Viscous Compressible Slip Flows. Part 1: Kinetic Flux Vector Splitting and its Variance Reduction form

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ABSTRACT

The work is in two parts: Part 1 deals with kinetic treatment of the slip flow and Part 2 deals with numerical modeling of the rarefied and rotating slip flow. The present paper containing Part 1 gives an overview of kinetic theory and its application to fluid flow, Bhatnagar–Gross–Krook (BGK) model and construction of Chapman-Enskog distribution. The paper describes the Kinetic Flux Vector Splitting (KFVS) scheme which performs upwinding in the Boltzmann level for viscous flows for three dimensional and axi-symmetric geometries. The paper also describes novel Variation Reduction Kinetic Flux Vector Splitting (VRKFVS) and kinetic treatment of the slip and far field boundary. Viscous split fluxes based on kinetic flux vector splitting satisfy the Onsager reciprocity relations and are treated in upwind manner for effective capture of slip phenomenon. Slip velocity not only depends on the velocity gradient in the normal direction but also on the fluid dynamic gradients in the tangential flow direction. Treatment of slip boundary using kinetic upwind fluxes based on diffuse reflection model considers these variations in the tangential flow direction.

Key words: kinetic, BGK model, Chapman-Enskog distribution, Boltzmann equation, BGK-Burnett, KFVS, VRKFVS, viscous, slip flow, Onsager reciprocity

Nomenclature

$f^{(N)}$	= particle distribution function in $6N$ dimensional phase space
$f(\vec{x}, \vec{v}, I, t)$	= molecular distribution function
$f^{`}, f^{`}_{a}$	= distribution functions of the molecules before collision and after collision
f_0	= Maxwellian distribution function
f_1, f_2	= first and second order Chapman-Enskog distribution function
$\bar{f}_i, \bar{f}_i^M$	= i^{th} Chapman-Enskog expansion term for Maxwellian f_0 and f_M
Δf, Δf_1	= difference in Maxwellian and difference in Chapman-Enskog term
$\Delta\hat{\bar{f}}_1$	= difference between first order Chapman-Enskog and Maxwellian distribution
$\Delta\bar{f}_1$	= difference in 1st Chapman-Enskog expansion term for Maxwellian f_0 and f_M
$f_0^{\infty}, f_1^{in}, f_0^{wc}$	= farfield, incident and distribution at wall condition.
f_1^{Σ}	= total distribution at the boundary
f_0^{wc}	= Maxwellian distribution function based on wall conditions
$\vec{x}$	= position vector
$\vec{v}$	= molecular velocity vector
I, I_0	= internal energy variable and average internal energy parameter
β	= thermal speed, $(2RT)^{-1}$
D_f	= the degree of freedom
t	= time
T	= temperature

$\vec{u}$ = macroscopic velocity vector
$\vec{c}$ = peculiar velocity
u_i, v_i, c_i = x, y and z components of macroscopic, molecular and peculiar velocity
s_i = spatial coordinate x, y and z
p = pressure
τ = shear stress tensor
ρ = density
R = specific gas constant
E = total energy, $\frac{RT}{\gamma-1}+\frac{1}{2}\left(\vec{u}^T\vec{u}\right)$
$J(f,f)$ = binary collision term
$K(f,f,f)$ = ternary collision term
$L(f,f,f,f)$ = quaternary collision term
$J_m(f,f)$ = binary collision model
Ψ, ψ_i = moment and its element
τ_s, τ_f = slow timescale and fast timescale in the evolution of the distribution function
Π = molecular cross section
g = magnitude of the relative velocity of the particles before collision
ε, Θ = scattering angles
δ = Dirac delta function
Ξ = linear subspace used in Levermore hierarchy
z = element of linear subspace used in Levermore hierarchy
Kn, Kn_{GL} = Knudsen number and gradient length Knudsen number
B_{NS} = breakdown matrix due to moment realizability
NS_B = breakdown parameter for Navier-Stokes equation
ς = macroscopic parameter
σ_P = entropy production
H , k_B = Boltzmann entropy function and dimensional Boltzmann constant ($k_B \approx 6.10^{-23}\, J/K$)
j, X = flux and thermodynamic force associated with Onsager reciprocity principle
Λ = Onsager's kinetic coefficients
μ, κ = viscosity and thermal conductivity
t_R = relaxation time
$t_{R,1}$, $t_{R,2}$ = relaxation time for momentum transport and energy transport
δo = exponent of the viscosity law of the gas
$\vec{q}$ = heat flux vector
Pr, Re = Prandtl number and Reynolds number
M = Mach number
λ, L = mean free path and length scale
$\xi_{1,\tau}$, $\tilde{\underset{\sim}{\xi}}_{\tau}$ = Chapman-Enskog polynomials associated with the shear stress
$\xi_{1,q}$, $\tilde{\xi}_q$ = Chapman-Enskog polynomials associated with the heat flux vector
$\vartheta_{\tau,1}$, $\vartheta_{\tau,2}$, $\vartheta_{\tau,3}$ = moment closure coefficients associated with the shear stress
$\vartheta_{q,1}$, $\vartheta_{q,2}$, $\vartheta_{q,3}$ = moment closure coefficients associated with the heat flux vector
φ = dissipation control function
ω = angular velocity
r, z, θ = radius, axial and azimuthal variable
U = state update vector or vector of conserved variable = $[\rho, \rho\vec{u}, \rho E]^T$
U_M = vector of conserved variable for Maxwellian f_M
GX, GY, GZ = flux components in x, y, z-direction
$GX_I^{\pm}$, $GY_I^{\pm}$, $GZ_I^{\pm}$ = inviscid flux components in x, y, z-direction

$GX_v^{\pm}$, $GY_v^{\pm}$, $GZ_v^{\pm}$ = viscous flux components in x, y, z-direction
GR = radial component of flux vector
S = source terms
v_z, v_r, v_θ = axial velocity, radial velocity, azimuthal velocity
μ_{num} = numerical viscosity
σ = diffuse reflection or accommodation coefficient
v_z^s, v_z^d = specularly reflected and the diffuse reflected z-component of the velocity

1. INTRODUCTION TO KINETIC FLUX VECTOR SPLITTING

Gudunov and Boltzmann schemes are broadly two approaches to solve hyperbolic system of conservation laws. Godunov scheme uses sound waves and streamlines to propagate information while Boltzmann scheme uses trajectories of individual particles and its distribution [1]. Godunov scheme relies on solving a Riemann's initial value problem with characteristics of the Euler equation. In this approach interaction amongst the neighboring cells is through discrete, finite amplitude waves. The numerical technique using this incoming and the outgoing waves is called the *flux differencing splitting* scheme. Examples are the methods of Roe [2] and Osher [3]. Whereas, in Boltzmann based approach interaction amongst the neighboring cells is through movement of the particles or its velocity distribution. The numerical technique based on this movement of incoming and outgoing particles is called *flux-vector splitting* scheme. One of the earliest examples is the Beam scheme of Sanders and Prendergast [4] and Steger and Warming [5].

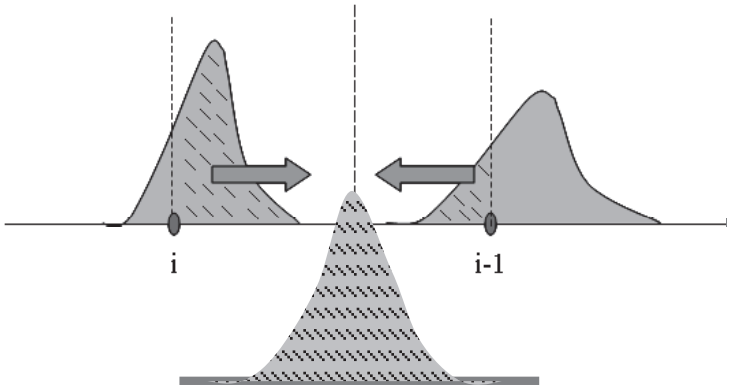


Figure 1. Upwinding using split velocity distribution in KFVS

A few years later to the Beam scheme [4], Harten *et al*. [1] developed an approach to construct a scheme for general hyperbolic systems of conservation laws. Equilibrium flux method (EFM) of Pullin [6] initiated the development of kinetic schemes for compressible Euler system based on Maxwellian distribution. Just after development of EFM Reitz [7] developed a kinetic scheme using Boltzmann equation. Deshpande [8] proposed Kinetic Flux Vector Splitting (KFVS) scheme which was further developed by Mandal and Deshpande [9] for solving Euler problems. At the same time Perthame [10] developed kinetic scheme and Prendergast and Xu [11] proposed a scheme based on BGK simplification of the Boltzmann equation. Xu [12] and May *et al*. [13] modified and further developed this scheme. The gas kinetic scheme of Xu [12] differs from the KFVS scheme mainly in the inclusion of particle collisions in the gas evolution stage. Numerical fluxes are calculated in the gas evolution stage as time dependent gas distribution function is computed at the cell interface by making use of local integral solution of the BGK model. Raghurama and Deshpande [14] proposed a scheme based on peculiar velocity based upwind method which splits the flux vector into acoustic and the transport part.

KFVS is based on moment-method strategy which operates in two levels: i) the Boltzmann level where upwind implementation is done, ii) the macroscopic (Euler or Navier-Stokes) level at which the state update operates. KFVS scheme for the viscous flows was proposed by Chou and Baganoff [15].

KFVS for viscous flows applies Courant splitting at the Boltzmann level followed by moment-method strategy using Chapman-Enskog distribution to obtain split Navier-Stokes fluxes based on the signs of the molecular velocity. Fig.1. shows upwinding in the Boltzmann level using the split velocity distribution based on the sign of the molecular velocity. Mahendra[16] and Mahendra *et al*. [17] used KFVS for simulating compressible, viscous flows. KFVS has also been applied to quantum gas dynamics for Bose-Einstein and Fermi-Dirac gases [18]. When it comes to resolving boundary layers and calculating adiabatic wall temperature the flux difference splitting is less dissipative compared to flux vector splitting [19]. KFVS is entropy consistent and do not suffer from the many pathological behavior of other flux differencing / splitting schemes. The dissipation in the KFVS can be controlled by incorporating the modified Courant splitting based on dissipation control parameter. Anil *et al*. [20] developed a modified KFVS with molecular velocity dependent dissipation control parameter. The paper also describes a novel scheme Variation Reduction Kinetic Flux Vector Splitting scheme (VRKFVS) which solves for the deviations over the chosen Maxwellian. Using this method the solver can capture very weak secondary flow features embedded in strong flow field. The paper also describes axi-symmetric formulation of KFVS.

Validity of the Navier-Stokes equation as well as diffusion equation requires sufficient collision of particles and relaxation of the distribution to weak spatial gradients and slow temporal variations. Flow can be classified as slip flow based on the Knudsen number defined by the extent of non-equilibrium effects and rarefaction. The most common approach to simulate slip flow is to couple the continuum solver with the slip boundary condition or slip models. Most of the slip models in the literature are for simple micro-channel flows. In such a scenario we require a more fundamental approach. The Part 1 of the paper also describes diffuse reflection model which uses kinetic upwind fluxes for slip boundary treatment. Kinetic flux vector splitting at the boundary generates the viscous split fluxes which satisfy the Onsager reciprocity relationship. The slip boundary is flux based and upwind treatment of such viscous split fluxes leads to effective capture of slip phenomenon.

