Time-dependent rarefied gas flow into vacuum from a long circular pipe closed at one end

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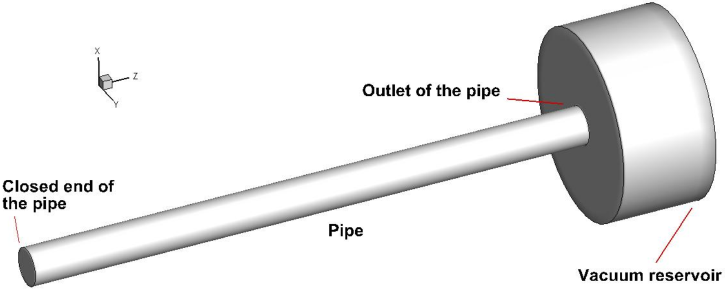
Specification of the problem

- At the initial time moment the rarefied gas at rest characterized by number density n_0 and temperature T_0 occupies a circular pipe of radius a and length L. The pipe is permanently closed at one end $z = -\text{L}$.
- At the outlet position $z = 0$ (other end of the pipe) a diaphragm separates the pipe and an infinitely large reservoir, in which there is no gas.
- At the start of the process $t = 0$ the diaphragm is removed and a non-stationary flow of the gas from the pipe into the reservoir starts.
- An example of geometry of the problem is shown here for $L/a = 30$.



BKE with the Shakhov model collision integral (1968)

- The three-dimensional equation for the velocity distribution function f takes the form

$$\xi_\alpha \frac{\partial f}{\partial x_\alpha} = \frac{p}{\mu}(f^+ - f), \quad f^+ = f_M\left[1 + \frac{4}{5}(1-\mathrm{Pr})\, S_\alpha c_\alpha \left(c^2 - \frac{5}{2}\right)\right],$$

$$f_M = \frac{n}{(2\pi R_g T)^{3/2}} \exp(-c^2), \quad S_i = \frac{1}{n}\int c_i c^2 f d\boldsymbol{\xi}, \quad \mathbf{c} = \frac{\mathbf{v}}{\sqrt{2R_g T}}, \quad c^2 = c_\beta c_\beta.$$

- Macroscopic quantities defined as

$$n = \int f d\boldsymbol{\xi}, \quad n\mathbf{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi}, \quad \frac{3}{2} mnR_g T + \frac{1}{2} mnu^2 = \frac{1}{2} m \int \xi^2 f d\boldsymbol{\xi},$$

$$\mathbf{q} = \frac{1}{2} m \int \mathbf{v} v^2 f\, d\boldsymbol{\xi}, \quad \mathbf{v} = \boldsymbol{\xi} - \mathbf{u}, \quad \rho = mn, \quad p = \rho R_g T,$$

$$u^2 = u_\alpha u_\alpha, \quad v^2 = v_\alpha v_\alpha, \quad \xi^2 = \xi_\alpha \xi_\alpha, \quad d\boldsymbol{\xi} = d\xi_x d\xi_y d\xi_z.$$

- Boundary condition on the surface:

$$f_w = \frac{n_w}{(2\pi R_g T_{\mathrm{sur}})^{3/2}} \exp\left(-\frac{\xi^2}{2R_g T_{\mathrm{sur}}}\right), \quad n_w = \sqrt{\frac{2\pi}{R_g T_{\mathrm{sur}}}} N_i, \quad N_i = -\int_{\xi_n<0} \xi_n f d\boldsymbol{\xi}.$$

- Here Prandtl number $\mathrm{Pr} = 2/3$, R_g is gas constant, m is molecular mass.

Non-dimensional form of the S-model equation

- Let us pass to non-dimensional variables as follows:

$$\mathbf{x}' = \frac{\mathbf{x}}{a}, \quad n' = \frac{n}{n_1}, \quad p' = \frac{p}{p_1}, \quad T' = \frac{T}{T_1},$$

$$\mathbf{u}' = \frac{\mathbf{u}}{v_*}, \quad \boldsymbol{\xi}' = \frac{\boldsymbol{\xi}}{v_*}, \quad \mathbf{q}' = \frac{\mathbf{q}}{mn_1 v_*^3}, \quad f' = \frac{f}{n_1 v_*^3}.$$

where $p_1 = mn_1 R_g T_1$, $v_* = \sqrt{2R_g T_1}$

- The degree of gas rarefaction is described by the so-called rarefication parameter δ_1, which is inversely proportional to the Knudsen number:

$$\delta = \frac{ap_1}{\mu(T_1)v_*} = \frac{8}{5\sqrt{\pi}}\frac{1}{\mathrm{Kn}}, \quad \mathrm{Kn} = \frac{\lambda_1}{a}.$$

Here λ_1 is the free molecular path at reference conditions.

