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Rapid communication

Comparative study for rarefied gas flow into vacuum through a short circular pipe

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ABSTRACT

The problem of rarefied gas flow into vacuum through a short circular pipe is studied numerically by solving the Boltzmann kinetic equation. Comparison of the results obtained with the exact and S-model collision integrals is presented across a large range of Knudsen numbers. Computed values of mass flow rate are also compared against the DSMC results and experimental data from existing literature.

A rarefied gas flow through a finite-length circular pipe with the constant cross sectional area is a popular problem in the rarefied gas dynamics [1–3]. Computational results for the complete geometrical setup with pipe and both reservoirs include Direct Simulation Monte Carlo (DSMC) studies [4,5] and deterministic calculations on the basis of the Boltzmann kinetic equation with model collision integrals [6–11]. A recent comparison of computational results with experimental data for the short tube with the length to radius ratio $L/R = 1$ can be found in Ref. [12].

The aim of this short communication is to compare different computational approaches for the particular case of the short pipe $L/R = 1$ and gas flow into vacuum. These approaches are the direct numerical solution of the Boltzmann kinetic equation with the exact collision integral and S-model collision integral [13,14]. The results of the kinetic studies are evaluated against the DSMC data [4] and experimental measurements [15]. The emphasis is to obtain well-resolved (converged) data on the basis of the kinetic equations in order to establish the relative accuracy of approaches. The work therefore complement the earlier review publication [12] and contributes to the proposed set of benchmark problem results.

Let us introduce a Cartesian coordinate system (x,y,z) with the origin located in the centre of the middle section of the pipe the Oz axes directed along the tube. A steady three-dimensional state of the rarefied gas is determined by the velocity distribution function $f(\boldsymbol{x},\boldsymbol{\xi})$, where $\boldsymbol{x} = (x,y,z)$ is the spatial coordinate, $\boldsymbol{\xi} = (\xi_x,\xi_y,\xi_z)$ is the molecular velocity vector. For the rest of the paper, the non-dimensional formulation is used, in which the spatial coordinates $\boldsymbol{x}$, mean velocity $\boldsymbol{u} = (u_1,u_2,u_3)$, number density n, temperature T, heat flux vector $\boldsymbol{q} = (q_1,q_2,q_3)$, viscosity μ and distribution function f are scaled using the following quantities:

$$R, \quad \beta, \quad n_1, \quad T_1, \quad mn_1\beta^3, \quad \mu_1 = \mu(T_1), \quad n_1\beta^{-3}, \tag{1}$$

where $n_1 = p_1/kT_1$ is the number density in the left reservoir, m is the mass of a molecule, $\beta = \sqrt{2kT_1/m}$ is the most probable speed, k is the Boltzmann constant. The degree of gas rarefaction is described by the so-called rarefaction parameter δ_1, which is inversely proportional to the Knudsen number:

$$\delta_1 = \frac{Rp_1}{\mu_1\beta}$$

Below, the non-dimensional variables are denoted by the same letters as the dimensional ones. The distribution function f is assumed to satisfy the Boltzmann kinetic equation

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$$\xi_x\frac{\partial f}{\partial x}+\xi_y\frac{\partial f}{\partial y}+\xi_z\frac{\partial f}{\partial z}=\delta_1 I(f,f) \tag{2}$$

Here $I(f,f)$ is the collision integral. The expression for the exact Boltzmann collision integral can be found in various references, e.g. Refs. [16,17], and is omitted here for the sake of brevity. For the S-model equation [13,14] the function $I(f,f)$ takes the following non-dimensional form:

$$I(f,f)=\frac{p}{\mu}\left(f^{(S)}-f\right),\quad f^{(S)}=f_M\left[1+\tfrac{4}{5}(1-\mathrm{Pr})S_\alpha c_\alpha\left(c^2-\tfrac{5}{2}\right)\right],$$
$$f_M=\frac{n}{(\pi T)^{3/2}}\exp(-c_\alpha c_\alpha),\quad S_i=\frac{2q_i}{nT^{3/2}},\quad v_i=\xi_i-u_i,\quad c_i=\frac{v_i}{\sqrt{T}} \tag{3}$$

Here summation over repeated Greek indices is assumed. For a monatomic gas the Prandtl number $\mathrm{Pr}=2/3$.