2. KINETIC THEORY AND FLUID FLOW

The detailed description of the classical gas system consisting of N particles in three dimensions is the Hamiltonian representation with $3N$ coordinates and $3N$ momenta. The alternative representation uses the Gibbs ensemble described by Liouville equation forming the basic statistical equation for conservation of N particle distribution function, $f^{(N)}$ in $6N$ dimensional phase space. BBGKY[1] hierarchy of equations are obtained after successive integration of the Liouville equation. There are kinetic theories which are not based on the BBGKY hierarchy like Prigogine-Balescu's method [21] and Markov's method of random flight [22]. Each chain in the BBGKY hierarchy involves reduced distribution function $f^{(H)}$ and higher order distribution function $f^{(H+1)}$. Boltzmann's molecular chaos ("Stosszahlansatz") assumption gives a closed equation for $f^{(1)}$ by introducing time irreversibility while asserting the absence of correlations between molecules entering a binary collision. In this case the gas system is described by the single particle distribution function governed by Boltzmann equation; it is this aspect of the Boltzmann equation that leads to entropy production.

2.1 Boltzmann equation

The Boltzmann transport equation describes the transient molecular distribution function $f(\vec{x}, \vec{v}, I, t)$: $R^N \times R^N \times R^+ \times R^+ \rightarrow R^+$. Additional internal energy variable $\mathrm{I} \in R^+$ is added as polyatomic gas consists of particles with additional degree of freedom. For a gas in absence of external force and without internal degrees of freedom, the Boltzmann equation with Bogoliubov's generalization is as follows

$$\frac{\partial f}{\partial t} + \nabla_{\vec{x}}.(\vec{v}f) = J(f,f) + K(f,f,f) + L(f,f,f,f) + \cdots \tag{1}$$

In above, $\vec{x}$, the position vector and $\vec{v}$, velocity vector of molecules are given in R^N, where $J(f, f)$ is binary or two particle collision, $K(f, f, f)$ being the ternary or three particle collision and $L(f, f, f, f)$ is quaternary or four particle collision. The binary collision integral $J(f, f)$ can be described as

[1] BBGKY equations are named after the five authors Bogoliubov, Born, Green, Kirkwood and Yvon who first suggested these equations.

$$J(f,f)=\int_{R^N}\int_{R^+}\int_{0}^{2\pi}\int_{0}^{\pi/2}\left(f^a f'^a - ff'\right)g\ \Pi\ d\vec{v}'\,dI\,d\varepsilon\,d\Theta \tag{2}$$

where $f=f(\vec{x},\vec{v},I,t)$ and $f=f'(\vec{x},\vec{v}',I,t)$ are the distribution functions of the molecules before collision and $f^a=f(\vec{x},\vec{v}_a,I,t)$ and $f'^a=f(\vec{x},\vec{v}'_a,I,t)$ are the distribution functions of the molecules after collision. Also, $g=|\vec{v}-\vec{v}'|$ is the magnitude of the relative velocity of the particles before collision and Π is the molecular collision cross section. Integration with respect to ε goes from 0 to 2π, while angle Θ varies from 0 (head-on collisions) to $\pi/2$ (grazing collisions). For hard sphere $\Pi = d^2/4$, where d is diameter of the hard sphere. HS model predict transport coefficients which are proportional to square root of temperature i.e. $T^{0.5}$ while real gases vary as $T^{0.7}$. With better collision model like Variable Hard Sphere (VHS) model in which $\Pi \propto g^{-\alpha}$ for a constant $\alpha > 0$ more realistic prediction of transport properties can be made. This binary collision integral vanishes in the Euler limit when the distribution becomes a Maxwellian, f_0.

The Boltzmann transport equation describes the transient molecular distribution. The moment of a function, $\Psi = \Psi(\vec{v},I,t) : R^N \times R^+ \times R^+ \rightarrow R^+$ is defined as the inner product

$$\Psi(\vec{x},t)=\left\langle \Psi(\vec{v},I,t),f\right\rangle \equiv \int_{R^N}\int_{R^+}\Psi(\vec{v},I,t)f(\vec{x},\vec{v},I,t)d\vec{v}dI\ . \tag{3}$$

The five moments function defined as $\Psi=\left[1,\vec{v},I+\frac{1}{2}\vec{v}^T\vec{v}\right]^T$ give the macroscopic mass, momentum, and energy densities. When we take moments of the Boltzmann equation we get the hyperbolic conservation equation. For example with $f = f_0$ we get Euler equations that are set of inviscid compressible coupled hyperbolic conservation equations written as

$$\int_{R^N}\int_{R^+}\Psi\left(\frac{\partial f_0}{\partial t}+\nabla_{\vec{x}}.(\vec{v}f_0)=0\right)d\vec{v}dI \equiv \frac{\partial U}{\partial t}+\frac{\partial GX}{\partial x}+\frac{\partial GY}{\partial y}+\frac{\partial GZ}{\partial z}=0 \tag{4}$$

where $U=[\rho,\rho\vec{u},\rho E]^T=\left\langle \Psi,f_0\right\rangle \equiv \int_{R^N}\int_{R^+}\Psi f_0(\vec{x},\vec{v},I,t)d\vec{v}dI$ is the vector of conserved variable and (GX, GY, GZ) are the Cartesian components of the flux vector defined as

$$GX=\int_{R^N}\int_{R^+}\Psi v_x f_0(\vec{x},\vec{v},I,t)d\vec{v}dI \equiv \begin{bmatrix}\rho u_x\\ p+\rho u_x^2\\ \rho u_x u_y\\ \rho u_x u_z\\ (\rho E+p)u_x\end{bmatrix}, \tag{5}$$

$$GY=\int_{R^N}\int_{R^+}\Psi v_y f_0(\vec{x},\vec{v},I,t)d\vec{v}dI \equiv \begin{bmatrix}\rho u_y\\ \rho u_y u_x\\ p+\rho u_y^2\\ \rho u_y u_z\\ (\rho E+p)u_y\end{bmatrix} \text{ and} \tag{6}$$

$$GZ=\int_{R^N}\int_{R^+}\Psi v_z f_0(\vec{x},\vec{v},I,t)d\vec{v}dI \equiv \begin{bmatrix}\rho u_z\\ \rho u_z u_x\\ \rho u_z u_y\\ p+\rho u_z^2\\ (\rho E+p)u_z\end{bmatrix}. \tag{7}$$

In the above equations ρ is the density, $\vec{u}$ = (u_x, u_y, u_z) is the fluid velocity, p is the pressure and $E=\frac{RT}{\gamma-1}+\frac{1}{2}\left(\vec{u}^T\vec{u}\right)$. For an ideal law we have $p = \rho RT$ where R is the gas constant and T is the absolute temperature.

2.2 Moments and extended thermodynamics

Levermore[23] proposed a procedure that generates hierarchy of closed systems of moment equations. The Levermore closure procedure ensures every member of the hierarchy is symmetric hyperbolic with an entropy, and formally recovers to Euler limit. Consider finite dimensional linear subspace Ξ of functions of $\vec{v}$ satisfying the following conditions :

$$\left.\begin{array}{ll} (I) & \Psi \equiv span\{1, \vec{v}, \vec{v}^T\vec{v}\} \subset \Xi \\ (II) & \Xi \quad follows\ Gallilean\ invariance \\ (III) & \Xi_c \equiv \{z \in \Xi : \langle \exp(z(\vec{v}))\rangle < +\infty\} \end{array}\right\}. \tag{8}$$

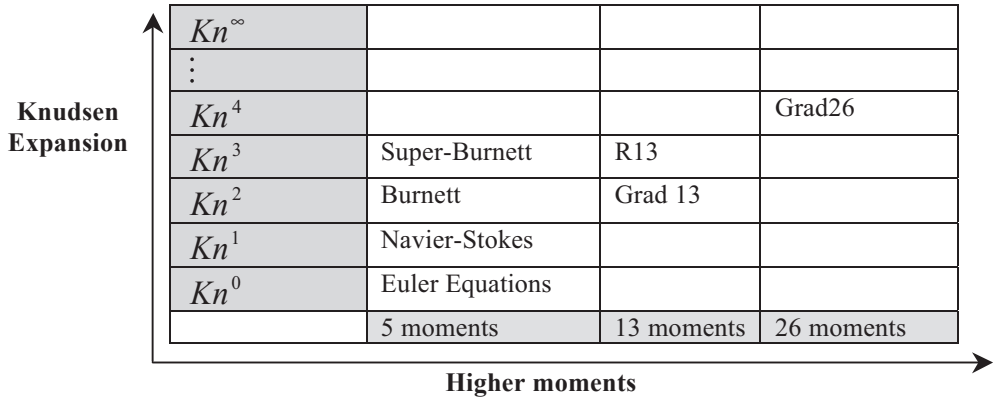
Examples of such admissible subspace with maximal degree two and four are

$$\left.\begin{array}{l} \Xi = span\{1, \vec{v}, \vec{v}^T\vec{v}\} \\ \Xi = span\{1, \vec{v}, \vec{v} \otimes \vec{v}\} \end{array}\right\} maximal\ degree = 2$$
$$\left.\begin{array}{l} \Xi = span\{1, \vec{v}, \vec{v} \otimes \vec{v}, \vec{v}(\vec{v}^T\vec{v}), (\vec{v}^T\vec{v})(\vec{v}^T\vec{v})\} \\ \Xi = span\{1, \vec{v}, \vec{v} \otimes \vec{v}, \vec{v} \otimes \vec{v} \otimes \vec{v}, (\vec{v}^T\vec{v})(\vec{v}^T\vec{v})\} \\ \Xi = span\{1, \vec{v}, \vec{v} \otimes \vec{v}, \vec{v} \otimes \vec{v} \otimes \vec{v}, \vec{v}(\vec{v}^T\vec{v}) \otimes \vec{v}\} \\ \Xi = span\{1, \vec{v}, \vec{v} \otimes \vec{v}, \vec{v} \otimes \vec{v} \otimes \vec{v}, \vec{v} \otimes \vec{v} \otimes \vec{v} \otimes \vec{v}\} \end{array}\right\} maximal\ degree = 4 \tag{9}$$

Thus there can be 5, 10, 14, 21, 26 and 35 equations with entropy based closures using Levermore procedure [24,25]. Closure based on Maxwellian (equilibrium solution) distribution will give us 13 and 20 moment equations. From the continuum mechanics perspective the flux in an equation becomes the density in the next one, as there can be infinite moments. Thus, there is a problem of the closure when we cut this hierarchy at the density with tensor of rank *n* as its flux and production term will require its balance as they become density in the next hierarchical step. According to the idea of rational extended thermodynamics Müller and Ruggeri[26] have treated this truncated system as a phenomenological system of continuum mechanics governed by universal principle of entropy, objectivity, causality and stability (convexity of entropy). The differential system is hyperbolic and classical constitutive equations are approximation of balance laws when relaxation times are negligible. (This avoids the *heat paradox*[2] observed in the classical theory.) The diffusion equation and the Navier-Stokes equation are valid only when particles have suffered many collisions and their distribution has relaxed to have weak spatial gradients and slow temporal variations. However, there are physical situations where gradients are large on the scale of a collisional mean free path or temporal changes are rapid relative to the mean collision time. Examples include radiation hydrodynamics in optically thin media (Levermore and Pomraning [27]), viscous angular momentum transport in boundary layers of accretion disks (Popham and Narayan [28]) and electron heat transport in laser produced plasma (Max [29]). It should be noted that Navier-Stokes equations do not have equations for evolution of shear stress and heat flux vectors as compared to 13-moments Grad system [30]. When relaxation time for evolution of shear stress and heat flux are negligible then 13-moments Grad system reduces to classical Navier-Stokes as illustrated by extended thermodynamics. Table 1 shows various hierarchies of equations due to Kundsen number expansion and number of moments compiled from Struchtrup [31].

