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Simple Formula for Calculation of Fluid Flows in Complex Microfluidic Networks

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Abstract

In this paper, we present simple formulae for prediction of the fluid flow and electric current through each of the channels connecting reservoirs and junctions in complex microfluidic networks that are commonly found in micro devices such as biochips. The shape of the cross-section of the channels we are concerned with is rectangular, and the series solutions for the Stokes' flow within the channel are represented by formulae that are very simple but accurate enough for the design of the channels. In particular, we for the first time propose the solution of the electroosmotic flow for the case where each side of the four walls has different zeta potential; this is also represented by a simple formula instead of the series form. Our code was validated by comparing the numerical solutions with the data reported in the literature and good agreement has been found.

Keywords: Microfluidic network, Pressure-driven flow, Electroosmotic flow

Introduction

Usually a microfluidic system or lab-on-a-chip is composed of a microfluidic network for the complex process including pumping, mixing, reaction, separation and detection, etc. As the number of functions to be performed in the system is increased, the configuration of the network becomes more complex, and the precise control of fluid flow in each part of the network in turn becomes more ambiguous and even difficult. This means that we need efficient and convenient design tools for predicting the hydrodynamical and electrochemical properties of the fluid flowing through each of the channels of the network.

The primary design tool needed for the chip designer is the computer program that can calculate the flow rate and the electric current through the channel; information on the pressure and the potential distribution at an arbitrary section of the channel may also be needed e.g. in order to predict the dispersion effect of the sample. Qiao and Aluru[1] proposed the so called compact model for calculating the pressure-driven and electroosmotic flows through microchannels of circular cross-section. The complex fluidic network was simplified by an electric circuit and the numerical results were in good agreement with the ones given by the full equations. Ajdari[2] proposed a linear system of equations to be solved for the pressure and the electric potential distribution in microchannels. Xuan and Li[3] presented the method of network calculation by using a linear system which can be applied not only to the microchannel but also to the nanochannel; hereinafter the word 'nanochannel' refers to the case where the thickness of the electric double layer (EDL) is comparable to the channel size whereas 'microchannel' refers to the case of negligible thin EDL. The configuration of the channel cross-section they treated was a circle and the Debye-Hückel linear analysis was employed in calculating the electroosmotic flows. Berli[4] also performed the network analysis and proposed a formula that can be applied to the microchannel as well as nanochannel for the cross-section of circular and slit shapes. They also followed the Debye-Hückel approximation in order to get the analytic solution for the electroosmotic flows. Later Berli[5] proposed the formula for the microchannel of the rectangular cross-section.

The fundamental formula needed for predicting the flow rate and the pressure and potential distributions in both the microchannels and nanochannels can be given analytically for the circular and slit cross-sections. However for the rectangular cross-section, we need a series form as the formula predicting the pressure-driven flow. In addition, when each side of the four walls surrounding the channel is made from different materials (for instance side/top walls from PDMS and the bottom wall from glass) we must use a series form as the formula predicting the electroosmotic flow.

This paper presents the fundamental formula that can predict the fluid flow rate, the electric current, and the pressure and potential distributions inside the

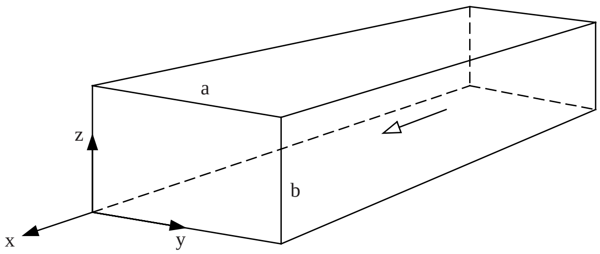

Figure 1. Geometry and coordinates for the analysis of the fluid flow and electric current through a microchannel with the cross-section of rectangular shape.

