Design of Gas Micro Distribution Systems Consisting of Long Tubes

Serafeim MISDANITIS, Dimitris VALOUGEORGIS*

* Corresponding author: Tel.: ++30 2421074058; Email: diva@mie.uth.gr*
Department of Mechanical Engineering, University of Thessaly, Volos, Greece

Abstract A novel algorithm is developed for the design of gaseous micro distribution systems consisting of long tubes based on linear kinetic theory. Provided that the geometry of the pipe network is fixed the algorithm is capable of estimating the mass flow rates through the pipes as well as the pressure heads at the nodes of the network. The pressure distribution along each pipe element may also be provided. The analysis is valid and the results are accurate in the whole range of the Knudsen number, while the involved computational effort is very small. This is achieved by successfully integrating the well known kinetic results for single tubes into a typical solver for designing gas pipe networks.

Keywords: Kinetic theory, Rarefied gases, Knudsen number, Pipe network

1. Introduction

Rarefied gas flows through long channels of various cross sections have been extensively investigated over the years based on linear kinetic theory (Valougeorgis and Thomas, 1986; Sharipov, 1999; Valougeorgis, 2007; Naris and Valougeorgis, 2008). It has been clearly shown that this approach is the most reliable one in the case of low speed flows providing very accurate results in the whole range of the Knudsen number with minimal computational effort. Very good agreement with corresponding experimental work developed in micro or either in vacuum experimental facilities has been obtained (Varoutis et al., 2009; Pitakarnnop et al., 2010; Szalmas et al., 2010).

However, in many microfluidics applications, the gaseous distribution system is consisting of single channels accordingly combined in order to form a microchannel network. The implementation of such micrometer-sized systems, made possible by modern micro-fabrication techniques, enable the reduction of weight, power consumption, and production costs of various systems in several engineering fields including vacuum technology, high altitude gas dynamics, aerosol industry, porous media, and microfluidics. Despite the fact that computational algorithms dedicated to the design of gas pipe networks in the continuum regime are well developed (Potter and Wiggert, 1997), corresponding tools for the design of gaseous pipe networks operating under rarefied conditions have not been developed so far. Obviously this is a serious drawback in the detailed design and optimization of complex gaseous micro electromechanical devices.

In the present work a computational approach is presented for the design of pipe networks consisting of long tubes. This is achieved by successfully integrating the kinetic results obtained for the rarefied flow through each tube of the network into a typical network algorithm solving the whole distribution system. Once the geometry of the network is fixed, the integrated algorithm may successfully handle gas pipe networks of any complexity operating under any rarefied conditions from the free molecular, through the transition up to the slip and hydrodynamic regimes.

2. Formulation of the problem

A typical pipe network may be considered as a directed linear graph consisting of a finite number of pipe sections (or edges) interconnected in a specified configuration.

Each pipe is characterized of its length L, diameter D and roughness. A point where two or more pipes are joined is known as a junction node or simply as a node. The closed path uniquely formed by adjacent pipes is a loop, while the open path connecting two fixed-grade nodes is a pseudo-loop. A fixed grade node is a node where a consistent energy grade is maintained (e.g. a constant pressure reservoir). For a well-defined network with p pipes, n junction nodes, l loops and f fixed-grade nodes the relation

$$p = n + l + f - 1 \tag{1}$$

holds. Usually the geometry of the network is specified and the objective is to compute the flow quantities, i.e., the mass flow rates through each tube and the pressure head at each node. In the present setup, the losses in the junctions of the network are considered negligible compared to the losses through the long piping elements and are not taken into account. This assumption seems reasonable for $L/D > 100$.

