taken at free-stream conditions.

$$\frac{L_{ref}}{\lambda_{ref}} = \frac{15\sqrt{\pi}}{(7-2\omega)(5-2\omega)} \sqrt{\frac{n_1 + \beta n_2}{n_1 + n_2}} \quad (24)$$

E. Normalized Values

The macroscopic quantities presented for the shock wave are normalized following Kosuge's approach²³, where y is the macroscopic variable, Y_- is the pre-shock value of y and Y_+ is post-shock:

$$\tilde{y} = \frac{y - Y_-}{Y_+ - Y_-} \quad (25)$$

Note that the tilde is omitted from here on for simplicity. Also, the origin of the plots ($X = 0$) is where the total number density is exactly half of the sum of the pre-shock and post-shock values.

IV. NORMAL SHOCK

A. Single Species Recovery

The numerical evaluation of the models begins with an investigation of the structure of a normal shock wave. The first step is to demonstrate that the two models collapse to a single-species model not only theoretically¹⁷, but also numerically. There are two main points to be made here.

First, a mixture of two gases with the same mass, initial velocity and temperature is inspected. Each gas is at 50% concentration. Numerically there is nothing to push the two gases to separate and we expect to observe equal species macroscopic properties through the shock, e.g. $n_1 = n_2$, $u_1 = u_2$, $T_1 = T_2$ etc.

In Fig. 1 (a) and (b) the Shakhov- and ES-based solvers respectively are tested to confirm that the species variables will collapse into one. The species number densities, species velocities and species temperature are plotted with a solid line for species 1 and dashed line for species 2. The results between species 1 and 2 match exactly for each solver, confirming that for identical species masses, the species do not separate from each other.

The second proof is to compare the total macroscopic properties of the gas ρ , u_0 , T and validate the results against single species results. This test case is well-studied and there are suitable experimental, e.g.⁴³, and numerical results, e.g.^{30,31,44}. As described earlier, the power law for the

FIG. 1. Profile of a normal shock wave with a free-stream Mach number 3.0, a mass ratio between species $\beta = 1$ and equal concentration between the species of 50%. Comparison of species macroscopic variables. Results for the Shakhov-based model shown in (a), with results for ES-based model in (b).

viscosity is used in the Shakhov- and ES-based solvers with a molecular potential ω . The results from Ohwada are for a hard-sphere and therefore $\omega = 0.5$, while the Sutherland law is found most suitable to compare against Alsmeyer's results. In Fig. 2 the results of the Shakhov-based and ES-based models in blue and green are validated with the results from Ohwada³¹ (red elements) for flow with free-stream Mach number $M_\infty = 3$. This also allows for a comparison between the two kinetic models. The mixture density ρ and velocity u_0 follow closely the results from Ohwada. The Shakhov- and ES-based results have a longer upstream tail, as can be expected in results of BGK-type models. This effect can also be observed in the early decrease of the mixture velocity u_0 of the models in comparison to the mixture velocity from Ohwada. It is further pronounced in the higher moment of the distribution function: the mixture temperature T , where the variation is more significant. The Shakhov-based model preserves the profile of the shock better than the ES-based model for a single species gas, which has been observed previously⁴⁵. The main goal of the investigation in this section was to demonstrate numerically that the mixture Shakhov- and ES-based kinetic models have the capability to reduce to single-species models. Indeed, the results show that for identical molecular mass of the species the single-species Shakhov and ES models are recovered.

FIG. 2. Profile of a normal shock wave with a free-stream Mach number 3.0, a mass ratio between species $\beta = 1$ and equal concentration between the species of 50%. Comparison of total mixture variables with the single-species full Boltzmann equation³¹.