- From now on, the non-dimensional variables are denoted by the same symbols as dimensional.

Non-dimensional form of the S-model equation (continued)

- In the non-dimensional variables the kinetic equation takes the form:

$$\xi_x \frac{\partial f}{\partial x} + \xi_y \frac{\partial f}{\partial y} + \xi_z \frac{\partial f}{\partial z} = \nu(f^{(S)} - f), \quad \nu = \frac{nT}{\mu(T)}\delta_1,$$

$$f^{(S)} = f_M \left(1 + \frac{4}{5}(1 - \mathrm{Pr})\mathbf{Sc}(c^2 - \frac{5}{2})\right), \quad f_M = \frac{n}{(\pi T)^{3/2}} e^{-c^2}, \quad \mathbf{S} = \frac{2\mathbf{q}}{nT^{3/2}}.$$

- Macroscopic quantities defined as

$$\left(n, n\mathbf{u}, \frac{3}{2}nT + nu^2, \mathbf{q}\right) = \int \left(1, \boldsymbol{\xi}, \xi^2, \frac{1}{2}\mathbf{v}v^2\right) f d\boldsymbol{\xi}.$$

  The non-dimensional pressure is given by $p = nT$.

- Boundary condition on the surface:

$$f(\mathbf{x}, \boldsymbol{\xi}) = f_w = \frac{n_w}{(\pi T_w)^{3/2}} \exp\left(-\frac{\xi^2}{T_w}\right), \quad \xi_n = (\boldsymbol{\xi}, \mathbf{n}) > 0,$$

$$n_w = N_i / N_r, \quad N_i = -\int_{\xi_n < 0} \xi_n f d\boldsymbol{\xi}, \quad N_r = +\int_{\xi_n > 0} \xi_n \frac{1}{(\pi T_w)^{3/2}} \exp\left(-\frac{\xi^2}{T_w}\right) d\boldsymbol{\xi}.$$

Numerical method of solution & Nesvetay-3D package

- Discrete velocity method conservative with respect to collision integral
  - Conservative calculations of macroscopic variables (number density, velocity, temperature, heat flux vector)
  - Euler explicit time marching
  - CFL number $\approx 0.25 \ldots 0.3$
- Second-order accurate Total Variation Diminishing method
  - Arbitrary cells in physical domain
  - Least-square or quasi-1D reconstructions
  - Various slope limiters
- Parallel solver
  - Either physical or velocity domains can be split
  - Calculations on up to 144 CPU cores (12 Intel Xeon Sandy Bridge CPUs)

Conservative discrete velocity framework

- Time marching:
$$\frac{\partial}{\partial t} f = -\boldsymbol{\xi}\nabla f + J(f), \quad J = \nu(f^{(S)} - f),$$
- Replace the infinite domain of integration in the molecular velocity space $\boldsymbol{\xi}$ by a finite computational domain.
- Let $\boldsymbol{\Xi}_k$ be a vector, made of k-th component of velocity nodes over the whole mesh:
$$\boldsymbol{\Xi}_k = (\xi_{k1}, \xi_{k2}, \xi_{k3}, \ldots \xi_{kN_\xi})^T.$$
- The kinetic equation is replaced by a system of N_ξ advection equations:
$$\frac{\partial}{\partial t}\mathbf{f} + \frac{\partial}{\partial x_\alpha}(\boldsymbol{\Xi}_\alpha \circ \mathbf{f}) = \mathbf{J}, \quad \mathbf{J} = \nu(\mathbf{f}^{(S)} - \mathbf{f}).$$

  Here operation $\circ$ corresponds to a component by component multiplication of vectors $c = a \circ b \quad \rightarrow \quad c_i = a_i b_i$.

One step explicit numerical method of Kolgan type

- Denote by $|V_i|$ the cell volume, $|A|_{il}$ area of face l. Integration over a control volume and use of calculus leads to the following implicit method:

$$\frac{\mathbf{f}_i^{n+1} - \mathbf{f}_i^n}{\Delta t} = \mathbf{R}_i^n = -\frac{1}{|V_i|} \sum_{l=1} \boldsymbol{\Phi}_{il}^n + \mathbf{J}_i^n,$$

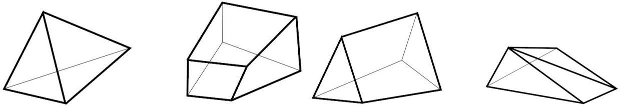
where $\mathbf{f}_i^n = \mathbf{f}(t^n, \mathbf{x}_i)$ - spatial average of distribution function in spatial cell V_i at time moment t^n.