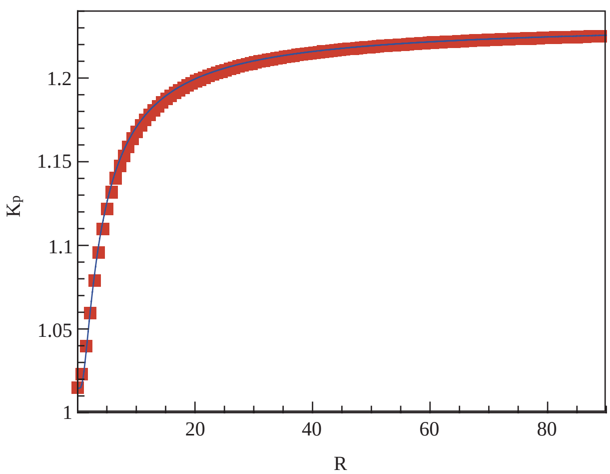

Figure 2. Comparison between the exact value (symbols) of $K_p(R)$ and that given from the approximation (4) (line).

microchannels of rectangular cross-section. Instead of using the series form we propose to use simple formulae for the pressure-driven and electroosmotic flows. Our method can be applied even to the case where the side walls are made from different materials. We also show that our code developed in this study can be used not only for calculating the flow rate and current with the pressures and potentials given at reservoirs and electrodes but also for the inverse problem, i.e. calculating the required pressure or potentials necessary to keep the given flow rate and current.

Results and Discussion

We developed a computer program that numerically constructs and solves the linear system of equations. In this section we present the numerical results obtained for a few example cases. All the details of the formulation and the numerical methods are given

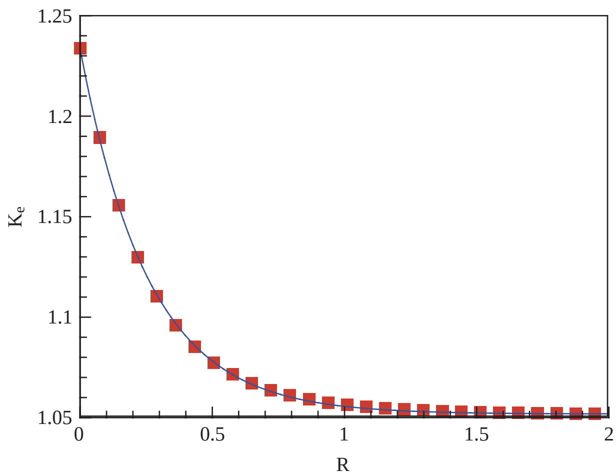

Figure 3. Comparison between the exact value (symbols) of $K_e(R)$ and that given from the approximation (11) (line).

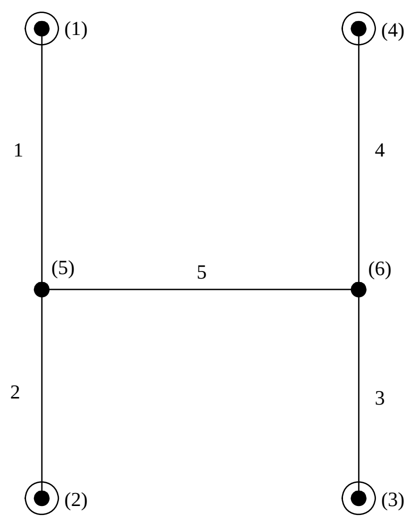

Figure 4. Typical example of a network composed of 5 channels and 6 junctions (including four set of reservoirs and electrodes marked by open circles).

in the section entitled "Materials and Methods" of this paper. As the first example, we consider the problem shown in Figure 4, which has been studied by Hu *et al.*[6] by using CFD with full equations and later by Berli[5] with equivalent circuit modeling. All the channels are composed of uniform cross-section with $a=100$ [μm] and $b=20$ [μm]. All the channel walls are also characterized by the uniform zeta potential with $\zeta=-18.3$ [mV]. Channel lengths are; $l_1=l_4=14$ [mm], $l_2=l_3=9$ [mm] and $l_5=10$ [mm]. The fluid used is HCl with $z=1$, $c_0=25$ [mM] and $\sigma_0=0.26$ [S/m]. We also assumed the following data; $T=298$ [K], $\rho=1000$ [kg/

Table 1. Applied potentials φ_j in [V] at four electrode junctions numbered j=1,2,3,4 during 6 operational steps of the immunoassay with the network of Figure 4.