Independent of the flow regime, the system of equations describing such a network is consisting of the pressure drop equations along each pipe element and the mass conservation equations at each node of the network. The pressure drop equations may be reduced to a set of the energy balance equations for the closed loops of the network, which along with the mass conservation equations form a closed set, which may be solved for the unknown mass flow rates. Then, the pressure heads at the nodes are estimated through the pressure drop equations. When the Knudsen number characterizing the flow through the network is very small and the flow is in the continuum or slip regimes, then the pressure drop equations along each channel are given by explicit algebraic expressions and their integration in the whole algorithm is straightforward. In contrary, when the flow is in the transition regime such expressions are not available. Here, this information is obtained from a data base, which has been developed for this purpose by solving a linearized kinetic equation in a wide range of the Knudsen number and obtaining the corresponding data.

Based on the above, in Subsection 2.1 all necessary information of the kinetic solution for rarefied flow through a single tube is provided, while in Subsection 2.2 the integrated algorithm for the flow solution of the whole network is described.

2.1 Single pipe formulation

The solution of a pressure driven rarefied gas flow through a long circular tube based on linear kinetic theory is a very well known problem (Sharipov and Seleznev, 1998) and therefore here, only information which is directly connected and needed to the solution of the whole network is reviewed. Since $D << L$, the flow is considered as fully developed and therefore the pressure (or density) varies only in the flow direction being constant at each cross section, while end effects at the connecting nodes of the channel are ignored. The mass flow rate at each cross section through the tube is given by

$$\dot{M} = 2\pi \int_0^R \rho(\tilde{z})\tilde{u}(\tilde{r})\tilde{r}d\tilde{r}, \tag{2}$$

where $0 \le \tilde{r} \le R$ is the radial direction, $0 \le \tilde{z} \le L$ is the flow direction, $\rho(\tilde{z})$ is the mass density and $\tilde{u}(\tilde{r})$ is the bulk velocity. By introducing into Eq. (1) the equation of state $\rho = 2P/\upsilon_0^2$, where $P = P(\tilde{z})$ is the local pressure along the tube υ_0 the most probable molecular velocity as well as the dimensionless variables $r = \tilde{r}/D$, $z = \tilde{z}/D$, $u = \tilde{u}/(\upsilon_0 X_P)$, where $X_P = (D/P)(dP/d\tilde{z})$ is the local pressure gradient and following a straightforward procedure (Sharipov, 1996; Sharipov and Seleznev, 1998; Varoutis et al., 2009) it is found that

$$\dot{M} = G^* \frac{\pi D^3}{4\upsilon_0} \frac{P_1 - P_2}{L}. \tag{3}$$

Here, P_1 and P_2 denote the pressure head at the two ends of the tube and

$$G^* = \frac{1}{\delta_1 - \delta_2} \int_{\delta_1}^{\delta_2} G(\delta) d\delta. \tag{4}$$

In Eq. (4),

$$\delta = \frac{PD}{\mu \upsilon_0} = \frac{\sqrt{\pi}}{2}\frac{1}{Kn} \tag{5}$$

with μ denoting the gas viscosity at some reference temperature, is the local rarefaction parameter which is proportional to the inverse Knudsen number. The values δ_1 , δ_2 correspond to P_1, P_2 and denote the rarefaction parameters at the two ends of the tube. Also, the quantity $G(\delta)$ is the dimensionless flow rate obtained by solving a suitably chosen linearized kinetic model equation subject to some boundary condition. For the purposes of the present work, the dimensionless flow rates are estimated based on the linearized BGK equation with Maxwell purely diffuse boundary conditions. It is noted that the later choice is related to the assumed roughness of the tube. The quantity $G(\delta)$ may easily be found in the literature (or computed) in the whole range of δ. These results are kept in a data base and are used in the solution of the network. In particular, in the process of solving the whole network the pressures P_1 , P_2 and therefore δ_1 , δ_2 are estimated and then the values of $G(\delta)$ obtained from the data base are used in the integration according to Eq. (4) to yield G^*, which is substituted next into Eq. (3) to deduce the mass flow rate for each pipe section of the network.