- The numerical flux through the face A_{il} is defined as

$$\boldsymbol{\Phi}_{il}^n = \int\limits_{A_{il}} (\boldsymbol{\xi}_{nil} \circ \mathbf{f}^n) ds, \quad \boldsymbol{\xi}_{nil} = n_{1l}\boldsymbol{\Xi}_1 + n_{2l}\boldsymbol{\Xi}_2 + n_{3l}\boldsymbol{\Xi}_3.$$

Here vector $\boldsymbol{\xi}_{nl}$ consists of projections of velocity nodes onto outward unit normal $\mathbf{n}_{il}$ of face l of cell V_i.

- We consider cells of various shapes.



Flux calculation

- As is usual in upwind methods, the numerical flux depends on boundary extrapolated values $\mathbf{f}^-$ (inner value) and $\mathbf{f}^+$ (external value):

$$\Phi_{il}^n = \mathbf{G}(\mathbf{f}_{i_l}^n, \mathbf{f}_{i_l,l_1}^n)|A_{il}|,$$

  Here l_1 is the number of the face of the cell $\sigma_l(i)$, adjacent to the face l of the cell i.

- The exact Riemann solver $\mathbf{G}(\mathbf{f}^-, \mathbf{f}^+)$ is given by

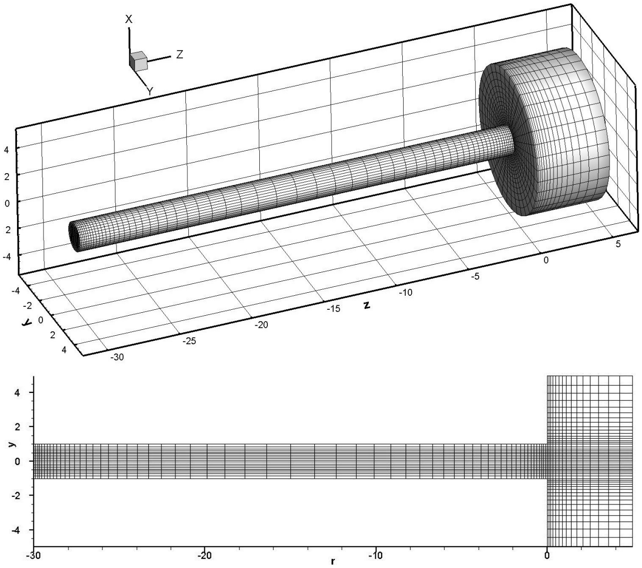
$$\mathbf{G}(\mathbf{f}^-, \mathbf{f}^+)^{\mathrm{exact}} = \frac{1}{2}\xi_{nil} \circ \left[(\mathbf{f}^- + \mathbf{f}^+)) - \mathrm{sign}(\xi_{nil}) \circ (\mathbf{f}^+ - \mathbf{f}^-)\right]$$

- For high-order method $\mathbf{f}^-$, $\mathbf{f}^+$ are found from a reconstruction procedure and depends on solution values in several neighboring cells.

Mesh parameters

- Calculations were performed for the pipe length $L = 10$ and $L = 30$ for $\delta_0 = 0$, 1 and 100. The reservoir size has the size of about five pipe radii.
- Verification: $L = 10$ and spatial meshes of 17 and 54 thousands hexahedrons, which differ in the radial resolution (clustering towards the pipe's surface) and longitudinal resolution inside the pipe.
- Spatial mesh is of O type, with a square patch in the centre of the cross section and clustering applied towards the pipe surface and its ends.
- The velocity domain is a cylinder and the velocity mesh is constructed in the cylindrical coordinate system. The velocity mesh resolution can be described by a group of three numbers, corresponding to the numbers of nodes in the radial, angular and ξ_z directions.
- For $\delta_0 \leq 10$ the mesh consists of $17 \times 16 \times 24$ cells whereas $21 \times 16 \times 32$ cells are used for $\delta_0 = 100$. The finer velocity mesh and slightly larger velocity domain size or $\delta_0 \gg 1$ are needed to properly resolve large temperature drops in the low-density region.
- Calculations have shown that the coarse of the two meshes is sufficient to obtain results with 2% accuracy. For the case $L = 30$ the mesh containing 27675 hexahedron cells is used, which is constructed by inserting the additional cells along the pipe