B. Normal Shock of a Gas Mixture

The numerical evaluation of the mixture models continues with an investigation of the structure of a normal shock wave for a binary gas mixture comprised of two different gases. In Fig. 3 and 4 we examine the flow at free-stream Mach numbers 1.5 and 3, mass ratio between species $m_2/m_1 = 2$, and concentration of the light gas (species 1) equals 90 percent. An example setup of a mixture of noble gases with that mass ratio is the mixture of neon and argon. A viscosity law with $\omega = 0.5$ is used for a hard-sphere mixture model. We evaluate the models by comparing the normalized species number densities n_1 and n_2 (Fig. 3 and 4 (a)) and species temperatures T_1 and T_2 (Fig. 3 and 4 (b)) through the shock. We validate against the results from the full Boltzmann equation²³, which are presented by the red elements- squares for species 1 and triangles for species 2. The figures show in solid (species 1) and dashed (species 2) black lines, how well Groppi et al.'s model¹² follows the Boltzmann results for the structure of the shock wave. The model is simulated by setting the Prandtl number to 1 in the Shakhov-based solver or $v_{ES} = 0$ in the ES-based solver. This eliminates the Shakhov-based or ES-based correction, respectively, and demonstrates the results that can be obtained by the original - Groppi et al.'s model. The figures also show the results obtained by the Shakhov-based model in blue and ES-based model in green.

The improvement of the slope for the species number density on Fig. 3 and 4 (a) is evident, but small for both models. However, the species temperature deviates significantly from the Groppi et al.'s model and follows much more closely the results of the full Boltzmann equation. This means that the significance of the two corrected models increases for higher order moments. We also notice that as every BGK-based model, upstream of the shock the models have longer tails than the Boltzmann results suggest and the models also deviate from each other. If we compare the two models, the Shakhov-based model performs slightly better upstream of the shock, especially for the higher Mach number, which is consistent with studies evaluating the Shakhov and ES models for a single species gas⁴⁵.

FIG. 3. Profile of a normal shock wave ((a) species number density, (b) species temperature). Validation and comparison between the model by Groppi et al.'s, Shakhov- and ES-based models with Kosuge's full Boltzmann model²³ for free-stream Mach number 1.5, mass ratio between species $\beta = 2$ and light-species concentration 90%¹⁷.

C. Heat Flux

The two models introduce changes that provide a correct third transport coefficient: the thermal conductivity in the continuum limit, leading to a correct Prandtl number for the gas mixture. This affects all variables, defining the flow, but mostly the heat flux. In the present work the difference of the heat flux prediction is demonstrated for the Groppi et al.'s, Shakhov-based and ES-based

FIG. 4. Profile of a normal shock wave ((a) species number density, (b) species temperature). Validation and comparison between the model by Groppi et al.'s, Shakhov- and ES-based models with Kosuge's full Boltzmann model²³ for free-stream Mach number 3, mass ratio between species $\beta = 2$ and light-species concentration 90%¹⁷.

models through the normal shock. Moreover, the results are evaluated against the results from the full Boltzmann equation²³. Figure 5 inspects the total heat flux variation through a normal shock wave of the same test cases: for free-stream Mach numbers 1.5 and 3, mass ratio of 2 and 90 percent light species concentration. On the plot we see the variation of the non-dimensionalized heat flux through the normal shock, defined as:

$$\tilde{q} = -\frac{q(x)}{p_r \sqrt{\frac{2kT_r}{m_2}}}, \quad (26)$$

where here $q(x)$ is the dimensional heat flux through the shock and the $\tilde{q}$ the heat flux non-dimensionalized as in the results provided by the full Boltzmann equation²³ and the tilde is omitted as we proceed. The reference pre-shock pressure and temperature are p_r and T_r with m_2 - the heavy species mass. This non-dimensionalization is done to match with the results of the full Boltzmann equation, provided to us by the authors of the paper showing normal shock wave results with the Boltzmann equation²³, shown with red elements. Note that heat flux is a combined effect between the thermal conduction and the Duffour effect. Our models fix only the thermal conductivity coefficient and the Duffour effect is not correctly fitted, which will offset the results for the total heat

