Multiobjective Strategies for Optimization of Microfluidic Mixing

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ABSTRACT

An investigation has been performed to determine the effect of various surface temperature distributions on the mixing of a binary fluid. Lattice Boltzmann simulations were conducted on a binary fluid in a micro channel having Re<10 and various wall temperature distributions. Also, optimization techniques were employed to determine acceptable solutions using mutltiobjectives and applied constraints. Good agreement was found between the "brute force" method of computing over 130 cases versus using the optimization scheme. It appears that this is the first application of optimization to micro channel surface directed flows.

Keywords: lattice Boltzmann,, microfluidics, mixing, simulations, multiobjective optimization

1 SEARCHING FOR OPTIMAL MIXERS

Recent computations[2-4] using the LBM to investigate surface temperature effects on fluid mixing in both 2D and 3D channels has demonstrated the complex nature of trying to find "optimum" wall temperature distributions. A long-term goal is to apply the optimal surface temperature distribution technique to surface property variations, for example temperature, hydrophobic and hydrophilic distributions, to manipulate channel flows. This technique is in contrast to many current studies utilizing flow control and fabricated, wall modifications to enhance mixing. Even with today's computers, finding "optimal" distributions is formidable. To address this issue, multiobjective optimization techniques were considered.

Optimizing a real-valued function - a single objective - is standard optimization theory while optimizing a vector-valued function is multiobjective optimization theory. When optimizing multiple objectives, it is rare to find a single solution that simultaneously optimizes all the objectives. Rather, one finds many solutions where improving one objective typically degrades at least one of the other objectives. By sweeping over all these solutions, the fluid engineer can make optimal trade-offs between the objectives. In other words, no solution from the set of optimal solutions can be determined as better than any other solution. Consequently, a complete multiobjective analysis is the collection of optimal solutions with a varying degree of objective values.

This paper examines such optimal mixer solutions for binary fluid flow in a 2D channel flow by varying wall temperature distributions. The applied wall temperatures had longitudinal variations along both the bottom and top channel walls. Additionally, the binary fluid model allowed fluid density ratios and various interaction strengths between fluid components. Next, multiobjective optimization techniques were applied to this binary mixing problem to determine solutions for "optimum mixing."

2 NUMERICAL METHOD

The technique used in computing incompressible flows with the LB method involves the time evolution of a density distribution function. The evolution of the Boltzmann equation has seen the development and adoption of the single relaxation Bhatnager, Gross and Krook (BGK) model for the collision operator which simplifies the operator and removes the Galilean invariance and dependence of pressure on velocity. It can be demonstrated that the Boltzmann equation recovers the Navier-Stokes equations via the Chapman-Enskog expansion. The LB method requires two steps, relaxation and streaming. During the relaxation step, distributions at the grid nodes relax to the equilibrium state according to the BGK rule. Then, in the streaming phase, the distribution advects freely at the characteristic velocity to the next node. It should be noted that the order of relaxation and streaming is not important. Once the distribution function is known, the macroscopic velocity and pressure can be calculated from its first two moments.

Building on previous work [2-4], the lattice Boltzmann BKG model in lattice units has the form

$$
\begin{aligned}
& f_{\alpha,m}(\vec{x}+\vec{e}_{\alpha}\Delta t, t+\Delta t) - f_{\alpha,m}(\vec{x},t) = \\
& (1/\tau_m)\left[\,(f_{\alpha,m}(\vec{x},t) - f^{eq}_{\alpha,m}(\vec{x},t)\right] \\
& + F_T(\vec{x},t) + \overrightarrow{G}_P \quad m = 1,2
\end{aligned}
$$

where f is the particle distribution, G_P is a body force and m=1,2 indicate equations for the density and temperature fields. The relaxation coefficients are given by τ_m and the coupling between the velocity and temperature fields is achieved via the force coupling term F_T.

The numerical simulations used a 9 bit (D9Q2) two-dimensional lattice. In this formulation the density, ρ,

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momentum, ρu, temperature, T, pressure, p, and sound speed, c_s, are determined using the expressions

$$\rho(\mathbf{x},t) = \sum_{\alpha=0}^{8} f_\alpha \qquad \rho\mathbf{u}(\mathbf{x},t) = \sum_{\alpha=0}^{8} f_{\alpha,1}\vec{e}_\alpha \quad T(\mathbf{x},t) = \sum_{\alpha=0}^{8} f_{\alpha,2}$$

$$p = c_s^2 \rho \qquad c_s = c/\sqrt{3} \qquad c = 1$$

The quantity c=1 indicates that in lattice Boltzmann units, the time and grid spacing are related by $\Delta x = c\Delta t$. Additionally, the viscosity and relaxation parameters for flow field, τ_v, and temperature, τ_T, have expressions which depend on the reference velocity and length, Reynolds number, viscosity and diffusion coefficient, D_T.