	φ_1	φ_2	φ_3	φ_4
Dispensing (P)	250	0	95	100
Incubating (P)	300	0	47.5	50
Washing (P)	120	0	500	300
Dispensing (S)	350	0	265	500
Incubating (S)	300	0	132.5	250
Washing (S)	300	0	500	0

Table 2. Calculated average velocity u_n in [μm/s] through each of the four channels numbered n=1,2,3,4 in comparison with the corresponding data (data within brackets) obtained by Hu *et al.*[6] with CFD for the electrode potentials given in Table 1. Here, the sign indicates the downward (positive) or upward (negative) motion of the fluid viewed from Figure 4.

	u_1	u_2	u_3	u_4
Dispensing (P)	141.9 (141)	141.3 (140)	3.2 (3)	2.6 (2)
Incubating (P)	70.9 (70.5)	70.7 (70)	1.6 (1.5)	1.3 (1)
Washing (P)	−102.6 (−102)	159.7 (159)	−273.0 (−271)	−10.7 (−10)
Dispensing (S)	−86.9 (−86)	135.1 (133)	−2.0 (−2)	220 (221)
Incubating (S)	−43.4 (−43)	67.6 (66.5)	−1.0 (−1)	110 (110.5)
Washing (S)	−74.1 (−74)	115.2 (114)	−398.5 (−396)	−209.3 (−208)

m^3], μ=0.001 [Pa.s] and $\varepsilon=80\varepsilon_0$ where ε_0 is the electric permittivity of the vacuum. This network has been actually used by Hu *et al.*[6] in immunoassay analysis. The analysis cycle consists of 6 operations and each operation has its own flow requirement; for instance, during the primary dispensing the fluid carrying antibody in the junction 1 is required to flow toward the junction 2 through the channels 1 and 2 while the fluids in the other channels remain stationary, and during the secondary incubating the fluid must flow from the junction 4 to the junctions 1 and 2 while the fluid in the channel 3 remain stationary, etc. In order to attain uniform velocity profiles, all the reservoirs are maintained at the ambient pressure, i.e. p_j=0 [Pa] for j=1, 2, 3, 4. Table 1 shows the six set-up of the electric potentials applied at the four electrodes constituting the boundary junctions in order to satisfy the flow requirement in each opera-tion. The numerical results calculated from the code are presented in Table 2 in comparison with the corresponding data obtained by Hu *et al.*[6] by using the CFD with the full equations. It can be seen that our data are in good agreement with

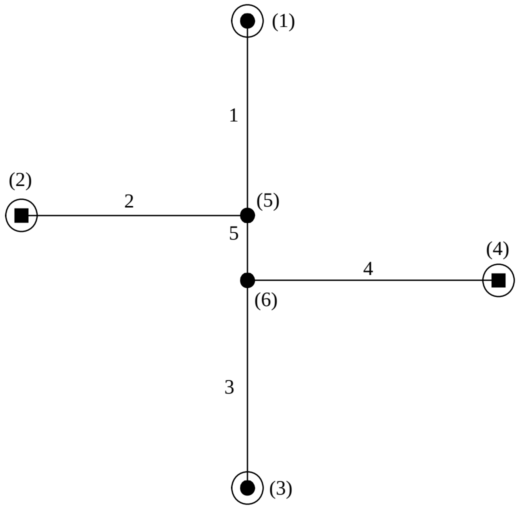

Figure 5. Second example of a network composed of 5 channels and 6 junctions. Here flow rates through the channels 2 and 4 are required to be zero, and the potentials at the two electrodes denoted by the junction numbers 2 and 4 are to be treated as unknowns, instead.