FIG. 5. Non-dimensional total heat flux for the gas mixture q for the Shakhov-based, ES-based and Groppi et al. models through a normal shock wave with free stream Mach numbers 1.5 (shown in (a)) and 3 (shown in (b)), mass ratio $\beta = 2$ and light-species concentration 90%. Results are evaluated against gas heat flux result from the full Boltzmann equation, provided to us by the authors of the paper showing normal shock wave results with the Boltzmann equation²³.

flux. However, for the described cases, this offset is small since the thermal effect is much stronger than the diffusion effect in the flow and is dominating the heat flux.

It is interesting to observe that macroscopic variables corresponding to higher order moments. e.g. the heat flux, vary over a more spread-out region, covering approximately 60% larger number of mean free paths. We observe a difference between the two new models of 4.1 percent, while the Shakhov-based and Groppi et al.'s models differ by a total of 20.5 percent. This emphasizes the importance of fitting correctly the transport coefficients and in particular the thermal conductivity. Comparing with results from the full Boltzmann equation, the results for the heat flux from the Shakhov- and ES-based models demonstrate the capability of the two models to capture the heat flux correctly through the shock and its maximum. Recovering the heat flux is a key advantage of the two new kinetic models.

When comparing the accuracy of the models, the same longer tail, inherent to BGK-style models, is evident through the shock as in the species temperature profile. This is an expected feature due to the relationship between the translational temperature and the heat flux. Note that the ES-based

model has an even longer upstream tail, which is further pronounced with the higher Mach number. In Fig. 5 we observe that the Shakhov-based model shows good agreement with the benchmark results, preserving the maximum and downstream tail of the heat flux.

Previously, we observed that the Shakhov-based model is matching the results for the single-species high speed flow more closely than the ES-based model. Furthermore, for both gas mixture cases, the Shakhov-based model performs better than the ES-based model. Therefore, the parametric study on the species mass variation and Mach number variation in the next sections will be performed with the Shakhov-based model.

D. Species Mass Ratio Variation

In this section a parametric study is conducted for a varying mass ratio between species. The Shakhov-based model is used to inspect the effect. The number of discrete velocities is 100 for the smaller mass ratios, but increases to 200 for mass ratios $\beta = 10, 20$ and 32.8 for better resolution of the velocity space. The solver is initialized at the same Mach number $M_\infty = 1.5$, concentration of light species gas 90% and varied mass ratio. The velocity is defined from a fixed Mach number, but the speed of sound a is defined with the mass of the gas mixture. Therefore $u_s = M_\infty a = M_\infty \sqrt{\gamma \frac{k}{m_{mix}} T}$, where $m_{mix} = \rho/n$. After non-dimensionalization the direct relationship between the velocity and the mass ratio β is clear. The velocity is initialized from the set Mach number and the initial macroscopic variables and the non-dimensional initial velocity is in the form:

$$u_s = M_\infty \sqrt{\frac{\gamma}{2} \frac{n_1 + n_2}{n_1 + \beta n_2} T}; \quad s = 1, 2, \quad (27)$$

where $\gamma = 5/3$ for a monoatomic gas. Therefore for a fixed Mach number and increasing mass ratio β , the initial velocity reduces. Note if the velocity is fixed instead, the Mach number will change for each mass ratio.

