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Numerical Modeling of Flow Distribution in Micro-Fluidics Systems

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Abstract

This paper describes an application of a general purpose computer program, GFSSP (Generalized Fluid System Simulation Program) for calculating flow distribution in a network of micro-channels. GFSSP employs a finite volume formulation of mass and momentum conservation equations in a network consisting of nodes and branches. Mass conservation equation is solved for pressures at the nodes while the momentum conservation equation is solved at the branches to calculate flowrate. The system of equations describing the fluid network is solved by a numerical method that is a combination of the Newton-Raphson and successive substitution methods. The numerical results have been compared with test data and detailed CFD (computational Fluid Dynamics) calculations. The agreement between test data and predictions is satisfactory. The discrepancies between the predictions and test data can be attributed to the frictional correlation which does not include the effect of surface tension or electro-kinetic effect.

Nomenclature

1. Introduction

Micro-fluidic channel networks [1,2] are being placed on lab-on-a-chip devices, the size of a postage stamp, to perform multi-step biochemical processes, or to perform parallel, arrayed biochemical experiments. Presently, typical micro fluidic channel networks are designed and developed in an iterative process involving very rudimentary modeling, followed by several fabrications and testing cycles. This is a costly and ineffective approach and often the process does not converge to a suitable system design. The reason the iterative process is used is that no commercially available tools exist for system-level micro fluidic network design and analysis. The purpose of the present paper is to describe the application of a finite-volume based general-purpose computer program developed for analyzing propulsion system [3] to model micro-fluidics network. The predictions have been compared with experimental data [4] and Navier-Stokes solution [5].

2. Mathematical Formulation

The finite volume formulation requires governing equations to be expressed in conservative form. The rate of change of a conserved property in a given control volume is expressed as the vector sum of transported property from neighboring control volumes

together with source or sink terms. The unknown variables in the flow circuit of figure 1 are pressure, temperature and flowrate. These variables are solved from the mass, momentum and energy conservation equations in conjunction with correlation of fluid friction.

Figure 1 shows the fluid nodes and branches. There are two types of fluid nodes: boundary nodes and internal nodes. The boundary nodes are designated by double rectangles (e.g. node 1, 2, 3 etc.). Internal nodes are designated by single rectangles (e.g. node 11, 12 etc.). The nodes are connected by branches designated by filled rectangle (e.g. 19, 39 etc.). The mass and energy conservation equations are solved at the internal nodes and the momentum conservation equations are solved at the branches.

2.1 Mass Conservation

The mass conservation equation at the i^{th} node (Figure 2) can be written as

$$\frac{m_{\tau+\Delta\tau} - m_{\tau}}{\Delta\tau} = -\sum_{j=1}^{j=n} \dot{m}_{ij} \qquad (1)$$

Equation 1 implies that the net mass flow from a given node must equate to rate of change of mass in the control volume. In the steady state formulation, the left side of the equation is zero, such that the total mass flow rate into a node is equal to the total mass flow rate out of the node.

2.2 Momentum Conservation

The momentum conservation equation at the *ij* branch can be written as

$$(p_i - p_j)A_{ij} - K_f \dot{m}_{ij}\left|\dot{m}_{ij}\right| A_{ij} = 0 \qquad (2)$$

Equation 2 implies that there is a balance between pressure and friction force. The frictional force is expressed as a product of friction parameter, K_f and square of flowrate. It may be noted that the square of flowrate was expressed as product of $\dot{m}_{ij}$ and $\left|\dot{m}_{ij}\right|$. This practice allows the pressure to increase or decrease depending upon the flow direction. It may be recalled that the flowrate is a vector property and the pressure is a scalar property. The friction parameter, K_f can be expressed as [6]

$$K_f = \frac{8fL}{\rho_u \pi^2 D^5 g_c} \qquad (3)$$

White [9] described a procedure to estimate the friction factor in non-circular duct (Figure 3). This procedure consists of the following steps:

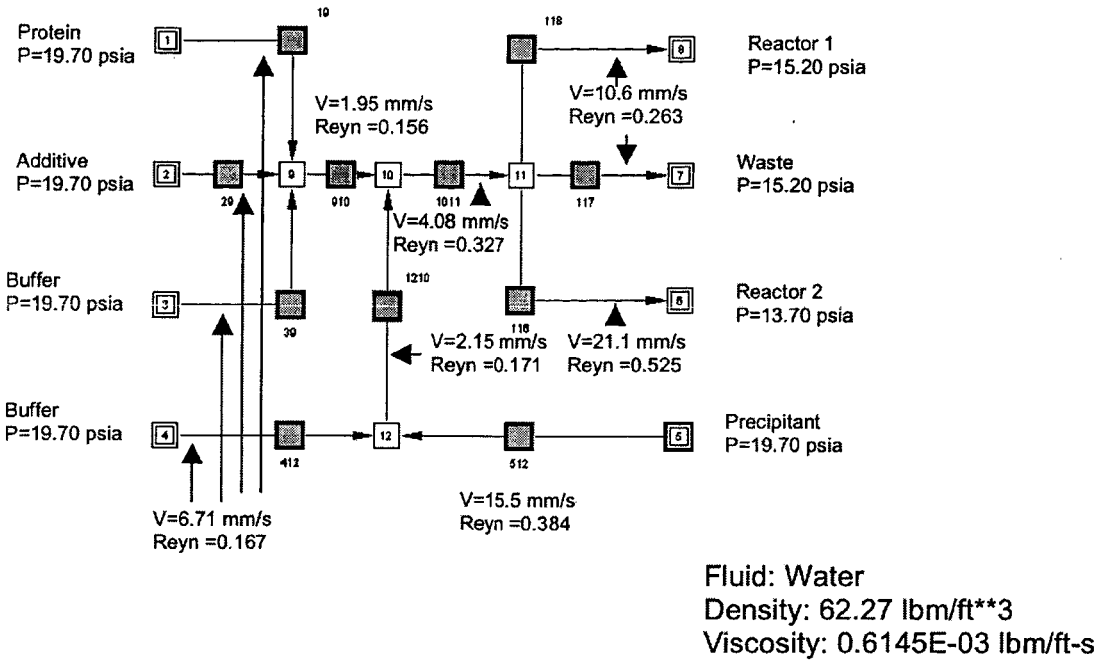


Figure 1. A typical micro-fluidics network system

1. Estimate the hydraulic diameter of the cross-section:

$$D_h = (4)(\text{Area}) / \text{Perimeter}$$

2. Estimate the Poiseuille Number for a particular cross-section. The Poiseuille Number can be expressed as a polynomial function of aspect ratio as shown in Equation 4. Table 1 provides the coefficients for different geometries.

$$Po = A_0 + A_1\left(\frac{b}{a}\right) + A_2\left(\frac{b}{a}\right)^2 + A_3\left(\frac{b}{a}\right)^3 + A_4\left(\frac{b}{a}\right)^4 \qquad (4)$$

Table 1. - Poiseuille Number Coefficients for Non-circular Duct Cross-sections

Coefficients	Rectangle	Ellipse	Concentric * Cylinder	Circular Section
A_0	23.9201	19.7669	22.0513	11.9852
A_1	-29.436	-4.53458	6.44473	3.01553
A_2	30.3872	-11.5239	-7.35451	-1.09712
A_3	-10.7128	22.3709	2.78999	0.0
A_4	0.0	-10.0874	0.0	0.0

* For b/a < 0.2508 $Po = A_0\left(\frac{b}{a}\right)^{A_1}$, where, $A_0 = 24.8272$, $A_1 = 0.0479888$