$$\nu = \frac{U_{in} L}{\mathrm{Re}} \qquad \tau_\nu = \frac{6\nu + 1}{2} \qquad \tau_T = \frac{6D_T + 1}{2}$$

The binary fluid model incorporated into the current formulation follows the development of Luo et al.[1] The lattice Boltzmann equation describing the binary fluid has the form

$$f_\alpha^\sigma(\mathbf{x} + \mathbf{e}_\alpha \Delta t, t + \Delta t) - f_\alpha^\sigma(\mathbf{x}, t) = \Omega_\alpha^\sigma$$

where the collision term contains the fluid-fluid interaction formulation. The mass density and momentum of the fluid mixture are

$$\rho = \rho_\sigma + \rho_\varsigma \qquad \rho u = \rho_\sigma u_\sigma + \rho_\varsigma u_\varsigma$$

$$\rho_\sigma(\mathbf{x},t) = \sum_\alpha f_\alpha^\sigma \qquad \rho_\sigma \mathbf{u}_\sigma(\mathbf{x},t) = \sum_\alpha f_\alpha^\sigma \mathbf{e}_\alpha$$

3 COMPUTATIONAL DOMAIN

The computational domain is composed of a two-dimensional channel that has four temperature zones with lengths, L, as shown in figure 1. The temperatures on the channel upper wall are specified to be some multiple of the bottom wall temperature

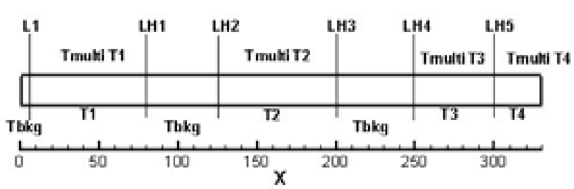


Figure 1. Sketch of the computational domain and wall temperature configuration.

The boundary conditions used in the simulations specify the Reynolds number, fluid viscosity and diffusion coefficient. Equating the Reynolds number at full scale with the Reynolds number in lattice units provides the reference velocity, U_{in}, and the viscosity, ν, can then be computed using the equations given above. The channel flow was pressure driven, and the inlet velocity, temperature and fluid components were specified. Also, the wall temperature distribution were specified using the scheme shown in figure 1.

4 QUALITY OF FLUID MIXING

To determine the quality, or degree of mixing, obtained for a particular temperature distribution and set of fluid properties, the difference in fluid density found at the upper and lower channel walls was used. The shape of the transverse (y) distribution of fluid densities was similar in all cases computed in this study. The general shape and measurement points are shown in figure 2.

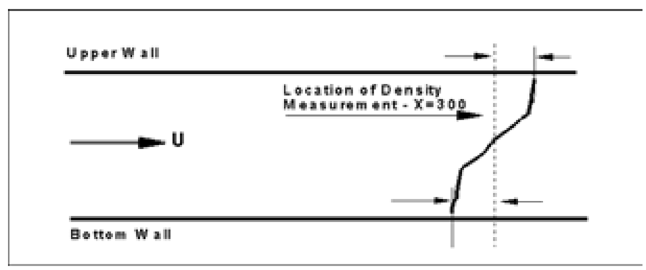


Figure 2. Sketch of the mixing quality measurement.

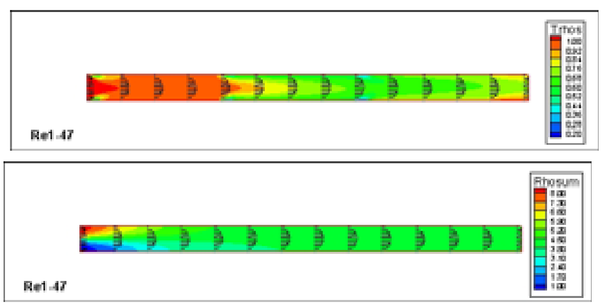
5 PARAMETRIC STUDY RESULTS

The following simulations demonstrate the effect of varying the temperature distribution along the channel. As shown in figure 1, the length and location of the various heated regions along the channel can be varied using the lengths *L*. Five distributions were considered, and the lengths are given in table 1. Also, the following parameters were used for a Reynolds number of Re=1.0: bottom wall temperatures of T_1=1.0, T_2=0.56, T_3=0.80 and T_4=1.0; top wall temperatures $T_{top}=0.90T_{bottom}$; a fluid-thermal coupling of C_T=0.0005; fluid density ratio of 1:10; and a fluid interaction coefficient of 0.025. The data in figure 3 presents the results at time t=10K for two cases. While the results do not show large differences in temperatures and fluid contours, the examples do suggest the difficulty of finding "optimum" temperature distributions. The transverse temperature distribution near the channel exit indicates a reasonably well mixed fluid.