Increasing the mass ratio between the two species would lead to a bigger difference between their velocities and temperatures due to different behavior of atoms with a weight difference. However, the initial velocity reduces due to the mass ratio increase and creates a counter-effect. In Fig. 6 the velocity variation u_{diff} through the shock is presented, where $u_{diff} = u_2 - u_1$. For the initial increase of mass ratio, the variation between the species increases as expected for species with bigger variation between their mass properties. However, the difference between the species velocity increases until it reaches its limit between mass ratios $\beta = 4$ and $\beta = 10$. The lower

initial velocity begins to counter this effect and for bigger and bigger mass ratios of 20 or 32.8 the velocity reduction is the dominating effect. Note that a simple substitution in Eq. 27 shows that the initial velocity at the specified conditions for $\beta = 32.8$ is close to half of the initial velocity for $\beta = 2$, due to the speed of sound change. Notice also that even though the peak of the difference

FIG. 6. Non-dimensional species velocity difference $u_2 - u_1$ through a normal shock wave with free stream Mach number 1.5, light species gas 90% and varied mass ratio from 2 to 32.8 between species.

between the species velocity decreases for a higher mass ratio, the number of mean free paths required for the velocities to become in equilibrium with each other increases. In Fig. 6 the shock wave with the mass ratio of 2 has difference in species velocities for approximately 24 mean free paths, while for a mass ratio of 32.8 the distance increases to 75 mean free paths for the velocities to equalize again to the gas mixture velocity behind the shock.

E. Mach Number Variation

The variation between species velocity and species temperature is tested in this section for a varied Mach number. Using the Shakhov-based model a parametric study is conducted based on a flow with light-species concentration 90% , mass ratio between species $\beta = 2$. In Fig. 7 the species velocity and temperature differences are plotted for Mach numbers $M_\infty = 1.5, 3$ and 6. The light species reacts first to the shock and u_1 decreases first, creating the difference between the two velocities. The species velocity difference increases with the increase of Mach number

(a) Species velocity difference

(b) Species temperature difference

FIG. 7. Non-dimensional species velocity difference $u_2 - u_1$ (in (a)) and species temperature difference $T_2 - T_1$ (in (b)) through a normal shock wave for a varied free stream Mach number of 1.5, 3 and 6, mass ratio between species $\beta = 2$ and light-species concentration 90%.

and for $M_\infty = 6$ it is represented by a sharp spike. Moreover, the highest Mach number creates a difference between the velocities in the flow for a bigger range of mean free paths, due to the light gas reacting to the shock wave very early to the shock. Meanwhile, the shock with $M_\infty = 1.5$ is spread out and gradual rather than steep. When the difference between velocities is normalized by the gas mixture velocity u_0 for each Mach number, the peak value of $M_\infty = 6$ is approximately 4.8 times the peak value of $M_\infty = 1.5$ test case, while $M_\infty = 3$ is approximately 3.7 times the peak value of $M_\infty = 1.5$ test case.

The temperature difference $T_{diff} = T_2 - T_1$ is presented as well in Fig. 7 (b). The relative variation in the temperature is bigger than the velocity. The lighter gas reacts quicker to the shock and the light species temperature T_1 increases first creating a negative $T_2 - T_1$ difference. The increase of the heavy gas is steep and the difference between $T_2 - T_1$ changes sign through the shock and becomes positive. The difference between temperatures is evident for the $M_\infty = 1.5$ test case, but quite small in comparison to the difference created by $M_\infty = 6$ test case. We confirm that increasing the Mach number has a significant effect on the species properties. Therefore, for higher velocities, the importance of modelling of the flow as a gas mixture is further emphasized.

In the next section, the middle Mach number $M_\infty = 3.0$ test case is investigated for a more complex

two-dimensional flow.