3. Calculate the friction factor for a non-circular pipe:

Laminar flow (Re<2300)

$$f = \frac{4Po}{\mathrm{Re}} \qquad (5)$$

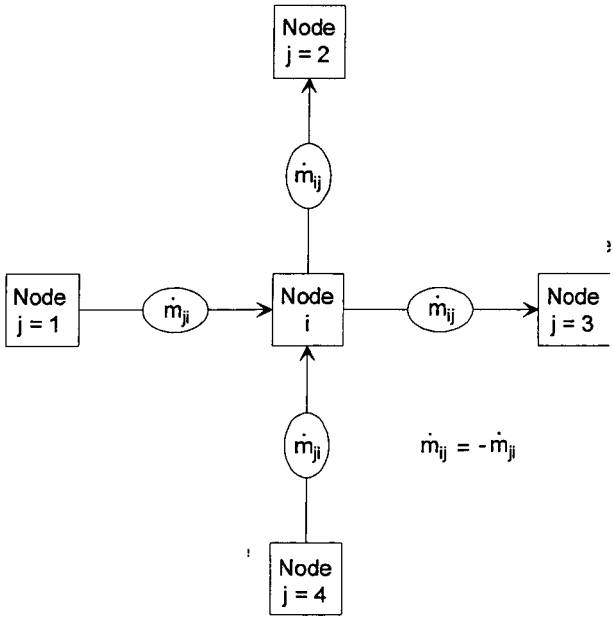
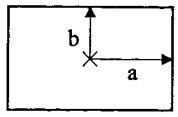
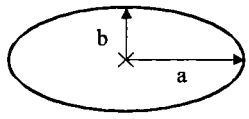


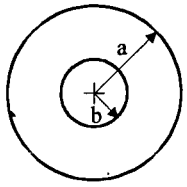
Figure 2. Schematic of connections between Nodes by Branches and the indexing practice



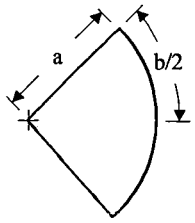
(a) - Rectangle



(b) - Ellipse



(c) - Concentric Annulus



(d) - Circular Sector

Figure 3. Non-circular duct cross-section

2.3 Energy Conservation Equation

The energy conservation equation for fluid node *i*, shown in Figure 2, can be expressed following the first law of thermodynamics and using enthalpy as the dependant variable. The energy conservation equation based on enthalpy can be written as

$$\frac{m\left(h-\frac{p}{\rho J}+\frac{1}{2}\frac{\rho u^2}{g_c J}\right)_{\tau+\Delta\tau}-m\left(h-\frac{p}{\rho J}+\frac{1}{2}\frac{\rho u^2}{g_c J}\right)_{\tau}}{\Delta\tau} \tag{6}$$

$$=\sum_{j=1}^{j=n}\left\{\mathrm{MAX}\left[-\dot{m}_{ij},0\right]\left(h_j+\frac{1}{2}\frac{\rho_j u_j^2}{g_c J}\right)-\mathrm{MAX}\left[\dot{m}_{ij},0\right]\left(h_i+\frac{1}{2}\frac{\rho_i u_i^2}{g_c J}\right)\right\}$$

The MAX operator represents the upwind formulation.

2.4 Equation of State

The resident mass in the ith control volume can be expressed from the equation of state for a real fluid as

$$m=\frac{pV}{RTz} \tag{7}$$

For a given pressure and enthalpy the temperature and compressibility factor in equation 6 is determined from the thermodynamic property program developed by Hendricks et al [7].

3. Solution Procedure

The pressure, enthalpy, and resident mass in internal nodes and flowrate in branches are calculated by solving equations (1), (6), (7), and (2) respectively. A combination of the Newton-Raphson method and the successive substitution method has been used to solve the set of equations. The mass conservation (1), momentum conservation (2) and resident mass (7) equations are solved by the Newton-Raphson method. The energy conservation equations for fluid and solid are solved by the successive substitution method. The temperature, density and viscosity are computed from pressure and enthalpy using a thermodynamic property program [7]. Figure 4 shows the flow diagram of the Simultaneous Adjustment with Successive Substitution (SASS) scheme. The iterative cycle is terminated when the normalized maximum correction Δ_{max} is less than the convergence criterion C_c. Δ_{max} Is determined from

$$\Delta_{max} = \max \left| \sum_{i=1}^{N_E} \frac{\phi_i'}{\phi_i} \right| \qquad (8)$$

The convergence criterion is set to 0.001 for all models presented in this paper. The details of the numerical procedure are described in Reference [6].

