Design of micro distribution systems consisting of long channels with arbitrary cross sections

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Abstract. Gas flows through long micro-channels of various cross sections have been extensively investigated over the years both numerically and experimentally. In various technological applications including microfluidics, these micro-channels are combined together in order to form a micro-channel network. Computational algorithms for solving gas pipe networks in the hydrodynamic regime are well developed. However, corresponding tools for solving networks consisting of micro-channels under any degree of gas rarefaction is very limited. Recently a kinetic algorithm has been developed to simulate gas distribution systems consisting of long circular channels under any vacuum conditions. In the present work this algorithm is generalized and extended into micro-channels of arbitrary cross-section etched by KOH in silicon (triangular and trapezoidal channels with acute angle of 54.74°). Since a kinetic approach is implemented, 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 kinetic results for the corresponding single channels into the general solver for designing the gas pipe network. To demonstrate the feasibility of the approach two typical systems consisting of long rectangular and trapezoidal micro-channels are solved.

1. Introduction

Rarefied gas flows through long channels of various cross sections have been extensively investigated over the years based on linear kinetic theory [1–3]. 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 [4–6].

However, in many microfluidics applications, the gaseous distribution system consists of single channels accordingly combined in order to form a pipe network. Despite the fact that computational algorithms dedicated to the design of gas pipe networks in the continuum regime are well developed, corresponding tools for the design of gaseous pipe networks operating under rarefied conditions have not been developed so far. Recently, a first attempt to deal with this problem has been performed for the design of pipe networks consisting of long tubes [7, 8]. 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. In the present work this methodology is generalized for gas distribution systems consisting of long channels with arbitrary cross sections. Results are provided for pipe networks consisting of rectangular and trapezoidal channels in a wide range of the Knudsen number.
It is emphasized that the present work is limited to long channels, i.e. when the ratio of the length over the hydraulic diameter is larger than about one hundred. Based on this assumption, the pressure drop due to the end effects as well as the junction elements such as bends, T junctions, cross junctions etc. may be considered negligibly small compared to the pressure drop through the channel and is not taken into account.

2. Formulation and Algorithm

A typical pipe network may be considered as a directed linear graph consisting of a finite number of channel elements interconnected in a specified configuration. Each element is characterized of its specific geometrical characteristics such as diameter \( D \) for cylindrical channels, width \( W \) and height \( H \) for rectangular channels, size of big base \( B \), small base \( b \), height \( h \) and the acute angle \( \phi \) for trapezoidal channels or side size \( a \) and acute angle \( \phi \) for triangular channels. All channels have a specific length \( L \), a cross section area \( A' \) and a perimeter \( \Gamma' \). At this point we introduce the hydraulic diameter \( D_h \), defined as

\[
D_h = \frac{4A'}{\Gamma'}
\]  

and it is used as the characteristic length of each piping element. In Table 1 the expressions for the hydraulic diameter, the cross section area and the perimeter for channels of various cross sections are shown. A point where two or more of the piping elements consisting a network 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). Usually the geometry of the network is specified and the objective is to compute the flow quantities, i.e., the mass flow rates \( \dot{M} \) through each tube and the pressure head \( P \) at each node.

Independent of the flow regime, the system of equations describing such a network consists 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 along the closed loops of the network. The latter ones, 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. In the case when the Knudsen number characterizing the flow through the network is very small and the flow is in the continuum or slip regimes, 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.

This is a well described methodology recently applied to the design of networks consisting of circular elements \[7, 8\] and in the present work it is extended into channels of various cross sections. As a result, the corresponding equations for the kinetic solution for rarefied flow through a single tube are generalized and presented in the next section, followed by the description of the integrated algorithm for the flow solution of the whole network.

2.1. Generalized formulation for single pipes with arbitrary cross sections

The solution of a pressure driven rarefied gas flow through long channels based on linear kinetic theory is a very well known problem \[1–4, 9–11\] and therefore here, only information which is directly connected and needed to the solution of the whole network is reviewed. Since \( D_h << L \), the flow is considered as fully developed and therefore the pressure (or density) varies only in
Table 1. Expressions of $D_h$, $A'$ and $\Gamma'$ for channels of various cross sections.

| Cross section            | $D_h$   | $A'$   | $\Gamma'$ |
|--------------------------|---------|--------|-----------|
| Cylindrical              | $D$     | $\frac{\pi D^2}{4}$ | $\pi D$ |
| Rectangular              | $\frac{2W \times H}{W+H}$ | $W \times H$ | $2(W+H)$ |
| Equilateral triangular   | $\frac{a}{\sqrt{3}}$ | $\frac{\sqrt{3}}{4} a^2$ | $3a$ |
| Equilateral trapezoidal  | $\frac{2(B+b)h}{B+b+\frac{2b}{\sin \phi}}$ | $\frac{B+b}{2}h$ | $B+b+\frac{2h}{\sin \phi}$ |