V. CYLINDER

A. Flow Past a Cylinder

A more complex test case - a two-dimensional flow with 48×48 and 64×64 (for the higher mass ratio) uniformly spaced discrete velocity meshes- is investigated. The Shakhov-based model is used to simulate the flow around the cylinder in this first section, while in the next section the two kinetic models are validated and compared. In Fig. 8 and 9 a flow with free-stream Mach number 3, Knudsen number 0.1, based on the radius of the cylinder and the reference length at free-stream conditions with light species concentration 90 percent of the gas is presented. The formed bow shock is well-resolved on the used mesh (27864 cells), i.e. with on average 25 cells covering the width of the shock. Fully-accommodating diffuse wall boundary conditions are used for the solid wall. We know from our previous simulations that the biggest differences between species occur in regions with strong non-equilibrium effects. We also know that the lighter species (species 1) reacts faster to those changes and then the heavier gas (species 2) has to catch up until they find a balance. In Fig. 8 the variation between species mean velocity is shown, while Fig. 9 focuses on the variation between species temperature. In the vicinity of the shock, the velocity of the lighter gas u_1 starts decreasing first and the difference between the two species $u_2 - u_1$ increases, until species 2 catches up post shock. Unlike the velocities, the heavy species temperature has a steeper slope, increases faster and crosses the lighter species temperature in the shock wave. This we can clearly observe in the plots. Temperature T_1 increases first, creating a negative $T_2 - T_1$ difference in blue and then T_2 catches up and surpasses T_1 leading to a positive temperature difference $T_2 - T_1$ in red.

Each figure contains three plots with varied conditions. In Fig. 8 (a) and (b) and Fig. 9 (a) and (b) the mass ratio between species is 2 and the assigned wall temperature is changed from $T_{wall} = 1.5T_\infty$ in (a) to $T_{wall} = 2.5T_\infty$ in (b) to inspect the sensitivity of the flow field with respect to the posed wall temperature. The non-equilibrium effect in the flow through the bow shock, expressed by the difference in species velocities and temperatures, is not affected by the changes of the wall temperature. For the considered wall temperatures, the shock stand-off distance is not significantly changed.

Changing the mass ratio between species to 4, however, affects the species mean velocities and

FIG. 8. Non-dimensional species velocity drift $u_2 - u_1$ in a binary mixture flow over a cylinder (velocity is non-dimensionalized with the most probable speed of the lighter gas) with initial Mach number 3, mass ratio between species $\beta = 2$ and 4, light-species concentration 90%, Knudsen number $Kn = 0.1$ and wall temperature $T_{wall} = 1.5$ and 2.5 . Results were obtained with the Shakhov-based model. (a) $m_2/m_1 = 2, T_{wall} = 1.5T_\infty$, (b) $m_2/m_1 = 2, T_{wall} = 2.5T_\infty$, (c) $m_2/m_1 = 4, T_{wall} = 1.5T_\infty$.

temperatures significantly, as we can see in Fig. 8 (c) and 9 (c). For the higher mass ratio, the non-equilibrium effects and species differences are stronger. The same is observed for the species temperature drift. This is consistent with the behavior observed previously for the normal shock simulations.

B. Validation with DSMC Simulations

Until now we were focused on emphasizing the difference between species mean properties as a way of establishing the non-equilibrium of the flow. The discussed results were obtained with the Shakhov-based kinetic model. We now consider the stagnation streamline (the streamline on which the stagnation point lies) for the same two flows past the circular cylinder with free-stream Mach number 3, Knudsen number 0.1 and a mass ratio of 2 and 4. The goal of this study is to

(a) $m_2/m_1 = 2$, $T_{wall} = 1.5T_\infty$ (b) $m_2/m_1 = 2$, $T_{wall} = 2.5T_\infty$ (c) $m_2/m_1 = 4$, $T_{wall} = 1.5T_\infty$

FIG. 9. Non-dimensional species temperature drift $T_2 - T_1$ in a binary mixture flow over a cylinder with initial Mach number 3, mass ratio between species $\beta = 2$ and 4, light-species concentration 90%, Knudsen number $Kn = 0.1$ and wall temperature $T_{wall} = 1.5$ and 2.5 . Results were obtained with the Shakhov-based model. (a) $m_2/m_1 = 2$, $T_{wall} = 1.5T_\infty$, (b) $m_2/m_1 = 2$, $T_{wall} = 2.5T_\infty$, (c) $m_2/m_1 = 4$, $T_{wall} = 1.5T_\infty$.