4. Computer Program

GFSSP (Generalized Fluid System Simulation Program) embodies the mathematical formulation and solution procedure described in the previous sections. The program structure is shown in Figure 5. The program consists of three modules: Graphical User Interface, Solver and User Subroutines. VTASC (Visual Thermofluid dynamics Analyzer for Systems & Components) is the Graphical User Interface (GUI). VTASC allows user to create a flow circuit using a point and click paradigm. It creates an ASCII data file that is read by the solver module and it reads the output data file for post processing the results. The solver module reads the data file generated by VTASC. It generates all governing equations from network data. The equations are solved by the iterative algorithm (SASS). It calls thermodynamic property programs to obtain the necessary properties during the iterative cycle.

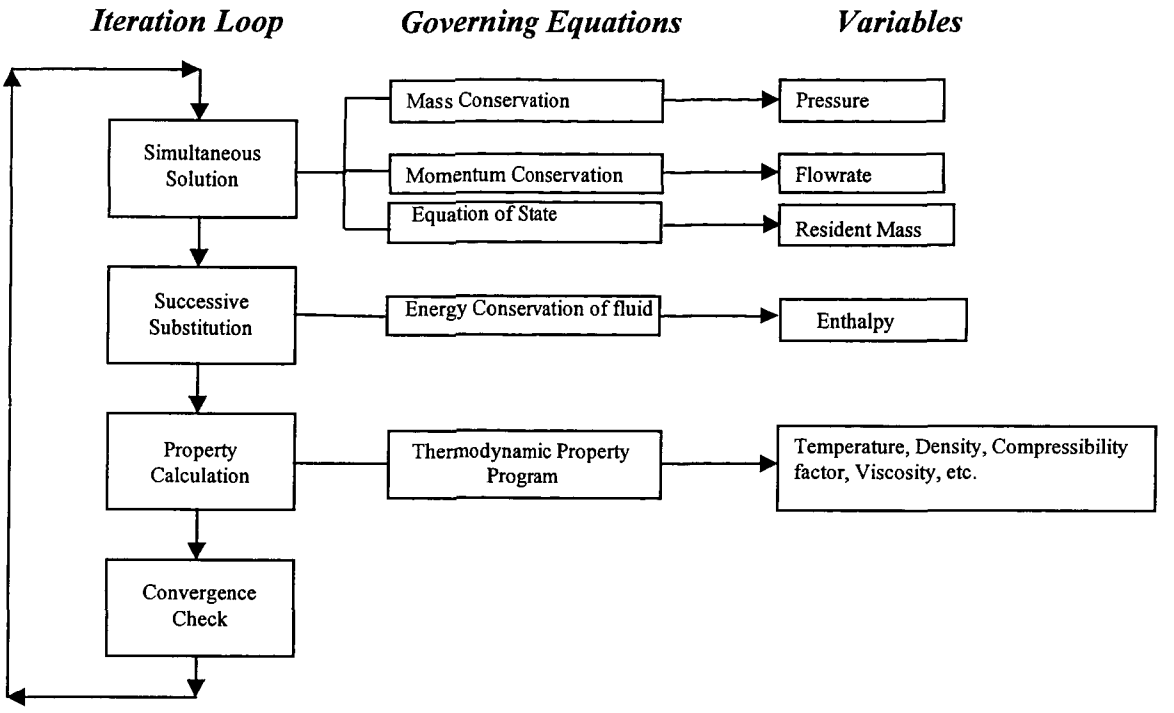


Figure 4. SASS (Simultaneous Adjustment with Successive Substitution) Scheme for solving Governing Equations

5. Computational Fluid Dynamics (CFD) Analysis

To assist validation of the GFSSP model for micro-fluidics network, a detailed 3-D CFD analysis was also carried out. Using CFD, the Navier-Stokes momentum differential equations are numerically solved. In this study, the CFD-ACE+ code [5], utilizing finite volume numerical method was used for calculating velocity and pressure fields within the 3-D micro channel configuration. The CFD method utilizes pressure-based SIMPLC algorithm and the incompressible flow equations are solved here on a multi-block structured grid system.