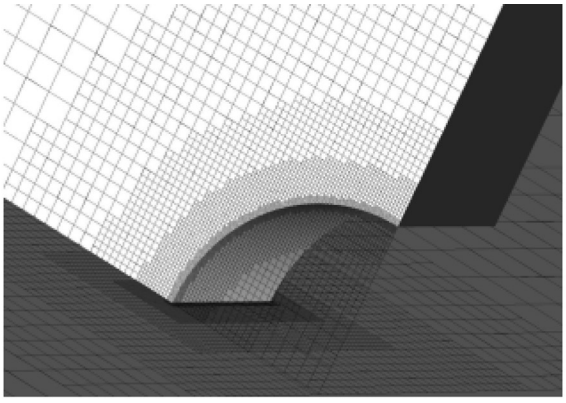
The non-dimensional macroscopic quantities are defined as the integrals of the velocity distribution function with respect to the molecular velocity:

$$(n,n\boldsymbol{u},n(\tfrac{3}{2}T+u^2),\boldsymbol{q})=\int\left(1,\boldsymbol{\xi},\xi^2,\frac{1}{2}\boldsymbol{v}v^2\right)f\mathrm{d}\boldsymbol{\xi},$$
$$u^2=u_\alpha u_\alpha,\quad v^2=v_\alpha v_\alpha,\quad \xi^2=\xi_\alpha\xi_\alpha,\quad p=nT. \tag{4}$$

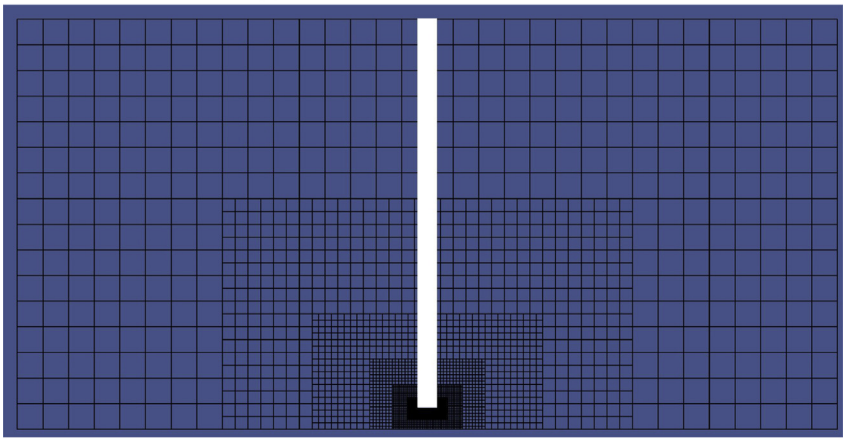
The kinetic Equation (3) has to be augmented with the boundary conditions on the pipe and reservoir walls. On the surface of the pipe the condition of diffuse molecular scattering on the pipe surface with complete thermal accommodation to the non-dimensional surface temperature $T_1\equiv 1$ is assumed. The density of reflected molecules n_w is found from the impermeability condition stating that the mass flux through the walls is equal to zero. The same condition is used for the parts of the reservoir walls directly adjacent to the pipe; these are located at $z=\pm L/2$. At the rest of the reservoir walls the distribution function of the molecules moving into the flow domain is specified as the locally Maxwellian one, with the parameters corresponding to the equilibrium values in each of the reservoirs.

The Boltzmann equation with the exact collision integral is solved using the Unified Flow Solver (UFS) [18–20]. The solution procedure consists of a second-order total variation diminishing (TVD) scheme on a semi-structured Cartesian grid with local mesh adaptation near pipe surface. The collision integral is evaluated with the Korobov's nodes on the equidistant Cartesian velocity grid. The calculations with the UFS solver are run on a quarter of the domain taking into account a symmetry relatively two orthogonal planes crossing the axis of the symmetry of the channel. In the most detailed computations the domain in physical space was a parallelepiped with sizes 20 × 20 × 40 units, a minimal cell size is approximately 0.01 in the direction normal to the pipe surface. A sequence of three spatial meshes is considered: 4.8, 32 & 245 thousand spatial cells for quarter of the domain. Graphical illustration of the finest spatial mesh can be found in Fig. 1.