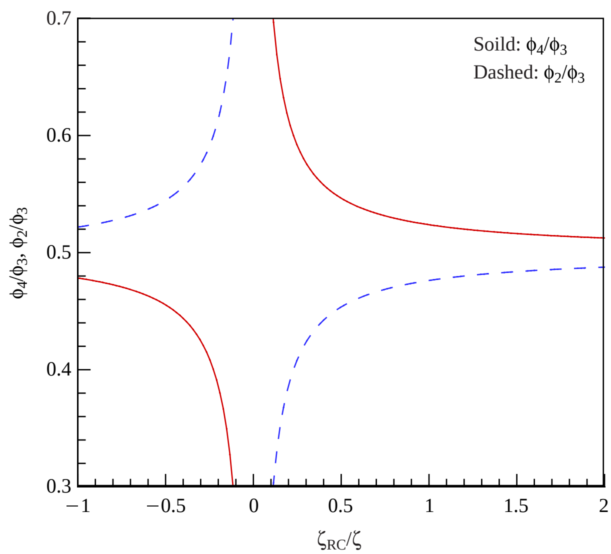

Figure 6. Effect of the ratio of the zeta potentials, ζ_{RC}/ζ, on the ratios of the applied potentials, φ_4/φ_3 and φ_2/φ_3, obtained numerically from the developed code for the second example of the network shown in Figure 5.

theirs for all operations. Except for the velocity data with low values, the maximum error is within 1%.

The second example treated in this study is shown in Figure 5, called double T-shape. This network has been used by Dodge *et al.*[7] in immunoassay and studied by Berli[5] in the network calculation. Here, all the reservoirs are set at the ambient pressure. The potentials at the junctions 1 and 3 are specified with $\varphi_1=0$ [V] and $\varphi_3=500$ [V]. The potentials at the junctions 2 and 4 are treated as unknown variables and the requirement is that the flow rate through the channel 2 and 4 become zero. All the channel cross-sections take the same configuration with $a=50$ [μm] and $b=20$ [μm]. The channel lengths are; $l_1=l_2=l_3=l_4=10$ [mm] and $l_5=1$ [mm]. The fluid used is KCl with $z=1$, $c_0=25$ [mM], $\sigma_0=0.37$ [S/m] and $T=293$ [K]. The zeta potential of each channel takes different value owing to the surface treatment. The channels 1 and 3 are given with the same value denoted by ζ and the other channels by ζ_{RC}. Berli[5] investigated the effect of the zeta potential ζ_{RC} on the potentials applied at the reservoir junctions 2 and 4 while the value of ζ was fixed at $\zeta=-60$ [mV]. Figure 6 shows the numerical results and they are in good agreement with the corresponding ones presented by Berli[5]. Because of different zeta potentials applied at each channel, the pressure gradients are built up at the channels, which in turn causes the velocity profile different from the plug type so that the dispersion effect may be significant.

During the test run of our code for several practical networks, it has been found that the current is almost dominated by the potential difference and the effect of the pressure difference is almost negligible. Besides, the convective current caused by the motion of ions within the EDL showing the non-equilibrium distribution, is negligibly small compared with the conductive current occurring in the bulk.

After the pressure and potential at each junction have been determined, we can estimate the total velocity profile from

$$u(y, z)=u_p(y, z)+u_e(y, z)$$

where the pressure-driven-flow velocity u_p and the electroosmotic-flow velocity u_e are calculated from Eqs. (1) and (6) presented in the section "Materials and Methods", respectively. From the velocity profile we can analyze the dispersion effect as proposed by Qiao and Aluru[1].

In order to generalize the code we must include not only the dispersion analysis but also the quantification of mixing and separation, etc. In a short future we expect such modules can be developed appropriately and added to the code.

Conclusions

We in this paper presented the methodology of the network calculation together with the formulae that are simple but accurate enough for the design of microfluidic devices. The simple formula can also treat the case where each side of the channel cross-section carries different zeta potential. We have shown by running the developed computer program for example cases that the algorithms as well as the simple formula indeed result in the data that are in good agreement with those reported in the literature.