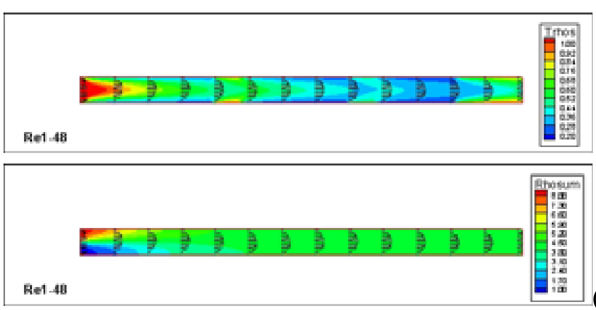
To determine if there exists a solution space where one could find acceptable solutions for a given channel flow configuration, over 130 channel flow simulations were made. The ranges of conditions considered are as follows. Re=1-250, fluid density differences of 1:1, 1:2, 1:5 and 1:10, fluid interaction coefficients ω_D= 0, 0.010 and 0.025, wall temperature multipliers of T_{multi}=0.50, 0.75, 0.90 and 1.0 where the channel top wall temperature was $T_{top}=T_{multi}T_{bottom}$ and the fluid thermal coupling varied from C_T =0, 0.00025 and 0.0005. Figure 4 shows the results for all the simulations conducted at Re=1.0.

Case No.	L1	LH1	LH2	LH3	LH4	LH5
46	5	80	125	200	250	300
47	10	100	110	200	210	300
48	100	120	200	220	280	300
49	100	160	170	230	240	300
50	30	70	130	200	230	300

Table 1. Lengths used to specify the temperature zones along the channel



(a)



(b)

Figure 3. Examples of the microcannel flow, with Re=1, using the five length distributions for temperature given in Table 1. Shown are the velocity vectors and contours of temperature (top) and total density (bottom) (a) Case 47; and (b) Case 48.

6 MULTIOBJECTIVE OPTIMIZATION FOR FLUID MIXING

Most engineering problems trade competing objectives to optimize system performance. For mixing fluids, a mixing process that delivers a good mix of fluid 1 may not mix fluid 2 very well. However, it may be possible to adjust the mixer to get a better mix of fluid 2 by accepting a slightly worse mix of fluid 1. That is, the mixing system is designed to simultaneously optimize the mixing of both fluids. The mathematics of trading these competing objectives is called *multiobjective optimization.*

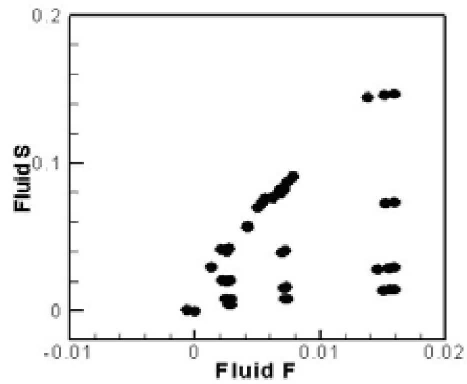


Figure 4. Quality of mixing for Re=1 computations.

The following simulations illustrate the quality of fluid mixing that can be obtained by varying the temperatures T_1, T_2, T_3, and T_4. Let $\boldsymbol{T}$ denote the temperature vector:

$$\boldsymbol{T} = [\ T_1\ \ T_2\ \ T_3\ \ T_4\ ] \quad (0 \leq T_n \leq 1).$$

The temperature multipliers are fixed at 0.9: $T_{top}=0.9T_{bot}$ and the heater layout is fixed and defined by:

$$\boldsymbol{L} = [\ 30\ \ 70\ \ 130\ \ 200\ \ 230\ \ 300\ ].$$

The LBM is run with all inputs held constant—only the temperature vector $\boldsymbol{T}$ is allowed to vary. Let $q_F(\boldsymbol{T})$ denote the quality of the mixing for fluid F. Let $q_S(\boldsymbol{T})$ denote the quality of mixing for fluid S. The mixing function is

$$\boldsymbol{q}(\boldsymbol{T}) = [\ |q_F(\boldsymbol{T})|\ \ |q_S(\boldsymbol{T})|\ ].$$

