Numerical modeling of nozzle gas flow using continuum approach in transition regime

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Abstract. This study is devoted to the numerical modelling of two-dimensional micro nozzle gas flow in continuum and transition regime with continuum mathematical models. Regularized 13-moment (R13) set of equations and Navier-Stokes-Fourier (NSF) equations are used as continuum approaches here. The numerical results for two-dimensional nozzle flow of the R13 equations and NSF equations have been compared for two cases of input and output pressures.

1. Introduction
It is known that the assumption of a continuum medium is valid in case where the mean free path of the molecules is much smaller than the characteristic linear size of the flow. In this case the Navier-Stokes-Fourier (NSF) equations are correct. If this condition is violated, the fluid will not be in thermodynamic equilibrium, then the result - occurrence a variety rarefied effects. The criterion of a flow rarefaction is a Knudsen number (Kn). Kn is defined as the ratio of the average mean free path to the typical length scale of the flow. Numerous analytical, experimental and numerical investigations have helped to make the classification of flow regimes of gas into the rarefied effects, based on the local Knudsen number. The range of Knudsen number Kn<10⁻³ corresponds to the continuum flow, 10⁻³<Kn<10⁻¹ is slip flow, 10⁻¹<Kn<10 is flow in the transitional regime, for Kn>10 is the free-molecular regime. So the formal area of the applicability of NSF equations with kinetic boundary conditions is Kn<10⁻¹ [1].

In micro-nozzles a continuum flow occurs in the combustor, transonic section, and the flow core of the supersonic section, while the slip and transition regimes are observed near the walls, at the nozzle exit, in high-gradient zones of shock-wave structures, and in the initial section of the jet. In the far-field region of the jet, we can observe a free-molecular flow. Due to the variety of flow regimes, flows in such devices are difficult to simulate in sense of mathematical approach and numerical methods. Accordingly, different medium models have to be used in different zones of the computational domain and the resulting solutions have to be matched at the boundaries of the zones or we need to use a universal approach to the entire problem, which is not always an optimal way out. Examples of universal approaches, in which all the flow regimes are computed using unified kinetic algorithms, include nonequilibrium flow simulation based on the direct solution of the Boltzmann equation [2,3] or model equations [4-7], the direct simulation Monte Carlo (DSMC) method [8-10]. However, for
low-velocity gas flows in three dimensions, an exact solution is difficult to compute by applying kinetic methods, and this task often lies beyond the capabilities of modern computers (e.g., the DSMC method yields a wide statistical scatter under such conditions, while the direct solution of the Boltzmann equation and molecular dynamics methods lead to high computational costs at low Knudsen numbers).

For processes in the transition regime, where, approximately, 0.01<Kn<10, extensions of the hydrodynamic equations are based either on the Chapman-Enskog method [1,11,12], or on Grad’s moment method [1,11,13,14]. In the given work we have stopped on the question of the applicability of 13 moment system of Grad with its proposed modification [14,15] to two-dimensional supersonic flows. The obtained system is here called the «regularized Grad’s set» (or R13). The choice of the system of thirteen moments indicates that all variables in this case have clear physical meaning (density, components of a vector of speed, pressure tensor and a vector of a heat flux).

2. Mathematical model

2.1. Bulk equations

The regularization of the Grad’s original 13-moment system [13] was derived in 2003 [15] by a Chapman-Enskog expansion [12] of higher moment equations only, based on the assumption of faster relaxation times for higher moments. Later derivations of the R13 equations were developed explicitly without this assumption (Order of Magnitude Method) [11]. The resulting equations contain higher order terms which behave well in the description of shocks [16-20] and some two dimensional supersonic flow simulations [21-23]. The tensor form of the regularized 13-moment system (R13) can be written as

\[
\frac{\partial \rho}{\partial t} + \rho \frac{\partial u_i}{\partial x_i} = 0, \tag{1}
\]