Materials and Methods

In this section we address the formulation and the numerical methods used in the simulation of the microfluidic network problems. Microfluidic networks are composed of reservoirs, electrodes and channels. The channels connect the reservoirs and electrodes. They are also connected to each other at junctions. In predicting the flow rates and electric currents inside the channels we need fundamental formulae that can compute the flow rate and current through a single channel. In this paper we are interested in a straight channel of rectangular cross-section as shown in Figure 1. We assume that the fluid and current flows remain at a steady state and fully-developed at low Reynolds numbers.

Pressure-driven Flow

The axial flow velocity u can be obtained from the following series formula[5].

$$u=\frac{4b^2}{\mu}\left(-\frac{dp}{dx}\right)\sum_{k=0}^{\infty}\frac{1}{\beta_k^3}\left\{1-\frac{\cosh[\beta_k(2y/a-1)/2R]}{\cosh[\beta_k/(2R)]}\right\}\sin(\beta_k z/b) \tag{1}$$

where μ is the fluid viscosity, $R=b/a$ the aspect ratio of the channel cross-section, dp/dx the pressure gradient along the channel axis and $\beta_k=(2k+1)\pi$. The average velocity $\bar{u}$ can be obtained from integration of Eq. (1) over the cross-section yielding

$$\bar{u}=\frac{8b^2}{\mu}\left(-\frac{dp}{dx}\right)\sum_{k=0}^{\infty}\frac{1}{\beta_k^4}\left\{1-\frac{2R}{\beta_k}\tanh[\beta_k/(2R)]\right\} \tag{2}$$

Instead of using this series form we in this paper propose to use a simple formula

$$\bar{u}=\frac{8b^2}{\mu}\left(-\frac{dp}{dx}\right)\frac{K_p}{\pi^4}\left\{1-\frac{2R}{\pi}\tanh[\pi/(2R)]\right\} \tag{3}$$

where the correction factor K_p is close to 1. We have found from a curve fitting that the empirical formula

$$K_p(R)=0.2190\exp(-3.4/R)+1.01468 \tag{4}$$

provided the average flow velocity with maximum error 0.7% over all the possible range of R. Figure 2 shows the comparison between the exact value of $K_p(R)$ obtained from the full equation (2) and that computed from the approximation (4). We can see that the difference between the two data is almost indistinguishable.

Electroosmotic Flow

We consider the electroosmotic flow driven for the moment only by the bottom wall of the channel with the zeta potential ζ. In this paper we assume that the Debye length

$$\lambda_D = \sqrt{\frac{\varepsilon k_B T}{2e^2 z^2 c_0}} \tag{5}$$

is much smaller than the channel size; that is, we confine ourselves to the microchannels. Here, we take the fluid as the binary liquid with the valence z. Further, ε is the electric permittivity of the fluid, k_B the Boltzmann constant, T the temperature, e the elementary charge and c_0 the number concentration of each ion in the bulk, i.e. the number density.

Then the electroosmotic-flow velocity is given as

$$u = u_s U(y, z; a, b, R) \tag{6}$$

where the dimensionless velocity U is defined as

$$U(y, z; a, b, R) = 4\sum_{k=0}^{\infty} \frac{\sinh[\beta_k(b-z)/a]}{\beta_k \sinh(\beta_k R)} \sin(\beta_k y/a) \tag{7}$$

and the slip velocity u_s as

$$u_s = \frac{\varepsilon\zeta}{\mu}\left(\frac{d\varphi}{dx}\right) \tag{8}$$

Equation (7) can be obtained by applying the technique of separation of variable to the axial momentum equation $\nabla^2 U=0$ with the boundary conditions, $U=1$ at $z=0$ and $U=0$ at $y=0$, a and $z=b$. Here, $d\varphi/dx$ is the gradient of the external potential along the channel axis (i.e. the negative electric field). The average velocity is given by

$$\bar{u} = \frac{8u_s}{R}\sum_{k=0}^{\infty} \frac{1}{\beta_k^3} \tanh(\beta_k R/2) \tag{9}$$

We also propose to use a simple formula instead of this series form;

$$\bar{u} = \frac{8u_s}{\pi^3 R} K_e \tanh(\pi R/2) \tag{10}$$

where the correction factor K_e is given as

$$K_e(R) = 0.1819\exp(-3.86R) + 1.0518 \tag{11}$$

This formula is again given from a curve fitting. It turned out that the maximum error is 0.1% over the whole range of R, see Figure 3.