2.2 Generalized network equations

As mentioned above the initial system of equations describing the network consists of the pressure drop equations along each piping element and the mass conservation equations at each node of the network. The former ones are given by solving Eq. (3) for the pressure difference to yield

$$\left(P_1 - P_2\right)_j = \Delta P_j = 4\frac{\dot{M}_j}{G_j^*}\frac{L_j \upsilon_0}{\pi D_j^3}, \tag{6}$$

where the index $1 \le j \le p$ denotes each of the p pipes of the network. The latter ones may be expressed as

$$\left[\sum_j (\pm)\dot{M}_j - Q\right]_i = 0 \tag{7}$$

where the index $1 \le i \le n$ denotes each of the n junction nodes of the network, while the summation index j refers to the pipes connected to the node i, while Q is the external demand (if any) at node i. The plus and minus signs are used for flow into and out of the node i respectively. Equations (6) and (7) are coupled and may be solved for the unknown pressure heads and mass flow rates.

However, it is convenient to reduce the number of equations by combining the pressure drop equations (6) along each uniquely determined closed loop of the network to derive the so-called energy balance equations (Potter and Wiggert, 1997):

$$\left[\sum_j (\pm)\left(\Delta P_j\right)\right]_k = 0 . \tag{8}$$

Here the summation index j pertains to the pipes that make up a loop, while the index $1 \le k \le l$, denotes each of the l loops. The plus sign is used if the flow in the element is positive in the clockwise sense; otherwise the minus sign is employed. By substituting Eqs. (6) into (8), the energy balance equations become

$$\left[\sum_j (\pm)\left(4\frac{\dot{M}_j}{G_j^*}\frac{L_j \upsilon_0}{\pi D_j^3}\right)\right]_k = 0 . \tag{9}$$

Following this procedure, the pressure heads have been eliminated from Eqs. (9), which along with Eqs. (7) form a well defined system having as unknowns only the mass flow rates $\dot{M}_j$. Once this system is solved for the mass flow rates then, the pressure heads are obtained from Eqs. (6). When there are fixed-grade nodes in the network then, the system of equations for the mass flow rates is amplified by the energy balance equation around each pseudo-loop connecting two fixed grade nodes:

$$\left[\sum_j (\pm)\left(4\frac{\dot{M}_j}{G_j^*}\frac{L_j \upsilon_0}{\pi D_j^3}\right) + \Delta H\right]_m = 0 . \tag{10}$$

Here, the summation index j pertains to the pipes that make up a pseudo-loop, the index

$1 \le m \le f-1$, denotes each of the $f-1$ pseudo-loops (f is the number of fixed grade nodes) and ΔH is the difference in magnitude of the fixed-grade nodes in the path ordered in a clockwise fashion across the imaginary pipe in the pseudo-loop. The plus and minus signs follow the same arguments given for Eqs. (8) and (9).

Based on the above the final system of equations will consist of $n+l+f-1$ equations to be solved for the p unknown mass flow rates $\dot{M}_j$. This clearly explains why for a well defined pipe network relation (1) must be satisfied. However, it is important to note that since in the system consisting of Eqs. (7), (9) and (10) the quantities G_j^* are not known a priori, an overall iterative algorithm incorporating Eqs. (6) is needed. The detailed description of this algorithm is presented in the next section

3. Numerical algorithm

The developed code includes the drawing of the network in a graphical environment and the formulation and solution of the governing equations describing the flow conditions of the micro distribution system. At the present stage the code is able of providing the input data and solving pipe networks of various complexity.

The drawing of the network and the input of the data are prepared on a graphical user interface (GUI). The development of the graphic interface is based on available GNU General Public License (GPL) libraries including some new libraries written in javascript to match the needs of the application. As a result, the user is able to draw the desired network by adding nodes and edges and the corresponding data, i.e., the coordinates of the nodes in a 3D space, the length and the diameter of the pipe elements, the pressure heads of the fixed-grade nodes and information for the type of the gas and its properties (viscosity, most probable molecular velocity, etc.). The demands (if any) at the nodes are also provided. A sample picture of the developed GUI is shown in Fig.1.