\[
\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = 0, \tag{2}
\]

\[
\frac{3}{2} \rho \frac{\partial \theta}{\partial t} + \frac{3}{2} \rho u_k \frac{\partial \theta}{\partial x_k} + \frac{\partial q_{ij}}{\partial x_j} + p \frac{\partial v_k}{\partial x_k} + \sigma_{ij} \frac{\partial \nu_{ij}}{\partial x_j} = 0, \tag{3}
\]

\[
\frac{\partial \sigma_{ij}}{\partial t} + \frac{\partial \sigma_{ij} \nu_k}{\partial x_k} + \frac{4}{5} \frac{\partial q_{ij}}{\partial x_j} + 2p \frac{\partial \nu_{ij}}{\partial x_j} + 2 \sigma_{ij} \frac{\partial \nu_{ij}}{\partial x_j} = \frac{\sigma_{ij}}{\tau}, \tag{4}
\]

\[
\frac{\partial q_i}{\partial t} + \frac{\partial q_i \nu_j}{\partial x_j} + \frac{5}{2} \rho \frac{\partial \theta}{\partial x_j} + \frac{5}{2} \sigma_{ik} \frac{\partial \theta}{\partial x_k} + \theta \frac{\partial \sigma_{ik}}{\partial x_k} - \sigma_{ik} \frac{\partial \rho}{\partial x_k} - \frac{\sigma_{ik}}{\rho} \frac{\partial \sigma_{ik}}{\partial x_k} + \frac{2}{3} \frac{\partial q_i}{\partial x_j} + \frac{2}{5} \frac{\partial q_i}{\partial x_j} + \frac{2}{5} \frac{\partial q_i}{\partial x_j} + \frac{1}{2} \frac{\partial R_{ik}}{\partial x_k} + \frac{1}{6} \frac{\partial \Delta}{\partial x_k} + m_{ik} \frac{\partial \nu_{ij}}{\partial x_j} = -\frac{2}{3} q_i \frac{\partial \tau}{\partial x_i}, \tag{5}
\]

where the mass density \( \rho \), velocity \( u_i \), temperature in energy units \( \theta = \frac{k}{\mu} T \) (\( k \) is the Boltzmann constant and \( m \) the particle mass), trace-free viscous stress tensor \( \sigma_{ij} \) (with \( \sigma_{ii} = 0 \)), and heat flux \( q_i (i=x, y, z) \) form 13 primitive variables. The pressure is given by the ideal gas law \( p = \rho \theta \), and \( \tau = \mu / p \) is the relaxation time, with the viscosity coefficient \( \mu \). The viscosity in this study is defined by combined law [24]

\[
\mu(T, \frac{T}{T}) = \begin{cases} 
\mu(T) \left( \frac{T}{T_0} \right)^{\nu}, & T < T_0, \\
\mu(T) \left( \frac{T}{T_0} \right)^{\nu_2}, & T \geq T_0 
\end{cases} \tag{6}
\]
where $T_c$ is the critical temperature ($T_c = 150K$, $S = 128.35K$ and $a = 0.945$ for argon) [24]. The angular brackets in the subscripts indicate the trace-free and symmetric part of the tensor [11]. Equations (1) – (3) are the conservation laws for mass, momentum and energy; equations (4) and (5) are the moment equations for stress tensor and heat flux vector, respectively. These 13 equations must be closed by constitutive relations for the higher moments $R_{ij}$, $\Delta$, $m_{ik}$, and these differ based on the method of (regularizing) closure [19,20]. For Grad’s original 13 moment equations [13], $R_{ij} = \Delta = m_{ik} = 0$. Higher-order moments have the following analytical form [15]:

$$m_{ij} = -2\tau \left[ \frac{k}{m} \frac{\partial \sigma_{ij}}{\partial x_j} - \frac{k}{m} \sigma_{ij} \frac{\partial \ln \rho}{\partial x_j} + \frac{4}{5} q_i \frac{\partial \sigma_{ij}}{\partial x_j} - \sigma_{ij} \frac{\partial \sigma_{ij}}{\partial x_j} \right].$$