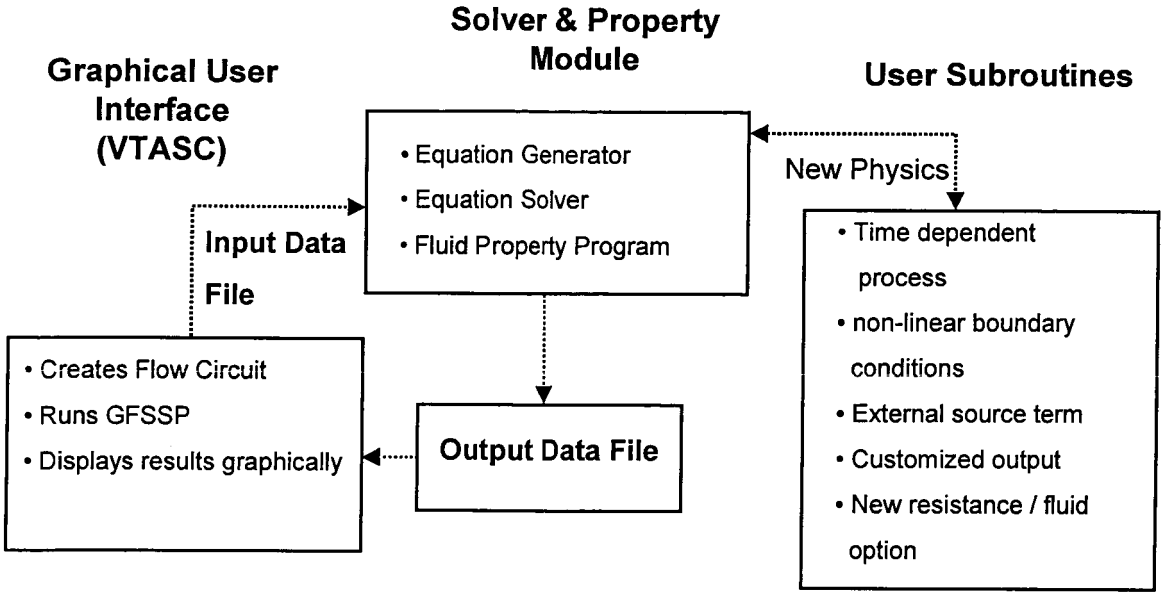


Figure 5. GFSSP Program Structure

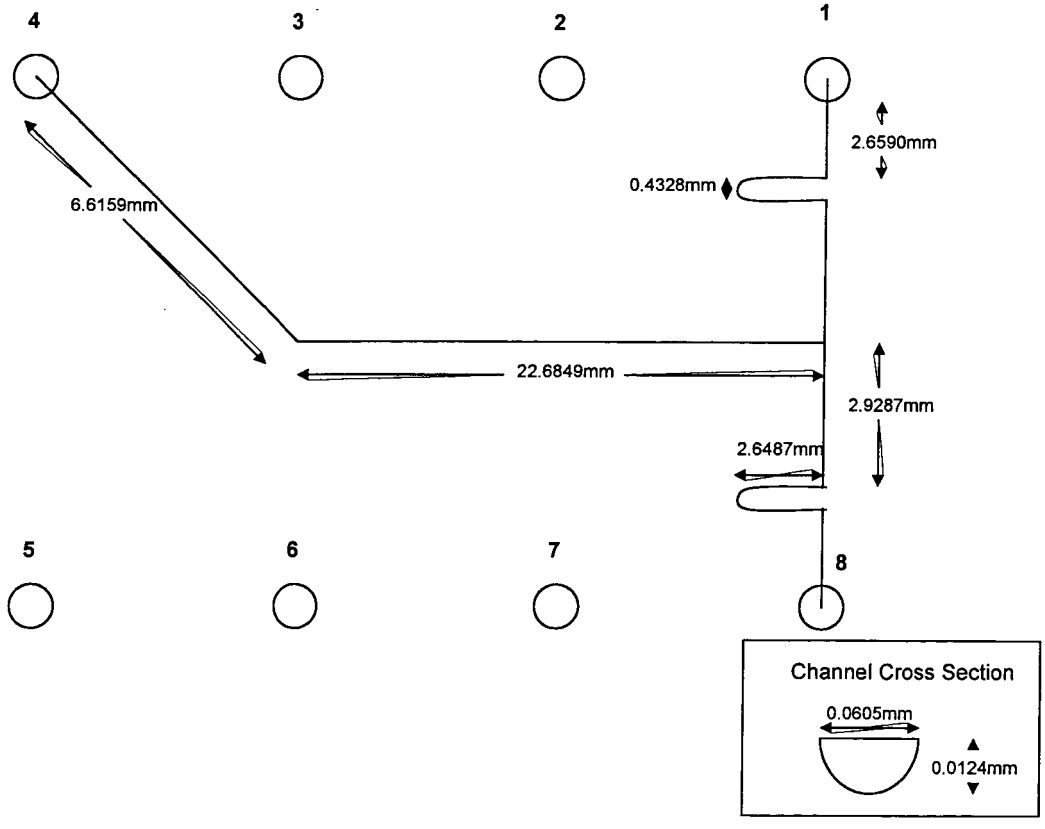


Figure 6. Micro-fluidic chip considered for model verification

6. Results & Discussion

The T-junction micro flow on the Caliper N145 chip was used for validation. Figure 6 shows the layout and dimensions of micro-fluidic chip considered in the present study. The glass chip was micro fabricated by isotropic etching with about 60 micrometer in width and 12.4 micrometer in depth. The modeled geometries used for CFD calculations are shown in Figure 7 for the cross-section and at the T-junction. The GFSSP model is shown in Figure 8. By adjusting the pressure difference among well number 1, 8 and 4, different flow fields across the T-junction can be set up. Dyes were introduced in well number 1 and well number 8 for flow velocity measurement [4] using vitalization technique. To accommodate flow visualization, pressure levels at well number 1, 8 and 4 were always different with well number 4 being the minimum. For micro-channel with this dimension, the electro-viscous effect [1] would be significant for water and low concentration ionic solution fluid flows due to the existence of electrical double layer (EDL). In addition to pure water, aqueous KCl solutions of concentration 10^{-4} and 10^{-2} M were used as the testing liquids. Following the studies of [1] and [2], the 10^{-2} M experiment was taken to be the case without EDL effects when compared to the numerical results.