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 piping element is given by

$$\dot{M} = \int \rho u' dA',$$  \hspace{1cm} (2)

where $\rho$ is the mass density and $u'$ is the bulk velocity. The equation of state is given by $\rho = \frac{2P}{v_0^2}$, where $P$ is the local pressure along the piping element and $v_0$ the most probable molecular velocity. By introducing into Equation 2 the equation of state as well as the corresponding dimensionless space variables along with the dimensional quantity for the bulk velocity $u = u'(v_0 X P)$, where $X P = \frac{D_h}{P} \left( \frac{dP}{dz'} \right)$ is the local pressure gradient and following a straightforward procedure \[4, 11, 12\] it is found that

$$\dot{M} = G^* A'D_h \frac{P_1 - P_2}{v_0} \frac{L}{L}.$$  \hspace{1cm} (3)

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

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

The local rarefaction parameter $\delta$ is proportional to the inverse Knudsen number and it is defined by

$$\delta = \frac{P D_h}{\mu v_0} = \frac{\sqrt{\pi}}{2} \frac{1}{Kn},$$  \hspace{1cm} (5)

with $\mu$ denoting the gas viscosity at some reference temperature. The values $\delta_1$, $\delta_2$ correspond to $P_1$, $P_2$ and denote the rarefaction parameters at the two ends of the tube. Finally, 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 latter choice is related to the assumed roughness of the tube. The quantity $G(\delta)$ may be easily found in the literature (or computed) in the whole range of $\delta$. 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 $\delta_1$, $\delta_2$ are estimated and then the values of $G(\delta)$, obtained from the data base, are used in the integration according to Equation 4 to yield $G^*$, which is substituted next into Equation 3 to deduce the mass flow rate for each piping 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 Equation 3 for the pressure difference to yield

\[(P_1 - P_2)_j = \Delta P_j = \frac{\dot{M}_j L_j v_0}{G^*_j A'_j D_{h_j}},\]

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

\[\sum_j (\pm) \dot{M}_j - Q_i = 0,\]

where the index \(1 \leq i \leq n\) denotes each of the \(n\) junction nodes of the network, while the summation index \(j\) refers to the pipes connected to the node \(i\) and \(Q_i\) 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 combing the pressure drop equations (Equation 6) along each uniquely determined closed loop of the network to derive the so-called energy balance equations:

\[\sum_j (\pm) (\Delta P_j) = 0.\]

Here the summation index \(j\) pertains to the pipes that make up a loop, while the index \(1 \leq k \leq l\), 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 Equations 6 into 8 the energy balance equations become

\[\sum_j (\pm) \left( \frac{\dot{M}_j L_j v_0}{G^*_j A'_j D_{h_j}} \right) = 0.\]

Following this procedure, the pressure heads have been eliminated from the set of Equations 9, which along with the set of Equations 7 form a well defined system having as unknowns only the mass flow rates. Once this system is solved for the mass flow rates, then the pressure heads are obtained from Equations 6. In the case when there are fixed-grade nodes in the network, 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:

\[\sum_j (\pm) \left( \frac{\dot{M}_j L_j v_0}{G^*_j A'_j D_{h_j}} \right) + \Delta H = 0.\]

Here, the summation index \(j\) pertains to the pipes that make up a pseudo-loop, the index \(1 \leq m \leq f - 1\), denotes each of the \(f - 1\) pseudo-loops (\(f\) is the number of fixed grade nodes) and \(\Delta H\) 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 Equations 8 and 9.

Based on the above, the final system of equations consists of \(n + l + f - 1\) equations to be solved for the \(p\) unknown mass flow rates \(\dot{M}_j\). However, it is important to note that since in the
system consisting of Equations 7, 9 and 10 the quantities $G^*_j$ are not known a priori, an overall iterative algorithm incorporating the set of Equations 6 is needed. The detailed description of this algorithm is presented in the next section.

2.3. 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 specific geometrical characteristics of each piping 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. Therefore, a connectivity matrix for each node and element of the network is formed providing all necessary information as input data.

Once the network is drawn, the resulting input file is introduced into a Fortran code. The code is scanning to find all possible closed loops, keeping finally 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. In addition, the code is based on an iterative process between the pressure drop equations (Equation 6) and the system of mass and energy conservation equations consisting of Equations 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 $\Delta P_j$ along each tube are stored.
2. The rarefaction parameter at each node is estimated by Equation 5.
3. The quantity $G^*_j$ is estimated by Equation 4 for each tube using the available data bank for the dimensionless flow rate $G(\delta)$. Cubic splines are used to interpolate if needed between the values provided in the data bank.
4. The system of mass conservation and energy balance equations (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 $\Delta P_j$.
6. The updated values of $\Delta P_j$ are compared with the ones in Step 1 and the whole process is repeated upon convergence.