(7)

$$R_{ij} = -\frac{24}{5} \left[ \frac{k}{m} \frac{\partial q_i}{\partial x_j} + \frac{k}{m} \frac{\partial \sigma_{ij}}{\partial x_j} + \frac{5}{7} \frac{k}{m} \left( \sigma_{ij} + \sigma_{ik} \frac{\partial \sigma_{ij}}{\partial x_i} - \frac{2}{3} \sigma_{ij} \frac{\partial \sigma_{ij}}{\partial x_i} \right) - \frac{k}{m} \frac{\partial \sigma_{ij}}{\partial x_i} \right].$$

(8)

$$\Delta = -12\tau \left[ \frac{k}{m} \frac{\partial q_i}{\partial x_i} + \frac{2}{5} \frac{k}{m} q_i \frac{\partial \sigma_{ij}}{\partial x_i} - \frac{k}{m} \frac{\partial q_i}{\partial x_i} + \frac{1}{\rho} q_i \frac{\partial \sigma_{ij}}{\partial x_i} + \frac{k}{m} \sigma_{ij} \frac{\partial \sigma_{ij}}{\partial x_i} \right].$$

In this paper we studied the behavior of the linear version [21] of this system. In the case, the calculation of high-order moments involves only terms that are responsible for the so-called gradient transport mechanism (GTM) [25] for the stress tensor and heat flux. It is these terms that ensure stabilization of the original Grad’s system of equations. The remaining terms omitted in the linear case form the so-called non-gradient transport mechanism (NGTM) [25].

In the linear case (GTM), higher-order moments have the following form:

$$m_{ij} = -2\tau \frac{k}{m} \frac{\partial \sigma_{ij}}{\partial x_j}, \quad R_{ij} = -\frac{24}{5} \frac{k}{m} \frac{\partial q_i}{\partial x_j}, \quad \Delta = -12\tau \frac{k}{m} \frac{\partial q_i}{\partial x_j}.$$  

(10)

The NSF equations of classical hydrodynamics can be obtained from the above by Chapman-Enskog expansion, which yields the Navier-Stokes and Fourier laws as

$$\sigma_{ij}^{\text{NSF}} = -2\mu \frac{\partial v_i}{\partial x_j}, \quad q_i^{\text{NSF}} = -\frac{15}{4} \mu \frac{\partial \theta}{\partial x_i}.$$  

(11)

In 2006 M. Torrilhon in work [21] has offered the divergent form of the R13 equations for the two-dimensional case. For the two-dimensional case (the number of the equations then decreases to nine) this system of the equations can be written down as follows:

$$\frac{\partial U(W)}{\partial t} + \text{div} F(W) = P(W), \quad W = \left\{ \rho, \rho v_i, \rho p, \rho p_i, \sigma, \rho q_i \right\}^T,$$

(12)

where $W$ is the vector of primitive variables, $\sigma = \sigma_{ij}$, $p = (p_x + p_y) / 3$. Vectors $U(W)$, $F(W)$ and $P(W)$ are vectors of conservative variables, fluxes and relaxation terms accordingly. The form of these vectors is presented in [21].