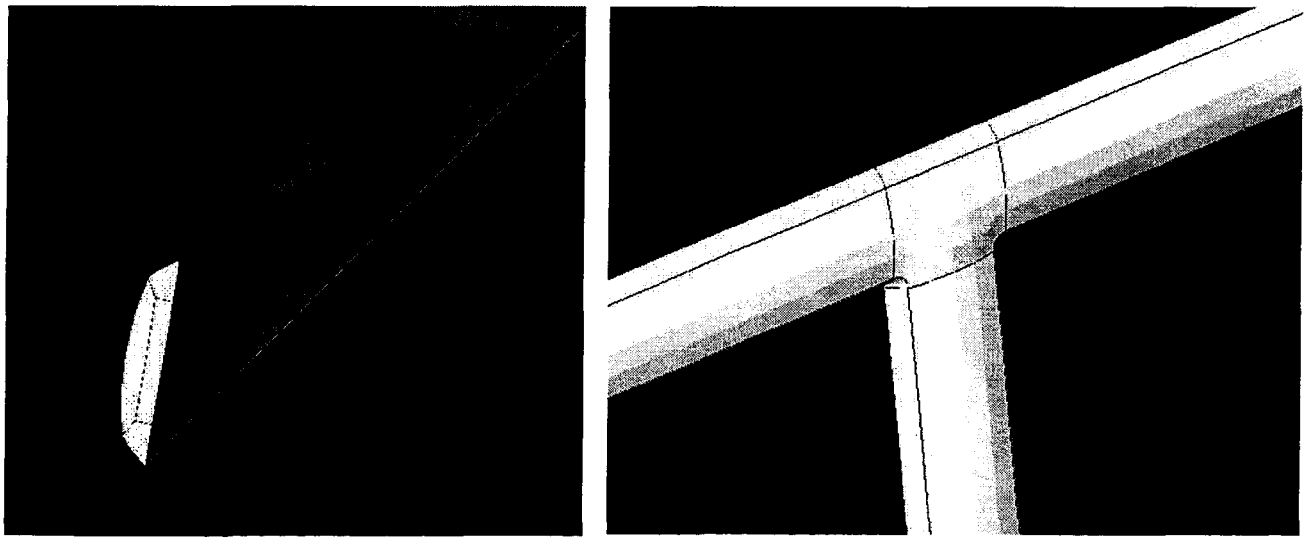


Figure 7. Modeled cross-section (a) and T-junction (b) geometries for CFD.

It may be noted that the node numbers in Figure 6 and 8 are not compatible. Node 8 of Figure 8 is equivalent to Node 1 of Figure 6. Similarly, Node 11 and 1 of Figure 8 are equivalent to Node 8 and 4 of Figure 6. The number of nodes and branches used in the numerical model was appropriate for representing resistances in the flow circuit. There were two types of resistances in the circuit. The filled rectangle represents flow in a rectangular pipe. The micro-channel cross section was assumed rectangular. The other type of resistance is denoted by 2K. This option considers the branch as a common

fittings or valves. The resistance in common fittings and valves can be computed by the two-K method [8]. For this option, K_f can be expressed as:

$$K_f = \frac{K_1 / Re + K_\infty (1 + 1/D)}{2 g_c \rho_u A^2} \qquad (9)$$

Where:

K_1= K for the fitting at Re =1;
K_∞ = K for the fitting at Re =∞;
D = Internal diameter of attached pipe, in.

The constants K_1 and K_∞ for common fittings and valves are listed in Reference [6].