[2] The parabolic nature of heat equation in classical theory implies an infinite speed of propagation of disturbance in temperature. This paradox is similar to paradox of diffusion and shear waves.

Table 1. Hierarchy of equations due to Knudsen number expansion and number of moments for Maxwell molecule.



Kn^{∞}			
⋮			
Kn^{4}			Grad26
Kn^{3}	Super-Burnett	R13	
Kn^{2}	Burnett	Grad 13	
Kn^{1}	Navier-Stokes		
Kn^{0}	Euler Equations		
	5 moments	13 moments	26 moments

2.3 Quasi Gas Dynamics (QGD) and hydrodynamic theory of Brenner

Quasi-gas-dynamics (QGD) of Elizarova[32] and Quasi-hydrodynamic of Sheretov[33] approach uses the time-spatial averaging procedure for the definition of the main gas dynamic quantities: density, velocity, and temperature as compared to spatial averaging used in conventional Navier-Stokes theory. Galileo transformation does not hold for the gas-dynamic equations based on spatial-time averages. For example consider continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \cdot \tag{10}$$

For spatial-time averages, the mass flux density may not be same as momentum of the volume unit [32] as

$$\int_{t}^{t+\Delta t} \rho_s(x,t')u_s(x,t')\,dt' \neq \int_{t}^{t+\Delta t} \rho_s(x,t')\,dt' \cdot \int_{t}^{t+\Delta t} u_s(x,t')\,dt' \ . \tag{11}$$

For spatial-time averages, the mass flux density may not be same as momentum of the volume unit as even for small time Δt, the instant value of density and momentum change.

For example in QGD an additional dissipative summands is introduced in the equations such that time-spatial averages are invariant under Galilieo transform. Due to this additional averaging (smoothing) in time the determination of the gas-dynamic parameters QGD formally differ from the Navier–Stokes system. This is similar to modification in hydrodynamic theory proposed by Brenner [34] by introducing a new mass diffusion contribution to the continuity equation. The equations were formalized by Ottinger [35] by providing thermodynamical basis. Greenshields and Reese [36] investigated monatomic gas shocks and found that results with Brenner's modifications are significantly better than those of the standard Navier–Stokes equations. Guo and Xu [37] studied gaseous micro flows using Brenner's hydrodynamic model and found that Brenner's model failed to give qualitative correct temperature profile.

2.4 BGK model

Boltzmann equation being a nonlinear integro-differential equation becomes difficult to handle. This requires some alternative simpler model to replace the collision term. Such models which replace the Boltzmann collision integral are called a kinetic model. These models should preserve the basic properties and characteristics of the Boltzmann equation. Kinetic model should satisfy the following properties :

a) Locality and Galilean invariance
Since the Boltzmann equation is invariant under Galilean transformation hence the collision term $J_m(f,f)$ should depend only on peculiar velocity $\vec{c} = \vec{v} - \vec{u}$.

b) Additive invariants of the collision
This property ensures conservation of mass, momentum and energy and is represented as

$$\int_{R^N}\int_{R^+}\Psi J_m(f,f)\,d\vec{v}\,dI = 0\,. \tag{12}$$

c) Uniqueness of equilibrium
The zero point of kinetic model $J_m(f, f) = 0$ representing collision term implies uniqueness of equilibrium.

d) Local entropy production inequality
This property represents non-negative entropy production by the kinetic model representing collision term.

$$\sigma_p = -k_B\int_{R^N}\int_{R^+} lnf\; J_m(f,f)\,d\vec{v}\,dI = -k_B\,\frac{dH}{dt} \geq 0 \tag{13}$$

where k_B is the dimensional Boltzmann constant ($k_B \approx 6.10^{-23}\ J/K$) and Boltzmann H-function is given by

$$H = \int_{R^N}\int_{R^+} flnf\,d\vec{v}\,dI\,. \tag{14}$$

e) Entropy production close to equilibrium satisfies the Onsager-Casimir reciprocal relations [38]. The moments of the distribution generate fluxes j_α which couples with its associated thermodynamic force X_φ as follows

$$j_\alpha = \sum_\varphi \Lambda_{\alpha\varphi} X_\varphi \tag{15}$$

where $\Lambda_{\alpha\varphi}$ are the kinetic coefficients such that entropy production σ_P satisfies the Onsager-Casimir reciprocity relations

$$\sigma_P = \sum_\alpha j_\alpha X_\alpha = \sum_{\alpha,\varphi}\Lambda_{\alpha\varphi} X_\alpha X_\varphi\,. \tag{16}$$

f) Positive distribution
The H-function of the kinetic model should decay monotonically such that Boltzmann equation gives positive distribution leading towards the unique equilibrium solution.

g) Correct transport coefficients in the hydrodynamic limit
In the hydrodynamic limit the kinetic model should generate correct transport coefficients such as viscosity, μ and thermal conductivity, κ and Prandtl number, $Pr = (5R/2)(\mu/\kappa)$. The Prandtl number should be is close to 2/3.

One of the simplest kinetic model is the Bhatnager-Gross-Krook (BGK) [39] model and there are various other models like Shakhov's model [40], the ellipsoidal statistical BGK (ES-BGK) model [41,42], Liu model [43], the BGK model with velocity dependent collision frequency ν(C)–BGK model of Mieussens and Struchtrup [44] which yield the proper Prandtl number. The Shakhov's model [40] or S-model is a generalization of the BGK model equation with correct relaxation of both the heat flux and stresses, leading thus to the correct continuum limit in the case of small Knudsen numbers. Model proposed by Shakhov provides reliable result for non-isothermal flows. Zheng and Struchtrup[45] have carried out detailed study on kinetic models. The Bhatnagar–Gross–Krook model (BGK) is preferred because of the low computational cost even though it yields an incorrect value of Prandtl number. This model assumes that

$$J_m(f,f) = \frac{f_0 - f}{t_R} \tag{17}$$

where t_R is the relaxation time for distribution f to reach the equilibrium Maxwellian distribution f_0.

2.5 Method of Reduced description : Chapman-Enskog expansion

Boltzmann's molecular chaos assumption gives a closed equation for $f^{(1)}$. The method of reduced description is required to find the closed set of equations. At each level of reduction the insignificant features are discarded for simplicity while retaining the essential physics. The closure problem becomes difficult because of the presence of higher order moments in the equation of lower order moment. Various methods have been developed to give a reduced description in terms of distribution function[46]. Some of the salient methods are: the Chapman-Enskog method [47], the Grad's method [48,49], the quasi-equilibrium method, and the method of the invariant manifold [50]. In the Grad's method [49] Boltzmann equation is projected onto Hermite basis i.e. we seek solution of mass, momentum and energy conservation equation by expanding the distribution function $f(\vec{x}, \vec{v}, I, t)$ in Hermite or Gram-Charlier polynomials. The unique feature of Hermite orthonormal polynomials forming the expansion basis is that its expansion coefficients correspond to the velocity moments. Thus, N^{th} order distribution function can be approximated by its projection onto a Hilbert subspace spanned by the first Hermite polynomials. Instead of searching for a perturbative solution of the Boltzmann equation in the neighbourhood of equilibrium. The Chapman-Enskog method makes use of the time scales present in the equation of motion and expands it in terms of slow and fast components. As the evolution of distribution function in Boltzmann's equation happens on slower timescale τ_s due to slow process of spatial gradients and at faster timescale τ_f due to the process of collisions. The five moments corresponding to mass, momentum and energy densities evolve slowly through spatial gradients as they are unaffected by collisions, whereas all the higher moments which include momentum and energy fluxes evolve on the faster timescale of collisions. In van Kampen's procedure [51] the slow variables are kept unexpanded while the fast variables are expanded in power of τ_f / τ_s. The combination of any slow and fast variables will give rise different, but asymptotically equivalent evolution equations for the slow variables at each stage in procedure laid out by van Kampen [52].In this paper we have followed Chapman-Enskog approach developed independently by Chapman and Enskog [47].

As described earlier the Boltzmann equation with the BGK model is

$$\frac{\partial f}{\partial t} + \nabla_{\vec{x}}.(\vec{v}f) = J_m(f,f) = \frac{(f_0 - f)}{t_R} \tag{18}$$

where f_0 is the Maxwellian, this can be written in the non-dimensional form [47] as

$$Kn\left[\frac{\partial f}{\partial \hat{t}} + \nabla_{\vec{\hat{x}}}.(\vec{\hat{v}}f)\right] = \frac{(f_0 - f)}{\hat{t}_R} \tag{19}$$

where $\hat{x} = x/L$, $\vec{\hat{v}} = \vec{v} / |v_{rms}|$, $\hat{t}_R = t_R |v_{rms}| / \lambda$, $\hat{t} = t |v_{rms}| / L$ and $Kn = \lambda/L$ is the local Knudsen number defined as a ratio of mean free path, λ and length scale, L and $|v_{rms}|$ is the root mean square velocity. The distribution function f can be written as the Chapman-Enskog perturbative expansion in terms of with Knudsen number as follows

$$f = f_0 + Kn\overline{f}_1 + Kn^2\overline{f}_2 + \cdots \tag{20}$$

where f_0 is the Maxwellian for the polyatomic gas given as

$$f_0 = \frac{\rho}{I_o}\left(\frac{\beta}{\pi}\right)^{\frac{D_f}{2}} exp\left(-\beta\left(\vec{v} - \vec{u}\right)^2 - \frac{I}{I_o}\right) \tag{21}$$

where thermal speed, $\beta = \frac{1}{2RT}$, D_f is the degree of freedom, I is the internal energy parameter and I_0 is the average internal energy parameter given as follows:

$$I_o =< I, f_0 >= \left(\frac{2 + D_f - \gamma\, D_f}{2(\gamma - 1)} \right) \frac{1}{2\beta} \,. \tag{22}$$

It should be noted that the perturbation terms satisfies the moment closure property, expressed as

$$< \Psi, Kn^i \bar{f}_i >_{\forall i \geq 1} = 0 \,. \tag{23}$$

In Chapman-Enskog expansion, the first term represents the Maxwellian equilibrium distribution function corresponding to the Euler equations. The first two terms in Chapman Enskog expansion, i.e., $(f_0 + \mathrm{Kn}\bar{f}_1)$ give a distribution function corresponding to the Navier–Stokes equations, which represent a first-order departure from equilibrium. Higher order expansion gives Burnett equations [53,54,55], and super-Burnett equations [56]. Boltzmann equation with higher order Chapman-Enskog distribution will express higher order constitutive relationship for shear and heat transfer terms. The higher order terms are proportional to the corresponding power of Knudsen number, Kn hence higher order terms become important in the Knudsen number dominated regime. Woods[53] has shown that both Chapman-Enskog theory and the physical models are based on an inppropriate definition of peculiar velocity. Woods [53] has suggested correction such that material frame-indifference holds. Using the non-dimensionless Boltzmann equation and Chapman-Enskog perturbation expansion, higher order distribution is generated by virtue of iterative refinement as follows:

$$\bar{f}_i = -\frac{t_R}{Kn} \left[\frac{\partial \bar{f}_{i-1}}{\partial t} + \nabla_{\vec{x}} . (\vec{v} \bar{f}_{i-1}) \right] \tag{24}$$

where Kn is the Knudsen number with $\bar{f}_0 = f_0$. In terms of substantative derivative $\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{u}.\nabla$ for inertial frame it can be written as

$$\frac{f_1}{f_0} = -\frac{t_R}{Kn} \left[\begin{array}{l} \frac{1}{\rho} \frac{D\rho}{Dt} - 2\beta^2 R \left(\frac{D_f + 2}{2\beta} - \frac{4(\gamma - 1) I}{2 - D_f(\gamma - 1)} - \sum_i^{D_f} c_i^2 \right) \frac{DT}{Dt} \\ + 2\beta \sum_j^{D_f} c_j \left(\frac{Du_j}{Dt} + \sum_i^{D_f} \left(c_i \frac{\partial u_i}{\partial s_j} \right) \right) \\ + \sum_j^{D_f} c_j \left\{ \frac{1}{\rho} \frac{\partial \rho}{\partial s_j} - 2\beta^2 R \left(\frac{D_f + 2}{2\beta} - \frac{4(\gamma - 1) I}{2 - D_f(\gamma - 1)} - \sum_i^{D_f} c_i^2 \right) \frac{\partial T}{\partial s_j} \right\} \end{array} \right] \tag{25}$$

where $c_i = v_i - u_i$ and $i = x, y, z$ with u_i and v_i being the fluid and molecular velocities, s_1, s_2 and s_3 are spatial coordinates x, y, z. After substitution of Euler equations

$$\int_{R^N} \int_{R^+} \Psi \left(\frac{\partial f_0}{\partial t} + \nabla_{\vec{x}} . (\vec{v} f_0) = 0 \right) d\vec{v} dI \Rightarrow \left. \begin{array}{l} \frac{D\rho}{Dt} = -\rho \frac{\partial u_i}{\partial s_i} \\ \frac{Du_i}{Dt} = \frac{\rho}{2\beta^2} \frac{\partial \beta \rho}{\partial s_i} \\ \frac{DT}{dt} = -(\gamma - 1) T \frac{\partial u_i}{\partial s_i} \end{array} \right\} . \tag{26}$$