compare the Shakhov- and the ES-based models with DSMC results. The DSMC solver used in this work is dsmcFoam+³². To remain consistent with the kinetic models the Mach number ($M_\infty = 3$) is based on the gas constant of the mixture and the Knudsen number is defined as for the kinetic models, as described in detail in Problems Setup section. In both cases, the light species is neon, with argon and krypton being used for the mass ratios of 2 and 4, respectively. Note that the molecular mass of krypton was slightly modified to get an exact ratio of 4. The variable hard sphere collision model is used ($\omega = 0.72$), with fully diffusive reflections considered for the cylinder surface interactions. As before, the cylinder wall temperature is held constant at $1.5T_\infty$. The DSMC simulation is set up as described. The numerical meshes consist of 40000 cells that are smaller near the stagnation point in order to ensure that all cells are smaller than the local mean free path. The total freestream number density is $3.11 \times 10^{19} m^{-3}$, which consists of 90% neon and 10% argon for the first test case at $\beta = 2$. A viscosity coefficient of 0.72 and a reference temperature of 273K is used for both species to maintain consistency with the kinetic models developed in this work. The variable hard sphere mean free path of the mixture is $8.54 \times 10^{-2} m$. A freestream

temperature of 300 K is used and a velocity of 1299.8m/s to give a Mach number of 3. A time step of $5 \times 10^{-6}\text{s}$ is used and 274000 samples were taken after steady state was reached to reduce the numerical scatter in the results. There are 70 DSMC particles per cell in the free-stream and approximately 3.04×10^6 particles in the simulation at steady state. All gas-surface interactions are considered to be fully diffusive with a wall temperature of 450 K. The described test setup is identical for the two mass ratios. The DSMC results are shown in black lines, while the Shakhov-based and ES-based solutions are in blue and green respectively. We plot the non-dimensional number densities and temperatures through the shock and until the solid is reached at $x/R = -1$, where R is the radius of the cylinder ($x = 0$ at the cylinder center).

In Fig. 10 the non-dimensionalized total number density n and the heavy gas number density n_2 are shown. Physically, the gas undergoes a compression effect through the shock and then towards the stagnation point of the cylinder, demonstrated by the increase in number density. Figure 10 shows good agreement in the stagnation streamline density profiles predicted by dsmcFoam+ and the kinetic models, with the ES-based model slightly closer to the DSMC than the Shakhov-based model for the total number density, while the heavy gas number density's profile is also matching closely with the ES-based model. Notice that the number density for both kinetic models reaches a maximum value of approximately 8 times the freestream number density in the center of the cell neighboring the wall of the cylinder, while DSMC predicts approximately 7.55 times the freestream value. A possible explanation for this effect is the better flow resolution in the near-wall region in the kinetic simulations, originating from the finer mesh used in this region as compared to the DSMC mesh.

The mixture temperature is shown on Fig. 11 (a). The temperature jump is caused by the shock and later on relaxes, going into the boundary layer of the cylinder towards the prescribed wall temperature $T_{wall} = 1.5T_\infty$. The figure shows a reasonable agreement in the stagnation streamline temperature profile for the gas mixture. The longer tail upstream of the shock appears for both models in comparison to DSMC, with a more pronounced effect in the solution by the ES-based model. In this first region of the bow shock the Shakhov-based model solution matches closer to the solution by DSMC. However, the peak of temperature provided by the ES-based model predicts the DSMC results better than the Shakhov-based model. Near to the solid wall the gas mixture temperature of the kinetic models closely approaches the fixed wall temperature $T_{wall} = 1.5T_\infty$ in the first cell above the wall in the stagnation point for the two kinetic models ($T = 1.75T_\infty$) and so does the DSMC solution ($T = 1.77T_\infty$).

FIG. 10. Comparison of the total number density (in (a)) and heavy species number density (in (b)) for the Shakhov and ES kinetic models with DSMC results for Mach number 3, mass ratio $\beta = 2$, light species concentration 90%, Knudsen number $Kn = 0.1$ and $T_{wall} = 1.5$.