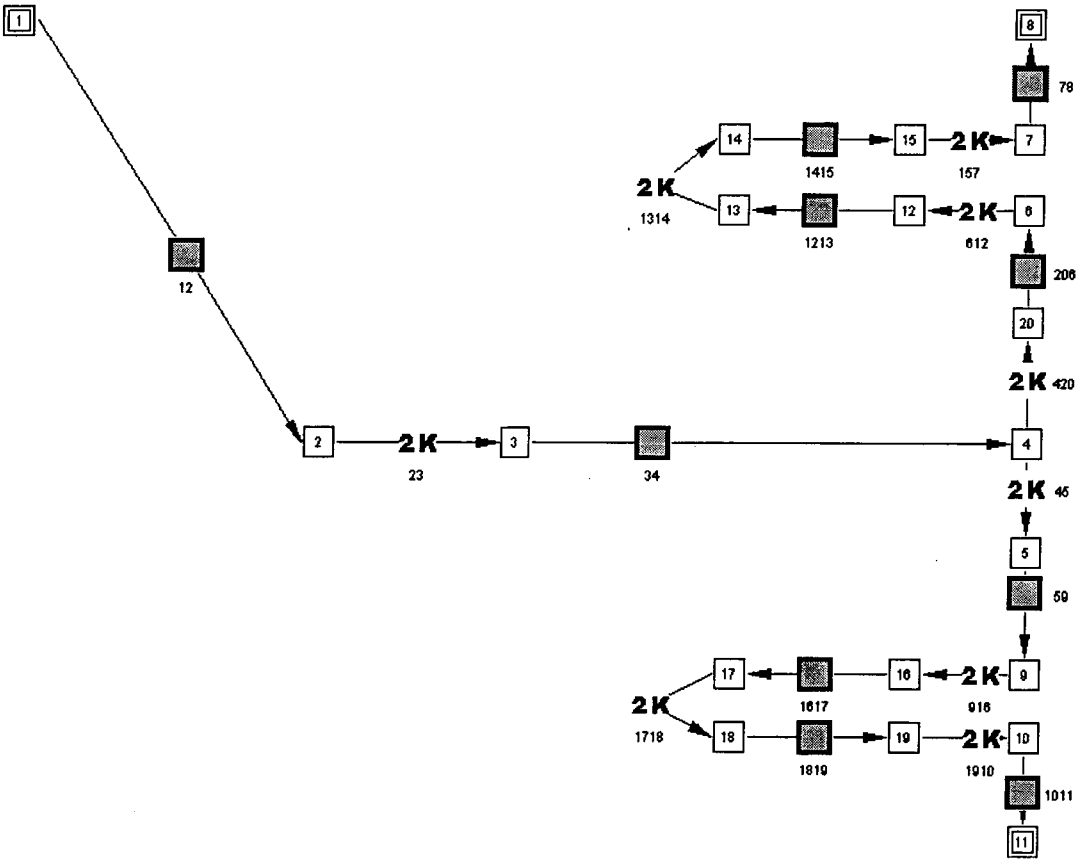


Figure 8. GFSSP model of flow network in chip with micro-channels

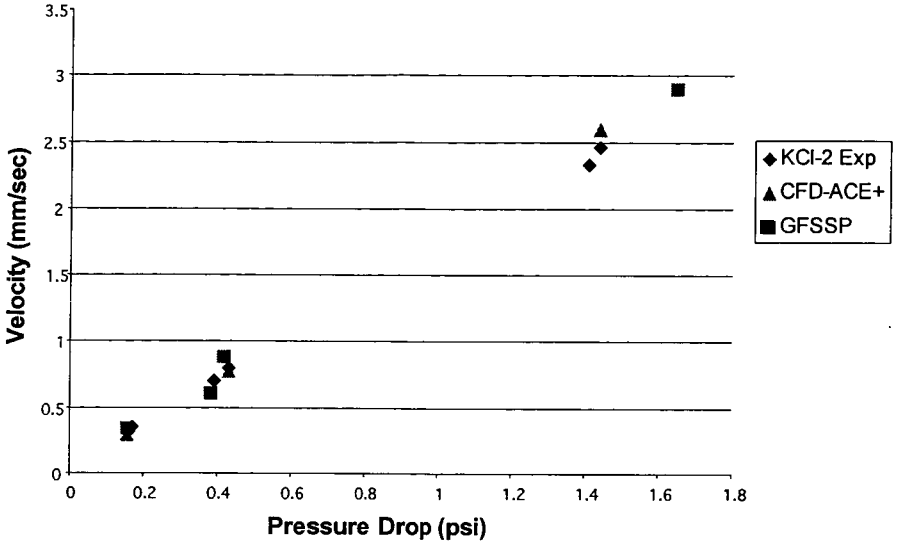


Figure 9. Comparison between numerical prediction and test data

Figure 9 shows the comparison between numerical prediction and test data. The velocity in branch 34 is plotted with the maximum pressure differential between inlet and outlet. Test data has been compared with GFSSP prediction and predictions by CFD-ACE+. It may be observed that at low flow velocity, test data, network flow analysis prediction by GFSSP and Navier-Stokes flow analysis compare well. However at higher flowrates, both predictions deviate from test data. The observed discrepancies could be attributed to electro-kinetic effect which has not been accounted for any of the analysis scheme. It may also be emphasized that pressure drop is quite accurately predicted by network analysis code which is evident from good comparison between GFSSP and CFD-ACE+ at all flowrates.

7. Conclusions

A numerical method for flow analysis in micro-fluid system has been described. The method solves the finite volume formulation of conservation equations for mass, momentum and energy in conjunction with friction correlation and thermodynamic equation of state. The numerical method is embodied into a general purpose computer program for modeling flow distribution in a generic network. The predicted numerical solution has been compared with test data as well as multi-dimensional Navier-Stokes solution. The network flow analysis results compare well with Navier-Stokes solution at different flowrates. Both numerical solutions (network system and Navier-Stokes) compare well with test data at low flowrates. Discrepancy with test data exists at higher flowrates. The observed discrepancy is attributed to the electro-kinetic effect which has

not been accounted for. The future research effort is directed to model electro-kinetic effect in micro-fluid system.

8. Acknowledgement

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9. References

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