The first-order Chapman-Enskog term can be written as

$$f_1 = f_0\left[1-\frac{\xi_{1,\tau}}{p}-\frac{\xi_{1,q}}{p}\right] \tag{27}$$

where $\xi_{1,\tau}$ and $\xi_{1,q}$ are Chapman-Enskog polynomials associated with the shear stress tensor and heat flux vector. For 3D geometry it can be written as follows:

$$\begin{aligned}\xi_{1,\tau} = {} & pt_R\left[\frac{5\gamma-7}{2}-\frac{(\gamma-1)I}{I_o}+c_x^2(3-\gamma)\beta-c_y^2(\gamma-1)\beta-c_z^2(\gamma-1)\beta\right]\frac{\partial u_x}{\partial x}\\ & +pt_R\left[\frac{5\gamma-7}{2}-\frac{(\gamma-1)I}{I_o}-c_x^2(\gamma-1)\beta+c_y^2(3-\gamma)\beta-c_z^2(\gamma-1)\beta\right]\frac{\partial u_y}{\partial y}\\ & +pt_R\left[\frac{5\gamma-7}{2}-\frac{(\gamma-1)I}{I_o}-c_x^2(\gamma-1)\beta+c_y^2(\gamma-1)\beta-c_z^2(3-\gamma)\beta\right]\frac{\partial u_z}{\partial z}\\ & +pt_R\left[2\beta c_x c_y\left(\frac{\partial u_x}{\partial y}+\frac{\partial u_y}{\partial x}\right)+2\beta c_y c_z\left(\frac{\partial u_y}{\partial z}+\frac{\partial u_z}{\partial y}\right)+2\beta c_x c_z\left(\frac{\partial u_x}{\partial z}+\frac{\partial u_z}{\partial x}\right)\right]\end{aligned} \tag{28}$$

$$\begin{aligned}\xi_{1,q} = {} & -2\beta^2 Rpt_R\left[\frac{7c_x}{2\beta}-\frac{c_x I}{I_o\beta}-c_x^3-c_y^2c_x-c_z^2c_x\right]\frac{\partial T}{\partial x}\\ & -2\beta^2 Rpt_R\left[\frac{7c_y}{2\beta}-\frac{c_y I}{I_o\beta}-c_x^2c_y-c_y^3-c_z^2c_y\right]\frac{\partial T}{\partial y}\\ & -2\beta^2 Rpt_R\left[\frac{7c_z}{2\beta}-\frac{c_z I}{I_o\beta}-c_x^2c_z-c_y^2c_z-c_z^3\right]\frac{\partial T}{\partial z}\end{aligned} \tag{29}$$

where Navier Stokes stress τ_{xx}, τ_{xy} and τ_{yy} and heat flux q_x, q_y and q_z are given as follows

$$\tau_{xx} = 2pt_R\frac{\partial u_x}{\partial x}+(1-\gamma)pt_R\left(\frac{\partial u_x}{\partial x}+\frac{\partial u_y}{\partial y}+\frac{\partial u_z}{\partial z}\right) \tag{30}$$

$$\tau_{yy} = 2pt_R\frac{\partial u_y}{\partial y}+(1-\gamma)pt_R\left(\frac{\partial u_x}{\partial x}+\frac{\partial u_y}{\partial y}+\frac{\partial u_z}{\partial z}\right) \tag{31}$$

$$\tau_{zz} = 2pt_R\frac{\partial u_z}{\partial z}+(1-\gamma)pt_R\left(\frac{\partial u_x}{\partial x}+\frac{\partial u_y}{\partial y}+\frac{\partial u_z}{\partial z}\right) \tag{32}$$

$$\tau_{xy} = \tau_{yx} = pt_R\left(\frac{\partial u_x}{\partial y}+\frac{\partial u_y}{\partial x}\right) \tag{33}$$

$$\tau_{xz} = \tau_{yz} = pt_R\left(\frac{\partial u_x}{\partial z}+\frac{\partial u_z}{\partial x}\right) \tag{34}$$

$$\tau_{yz} = \tau_{zy} = pt_R\left(\frac{\partial u_y}{\partial z}+\frac{\partial u_z}{\partial y}\right) \tag{35}$$

$$q_x = -pt_R R\frac{\gamma}{\gamma-1}\frac{\partial T}{\partial x} \tag{36}$$

$$q_y = -pt_R R\frac{\gamma}{\gamma-1}\frac{\partial T}{\partial y} \tag{37}$$

$$q_z = -pt_R R\frac{\gamma}{\gamma-1}\frac{\partial T}{\partial z}\,. \tag{38}$$

From the expression of shear stress it can also be deduced that Stokes hypothesis is only valid for monatomic gases. Macroscopic dynamic viscosity is directly related to molecular collision process by virtue of collision time. Chapman–Enskog expansion gives a viscosity coefficient of

$$\mu = t_R p \tag{39}$$

and thermal conductivity as

$$\kappa = pt_R R\frac{\gamma}{\gamma-1}\,. \tag{40}$$

The relaxation time of the BGK model is defined by

$$t_R^{-1} = \left(\frac{RT_{ref}^{\delta o}}{\mu_{ref}}\right)\rho T^{1-\delta o} \tag{41}$$

where μ_{ref} is the viscosity of the gas at the reference temperature, T_{ref}, δo is the exponent of the viscosity law of the gas, which depends on the molecular interaction potential and on the type of the gas. The single relaxation time in the BGK model used for the collision operator leads to incorrect values of the transport coefficients at the hydrodynamic limit. This approach gives Prandtl number as unity. This is a major drawback of this model but solution of Navier-Stokes are not affected by this variation [57]. Some drawbacks of this model, such as the incorrect value of the Prandtl number, can be corrected by modified models. Woods [53] suggested a method which appears to be *ad hoc* in which two distinct collision interval $t_{R,1}$ for momentum transport and $t_{R,2}$ for energy transport are adopted. These collision intervals are related as

$$t_{R,1} = \mathrm{Pr}\, t_{R,2} = \frac{2}{3}t_{R,2}\,. \tag{42}$$

Chae *et al*. [59] and Xu [12] have suggested following modification of energy flux for accurate heat transfer prediction

$$\left[\rho E\right]^{corrected} = \rho E + \left(\frac{1}{\mathrm{Pr}} - 1\right)\vec{q} \tag{43}$$

where $\vec{q}$ is the heat flux vector. May *et al*.[13] have proposed Prandtl number correction methodology which operates at the level of the partial differential equations and is also significantly cheaper in terms of computation requirement. It is important to understand that there are very few models which respect each constraint of positivity, conservation of moments, and dissipation of entropy, while being computationally inexpensive. With an assumption that the departure from equilibrium is small, the Chapman-Enskog distribution function can be derived by implementing the method of Prandtl number correction suggested by Woods [53]. The corrected Chapman-Enskog polynomial $\xi_{1,\tau}$ and $\xi_{1,q}$ associated with the shear stress tensor and heat flux vector can be written as

$$\begin{aligned}\xi_{1,\tau} = &\left[\frac{5\gamma-7}{2(5-3\gamma)} - \frac{I}{4\beta I_o^2} + \beta c_x^2\right]\tau_{xx} + \left[\frac{5\gamma-7}{2(5-3\gamma)} - \frac{I}{4\beta I_o^2} + \beta c_y^2\right]\tau_{yy} \\ &+ \left[\frac{5\gamma-7}{2(5-3\gamma)} - \frac{I}{4\beta I_o^2} + \beta c_z^2\right]\tau_{zz} + 2\beta c_x c_y \tau_{xy} + 2\beta c_x c_z \tau_{xz} + 2\beta c_y c_z \tau_{yz}\end{aligned} \tag{44}$$

$$\begin{aligned}\xi_{1,q} = 2\beta\left(\frac{\gamma-1}{\gamma}\right)&\left[\frac{7}{2}c_x - \frac{c_x I}{I_o} - \beta c_x^3 - \beta c_x c_y^2 - \beta c_x c_z^2\right] q_x \\ +2\beta\left(\frac{\gamma-1}{\gamma}\right)&\left[\frac{7}{2}c_y - \frac{c_y I}{I_o} - \beta c_x^2 c_y - \beta c_y^3 - \beta c_y c_z^2\right] q_y \\ +2\beta\left(\frac{\gamma-1}{\gamma}\right)&\left[\frac{7}{2}c_z - \frac{c_z I}{I_o} - \beta c_x^2 c_z - \beta c_y^2 c_z - \beta c_z^3\right] q_z\end{aligned} \tag{45}$$

where $I_o = \frac{5-3\gamma}{2(\gamma-1)}RT$ and $c_i = v_i - u_i$ where $i = x, y, z$ with u_i and v_i being the fluid and molecular velocity. Appendix gives the one dimensional second order Chapman Enskog derivation for BGK-Burnett equation. It should be noted that Chapman-Enskog theory and the physical models are based on an inappropriate definition of the peculiar velocity leading to frame dependence of the Burnett equations [53].