The S-model kinetic Equation (3) is solved using an implicit time-marching algorithm conservative with the respect to the model collison integral. A summary of the numerical method and the corresponding computer program "Nesvetay 3D" can be found



(a) Three-dimensional close-up view



(b) Cross-sectional cut in the symmetry plane

Fig. 1. The finest spatial mesh 245 thousand spatial cells used for the UFS solver.

in Refs. [21], see also Refs. [22,9,23] and references therein. In the present study the most accurate locally one-dimensional TVD scheme implemented in the solver is employed.

The computational setup and most of the results for the S-model equation are taken from Ref. [23]. Reservoirs of length and radius 10 are used and a sequence of three spatial meshes (5.6, 41 & 350 thousand spatial cells) is considered. The complete geometry of the problem (whole pipe and reservoirs) is discretized. The non-uniform velocity mesh consisted of $25 \times 16 \times 32$ nodes with the extended domain size $-4 \le \xi_z \le 4$. It can be stated that for the range of δ_1 values used in the present work the accuracy of calculations for the S-model kinetic equation is within 1%. Further details can be found in Ref. [23].

Overall, the computational effort to solve the exact Boltzmann equation is at least 10 times larger as compared to the S-model kinetic equation. The difference is due to the higher complexity of the exact collision integral and as well as different time evolution methods. The "Nesvetay 3D" employs an implicit temporal discretization method allowing to run with large time step as compared to the explicit method in the UFS solver.

It should also be noted that two sets of calculations use differently sized spatial domains, which needs to be taken into account while comparing spatial resolution and spatial cell count.

For large-scale problems such as the ones reported here the calculations are carried out on modern high-performance clusters using Message Passing Interface (MPI). The calculations for "Nesvetay 3D" code are run on the high-performance computer "Lomonosov" of Lomonosov Moscow State University, Russia, using up to 128 cores of the machine. The UFS solver runs were executed on the MVS100K machine of the Joint Supercomputer Centre of the Russian Academy of Sciences (JSCC RAS) using 1000 cores.

The main computed quantity is the mass flow rate $\dot{M}$ through the pipe. In the presentation of the results, it is more convenient to use the so-called reduced mass flow rate Q, which is defined as a ratio of the mass flow rate $\dot{M}$ at given value of the rarefaction parameter δ_1 and L/R_1 to its values M_0 in the free-molecular orifice flow [24,5]. In the non-dimensional variables Q is calculated as

$$Q = \frac{\dot{M}}{\dot{M}_0}, \quad M = \int\limits_{A(z)} \rho(x,y,z) w(x,y,z) \mathrm{d}x\mathrm{d}y, \quad \dot{M}_0 = \frac{\sqrt{\pi}}{2}. \quad (5)$$

For the free-molecular case $\delta_1 = 0$ the solution can be obtained using the integral equation of Clausing [25]. There are a number of numerical solutions of this equation obtained by other authors afterwards as well as statistical solutions; for discussions see e.g. Ref. [16]. For $L/R = 1$ and $p_2 = 0$ the free-molecular value of the flow rate is $Q_{\mathrm{fm}} = 0.672$.

Table 1 contains the present numerical results, previous kinetic studies [6], DSMC data from Ref. [4] and experimental data from Ref. [15]. The numerical results cover the range $0 \le \delta_1 \le 100$, corresponding to flow regimes from the free-molecular one to the nearly continuum. It is seen that the free-molecular and nearly free-molecular solutions are computed by "Nesvetay 3D" solver with high accuracy even on the coarsest mesh. The UFS package overestimates the flow rate quite significantly on coarsest meshes, but converges as the spatial mesh is refined. For the medium and large values of δ_1 both solvers converge to the resolved value of the flow rate from below. It should be noted that the overall discrepancy of all three computational set of data (BKE, S-model and DSMC) at the nearly continuum regime $\delta_1 = 100$ is below 1%, which is within the computational error of simulations. The slightly larger flow rate value obtained by "Nesvetay 3D" solver can be explained by the generally higher-accuracy of its body-fitted spatial mesh and second-order accurate TVD advection scheme. The deviation of the S-model equation from the DSMC data is around 2% for $\delta_1 = 1$ and well below 1% for other values of the rarefaction parameter. The results of the BKE solver are close to the DSMC data from Ref. [4] for all δ_1 values.