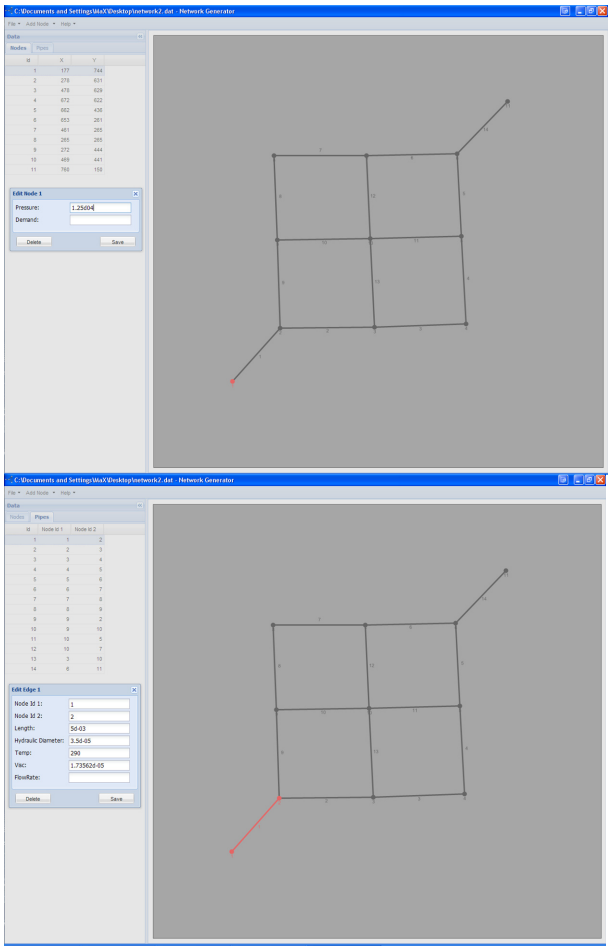

Figure 1: Sample picture of the GUI interface developed for the input data, with numbering of nodes (up) and pipes (down).

Therefore, a connectivity matrix for each node and tube of the network is formed providing all necessary information as input data. In addition, the code is scanning to find all possible closed loops, keeping finally only the l uniquely determined loops consisting of the least number of piping elements and the $f-1$ pseudo-loops between the f fixed-grade nodes.

Once the network is drawn, the resulting input file is introduced into a Fortran code. The code is based on an iterative process between the pressure drop equations (6) and the system of mass and energy conservation equations consisting of Eqs. (7), (9) and (10), which may be summarized as follows:

1. At all nodes of the network, where the pressure head is unknown it is initially assumed and the pressure differences ΔP_j along each tube are stored.

2. The rarefaction parameter at each node is estimated by Eq. (5).
3. The quantity G_j^* is estimated by Eq. (4) for each tube using the available data base for the dimensionless flow rate $G(\delta)$. Cubic splines are used to interpolate if needed between the values provided in the data base.
4. The system of mass conservation and energy balance equations (7), (9) and (10) is solved by applying Gauss elimination with full pivoting to compute the mass flow rates $\dot{M}_j$ through each pipe section.
5. Equations (6) are solved to estimate the updated pressure drops ΔP_j.
6. The updated values of ΔP_j are compared with the ones in Step 1 and the whole process is repeated upon convergence.

A detailed flow diagram of the developed algorithm including both the graphical interface and the solver is shown in Fig. 2.