2.2. Boundary conditions

The first attempt to derive the boundary conditions on a solid wall for R13 system was done by Gu and Emerson in [26]. Further a similar method was used by Struchtrup and Torrilhon to derive their version of the boundary conditions [27] on the solid wall. In both cases, Maxwell’s accommodative model [28] was the base for derivation these boundary conditions. The idea of such formulation of the boundary conditions is that some part ($1 - \alpha$) of the molecules reflects specularly from the wall. The rest $\alpha$ part of the molecules diffusely reflects with a Maxwellian distribution $f^{\text{tr}}_{\omega}$ at the temperature of the wall. As result the compound «wall» distribution function is as follows:
f^{w}(v_{i},v_{j},v_{k})=egin{cases} \alpha f^{w}_{m}+(1-\alpha)f\left(v_{i},-v_{j},v_{k}\right), & v_{i} \geq 0, \\ f\left(v_{i},v_{j},v_{k}\right), & v_{i} \leq 0. \end{cases}
(13)

Then, in order to obtain conditions for each moment on the wall, it is necessary to make the integration of the equations for the corresponding weight of each moment. After integration the following boundary conditions for the solid isothermal wall were obtained [27]:

\[ u = u_{w} - \frac{1}{p_{a}} \left( n_{y} \sqrt{2 \theta \frac{2-\alpha}{\alpha} \gamma_{y} + \frac{m_{yy} + q_{k}}{2}} \right), \]
(14)

\[ \theta = \theta_{w} - \frac{1}{p_{a}} \left( n_{y} \sqrt{2 \theta \frac{2-\alpha}{\alpha} q_{s} + \frac{\partial \gamma_{y}}{4} + \frac{5R_{yy}}{56} + \frac{\Delta}{30}} \right) \left( u - u_{w} \right)^{2}, \]
(15)

\[ R_{y} = n_{y} \sqrt{2 \pi \theta 2-\alpha} \left[ p_{a} \frac{\partial u}{5} - \frac{1}{\alpha} \frac{\partial m_{yy}}{2} - \frac{11}{5} \frac{\partial q_{s} - p_{a} (u - u_{w})^{3}}{2} + 6 p_{a} \left( \theta - \theta_{w} \right) (u - u_{w}) \right], \]
(16)

\[ m_{xx} = -n_{y} \sqrt{2 \pi \theta 2-\alpha} \left[ \frac{p_{a}}{5} \left( \theta - \theta_{w} \right) - \frac{4 p_{a} \gamma}{5} (u - u_{w})^{2} + \frac{R_{y}}{14} + \theta \left( \gamma_{y} - \frac{\partial \gamma_{y}}{5} \right) + \frac{\Delta}{50} \right], \]
(17)

\[ m_{yy} = n_{y} \sqrt{2 \pi \theta 2-\alpha} \left[ \frac{2 p_{a}}{5} \left( \theta - \theta_{w} \right) - \frac{R_{y}}{14} + \frac{\Delta}{75} - \frac{7}{5} \frac{\partial \gamma_{y}}{5} + \frac{3 p_{a}}{5} (u - u_{w})^{2} \right]. \]
(18)

where \( n_{y} \) is the normal to wall surface directed into gas, \( \alpha \) is the factor of accommodation of a surface, \( u_{w} \) and \( \theta_{w} \) are the tangential velocity and wall temperature respectively.

These equations represent the five so-called kinetic boundary conditions. The integrals for the moments, which weight is proportional to the weight of even degree of the normal component of particle velocity are equal to zero [27]. The first equation determines the slip velocity on the wall, the second boundary condition - the temperature jump. The remaining equations are expressions for the moments of higher order (the new moments in comparison with Grad’s 13-moment system). Missing relations for the determination of the remaining variables can be obtained from the main flow equations. The question of formulating proper boundary conditions for the R13 equations is under ongoing investigation [29].

The variant of kinetic boundary conditions [30] for NSF equations is used for numerical simulation of solid wall [30]

\[ u = u_{w} + \frac{2 - \alpha}{\alpha} \frac{\partial u}{\partial y} + \frac{3}{4 \rho T} \frac{\partial T}{\partial x}, \]
(19)

\[ T = T_{w} + \frac{2 - \alpha}{\alpha} \frac{2 \gamma}{\gamma + 1 Pr} \frac{\partial T}{\partial y}, \]
(20)

where \( \lambda \) is the mean of the average free path, \( \gamma \) is the ratio of specific heats and \( Pr \) is Prandtl number.