The final velocity profile must encompass the contributions from all the surrounding walls and can be obtained by the algebraic sum as follows.

$$u = \sum_{i=1}^{4} u_{s,i} U_i \tag{12}$$

where the subscripts $i=1, 2, 3, 4$, indicate the bottom, top, left and right walls, respectively. Each of U_i can be obtained from (7) simply by switching coordinates and constants as follows; $U_1=U(y, z; a, b, R)$, $U_2=U(y, b-z; a, b, R)$, $U_3=U(z, y; b, a, R^{-1})$, $U_4=U(z, a-y; b, a, R^{-1})$. The slip velocity at the i-th wall of the channel, $u_{s,i}$, is obtained from (8) with the corresponding zeta potential $\zeta=\zeta_i$ there. The flow rate can also be obtained by using the formula in a form similar to (12) as follows.

$$\bar{u} = \sum_{i=1}^{4} M_i u_{s,i} \tag{13}$$

where

$$M_i = \begin{cases} 8\pi^{-3}R^{-1}K_e(R)\tanh(\pi R/2) & \text{for } i=1, 2 \\ 8\pi^{-3}RK_e(R^{-1})\tanh(\pi R^{-1}/2) & \text{for } i=3, 4 \end{cases} \tag{14}$$

Flow Rate and Electric Current

The flow rate passing through the channel is given by $Q=A\bar{u}$, where $A=ab$ is the cross-sectional area of the channel. When both the pressure difference Δp and the potential difference $\Delta\varphi$ exist over the channel length l, the flow rate is determined from the following equation.

$$Q = L_{11}\Delta p + L_{12}\Delta\varphi \tag{15}$$

where

$$L_{11} = -\frac{8A^2RK_p}{\pi^4\mu l}\left[1 - \frac{2R}{\pi}\tanh\left(\frac{\pi}{2R}\right)\right]$$

$$L_{12} = \frac{\varepsilon A}{\mu l}\sum_{i=1}^{4} M_i\zeta_i$$

In order to determine the electric potential at each junction or reservoir, we employ the Kirchhoff's junction law by using the current flowing through each of the channels connected to the junction or reservoir; so we need the formula relating the potential difference to the current for a given channel. Neglecting the diffusive effect along the x-direction, we can obtain the total current density $j(y, z)$ along a channel as the sum of the convection effect $\rho_e u(y, z)$ and the conduction effect $-\sigma(y, z)d\varphi/dx$, where ρ_e is the volume charge density $\sigma(y, z)$ and is the electric conductivity of the fluid. For microchannels the thickness of EDL is much smaller than the channel size and ρ_e is non-zero only within the EDL. Therefore it is allowed to assume that the convective current is confined to EDL. Conversely, in considering the conduction current, we can neglect the effect of EDL and assume that the conductivity remains uniform over the cross-section, i.e. $\sigma=\sigma_0=$constant. Derivation of the formula for the current requires some algebraic works and we here show only the results. The total current I passing a channel is given by

$$I=L_{21}\Delta p+L_{22}\Delta\varphi \tag{16}$$

where

$$L_{21}=L_{12}=\frac{\varepsilon A}{\mu l}\sum_{i=1}^{4}M_i\zeta_i \tag{17a}$$

$$L_{22}=-\frac{\sigma_0 A}{l}-\frac{8\varepsilon^2\psi_T^2}{z^2\mu\lambda_D l}\sum_{i=1}^{4}s_i\sinh^2(z\zeta_i\psi_T^{-1}/4) \tag{17b}$$