A better mix is characterized by simultaneously forcing $|q_F(\boldsymbol{T})|$ and $|q_S(\boldsymbol{T})|$ as small as possible. Figure 5 shows the MATLAB results of randomly sampling the temperature vector $\boldsymbol{T}$ and plotting the mixing function $\boldsymbol{q}(\boldsymbol{T})$. The tight correlation between the two fluids gives the linear shape. The minimal elements are the small base of the “L”. On the left side of the minimal elements, we see that q_F=0 or that perfect mixing is achieved for fluid F. Figure 5 also verifies that the minimizer can recognize a Pareto point. Indeed, the problem of numerically identifying a Pareto point, and the more general problem of *halting* a minimizer, are non-trivial problems. The minimizer was started at the temperature vector

$$\boldsymbol{T}_0 = [\ 0.1146\ \ \ 0.02374\ \ \ 0.01779\ \ \ 0.9523]$$

corresponding to the bottom of the "L." Only 6 function evaluations were made before the minimizer determined a Pareto point had been *numerically* obtained and terminated at the point marked with the $\boldsymbol{q}_{\mathrm{MO,opt}}$. The associated optimal temperatures are listed on the right and vary slightly from starting temperatures.

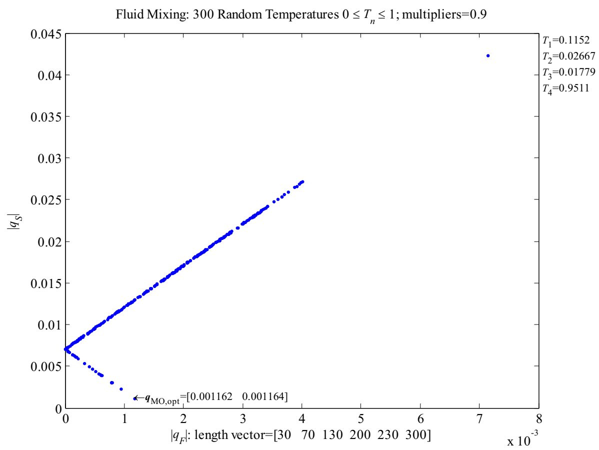


Figure 5: Mixing as a function of temperature.

Figure 6 tests the multiobjective minimizer by asking—does it find a minimal element when started from a non-minimal element? The non-optimal point was

$$\boldsymbol{T}_0 = [\ T_1 \ \ T_2 \ \ T_3 \ \ T_4\ ] = [\ 0.5 \ \ \ 0.5 \ \ 0.5 \ \ 0.5].$$

Figure 6 marks the mixing performance of $\boldsymbol{T}_0$ by the point labeled $\boldsymbol{q}_0$. The minimizer converged to a Pareto point $\boldsymbol{q}_{\mathrm{MO,opt}}$ in only 41 function calls.

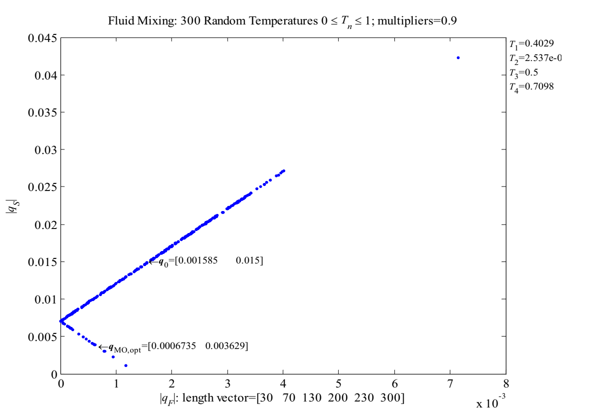


Figure 6: A minimal element determined from a non-optimal starting point

7 SUMMARY

A lattice Boltzmann method has been implemented to provide solutions for the velocity field, temperature distribution and binary fluid transport in 2D channel flows typical of microfluidic systems. Solutions using various Reynolds numbers, wall temperature distributions and fluid properties has clearly shown the difficulty in finding an "optimum" distribution of wall temperatures to provide maximum binary fluid mixing. Over 130 cases were computed and show that zones of acceptable fluid mixing can be defined. To provide a numerical technique to find the range of acceptable solutions for the mixing of two fluid components, multiobjective optimization techniques were used. The results show that, by optimizing on either heater geometry or heater temperature, a distribution of mixing quality (the mixing of fluid 1 and 2) can be obtained. This data has the same trend as found by using the "brute force" method. Also, the data provides a guideline to determining what level of mixing of two fluids will satisfy the device constraints. Additional work involves the application of a multiobjective optimizer to obtain the "optimum" mixing via the simultaneous specification of both heater geometry and temperature.

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