Table 1
Mesh convergence studies for the reduced flow rate Q defined in Equation (5). Mesh resolution: for the BKE (i), (ii), (iii) correspond to 4.8, 32 & 245 thousand spatial cells for quarter of the domain; for the S-model – 5.6, 41 & 350 thousands cell for the whole domain.

δ_1	Exact BKE			S-model, Ref. [23]			DSMC,	Exp. Data,
	(i)	(ii)	(iii)	(i)	(ii)	(iii)	Ref. [4]	Ref. [15]
0.	0.690	0.679	0.674	0.666	0.670	0.672		
0.1	0.700	0.689	0.683	0.678	0.683	0.684	0.680	0.675
1.	0.767	0.762	0.756	0.758	0.766	0.768	0.754	0.743
10.	1.007	1.048	1.058	1.035	1.061	1.066	1.062	1.06
100.	1.211	1.322	1.358	1.290	1.351	1.367	1.358	1.33

Fig. 2 shows the axial distributions of density, temperature and axial velocity for $\delta_1 = 1$ and both the BKE and S-model equations. In order to improve the resolution of low-pressure region, a finer velocity mesh is used for this particular calculation by both codes. The solution is not sensitive to the spatial mesh for this value of the rarefaction parameter. Unlike the case of a longer pipe $L/R \ge 10$, in which the pressure profile becomes convex [7,11], the axial distribution of pressure remains almost linear inside the pipe for all values of δ_1. The temperature profile exhibits a typical behaviour, similar to that of the source flow. Namely, temperature drops as $z \to \infty$. Overall, there is a good agreement between solutions inside the pipe and its whereas some differences exist in velocity and temperature profiles downstream in the vacuum region, which can be due to both difference in the governing equations as well as accuracy of calculations for such a low pressure.

In conclusion, it can be stated that for the considered problem the use of the S-model kinetic equation provides good accuracy across all flow regimes as compared to the DSMC and BKE solutions. The largest discrepancy in the mass flow rate occurs in the rarefied regime $\delta_1 = 1$ and is below 2%. The computational cost to solve the S-model equation by "Nesvetay 3D" is significantly lower than that of the Unified Flow Solver for the Boltzmann equation with the exact collision integral. Future work will include the assessment of the relative accuracy of kinetic equations and corresponding solvers on more demanding flow problems.

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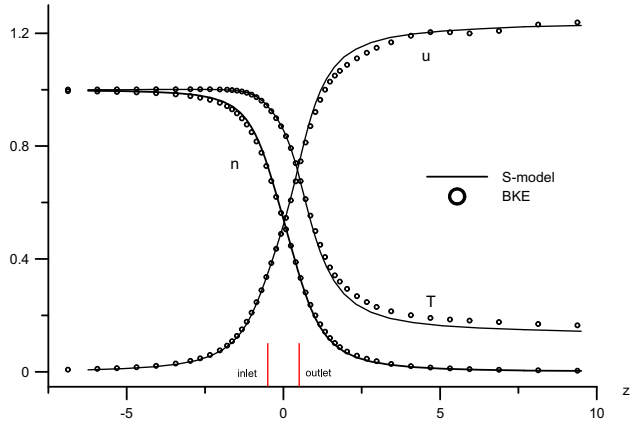

Fig. 2. Axial distributions of flow variables for $\delta_1 = 1$. The pipe corresponds to $-1/2 \le z \le 1/2$.