3. Numerical scheme

Implemented numerical method for R13 and NSF equations is a version of high resolution Godunov method with a linear reconstruction of the flow parameters [31]. To approximate both systems of equations we introduce a regular computational grid consisting of convex quadrilateral cells.

The second-order accuracy in space for smooth solutions is achieved using essentially two-dimensional reconstruction procedures [32,33] for the primitive variables within each computational cell. For a discretization "elliptical" part of the fluxes (diffusion terms) the standard central difference approximation is used.

A modified second order Runge-Kutta method [32-34] is used to approximate the equation system in time. So the divergent term is approximated explicitly, and the relaxation term - implicitly. Therefore, in each cell at each time stage of the method a system of nonlinear equations has to be
solved. But it doesn’t increase computational time too much, because this nonlinear system can be easily solved due to structure of the relaxation terms. Numerical scheme based on Newton’s method is used for solid wall boundary conditions modeling for R13 equations [32-34].

4. Numerical results

4.1. Formulation of the problem

The two dimensional argon nozzle flow is considered. The half-angle of the solution of the nozzle confuser part is 30° and the half-angle of the diffuse one is 45°. The width of critical cross section is 2 mm. The input temperature is 300 K. The ratio of input and output pressure is equal to 10³. The numerical results for both methods have been obtained for three variants of input pressure \( p_{\text{in}} = 10 \text{ atm.}, p_{\text{up}} = 1 \text{ atm.} \text{ and } p_{\text{up}} = 10^{-1} \text{ atm.} \)

4.2. Continuum and slip flow regime

The numerical results for the variant of deep continuum regime (with \( p_{\text{up}} = 10 \text{ atm.} \)) are almost the same for R13 and NSF approaches. This fact just proves that R13 equations give the same physical result for supersonic nozzle flow in continuum regime as NSF equations. With the increase of input pressure in ten times the small difference in Mach number distribution fields can be seen (see figure 1). The flow inside of the nozzle is same and the difference grows with the distance from the nozzle edge.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Mach number distribution for NSF (a) and R13 (b) equations for \( p_{\text{up}} = 1 \text{ atm.} \).
\end{figure}

The figure 2 presents the field of local Knudsen number for this case counted by the average free path for Maxwell molecules

\[
Kn = \frac{\lambda}{\hbar} = \sqrt{\frac{\pi \mu(\Theta)\sqrt{\Theta}}{ph}}
\]  \hspace{1cm} (21)

where \( \hbar \) is the critical cross section size. As it can be seen, Knudsen number is moderate for the applicability of NSF approach here. The area of moderately rarefied gas (\( Kn > 0.1 \)) is outside of the interest for the nozzle flow problem here.
Figure 2. The distribution of Knudsen number for $p_{\text{up}} = 1$ atm.

4.3. Transition regime

The further increasing of pressure ($p_{\text{up}} = 10^{-1}$ atm.) has obvious influence to the flow in the low pressure chamber (figure 3). The difference between numerical results can be seen inside the nozzle. The width of boundary layers is different. So we have the difference of Mach number function along the symmetry plane. The field of local Knudsen number (figure 4) shows that rarefaction nonequilibrium effect can be observed inside the nozzle geometry. The level of $Kn = 0.1$ (formal boundary of transitional regime) is overstepped for significant part of considered flow.

Figure 3. Mach number distribution for NSF (a) and R13 (b) equations for $p_{\text{up}} = 0.1$ atm.

5. Conclusion

A numerical method for regularized 13-moment equations has been tested for supersonic nozzle flow. The numerical results presented here show the capability of R13 equations to extend the area of continuum approach applicability. In contrast with the kinetic methods, this approach is applicable for as an efficient numerical tool for simulation of transitional-regime gas flows in micro scale devices.
Figure 4. The distribution of Knudsen number for $p_{up} = 0.1$ atm.

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