Example of computational mesh



Definitions of computed integral data

- Reduced flow rate at any inside position: $Q(z) = \frac{2}{\sqrt{\pi}}\dot{M}, \quad \dot{M}(z) = \int\limits_{A(z)} nu_3 dxdy.$
- We need the time-dependent value at the outlet position $Q^{\text{outlet}}(t) = Q(t, 0)$.
- At initial time $t = 0$ it is obvious that $Q^{\text{outlet}}(0) \equiv 1$.
- The gas dynamics solution of a rarefaction wave (expansion into vacuum) gives

$$u_z - c = \frac{z}{t}, \quad u_z + 3c = 3c_0, \quad c_0 = \sqrt{5/6}, \quad T = n^{2/3}, \quad -L < z < 0, \quad t < \frac{L}{c_0}$$

From here the explicit expression for the solution is given by

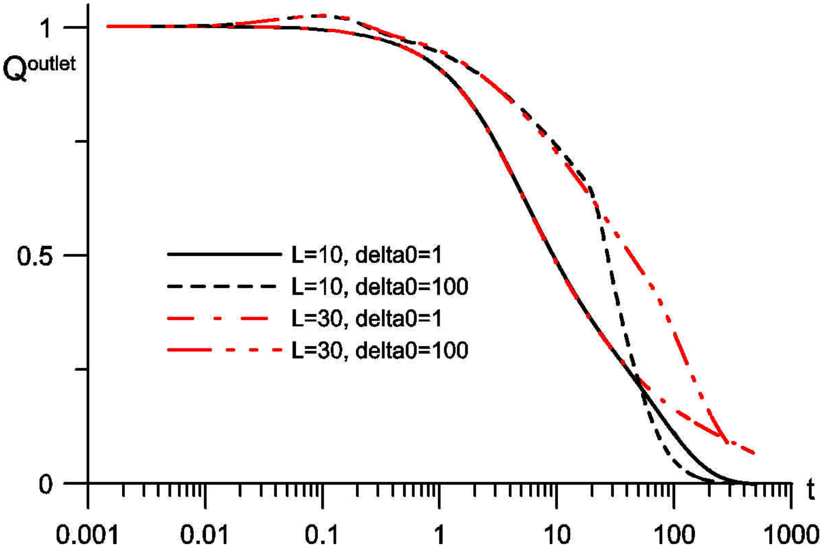
$$u_z = \frac{3}{4}(c_0 + \frac{z}{t}), \quad c = u_z - z/t, \quad T = \frac{6}{5}c^2, \quad n = T^{3/2}.$$

Gas dynamics flow rate through a circular pipe in the non-stationary expansion into vacuum:

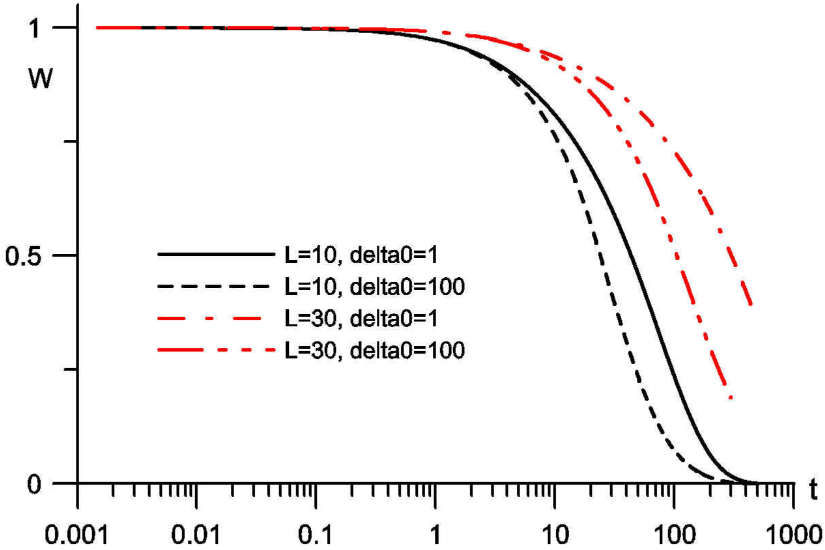
$$u_* = \frac{3}{4}c_0, \quad n_* = \frac{27}{64}, \quad \dot{M}_* = n_* u_* \pi \approx 0.907, \quad Q_* \approx 1.02$$

- Reduced total mass: $W(t) = \frac{M_{tot}(t)}{M_{tot}(0)}$, where $M_{tot}(t) = \int\limits_{-L \le z \le 0} n(t, \mathbf{x}) d\mathbf{x}$.