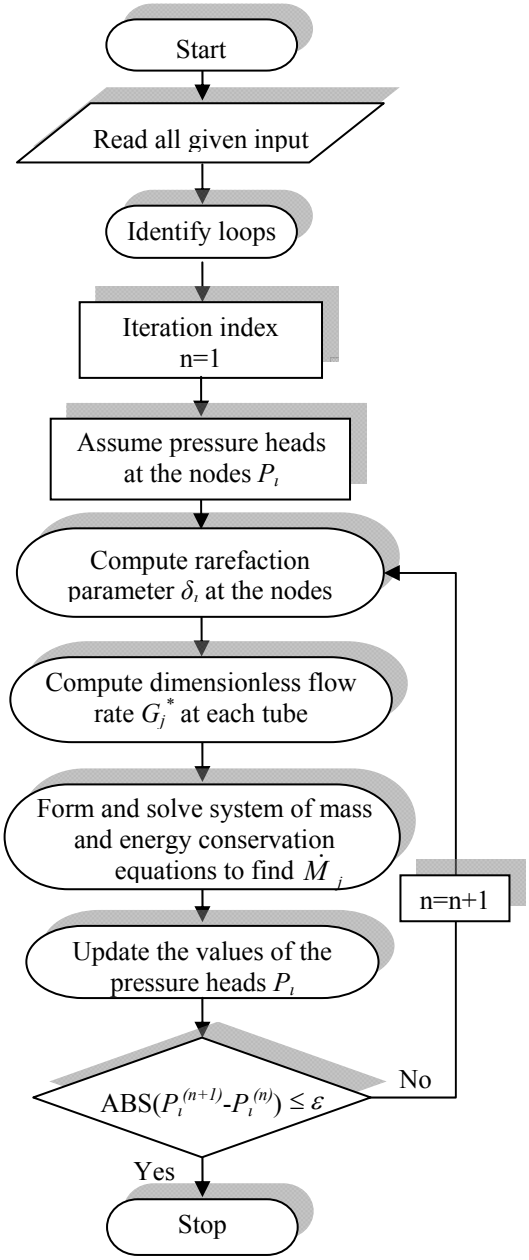

Figure 2: Flow diagram of the algorithm.

4. Results

To demonstrate the feasibility and the effectiveness of the proposed methodology the sample network shown in Fig. 3 is simulated. The network consists of $p=14$ tubes, $n=9$ junction nodes, $f=2$ fixed-grade nodes and $l=4$ loops. All tubes have length $L=5000$ μm and diameter $D=35$ μm. Nodes 1 and 11 refer to two reservoirs, where the pressure is held constant equal to $P_1=1.25\times10^4$ Pa and $P_{11}=1.40\times10^4$ Pa. The micro distribution system is characterized by the demands at nodes 4 and 8 equal to $Q_4=7.1\times10^{-11}$ kg/s and $Q_8=1.8\times10^{-11}$ kg/s respectively. The conveying gas is argon and the temperature of the flow is constant and equal to 293K.

The system of governing equations includes nine mass conservation equations at nodes {2,3,…,10}, four energy balance equations along the closed loops {I, II, III, IV} and one energy balance equation along the open pseudo-loop formed along the nodes {1,2,3,4, 5,6,11}. The total number of equations of the system is 14 and its solution returns the 14 unknown mass flow rates $\{\dot{M}_1,...,\dot{M}_{14}\}$. Then, from the pressure drop equations the pressure heads $\{P_2,...,P_{10}\}$ are found. The arrows in the left and right parts of Fig. 3 indicate the initially assumed and finally computed flow directions respectively.