It is very interesting to observe the variation between species temperature $T_2 - T_1$ (Fig. 11 (b)). As in the normal shock study, the increase in T_1 is faster and therefore negative difference between the temperatures $T_2 - T_1$ is seen in the first part of the shock. Then a steeper growth of the heavy species temperature, creates a positive $T_2 - T_1$ difference, until we reach equilibrium, where the species temperatures are equalized. We see that the kinetic models follow qualitatively the results by DSMC, but the increase of the temperature of the light species is bigger. The DSMC results display some statistical scatter, since the heavy gas species is only 10% of the gas mixture and therefore a trace species in the DSMC simulation. This means the number of particles for the heavy species is only 10% of the total number of particles at the imposed boundary condition in the free-stream. This makes reducing the statistical scatter challenging with the use of constant particle weighting factors. Here we observe one of the benefits and motivations of kinetic modelling with DVM - the lack of statistical scatter for these type of flows with small concentrations of one of the species.

Considering the higher mass ratio $\beta = 4$, a gas mixture of neon and krypton is simulated by DSMC. The setup is very similar to the neon-argon mixture. Again, the total freestream number density is $3.11 \times 10^{19} m^{-3}$, which consists of 90% neon and 10% krypton. The variable hard sphere

FIG. 11. Comparison of the mixture temperature (in (a)) and the species temperature drift (in (b)) for the Shakhov and ES kinetic models with DSMC results for Mach number 3, mass ratio $\beta = 2$, light species concentration 90%, Knudsen number $Kn = 0.1$ and $T_{wall} = 1.5$.

mean free path of the mixture is $8.31 \times 10^{-2} m$. The freestream velocity to achieve Mach number 3 is $1194.51 m/s$ with this gas mixture. Note that for the same Mach number and different mass ratios, the freestream velocity has decreased. This is consistent with the findings from the normal shock wave results in Section (D). All other simulation parameters are the same as for the neon-argon mixture described above. Figure 12 shows very good agreement in the stagnation streamline density profiles predicted by dsmcFoam+ and the kinetic models.

Figure 13 (a) shows good agreement in the stagnation streamline temperature profile for the gas mixture. The shock stand-off distances of the two kinetic models are similar to each other and to the DSMC results. The peak temperature is also lower in the DSMC results than for the kinetic models, while the Shakhov-based model is closer to the DSMC prediction.

The difference between species temperatures in Fig. 13 (b) is well captured by the kinetic models and DSMC in its decrease, while the increase predicted by dsmcFoam+ has a significantly greater peak temperature difference than the kinetic models. The DSMC results do not exhibit as much scatter as the lower mass ratio, because the non-dimensional temperature differences between the species are greater at the higher mass ratio. For the higher mass ratio, the two kinetic models are fairly close to each other, while the Shakhov-based model matches DSMC slightly

FIG. 12. Comparison of the total number density (in (a)) and heavy species number density (in (b)) for the Shakhov and ES kinetic models with DSMC results for Mach number 3, mass ratio $\beta = 4$, light species concentration 90%, Knudsen number $Kn = 0.1$ and $T_{wall} = 1.5$.

better than the ES-based model in first part of the bow shock region.

Even though the differences between DSMC and the kinetic models are discussed in detail, they are very small and we consider the validation of the kinetic models with DSMC successful. Overall, the comparison between Shakhov-based, ES-based and DSMC shows good agreement and further inspection of different parameters like Mach number and concentration are considered part of future work.