Here $\psi_T=k_BT/e$ is the thermal potential and s_i indicates the length of the i-th side of the rectangle, i.e., $s_1=s_2=a$ and $s_3=s_4=b$. Depending the specific network problem, the conductivity σ_0 may be directly given or the diffusivity D may be instead given. For the latter case, we can get the conductivity formula by employing the Einstein equation linking the mobility and the diffusivity reading

$$\sigma_0=\frac{2z^3e^2Dc_0}{k_BT}$$

Linear System of Equations for the Junction Pressure and Potential

Our first target in the network calculation is to obtain the pressures and potentials at all the junctions. A typical network is shown in Figure 4, where 5 channels are connected by 6 junctions. In order to derive the relevant equations, we first apply the conservation of the fluid mass and the electric charge at each junction. Consider a generalized junction where multiple channels are connected. By the term 'generalized' we mean that the reservoir or the electrode (or both) is also considered as one of the junctions; the only difference is that the reservoir and the electrode can supply the fluid mass and the charge without bound, respectively.

Suppose there are multiple channels connected to a junction with a sequential number j; in Figure 4, the junction $j=5$ has three channels numbered $n=1, 2, 5$. The flow rate and the current through the channel number n are given respectively by

$$\begin{aligned} Q_n&=L_{11,n}\Delta p_{j,k}+L_{12,n}\Delta\varphi_{j,k},\\ I_n&=L_{21,n}\Delta p_{j,k}+L_{22,n}\Delta\varphi_{j,k} \end{aligned} \tag{18}$$

Here, $\Delta p_{j,k}$ and $\Delta\varphi_{j,k}$ denote the pressure and potential differences between the present junction j and the junction k at the other end of the channel n; $\Delta p_{j,k}=p_j-p_{k(j,n)}$, $\Delta\varphi_{j,k}=\varphi_j-\varphi_{k(j,n)}$. The total amount of flow rate and current coming into the junction are given by

$$Q=\sum_{n\in N_j}Q_n,\quad I=\sum_{n\in N_j}I_n \tag{19}$$

where N_j stands for the subset of the channel's serial numbers connected to the junction j; in Figure 4, $N_j=\{1,2,5\}$ for the junction $j=5$. If there is no further input of fluid and charge, then LHS of the above must become zero following the conservation principle. If there is separate input of the flow rate Q_{in} and the current I_{in}, LHS of the above equations must be replaced by $-Q_{in}$ and $-I_{in}$, respectively. On the other hand the main variables to be obtained by applying the equations (19) are the pressure p_j and the potential φ_j. Since p_k and φ_k are also unknown, we need a linear system of equations coupling all the junction variables. As an example we consider Figure 4 and assumes that at four boundary junctions $j=1,2,3,4$ the pressures and potentials are given. Then we have four unknown variables, p_5, p_6, φ_5 and φ_6 that are to be determined by solving the following equations.

$$\sum_{n=1,2,5}L_{11,n}(p_5-p_{k(5,n)})+\sum_{n=1,2,5}L_{12,n}(\varphi_5-\varphi_{k(5,n)})=0$$

$$\sum_{n=1,2,5}L_{21,n}(p_5-p_{k(5,n)})+\sum_{n=1,2,5}L_{22,n}(\varphi_5-\varphi_{k(5,n)})=0$$

$$\sum_{n=3,4,5}L_{11,n}(p_6-p_{k(6,n)})+\sum_{n=3,4,5}L_{12,n}(\varphi_6-\varphi_{k(6,n)})=0$$

$$\sum_{n=3,4,5}L_{21,n}(p_6-p_{k(6,n)})+\sum_{n=3,4,5}L_{22,n}(\varphi_6-\varphi_{k(6,n)})=0$$

We move the terms multiplied by the four sets of known variables (p_j,φ_j) (for $j=1,2,3,4$) to RHS and solve the resultant system of equations to obtain the four unknown variables. We used the Gauss elimination method with pivoting as the solver.

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