The results are shown in Tables 1 and 2. In Table 1, the computed Knudsen number and pressure at each node of the network are tabulated. In Table 2, the average Knudsen number and the mass flow rate along each tube

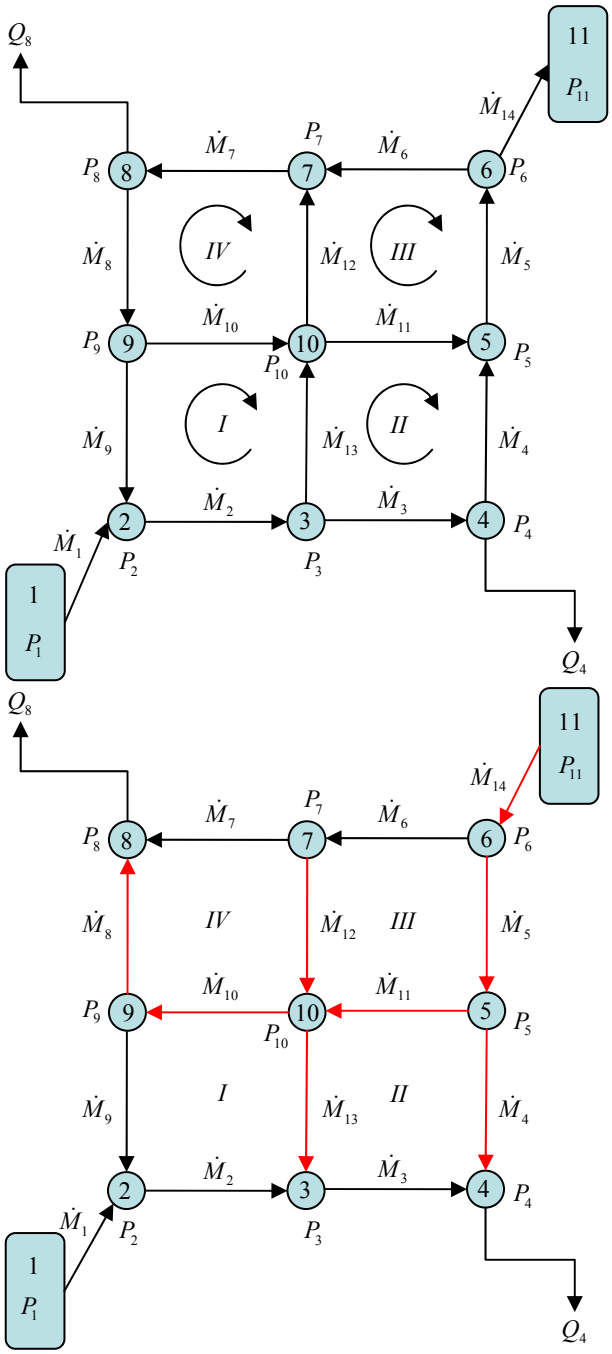

Figure 3: Schematic representation of pipe network showing the initially assumed flow directions (up) and the ones derived after the completion of the code (down).

of the network are presented. The negative values at some of the mass flow rates indicate that the final direction of the flow in this tube is opposite to the one initially assumed. The red arrows shown in Fig. 3 (down) indicate the corrected flow direction obtained after convergence of the code. In this test case the flow happens to be in the slip regime.

Table 1

Pressure head and Knudsen number at each node of the network.

Node number	*Local Kn*	*Pressure head [Pa]*
1	1.61(-2)	1.250(4)
2	1.62(-2)	1.237(4)
3	1.64(-2)	1.222(4)
4	1.69(-2)	1.186(4)
5	1.61(-2)	1.245(4)
6	1.54(-2)	1.304(4)
7	1.59(-2)	1.262(4)
8	1.62(-2)	1.239(4)
9	1.62(-2)	1.239(4)
10	1.62(-2)	1.242(4)
11	1.43(-2)	1.400(4)

Table 2

Mass flow rates and average Knudsen number at each tube of the network.