C. Surface Heat Flux and Pressure

The heat flux and pressure along the surface of the cylinder are of particular interest for industrial applications. Two cases are inspected for the same conditions as in the previous section and the results from the Shakhov-based mixture model and the DSMC method are compared. The kinetic model is presented by red elements and DSMC with black elements for both heat flux (Fig. 14) and pressure (Fig. 15) results. Note that the heat flux non-dimensionalization is consistent with the Kosuge's²³ and is described in section IV (C), while pressure is scaled with the free-stream pressure. In the figures the heat flux and pressure are plotted on the ordinate, while the abscissa shows the cylinder angle as measured from the center ($X = 0.0$), where the stagnation

FIG. 13. Comparison of the mixture temperature (in (a)) and the species temperature drift (in (b)) for the Shakhov and ES kinetic models with DSMC results for Mach number 3, mass ratio $\beta = 4$, light species concentration 90%, Knudsen number $Kn = 0.1$ and $T_{wall} = 1.5$.

streamline is in line with 0 degrees and 90 degrees is the point where the cylinder surface is parallel to the free-stream.

The results from the DVM show good agreement with results from DSMC. The value of the non-dimensional heat flux at the stagnation point is greater for the larger mass ratio. The peak of the heat flux is at the stagnation point where the difference between DVM and DSMC results is 0.73% for $\beta = 2$ and 1.85% for $\beta = 4$. The difference between the results from the kinetic model and DSMC decreases along the cylinder surface. At the top of the cylinder (90deg) the non-dimensional heat flux has values under 1 (for $\beta = 2$, $q = 0.86$) and just above 1 (for $\beta = 4$, $q = 1.12$), as observed in Fig. 14 (a) and (b). Some discrepancies are observed in the last few cells, most likely due to the imposed boundary conditions. This is further pronounced in the results for the pressure on the cylinder surface and discussed in more detail below.

The gas mixture pressure along the cylinder surface for the two mass ratios is shown in Fig. 15 (a) and (b). There is a good comparison between the kinetic model and DSMC from the stagnation line to approximately 70deg. Beyond that, for both mass ratios the surface pressure predicted by the kinetic model is higher than the DSMC prediction. Most likely this is due to the outflow boundary conditions imposed by the two solvers for a flow that is not supersonic in this region. For

(a) Heat flux at $\beta = 2$

(b) Heat flux at $\beta = 4$

FIG. 14. Comparison of the surface heat flux along the cylinder for the Shakhov-based kinetic model with DSMC results for Mach number 3, mass ratio $\beta = 2$ (in (a)) and $\beta = 4$ (in (b)), light species concentration 90%, Knudsen number $Kn = 0.1$ and $T_{wall} = 1.5$.

DVM the extrapolation boundary condition is applied on the outflow boundary face. Meanwhile, the vacuum boundary condition imposed for DSMC is only strictly accurate for Mach number $\gg 1$. Close to the cylinder surface, the flow is subsonic and therefore both boundary conditions are not strictly valid, although both are widely used for this kind of cylinder test cases.

(a) Pressure at $\beta = 2$

(b) Pressure at $\beta = 4$

FIG. 15. Comparison of the surface pressure along the cylinder for the Shakhov-based kinetic model with DSMC results for Mach number 3, mass ratio $\beta = 2$ (in (a)) and $\beta = 4$ (in (b)), light species concentration 90%, Knudsen number $Kn = 0.1$ and $T_{wall} = 1.5$.

VI. CONCLUSION

Two newly introduced kinetic models for binary gas mixtures were tested and evaluated through simulations examining the structure of a normal shock wave and the high speed flow over a cylinder. The comparisons with the benchmark results for the full Boltzmann equation and DSMC respectively, show promising results from both models for a range of Mach numbers, species mass ratios and imposed wall temperature in the cylinder case. The Shakhov-based mixture model generally demonstrates higher accuracy than the ES-based model for both the single-species and multi-species flows considered here. In future work, further validation for low speed flows and variety of rarefaction levels will be presented. The next big step in terms of kinetic modelling is the extension to diatomic gas flows with different rotational and vibration temperatures per species and gas diffusion effects between species. This will enable the modelling the components of air as a mixture of gases and simulate rarefied flows of aerospace interest.

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