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References

[1] Sharipov F, Seleznev V. Data on internal rarefied gas flows. J Phys Chem Ref Data 1998;27(3):657–706.
[2] Koppenwallner G, Lips T, Dankert C. Discharge coefficients and on-axis flow properties in small sonic orifices at low Reynolds numbers. In: Ivanov M, Rebrov A, editors. Rarefied gas dynamics: 25-th international symposium, Novosibirsk 2007. p. 585–91.
[3] Jousten K, editor. Handbook of vacuum technology. Berlin: Wiley-VCH; 2008.
[4] Varoutis S, Valougeorgis D, Sazhin O, Sharipov F. Rarefied gas flow through short tubes into vacuum. J Vac Sci Technol 2008;26(1):228–38.
[5] Varoutis S, Valougeorgis D, Sharipov F. Simulation of gas flow through tubes of finite length over the whole range of rarefaction for various pressure drop ratios. J Vac Sci Technol A 2009;27(6):1377–91.
[6] Titarev V, Shakhov E. Computational study of a rarefied gas flow through a long circular pipe into vacuum. Vacuum, Special Issue “Vacuum Gas Dynamics: Theory, Experiments and Practical Applications” 2012;86(11): 1709–16.
[7] Titarev V, Shakhov E. Rarefied gas flow through a long circular pipe into vacuum. In: Rarefied gas dynamics. Proc. 28th int. symp., AIP conf. proc. 1501 2012. p. 465–72.
[8] Titarev V, Shakhov E. End effects in rarefied gas outflow into vacuum through a long tube. Fluid Dynamics 2013;48(5):697–707.
[9] Titarev V. Rarefied gas flow in a circular pipe of finite length. Vacuum 2013;94:92–103.
[10] Pantazis S, Valougeorgis D. Rarefied gas flow through a cylindrical tube due to a small pressure difference. Eur J Mech B Fluids 2013;38:114–27.
[11] Titarev V, Shakhov E, Utyuzhnikov S. Rarefied gas flow through a diverging conical pipe into vacuum. Vacuum 2014;101:10–7.
[12] Sharipov F. Benchmark problems in rarefied gas dynamics. Vacuum, Special Issue “Vacuum Gas Dynamics: Theory, Experiments and Practical Applications” 2012;86(11):1697–700.
[13] Shakhov E. Generalization of the Krook kinetic relaxation equation. Fluid Dynamics 1968;3(5):95–6.
[14] Shakhov E. Kinetic model equations and numerical results. In: Proc. XIVth intern. symp. rarefied gas dynamics. University of Tokyo Press; 1984. p. 137–48. invited paper.
[15] Fujimoto T, Usami M. Rarefied gas flow through a circular orifice and short tubes. J. Fluids Eng Tran ASME 1984;106(4):367–73.
[16] Koshamarov Y, Ryzhov Y. Applied rarefied gas dynamics. Moscow: Mashinostroenie; 1977 [in Russian].
[17] Aristov V. Direct methods for solving the Boltzmann equation and study of nonequilibrium flows. Dordrecht/Boston/London: Kluwer Academic Publishers; 2001.
[18] Kolobov V, Bayyuk SA, Arslanbekov R, Aristov V, Frolova A, Zabelok S. Construction of a unified continuum/kinetic solver for aerodynamic problems. AIAA J Space Rocket 2005;42(4):598.
[19] Kolobov V, Arslanbekov R, Aristov V, Frolova A, Zabelok S. Unified solver for rarefied and continuum flows with adaptive mesh and algorithm refinement. J Comput Phys 2007;223:589–608.
[20] Aristov V, Frolova A, Zabelok S, Arslanbekov R, Kolobov V. Simulations of pressure-driven flows through channels and pipes with unified flow solver. Vacuum, Special Issue “Vacuum Gas Dynamics: Theory, Experiments and Practical Applications” 2012;86(11):1717–24.
[21] Titarev V. Direct numerical solution of model kinetic equations for flows in arbitrary three-dimensional geometries. In: Rarefied gas dynamics. proc. 28th int. symp., AIP conf. proc. 1501 2012. p. 262–71.
[22] Titarev V. Efficient deterministic modelling of three-dimensional rarefied gas flows. Commun Comput Phys 2012;12(1):161–92.
[23] Titarev V, Dumbser M, Utyuzhnikov S. Construction and comparison of parallel implicit kinetic solvers in three spatial dimensions. J Comp Phys;256: 17–33.
[24] Shakhov E. The axisymmetric non-linear steady flow of a rarefied gas in a pipe of circular cross section. Comput Math Math Phys 1996;36(8):1123–31.
[25] Clausing P. Über die stromung sehr verdunnter gase durch röhren von beliebiger länge. Annalen der Physik 1932;(32):961–89.