Tube #	*From Node*	*To Node*	*Average Knudsen*	$\dot{M}_j$ *[kg/s]*
1	1	2	1.61(-2)	9.87(-12)
2	2	3	1.63(-2)	1.16(-11)
3	3	4	1.67(-2)	2.68(-11)
4	4	5	1.65(-2)	-4.42(-11)
5	5	6	1.58(-2)	-4.62(-11)
6	6	7	1.56(-2)	3.29(-11)
7	7	8	1.61(-2)	1.77(-11)
8	8	9	1.62(-2)	-3.41(-13)
9	9	2	1.62(-2)	1.69(-12)
10	9	10	1.62(-2)	-2.03(-12)
11	10	5	1.61(-2)	-2.03(-12)
12	10	7	1.60(-2)	-1.53(-11)
13	3	10	1.63(-2)	-1.53(-11)
14	6	11	1.48(-2)	-7.91(-11)

In order to provide an estimation of the involved computational effort it is noted that the solution of the sample network requires the CPU time of only 0.63 sec on a 3 Ghz dual core system. It is obvious that the involved computational effort is negligible. For more complex networks consisting of hundreds of tubes the computational effort it will be

increased but not significantly.

In the short future the "in house" developed algorithm will be extended to include channels of any cross section and more important, channels of short length. In the latter case the pressure drop through the junctions is taken into account. Also, it may be further developed to include optimization of gaseous micro distribution networks in order to be used as an engineering tool in the design of gas micro network systems.

5. Conclusions

A novel algorithm has been developed for the design of gaseous micro distribution systems consisting of long tubes based on linear kinetic theory. The drawing of the microchannel network is aided by a GUI interface, the output of which is directly linked to the iterative algorithm.

The integrated algorithm may successfully handle gas pipe networks of any complexity operating under any rarefied conditions from the free molecular, through the transition up to the slip and hydrodynamic regimes. This is achieved by successfully integrating the well known kinetic results for single tubes, based on the linearized BGK equation with Maxwell purely diffuse boundary conditions, into a typical solver for designing gas pipe networks. The systematic computational approach yields the mass flow rates through the pipes as well as the pressure heads at the nodes of the network. The effectiveness of the methodology has been demonstrated by solving a network of moderate complexity in the slip regime. It has been shown that the approach is computationally efficient.

It is hoped that the developed code may be used as an engineering tool in the design of networks consisting of long microchannels.

Acknowledgments

This work has been supported by the European Communities under the contract of Association EURATOM / Hellenic Republic. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

References

Naris S. and Valougeorgis D., 2008. Rarefied gas flow in a triangular duct based on a boundary fitted lattice, Eur. J. Mech. B/Fluids, 27, 810-822.

Pitakarnnop J., Varoutis S., Valougeorgis D., Geoffroy S., Baldas L. and Colin S., 2010. A novel experimental setup for gas microflows, Microfluid & Nanofluid, 8 (1), 57-72.

Potter M. C. and Wiggert D. C., 1997. Mechanics of Fluids, 2nd edition, Prentice Hall.

Sharipov F., 1996. Rarefied gas flow through a long tube at any temperature ratio, J. Vac. Sci. & Tech. A, 14 (4), 2627-2635.

Sharipov F. and Seleznev V., 1998. Data on internal rarefied flows, J. Phys. Chem. Ref. Data, 27, 657-706.

Sharipov F., 1999. Rarefied gas flow through a long rectangular channel, J. Vac. Sci. & Tech. A, 17, 3062-3066.

Szalmas L., Pitakarnnop J., Geoffroy S., Colin S. and Valougeorgis D., 2010. Comparative study between computational and experimental results for binary rarefied gas flows through long microchannels, Microfluid & Nanofluid, 9 (6), 1103–1114.

Valougeorgis D. and Thomas J. R., 1986. Exact numerical results for Poiseuille and thermal creep flow in a cylindrical tube, Phys. Fluids, 29, 423-429.

Valougeorgis D., 2007. The friction factor of a rarefied gas flow in a circular tube, Phys. Fluids, 19, 091702-4.

Varoutis S., Naris S., Hauer V., Day C. and Valougeorgis D., 2009. Computational and experimental study of gas flows through long channels of various cross sections in the whole range of the Knudsen number, J. Vac. Sci. & Tech. A, 27 (1), 89-100.