2.6 Breakdown of Navier-Stokes and flow regimes

Predicting fluid transport for rarefied flows or in micron-sized devices becomes difficult due to breakdown of continuum flow assumption embedded in conventional fluid dynamics. Validity of the Navier-Stokes equation as well as diffusion equation requires sufficient collision of particles and relaxation of the distribution to weak spatial gradients and slow temporal variations. Continuum also breaks down when gradients are substantial on the scale of mean free path or temporal changes are relatively rapid compared to mean collision time encountered in astrophysics. For rarefied flow the Navier-Stokes description for simple fluids breaks down when the characteristic length scale associated with flow approaches the molecular mean free path. For Navier–Stokes equations to remain valid it has also to operate within the framework of Newtonian mechanics following continuum approximation and satisfying constitutive relationships due to collision dominated transport models of stress tensor and heat flux vector. Levermore *et al*. [25] have applied the idea of moment realizability to derive criteria for the validity of the Navier-Stokes equation. These criteria is given in terms of the eigenvalues of the nondimensional 3×3 matrix given as follows

$$B_{NS} = I - \frac{\mu}{p}\left[\nabla\vec{u} + (\nabla\vec{u})^T - \frac{2}{3}\nabla\cdot\vec{u}I\right] - \frac{2}{3}\frac{\rho\kappa}{p^3}\nabla\left(\frac{p}{\rho}\right)\left[\nabla\left(\frac{p}{\rho}\right)\right]^T . \tag{46}$$

Significant deviations of the eigenvalues of this breakdown matrix from unity indicate large gradients and significant departure from the equilibrium state. The determination of non-equilibrium and continuum regions is generally carried out using a local continuum breakdown parameter called the gradient-length Knudsen number [60] defined as

$$Kn_{GL,\varsigma} = \frac{\lambda}{\varsigma}|\nabla\varsigma| \tag{47}$$

where ς is the parameter of interest, such as density (ρ), bulk velocity magnitude ($|V| = \sqrt{u^2 + v^2 + w^2}$), or temperature (T). λ is the mean free path given as

$$\lambda = \mu\sqrt{\frac{\pi}{2\rho p}} . \tag{48}$$

The actual continuum breakdown parameter is then the maximum of these, that is:

$$Kn_{GL} = \max(Kn_\rho, Kn_{|V|}, Kn_T) . \tag{49}$$

Schwartzentruber and Boyd [60] have recommended values of $Kn_{GL} > 0.05$ to signify continuum breakdown for representative hypersonic flows. In order to prevent a non-positive distribution function when the Navier Stokes solution is coupled with the Boltzmann solution Kolobov *et. al*. [61] have used switching criterion which is function of density gradient as well as velocity magnitude defined as follows:

$$NS_B = Kn\sqrt{\left(\frac{\nabla p}{p}\right)^2 + \frac{1}{|V|^2}\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2\right]}\ . \tag{50}$$

Most of the breakdown criteria which are valid for micro flows are not suitable for hypersonic flows. Breakdown criteria can also be formulated based on departure of flow from its equilibrium state. Lockerby et. al [62] have suggested breakdown criteria based on fractional relative departure from Navier-Stokes non-equilibrium given by Chapman-Enskog first order distribution. A local Knudsen number based on the degree of departure from the non-equilibrium flow state is expressed as

$$Kn = \frac{\int_{R^N}\int_{R^+} \psi_i (f - f_1)\, d\vec{v}\, dI}{\int_{R^N}\int_{R^+} \psi_i (f_1 - f_0)\, d\vec{v}\, dI} \tag{51}$$

where moment variable $\psi_i \in \Psi \equiv \{1, \vec{v}, \vec{v}^T\vec{v}\}$ or any other admissible $\psi_i \in \Psi \equiv \{1, \vec{v}, \vec{v}\otimes\vec{v}, \cdots\}$ and f is a higher order distribution function and f_1 is the Chapman-Enskog distribution function corresponding to Navier-Stokes equation. The Knudsen number can also be expressed in terms of Reynolds number (Re) and Mach number (M) as

$$Kn = \sqrt{\frac{\pi\gamma}{2}}\frac{M}{\mathrm{Re}}\ . \tag{52}$$

Different (M,Re) combination will give rise to different types of flow regimes [63]. Based on extent of non-equilibrium effects and rarefaction the flow regime can be broadly classified [64] as

1. No-slip continuum regime : This regime is valid for Kn < 0.001, since continuum and thermodynamic equilibrium prevails hence conventional no-slip is used along with Navier-Stokes equations.
2. Slip-Flow regime: This regime is valid in the range 0.001<Kn<0.1. The non-equilibrium effects occur in the close proximity of the wall, Navier-Stokes coupled with slip boundary conditions can effectively model velocity slip and temperature jump.
3. Transition regime: In the range 0.1 <Kn<10 the gas is very rarefied and Navier-Stokes is no longer valid. Flow modelling approach may require molecular or hybrid solvers.
4. Free-molecular flow: The regime is valid beyond Kn>10, in this regime collision frequency is very low as the flow is characterised by large mean free path compared to characteristic length scale. This regime can be modelled by collision less form of Boltzmann equation.

3. KINETIC FLUX VECTOR SPLITTING (KFVS)

In the Kinetic Flux Vector Splitting (KFVS) for Navier-Stokes upwinding is implemented using Courant split Boltzmann equation [9,16] as follows :

$$\begin{aligned}\frac{\partial f_1}{\partial t} + \frac{v_x + |v_x|}{2}\frac{\partial f_1}{\partial x} + \frac{v_x - |v_x|}{2}\frac{\partial f_1}{\partial x} + \frac{v_y + |v_y|}{2}\frac{\partial f_1}{\partial y} + \frac{v_y - |v_y|}{2}\frac{\partial f_1}{\partial y} \\ + \frac{v_z + |v_z|}{2}\frac{\partial f_1}{\partial z} + \frac{v_z - |v_z|}{2}\frac{\partial f_1}{\partial z} = 0\end{aligned}\ . \tag{53}$$

Taking Ψ moment and writing in terms of inner product

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\int_{R^N}\int_{R^+}\Psi f_1 d\vec{v}dI\right)\\
&+\frac{\partial}{\partial x}\left(\int_{R^\pm}\int_{R}\int_{R}\int_{R^+}\Psi\left(\frac{v_x\pm|v_x|}{2}\right)f_0 dv_x dv_y dv_z dI\right)+\frac{\partial}{\partial x}\left(\int_{R^\pm}\int_{R}\int_{R}\int_{R^+}\Psi\left(\frac{v_x\pm|v_x|}{2}\right)Kn\bar{f}_1 dv_x dv_y dv_z dI\right)\\
&+\frac{\partial}{\partial y}\left(\int_{R}\int_{R^\pm}\int_{R}\int_{R^+}\Psi\left(\frac{v_y\pm|v_y|}{2}\right)f_0 dv_x dv_y dv_z dI\right)+\frac{\partial}{\partial y}\left(\int_{R}\int_{R^\pm}\int_{R}\int_{R^+}\Psi\left(\frac{v_y\pm|v_y|}{2}\right)Kn\bar{f}_1 dv_x dv_y dv_z dI\right)\\
&+\frac{\partial}{\partial z}\left(\int_{R}\int_{R}\int_{R^\pm}\int_{R^+}\Psi\left(\frac{v_z\pm|v_z|}{2}\right)f_0 dv_x dv_y dv_z dI\right)+\frac{\partial}{\partial z}\left(\int_{R}\int_{R}\int_{R^\pm}\int_{R^+}\Psi\left(\frac{v_z\pm|v_z|}{2}\right)Kn\bar{f}_1 dv_x dv_y dv_z dI\right)=0
\end{aligned} \quad .(54)$$

Inviscid fluxes are based on Maxwellian, f_0 and viscous fluxes are based on perturbation $Kn\bar{f}_1$

$$\begin{aligned}
[GX,GY,GZ]_I &\equiv \int_{R^N}\int_{R^+}\Psi\vec{v}f_0 d\vec{v}dI \quad \text{and}\\
[GX,GY,GZ]_V &\equiv \int_{R^N}\int_{R^+}\Psi\vec{v}Kn\bar{f}_1 d\vec{v}dI \,.
\end{aligned} \tag{55}$$

This leads to split flux Navier-Stokes equations.

$$\frac{\partial U}{\partial t}+\frac{\partial GX_I^\pm}{\partial x}+\frac{\partial GX_V^\pm}{\partial x}+\frac{\partial GY_I^\pm}{\partial y}+\frac{\partial GY_V^\pm}{\partial y}+\frac{\partial GZ_I^\pm}{\partial z}+\frac{\partial GZ_V^\pm}{\partial z}=0 \tag{56}$$

where U is the state vector and, $GX_I^\pm$, $GX_V^\pm$, $GY_I^\pm$, $GY_V^\pm$, $GZ_I^\pm$ and $GZ_V^\pm$ represents the split inviscid and viscous fluxes. Expressions of these fluxes are given in Mahendra[16]. Viscous fluxes are upwinded and treated similar to inviscid fluxes. For example for two-dimensional case the x-component of the mass split fluxes due to viscous contribution can be derived as

$$GX_V^\pm(1)=\mp\frac{\rho}{p\sqrt{\beta}}\left[\frac{e^{-u_x^2\beta}}{2\sqrt{\pi}}\left(\frac{\tau_{xx}}{2}+q_x u_x\beta\frac{(\gamma-1)}{\gamma}\right)\right]. \tag{57}$$

Split fluxes should satisfy the Onsager reciprocity principles. For example viscous part of the mass flux contains terms of shear stress tensor as well as heat flux vector because the Chapman-Enskog polynomials $\xi_{1,\tau}$ and $\xi_{1,q}$ associated with the shear stress tensor and heat flux satisfy the Onsager reciprocal relation [38]. The upwind treatment of the viscous term is required for effective capture of cross phenomena of thermal transpiration or thermal creep and the mechanocalorific effect [17]. In the vicinity of equilibrium Chapman-Enskog polynomial, $\xi_{1,\tau}$ associated with shear stress and heat flux $\xi_{1,q}$ will give rise to thermodynamic forces which couples with its conjugate split fluxes satisfying the Onsager reciprocal relationship.

3.2 Modified KFVS

In modified KFVS [20] Boltzmann equation with Courant splitting [9,16] is expressed as

$$\begin{aligned}
&\left\langle\Psi,\frac{\partial f_1}{\partial t}\right\rangle+\left\langle\Psi,\frac{v_x+\varphi|v_x|}{2}\frac{\partial f_1}{\partial x}\right\rangle+\left\langle\Psi,\frac{v_x-\varphi|v_x|}{2}\frac{\partial f_1}{\partial x}\right\rangle\\
&+\left\langle\Psi,\frac{v_y+\varphi|v_y|}{2}\frac{\partial f_1}{\partial y}\right\rangle+\left\langle\Psi,\frac{v_y-\varphi|v_y|}{2}\frac{\partial f_1}{\partial y}\right\rangle+\left\langle\Psi,\frac{v_z+\varphi|v_z|}{2}\frac{\partial f_1}{\partial z}\right\rangle+\left\langle\Psi,\frac{v_z-\varphi|v_z|}{2}\frac{\partial f_1}{\partial z}\right\rangle=0.
\end{aligned} \tag{58}$$

Numerical schemes introduce artificial dissipation which will leads to loss of accuracy in the solution.

Modified partial differential equation (MPDE) analysis for one dimensional Boltzmann equation reveals a numerical kinetic viscosity as

$$\mu_{num} = \frac{\Delta x}{2}\sqrt{\frac{\beta}{\pi}}\int_R |v|\varphi e^{-\beta(v-u)^2}\, dv \quad . \tag{59}$$

With $\varphi = 0$ the formulation becomes central difference and with $\varphi = 1$ the formulation is in the KFVS upwind form. For the case when dissipation control function $\varphi = 1$ the numerical viscosity is maximum when molecular velocity v is closed to u. In modified KFVS, Anil *et al*.[20] introduces dissipation control function in order to resolve the discontinuity more sharply with less dissipation. The order of accuracy can be improved with the proper choice of dissipation control function φ such that $0 < \varphi < 1$. Analysis by Anil *et al*.[20] also revealed that particles with large peculiar velocity contribute little to the dissipation hence Anil *et al*.[20] considered dissipation control function, φ to be function of molecular velocity.