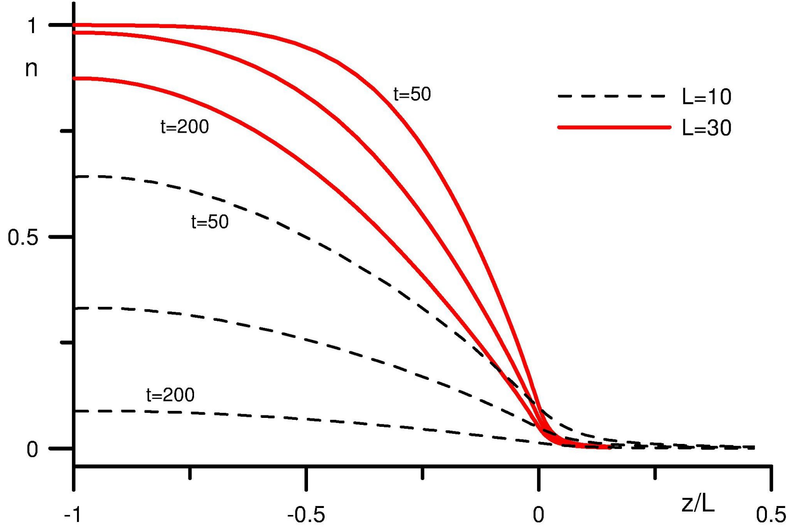
Computed reduced flow rate data for $L = 10, 30$.



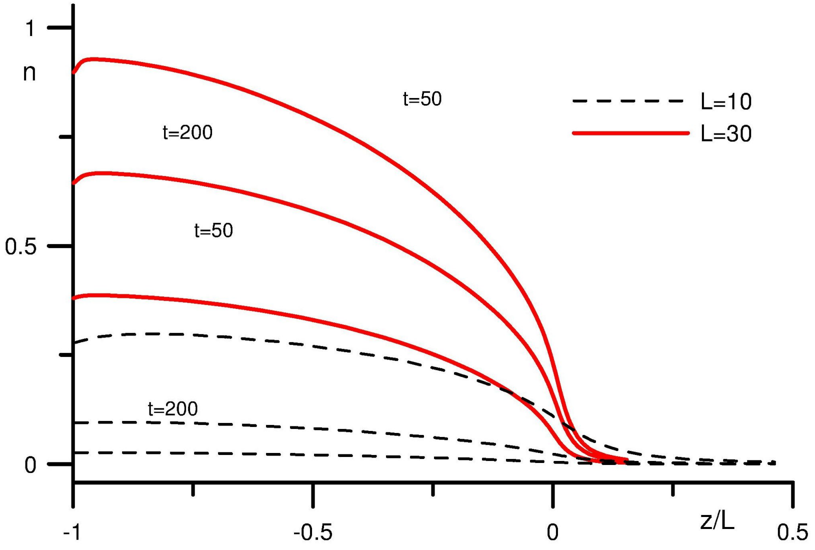
Computed reduced total mass



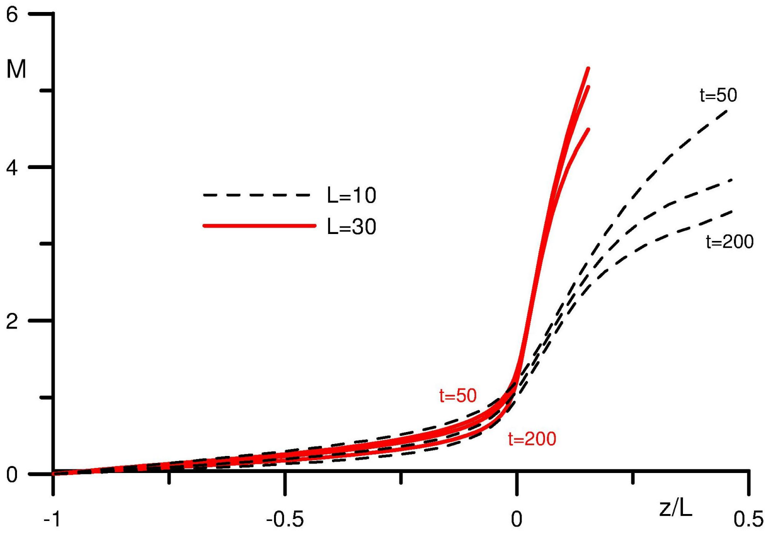
Axial distributions of density for $\delta_0 = 1$