3. Results

To demonstrate the feasibility and the effectiveness of the proposed methodology the sample network shown in Figure 1 is simulated. The network consists of $p = 14$ tubes, $n = 9$ junction nodes, $f = 2$ fixed-grade nodes and $l = 4$ loops. Nodes 1 and 11 refer to two reservoirs, where the pressure is held constant. The micro distribution system is characterized by the availability of introducing demands at nodes 4 and 8, however, for comparison reasons these two values are set to 0. The reference temperature is set to $T_0 = 293.7$ K. The conveying gas is argon (Ar), with molar mass $m = 0.039948$ kg/mol, gas constant $R = 208$ J/(kg · K), most probable molecular velocity $v_0 = 347.74$ m/s and viscosity $\mu = 22.7985$ µPa · s.
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 \( \dot{M}_1, \ldots, \dot{M}_{14} \).

Then, from the pressure drop equations, the pressure heads \( P_2, \ldots, P_{10} \) are found.

Two typical simulations are performed. The first one by simulating a network which consists of rectangular micro-channels with \( H = 2.00 \) \( \mu \)m and \( W = 20.00 \) \( \mu \)m, leading to an aspect ratio of \( H/W = 0.1 \) and a hydraulic diameter \( D_h = 3.63 \) \( \mu \)m and the second one where the micro-distribution system consists of equilateral trapezoidal elements with size of big base \( B = 6.87 \) \( \mu \)m, small base \( b = 1.80 \) \( \mu \)m, height \( h = 3.60 \) \( \mu \)m and acute angle \( \phi = 54.74^\circ \), leading to a hydraulic diameter \( D_h = 3.56 \) \( \mu \)m. In all cases considered, the length of the piping elements is kept constant and equal to \( L = 5.00 \) mm, while the pressures at both the upstream and downstream reservoirs are fixed to \( P_1 = 0.125 \) MPa and \( P_{11} = 140 \) Pa, respectively. Both networks simulated are compared, while keeping the same configuration, to a network consisting of cylindrical tubes of the equivalent hydraulic diameter \( D_h \).

The results are shown in Figure 2 for the rarefaction parameter, the pressure heads [Pa] and the mass flow rates [kg/s] for both networks simulated. The corresponding results using the hydraulic diameter concept are also included. The rarefaction parameter covers the range \( 0.0642 \leq 1/Kn \leq 57.33 \) for the rectangular case and \( 0.0630 \leq 1/Kn \leq 56.28 \) for the trapezoidal one. The flow in the network covers the slip, transition and free molecular regimes. The negative values at some of the mass flow rates indicate that the final direction of the flow in this piping element is opposite to the one initially assumed. The red arrows shown in Fig. 1 indicate the corrected flow direction obtained after convergence of the code.

Next, we comment on the comparison of the simulated networks with the corresponding ones consisting of cylindrical channels with the equivalent hydraulic diameter. In the case where all channels have the same hydraulic diameter, the friction factor is the same and therefore the pressure drop is similar. As a result, the rarefaction parameter is close for every node of the

Figure 1. Schematic representation of pipe network showing a) the initially assumed flow directions (left) and b) the flow directions derived after the completion of the code (right).
Figure 2. Rarefaction parameter (top), pressure heads (middle) and flow rates (bottom) for a network consisting of rectangular (left) and trapezoidal (right) channels. The corresponding results with the hydraulic diameter concept are also shown.

network in both geometries simulated. The relative error between the rectangular channels and the cylindrical ones is less than 4.11% for the pressure heads. Similar results can be seen for the comparison between the trapezoidal and the cylindrical channels, where the relative error is less than 0.09% for the pressure heads. However, in both comparisons, despite the good agreement between the rarefaction at the nodes and the pressure heads, the comparison with regard to the mass flow rate through each of the piping elements of the networks shows that there are significant differences. For the case of the rectangular channels there is a discrepancy around 220% for the flowrates and for the case of the trapezoidal channels around 85%.

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 seconds 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.

4. Concluding remarks

An existing "in house” algorithm for the design of gaseous distribution systems consisting of long channels has been generalized by taking into account channels with arbitrary cross sections. A graphical interface is developed in order to draw the network and create the output file which is directly linked to the main iterative algorithm. The algorithm is based on the integration of a data base created for this purpose by solving the linearized BGK equation with Maxwell purely diffuse boundary conditions in the whole range of the Knudsen number. As a result the integrated algorithm may successfully handle gas pipe networks of any complexity operating under any vacuum conditions from the free molecular, through the transition up to the slip and hydrodynamic regimes yielding the mass flow rate through the piping elements as well as the pressure heads and the Knudsen number at the nodes of the network. The effectiveness of the methodology has been demonstrated by solving a network consisting of rectangular channels and one of trapezoidal channels and comparing them with the equivalent network consisting of cylindrical channels of the same hydraulic diameter.

The developed algorithm may be further extended to pipe networks consisting not only of long channels but also of channels of finite length. This goal is going to be achieved once the available kinetic data base is enhanced with the corresponding results. It is hoped that present algorithm will constitute a significant engineering tool in the design and optimization of gaseous micro distribution networks operating under any rarefied conditions.

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