3.3 KFVS for axi-symmetric geometries

The velocity discretization of the transport operator is no longer trivial in the cylindrical system as inertia terms are velocity derivatives of the distribution function. It should be noted that characteristic curves of this form of Boltzmann equation are curves of R^4 and certainly more complex compared to the Cartesian form [65]. The characteristic curves are defined by

$$\dot{z}(t) = v_z, \qquad \dot{r}(t) = v_r, \qquad \dot{v}_r(t) = \frac{v_\theta^2}{r}, \qquad \dot{v}_\theta(t) = -\frac{v_r v_\theta}{r} \cdot \tag{60}$$

Mieussens[65] and Sugimoto and Sone[66] have used variables ζ and ω to replace (v_r, v_θ) by ($\zeta\cos\omega$, $\zeta\sin\omega$) to obtain completely conservative form of Boltzmann equation as follows

$$\frac{\partial rf}{\partial t} + v_z\frac{\partial rf}{\partial z} + \zeta\cos\omega\frac{\partial rf}{\partial r} - \zeta\frac{\partial \sin\omega f}{\partial \omega} = rJ(f,f) \cdot \tag{61}$$

Mieussens [65] used discrete-velocity models for the collision and transport operators, for plane and axisymmetric geometries satisfying positivity, entropy and conservation. The paper uses Boltzmann equation in the cylindrical coordinate system [67,68] with the following axi-symmetric form

$$\begin{aligned} &\frac{\partial f}{\partial t} + v_z\frac{\partial f}{\partial z} + v_r\frac{\partial f}{\partial r} + \frac{\partial v_r}{\partial t}\frac{\partial f}{\partial v_r} + \frac{\partial v_\theta}{\partial t}\frac{\partial f}{\partial v_\theta} = J(f,f) \\ \Leftrightarrow\ &\frac{\partial f}{\partial t} + v_z\frac{\partial f}{\partial z} + \frac{v_r}{r}\frac{\partial rf}{\partial r} + \left\{\frac{-fv_r}{r} + \frac{v_\theta^2}{r}\frac{\partial f}{\partial v_r} - \frac{v_r v_\theta}{r}\frac{\partial f}{\partial v_\theta}\right\} = J(f,f) \cdot \end{aligned} \tag{62}$$

The terms in the curly bracket correspond to the source terms. Taking Ψ moments with Chapman-Enskog distribution leads to split Navier—Stokes equations as

$$\begin{aligned} &\left\langle \Psi, \frac{\partial f_1}{\partial t} + \frac{v_z + \varphi|v_z|}{2}\frac{\partial f_1}{\partial z} + \frac{v_z - \varphi|v_z|}{2}\frac{\partial f_1}{\partial z} + \frac{v_r + \varphi|v_r|}{2r}\frac{\partial rf_1}{\partial r} + \frac{v_r - \varphi|v_r|}{2r}\frac{\partial rf_1}{\partial r}\right\rangle \\ &\qquad + \left\langle \Psi, \left\{\frac{-f_1 v_r}{r} + \frac{v_\theta^2}{r}\frac{\partial f_1}{\partial v_r} - \frac{v_r v_\theta}{r}\frac{\partial f_1}{\partial v_\theta}\right\}\right\rangle = 0 \\ &\Leftrightarrow \frac{\partial U}{\partial t} + \frac{\partial GZ^+}{\partial z} + \frac{\partial GZ^-}{\partial z} + \frac{1}{r}\frac{\partial rGR^+}{\partial r} + \frac{1}{r}\frac{\partial rGR^-}{\partial r} + S = 0 \end{aligned} \tag{63}$$

where $GZ^{\pm}$ and $GR^{\pm}$ represents axial and radial split fluxes and un-split source term $S=\left[0,0,-\frac{P}{r}-\frac{\rho u_{\theta}^{2}}{r}-\frac{\tau_{\theta\theta}}{r},\frac{\rho u_{r}u_{\theta}}{r}+\frac{\tau_{r\theta}}{r},0\right]^{T}$. For axi-symmetric geometries the dissipation control function, φ can either be a function of molecular velocity or any suitable macroscopic parameter depending on the type of flow.

4. VARIANCE REDUCTION KINETIC FLUX VECTOR SPLITTING (VRKFVS)

In this variant of kinetic flux vector splitting the Boltzmann equation uses distribution in a Chapman-Enskog perturbative form. The Boltzmann equation with distribution function written in Chapman-Enskog perturbative form with respect to Maxwellian f_0 is expressed as

$$\frac{\partial\left(f_0+\sum_{i}^{\infty}Kn^{i}\bar{f}_{i}\right)}{\partial t}+\frac{\partial\vec{v}\left(f_0+\sum_{i}^{\infty}Kn^{i}\bar{f}_{i}\right)}{\partial\vec{x}}=0\ \cdot \tag{64}$$

Assuming that f in the vicinity of f_0 as well as another chosen Maxwellian f_{M}. In such a case the Boltzmann equation can also be written based on Chapman-Enskog perturbative form with respect to f_{M}

$$\frac{\partial\left(f_M+\sum_{i}^{\infty}Kn^{i}\bar{f}_{i}^{M}\right)}{\partial t}+\frac{\partial\vec{v}\left(f_M+\sum_{i}^{\infty}Kn^{i}\bar{f}_{i}^{M}\right)}{\partial\vec{x}}=0\cdot \tag{65}$$

Taking Ψ moment of the difference of these two Boltzmann equations we get

$$<\psi,\frac{\partial(\Delta f)}{\partial t}+\frac{\partial\vec{v}\left(\Delta f+\sum_{i}^{\infty}Kn^{i}\bar{f}_{i}-\sum_{i}^{\infty}Kn^{i}\bar{f}_{i}^{M}\right)}{\partial\vec{x}}=0>\cdot \tag{66}$$

The term $\Delta f=f_0-f_M$ is the difference in the Maxwellians. It should be noted that the terms $\sum_{i}^{\infty}Kn^{i}\bar{f}_{i}$ and $\sum_{i}^{\infty}Kn^{i}\bar{f}_{i}^{M}$ associated with time derivative vanishes as these perturbation terms satisfy the moment closure property, expressed as

$$<\Psi,Kn^{i}\bar{f}_{i}>_{\forall i\geq 1}=<\Psi,Kn^{i}\bar{f}_{i}^{M}>_{\forall i\geq 1}=0\cdot \tag{67}$$

The difference in the perturbation terms for the two Maxwellians can be simplified for first order Chapman-Enskog as

$$Kn\bar{f}_{1}-Kn\bar{f}_{1}^{M}=-t_{R0}\left[\frac{\partial f_0}{\partial t}+\nabla_{\vec{x}}.(\vec{v}f_0)\right]+t_{RM}\left[\frac{\partial f_M}{\partial t}+\nabla_{\vec{x}}.(\vec{v}f_M)\right] \tag{68}$$

where t_{R0} and $t_{R\mathrm{M}}$ are relaxation time for f_0 and f_{M}.
Assuming $t_R=t_{R0}=t_{R\mathrm{M}}$ as the chosen distribution f_0 is in the vicinity of f_{M}. With this the difference in the perturbation terms can be approximated for the first order expansion as

$$Kn\Delta\bar{f}_{1}=Kn\bar{f}_{1}-Kn\bar{f}_{1}^{M}\approx-t_{R}\left[\frac{\partial\Delta f}{\partial t}+\nabla_{\vec{x}}.(\vec{v}\Delta f)\right] \tag{69}$$

where $\Delta\bar{f}_{1}=\bar{f}_{1}-\bar{f}_{1}^{M}$ and with its substitution the Boltzmann equation in this variance reduction form

based on first order Chapman-Enskog distribution is expressed as

$$\frac{\partial(\Delta f)}{\partial t}+\frac{\partial \vec{v}(\Delta f_1)}{\partial \vec{x}}=0 \quad or \quad \frac{\partial(\Delta \hat{f})}{\partial t}+\frac{\partial \vec{v}(\Delta f_1)}{\partial \vec{x}}=0 \tag{70}$$

where $\Delta f_1 = \Delta f + Kn\ \Delta \bar{f}_1$ and $\Delta \hat{f} = f_1 - f_M$ and $f_1 = f_0 + Kn\bar{f}_1$ as $<\Psi, Kn\ \bar{f}_1>=0$.
This method basically evaluates the "variance-reduced" form of the collision integral as in the variance reduction technique of Baker and Hadjiconstantinou [69] and Homolle and Hadjiconstantinou [70]. The collision integral can also be expressed as

$$J(f,f)=\frac{1}{2}\int_{R^N}\int_{R^N}\int_{R^+}\int_0^{2\pi}\int_0^{\pi/2}\left(\delta_1^a+\delta_2^a-\delta_1-\delta_2\right)f^{(1)}f^{(2)}g\ \Pi\ d\vec{v}_1\,d\vec{v}_2\,dI\,d\varepsilon\,d\Theta \tag{71}$$

where $\delta_1^a=\delta^3(\vec{v}_1^a-\vec{v})$, $\delta_2^a=\delta^3(\vec{v}_2^a-\vec{v})$, $\delta_1=\delta^3(\vec{v}_1-\vec{v})$ and $\delta_2=\delta^3(\vec{v}_2-\vec{v})$, δ is the Dirac delta function and subscript 'a' denotes after collision state. If the distributions $f^{(1)}=f_0+\Delta f^{(1)}$ and $f^{(2)}=f_M+\Delta f^{(2)}$ are perturbations around Maxwellians f_0 and f_M, then the collision integral in the variance-reduced form can be expressed as

$$\begin{aligned}J(f,f)&=\frac{1}{2}\int_{R^N}\int_{R^N}\int_{R^+}\int_0^{2\pi}\int_0^{\pi/2}\left(\delta_1^a+\delta_2^a-\delta_1-\delta_2\right)(2f_0\Delta f^{(2)}+\Delta f^{(1)}\Delta f^{(2)})\zeta\ \phi\ d\vec{v}_1\,d\vec{v}_2\,dI\,d\varepsilon\,d\Theta\\&=L(\Delta f)+\Gamma(\Delta f,\Delta f)\,.\end{aligned} \tag{72}$$

Thus the integral can be written as the sum of linear $L(\Delta f)$ and a quadratic $\Gamma(\Delta f, \Delta f)$ term.

In Variance Reduction Kinetic Flux Vector Splitting (VRKFVS) for Navier-Stokes upwinding is implemented in a similar way as in KFVS using Courant split Boltzmann equation as follows :

$$\frac{\partial \Delta\hat{f}}{\partial t}+\frac{v_x\pm|v_x|}{2}\frac{\partial \Delta f_1}{\partial x}+\frac{v_y\pm|v_y|}{2}\frac{\partial \Delta f_1}{\partial y}+\frac{v_z\pm|v_z|}{2}\frac{\partial \Delta f_1}{\partial z}\,. \tag{73}$$

Taking Ψ moments of the resulting variant of Boltzmann equation leads to Navier-Stokes equation based on Variance Reduction Kinetic Flux Vector Splitting (VRKFVS)

$$\begin{aligned}&\frac{\partial}{\partial t}(\Delta U)+\frac{\partial}{\partial x}\left[\Delta\left(GX_I^{\pm}\right)+\left(GX_V^{\pm}\right)_\Delta\right]+\frac{\partial}{\partial y}\left[\Delta\left(GY_I^{\pm}\right)+\left(GY_V^{\pm}\right)_\Delta\right]\\&\qquad+\frac{\partial}{\partial z}\left[\Delta\left(GZ_I^{\pm}\right)+\left(GZ_V^{\pm}\right)_\Delta\right]=0\end{aligned} \tag{74}$$

where $\Delta U = U - U_M$ is the deviation of the state update vector U over U_M based on Maxwellian distribution, f_M. The inviscid fluxes are also deviations over the inviscid fluxes based on the chosen distribution, f_M. Thus $\Delta(GX_I^{\pm}) = (GX_I^{\pm}) - (GX_I^{\pm})_M$, $\Delta(GY_I^{\pm}) = (GY_I^{\pm}) - (GY_I^{\pm})_M$ and $\Delta(GZ_I^{\pm}) = (GZ_I^{\pm}) - (GZ_I^{\pm})_M$, where $(GX_I^{\pm})_M$, $(GY_I^{\pm})_M$ and $(GZ_I^{\pm})_M$ are the inviscid split fluxes based on the Maxwellian distribution, f_M associated with the chosen state of equilibrium. The viscous fluxes $(GX_V^{\pm})_\Delta$, $(GY_V^{\pm})_\Delta$ and $(GZ_V^{\pm})_\Delta$ are computed based on relative velocity field over the chosen Maxwellian f_M. Thus we solve for the deviations over a state variable, U_M using the fluxes over a relative the flow field based on chosen Maxwellian, f_M. The selection of the state of equilibrium, f_M can be based on i) free stream condition, or ii) wall conditions, or iii) the mean equilibrium based on the neighborhood values, or iv) combination of all the three in the solution domain. This variant of KFVS based on variance reduction form of BGK-Boltzmann equation was found extremely useful in capturing weak secondary flow in a strong flow field environment. Part 2 of the paper describes the numerical implementation of VRKFVS.