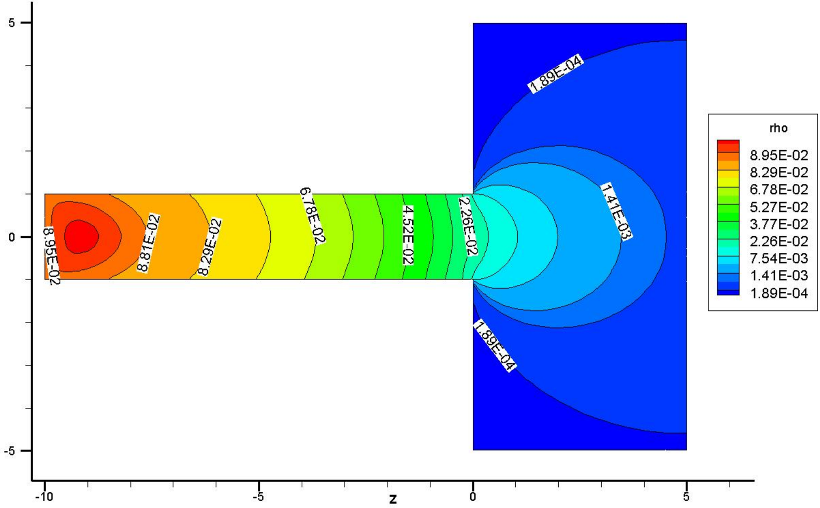
Axial distributions of density for $\delta_0 = 100$



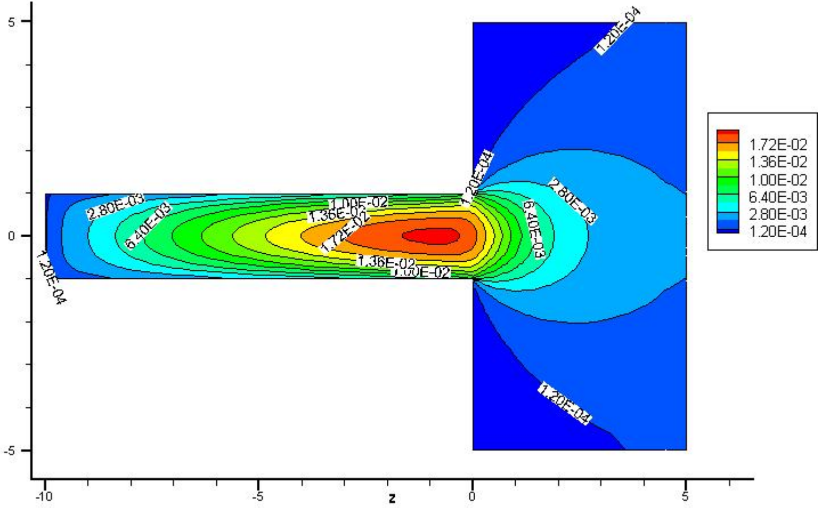
Axial distributions of Mach number for $\delta_0 = 100$



Density contour lines for $L = 10$, $\delta_0 = 100$ and $t = 100$.



Mass flow nu_3 for $L = 10$, $\delta_0 = 100$ and $t = 100$.



Conclusions

Some recent publications for 3D rarefied gas flows:

1. V.A. Titarev. Efficient deterministic modelling of three-dimensional rarefied gas flows // *Comm. Comp. Phys.* 2012. V. 12. N. 1. p. 162-192.
2. V.A. Titarev and E.M. Shakhov. Computational study of a rarefied gas flow through a long circular pipe into vacuum //*Vacuum, Special Issue "Vacuum Gas Dynamics"*. 2012. V. 86. N. 11. p. 1709-1716.
3. V. Titarev, M. Dumbser and S. Utyuzhnikov. Construction and comparison of parallel implicit kinetic solvers in three spatial dimensions // *J. Comp. Phys.* 2014. V. 256. p. 17-33.
4. E.V. Shakhov and V.A. Titarev. Non-stationary rarefied gas flow into vacuum from a circular pipe closed at one end // *Vacuum. 2014*, in press.
5. V.A. Titarev. Computer package Nesvetay-3D for modelling three-dimensional flows of monatomic rarefied gases // *Science & Education*. 2014. N. 6.

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