5. KINETIC TREATMENT OF BOUNDARY CONDITIONS

The boundaries conditions should be as physically meaningful as possible. Both in KFVS and VRKFVS the boundary conditions are implemented by constructing the distribution function. Once the distribution function is constructed based on the boundary data the second step is to take moments and obtain the state update equation. The various steps involved in implementing the boundary conditions are illustrated in the following sub-sections.

5.1 Treatment of far field boundary condition.

At the far field the distribution is Maxwellian as equilibrium prevails. This Maxwellian is split into two parts based on the direction of propagation. Similarly, the Chapman-Enskog distribution is split into two parts i.e. part escaping out of the flow domain and the part which remains in the flow domain. Thus, distribution function $f_1^{\Sigma}(v_x, v_y, v_z, I)$ at the far field boundary is constructed as the union of a Maxwellian distribution $f_0^{\infty}(v_x, v_y, v_z, I)$ corresponding to the incoming particle from the far field domain and Chapman-Enskog distribution $f_1(v_x, v_y, v_z, I)$ corresponding to outgoing particles from the computing domain. Thus,

$$f_1^{\Sigma}(v_x, v_y, v_z, I) = f_0^{\infty}(v_x, v_y, v_z, I)_{v_z \geq 0} \cup f_1(v_x, v_y, v_z, I)_{v_z < 0} \tag{75}$$

$$\begin{aligned} \left\langle \Psi, f_1^{\Sigma}(v_x, v_y, v_z, I) \right\rangle &= \left\langle \Psi, f_0^{\infty}(v_x, v_y, v_z, I)_{v_z \geq 0} \right\rangle \cup \left\langle \Psi, f_1(v_x, v_y, v_z, I)_{v_z < 0} \right\rangle \\ &\equiv \int_R \int_R \int_{R^+} \int_{R^+} \Psi f_0^{\infty} \, dv_x \, dv_y \, dv_z \, dI \cup \int_R \int_R \int_{R^-} \int_{R^+} \Psi f_1 \, dv_x \, dv_y \, dv_z \, dI \end{aligned} . \tag{76}$$

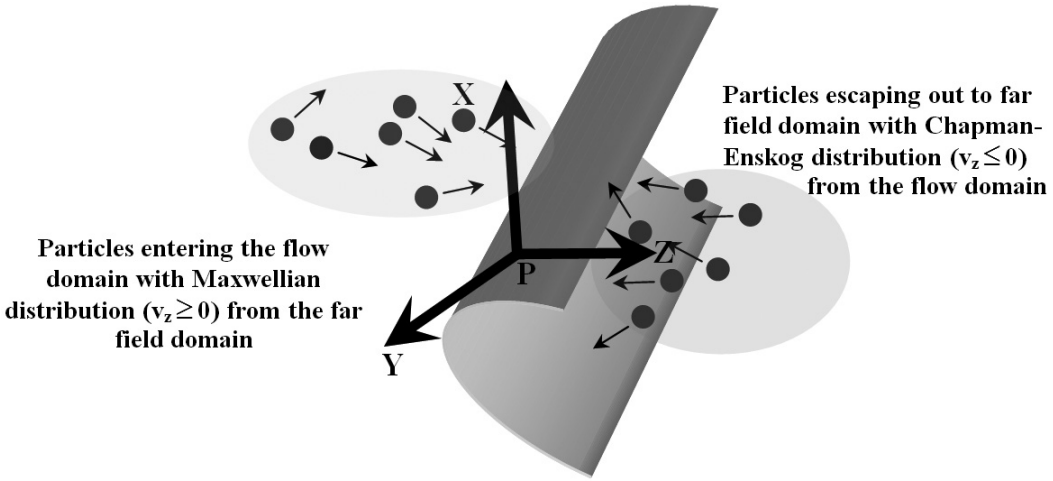


Figure 2. Distribution function constructed from the truncated Maxwellian from the far field and Chapman-Enskog distribution from the flow domain

The state update based on KFVS implementation at the boundary after taking Ψ moment and writing in terms of inner product can be expressed as

$$U^{n+1} = \bar{U}^n - \Delta t \left[\left(\frac{\partial GX^{\pm}}{\partial x} \right)^n + \left(\frac{\partial GY^{\pm}}{\partial y} \right)^n + \left(\frac{\partial GZ^{-}}{\partial z} \right)^n \right] \tag{77}$$

where

$$\bar{U}^n = \left(\int_{R^N} \int_{R^+} \Psi f_1^{\Sigma} d\vec{v} dI \right)^n , \tag{78}$$

$$\left(\frac{\partial GX^{\pm}}{\partial x}\right)^n = \frac{\partial}{\partial x}\left(\int_{R^{\pm}}\int_{R}\int_{R^-}\int_{R^+}\Psi\left(\frac{v_x \pm \varphi|v_x|}{2}\right) f_1\, dv_x dv_y dv_z dI\right)^n, \tag{79}$$

$$\left(\frac{\partial GY^{\pm}}{\partial y}\right)^n = \frac{\partial}{\partial y}\left(\int_{R}\int_{R^{\pm}}\int_{R^-}\int_{R^+}\Psi\left(\frac{v_y \pm \varphi|v_y|}{2}\right) f_1\, dv_x dv_y dv_z dI\right)^n \tag{80}$$

$$\text{and } \left(\frac{\partial GZ^{-}}{\partial z}\right)^n = \frac{\partial}{\partial z}\left(\int_{R}\int_{R}\int_{R^-}\int_{R^+}\Psi v_z f_1\, dv_x dv_y dv_z dI\right)^n \cdot \tag{81}$$

5.2 Treatment of slip boundary condition using diffuse reflection model.

The determination of non-equilibrium and continuum regions in the rarefied region is carried out using a local continuum breakdown parameter based on gradient-length Knudsen number. Cercignani and Lampis[71] introduced a phenomenological model which was latter on extended by Lords[72]. This model is called CLL (Cercignani, Lampis, Lord) reflection model is more physically meaningful and satisfies the reciprocity principle.

Diffuse reflection model is the most preferred approach for engineering applications, in this model molecules partially undergo specular reflection and the remainder reflect in diffuse manner. The boundary conditions at the surface of the solid object define the distribution function of the reflected particles as a sum of diffuse and specular reflections [73,17]. With a diffuse reflection or accommodation coefficient σ, distribution function can be written as

$$\begin{aligned} f_1^{\Sigma}(v_x, v_y, v_z, I) &= f_1^{in}(v_x, v_y, v_z, I)_{v_z \le 0} \\ &+(1-\sigma) f_1^{in}(v_x, v_y, v_z^s, I)_{v_z>0} + \sigma f_0^{wc}(v_x, v_y, v_z^d, I)_{v_z>0} \end{aligned} \tag{82}$$

where $f_1^{\Sigma}(v_x, v_y, v_z, I)$ is the total, $f_1^{in}(v_x, v_y, v_z, I)$ is the incident, $f_1^{in}(v_x, v_y, v_z^s, I)$ is the specularly reflected Chapman-Enskog distribution and $f_0^{wc}(v_x, v_y, v_z^d, I)$ is the diffuse reflected Maxwellian distribution evaluated at the wall conditions denoted by supescript ^{wc} such that no particles penetrate the wall. v_z^s is the specularly reflected and v_z^d is the diffuse reflected z-component of the velocity. With $v_z^s = -v_z$ and T^{wc} as the wall temperature, the density at the wall ρ^{wc} used in distribution $f_0^{wc}(v_x, v_y, v_z^d, I)$ can be obtained based on mass conservation as

$$\begin{aligned} &\int_R\int_R\int_{R^+}\int_{R^+} v_z^d f_0^{wc}\, dv_x\, dv_y\, dv_z\, dI + \int_R\int_R\int_{R^-}\int_{R^+} v_z^s f_1^{in}\, dv_x\, dv_y\, dv_z\, dI = 0 \\ &\frac{\rho^{wc}\sqrt{RT^{wc}}}{\sqrt{2\pi}} = \frac{\rho\sqrt{RT}}{\sqrt{2\pi}}\left(1-\frac{\tau_{zz}}{2p}\right) \Leftrightarrow \rho^{wc} = \rho\sqrt{\frac{T}{T^{wc}}}\left(1-\frac{\tau_{zz}}{2p}\right) \end{aligned} \cdot \tag{83}$$

The slip velocity expression can be obtained as

$$\vec{u}_{slip}(u_x, u_y, 0) = \frac{\int_{R^N}\int_{R^+}\vec{v} f_1^{\Sigma}\, d\vec{v}\, dI}{\int_{R^N}\int_{R^+} f_1^{\Sigma}\, d\vec{v}\, dI} \cdot \tag{84}$$

Similarly expressions of temperature jump can be obtained by equating the energy flux in the limit $\Delta z \to 0$. Thus,

$$\sigma\left[\begin{array}{l}\int_R\int_R\int_{R^+}\int_{R^+} f_0^{wc}\left(I+\frac{v^2}{2}\right)v_z\,dv_x\,dv_y\,dv_z\,dI \\ +\int_R\int_R\int_{R^-}\int_{R^+} f_1\left(I+\frac{v^2}{2}\right)v_z\,dv_x\,dv_y\,dv_z\,dI\end{array}\right]_{z=0} = \left[\int_R\int_R\int_{R^-}\int_{R^+}\left(I+\frac{v^2}{2}\right)v_z f_1\,dv_x\,dv_y\,dv_z\,dI\right]_{z=\Delta z} \tag{85}$$

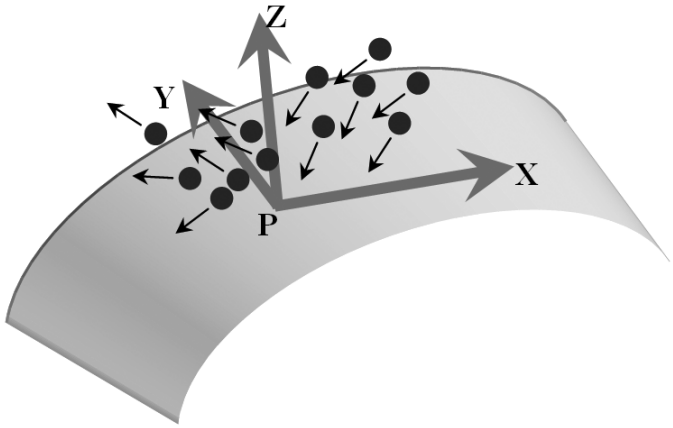


Figure 3. Distribution function as a sum of specular as well as diffuse reflections

These expressions of slip velocity and temperature jump are similar to Maxwell's velocity slip boundary condition [74] and von Smoluchowski's temperature jump boundary condition [75]. It is should be noted that these expressions are valid only in slip flow regime when there are insignificant fluid dynamic variations in the tangential direction. Slip velocity not only depends on the velocity gradient in the normal direction but also on the pressure gradient in the tangential flow direction [76]. Using the diffuse reflection model and accounting the split fluxes in the tangential direction a more accurate estimate of slip velocity and temperature jump can be made. The state update based on KFVS implementation at the boundary after taking Ψ moment and writing in terms of inner product can be expressed as

$$U^{n+1} = U^n - \Delta t\left[\left(\frac{\partial GX^{\pm}}{\partial x}\right)^n + \left(\frac{\partial GY^{\pm}}{\partial y}\right)^n + \left(\frac{\partial GZ^{-}}{\partial z}\right)^n\right] \tag{86}$$

where

$$\left(\frac{\partial GX^{\pm}}{\partial x}\right)^n = \frac{\partial}{\partial x}\left(\int_{R^{\pm}}\int_R\int_{R^-}\int_{R^+}\Psi\left(\frac{v_x \pm |v_x|}{2}\right)f_1^{\Sigma}dv_x dv_y dv_z dI\right)^n, \tag{87}$$

$$\left(\frac{\partial GY^{\pm}}{\partial y}\right)^n = \frac{\partial}{\partial y}\left(\int_R\int_{R^{\pm}}\int_{R^-}\int_{R^+}\Psi\left(\frac{v_y \pm |v_y|}{2}\right)f_1^{\Sigma}dv_x dv_y dv_z dI\right)^n, \tag{88}$$

$$\text{and } \left(\frac{\partial GZ^{-}}{\partial z}\right)^n = \frac{\partial}{\partial z}\left(\int_R\int_R\int_{R^-}\int_{R^+}\Psi v_z f_1^{\Sigma}dv_x dv_y dv_z dI\right)^n. \tag{89}$$

6. CONCLUDING REMARKS

Solution of Boltzmann equation because of its complex collision integral becomes a formidable task. The kinetic model and its corresponding discretization scheme should preserve the basic properties and characteristics of the Boltzmann equation. One of the important property is the entropy production close to equilibrium should satisfy the Onsager-Casimir reciprocal relationship. With an assumption of local equilibrium when spatial gradients and temporal variations are small, Navier-Stokes equation can be derived from the Boltzmann equation using first order Chapman-Enskog expansion. It is more rational to apply discretization in the Boltzmann level rather than the derived quantities i.e. macroscopic variables. KFVS is one such method which is based on moment-method strategy which operates in two levels: i) the Boltzmann level where upwind implementation is done, ii) the macroscopic (Euler or Navier-Stokes) level at which the state update operates. Modified KFVS based on dissipation control function adds to the accuracy. Variance reduction based Kinetic Flux Vector Splitting (VRKFVS) can effectively capture weak secondary flow features invoked due to perturbation of strong primary flow field. Kinetic boundary condition naturally leads to velocity slip and temperature jump. Diffuse reflection model based KFVS viscous fluxes satisfy the Onsager-Casimir reciprocity relations and uses kinetic upwind fluxes for slip boundary treatment. Slip velocity not only depends on the velocity gradient in the normal direction but also on the fluid dynamic gradients in the tangential flow direction. Treatment of slip boundary using kinetic upwind fluxes based on diffuse reflection model considers these variations in the tangential flow direction.

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APPENDIX

Second order Chapman-Enskog perturbation expansion can be written as

$$\begin{aligned} f &= f_0 + Kn\bar{f}_1 + Kn^2\bar{f}_2 \\ &= f_0 + Knf_0\xi_1 + Kn^2\bar{f}_1\,\xi_2 \end{aligned} \tag{A-1}$$

where Kn is the Knudsen number and ξ_1 and ξ_2 are the first and second order Chapman-Enskog polynomials. Expressing in terms of substantative derivative $\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{u}.\nabla$ and relaxation time t_R using the proceedure of iterative refinement we get

$$\frac{Kn^2\bar{f}_2}{f_0} = t_R^2 \left[\begin{array}{l} \left[\left(\frac{25}{4\beta^2} - \frac{I^2}{\beta^2 I_o^2} - \frac{5I}{\beta^2 I_o}\right)c_x^2 + \left(\frac{2I}{\beta I_o} - \frac{5}{\beta}\right)c_x^4 + c_x^6\right]\left(\frac{\partial\beta}{\partial x}\right)^2 \\ +2\left[\begin{array}{l}\left(\frac{5(3\gamma-5)}{4\beta} - \frac{(4\gamma-5)I}{\beta I_o} + \frac{(\gamma-1)I^2}{\beta\, I_o^2}\right)c_x + \\ \left((10-4\gamma) + \frac{(2\gamma-4)I}{I_o}\right)c_x^3 - (3-\gamma)\beta c_x^5\end{array}\right]\left(\frac{\partial\beta}{\partial x}\right)\left(\frac{\partial u_x}{\partial x}\right) \\ +\left[\begin{array}{l}\left(\frac{(3\gamma-5)^2}{4} - \frac{(3\gamma-5)(\gamma-1)I}{I_o} - \frac{(\gamma-1)^2 I^2}{I_o^2}\right) + \\ \left((3-\gamma)(3\gamma-5)\beta - \frac{(\gamma-1)(3-\gamma)2\beta I}{I_o}\right)c_x^2 + (3-\gamma)^2\beta^2 c_x^4\end{array}\right]\left(\frac{\partial u_x}{\partial x}\right)^2 \end{array} \right]$$

$$+t_R^2\left[\begin{array}{l}\left(\frac{5c_x}{2\beta}-\frac{I\ c_x}{I_o\beta}-c_x^3\right)\frac{D}{Dt}\left(\frac{\partial\beta}{\partial x}\right)+\left\{\begin{array}{l}\left(-\frac{5}{2\beta}+\frac{I}{I_o\beta}+3c_x^2\right)\frac{Du_x}{Dt}\\ -\frac{5c_x}{2\beta^2}\frac{D\beta}{Dt}\end{array}\right\}\left(\frac{\partial\beta}{\partial x}\right)\\ +\left((3-\gamma)\beta c_x^2-\frac{(\gamma-1)\ I}{I_o}c_x+\frac{(3\gamma-5)}{2}\right)\frac{D}{Dt}\left(\frac{\partial u_x}{\partial x}\right)+\\ \left\{\left((3-\gamma)c_x^2-\frac{(\gamma-1)}{\beta I_o}\right)\frac{D\beta}{Dt}-2(3-\gamma)\beta c_x\frac{Du_x}{Dt}\right\}\left(\frac{\partial u_x}{\partial x}\right)\end{array}\right]$$

$$+t_R^2\left[\begin{array}{l}\left(\frac{5c_x^2}{2\beta}-\frac{I\ c_x^2}{I_o\beta}-c_x^4\right)\frac{\partial^2\beta}{\partial x^2}+\left(\begin{array}{l}-\frac{5c_x}{2\beta}\frac{\partial u_x}{\partial x}+\frac{I\ c_x}{I_o\beta}\frac{\partial u_x}{\partial x}+3c_x^3\frac{\partial u_x}{\partial x}\\ -\frac{5c_x^2}{2\beta^2}\frac{\partial\beta}{\partial x}\end{array}\right)\frac{\partial\beta}{\partial x}\\ +\left((3-\gamma)\beta c_x^3-\frac{(\gamma-1)\ I}{I_o}c_x+\frac{(3\gamma-5)}{2}c_x\right)\frac{\partial^2 u_x}{\partial x^2}+\\ \left(-2(3-\gamma)\beta\frac{\partial u_x}{\partial x}+(3-\gamma)c_x^2\frac{\partial\beta}{\partial x}-\frac{(\gamma-1)\ I}{\beta I_o}\frac{\partial\beta}{\partial x}\right)\left(\frac{\partial u_x}{\partial x}\right)\end{array}\right]. \qquad \text{(A-3)}$$

This perturbation term has to satisfy the moment closure property, expressed as

$$<\Psi, Kn^i\overline{f}_i>_{1\le i\le 2}=0. \qquad \text{(A-4)}$$

Evaluation shows that $<\Psi, Kn^2\overline{f}_2>\neq 0$ so we require additional moment closure terms thus making the determination of f_2 non-unique [54]. The complete second order can be evaluated in terms of moment closure coefficients $\vartheta_{\tau,\mathrm{k}}$ and $\vartheta_{q,\mathrm{k}}$ as

$$f_2=f_0+Kn\overline{f}_1-Knt_R\left[\frac{D\overline{f}_1}{Dt}+\frac{\partial f_0\tilde{\xi}_1}{\partial x}\right] \qquad \text{(A-5)}$$

$$\tilde{\xi}_1=-\frac{1}{Kn}\left(\frac{\tilde{\xi}_\tau}{P}\tau+\frac{\tilde{\xi}_q}{P}q\right) \qquad \text{(A-6)}$$

$$\tilde{\xi}_\tau=\left(\frac{3\gamma-5}{2(3-\gamma)}\vartheta_{\tau,1}-\frac{I}{I_o^2}\frac{1}{4\beta}\vartheta_{\tau,2}+\beta c_x^2\vartheta_{\tau,3}\right) \qquad \text{(A-7)}$$

$$\tilde{\xi}_q=2\beta\left(\frac{\gamma-1}{\gamma}\right)\left(-\frac{I}{I_o}c_x\vartheta_{q,1}+\frac{5}{2}c_x\vartheta_{q,2}-\beta c_x^3\vartheta_{q,3}\right) \qquad \text{(A-8)}$$

Table A-1 Closure coefficients

$\vartheta_{\tau,1}$	$\vartheta_{\tau,2}$	$\vartheta_{\tau,3}$	$\vartheta_{q,1}$	$\vartheta_{q,2}$	$\vartheta_{q,3}$
3	3	1	1	$\frac{1}{5}\left(\frac{3\gamma-5}{\gamma-1}\right)$	$-\frac{1}{3}\left(\frac{3-\gamma}{\gamma-1}\right)$
3	3	1	$-3\left(\frac{\gamma-1}{3-\gamma}\right)$	$-\frac{3}{5}\left(\frac{3\gamma-5}{3-\gamma}\right)$	1
1	1	3	1	$\frac{1}{5}\left(\frac{3\gamma-5}{\gamma-1}\right)$	$-\frac{1}{3}\left(\frac{3-\gamma}{\gamma-1}\right)$
1	1	3	$-3\left(\frac{\gamma-1}{3-\gamma}\right)$	$-\frac{3}{5}\left(\frac{3\gamma-5}{3-\gamma}\right)$	1

where closure coefficients $\vartheta_{\tau,\,k}$ and $\vartheta_{q,\,k}$ $\forall k = 1,2,3$ differ from the closure coefficients given by Balakrishnan [54]. Table A-1 shows the closure coefficients. It should be noted that Burnett equations are embedded within Grad's 13 moment method [48] and can easily be extracted using Chapman-Enskog theory. Another alternative to extract Burnett equations from moment systems is Maxwellian iteration of Ikenberry and Truesdell [77]. For more details on second order Chapman-Enskog expansion and Burnett equation refer Struchtrup[31].

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