Modelling Annular Micromixers

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Abstract

Magnetohydrodynamic mixing of two fluids in an annular microchannel is modelled as a two-dimensional, laminar, convection-diffusion problem, and examined using asymptotic analysis and numerical simulation. The time T required for mixing of a plug of solute depends on the Peclét number Pe, and on the geometry of the annulus. Three scaling regimes are identified: purely diffusive, Taylor-dispersive, and convection-dominated; each with a characteristic power-law dependence of T upon Pe. Consequences of these results for optimal micromixer design are discussed.

Keywords: Mixing, microfluidics, Taylor dispersion, Peclét number, convection-diffusion.

1 Introduction

Recent advances in microfluidic and lab-on-a-chip technology have led to increased interest in laminar mixing of fluids [1], [2]. Efficient mixing is vital for chemical reactions, but turbulence is absent at the low Reynolds numbers common in microscale devices, and molecular diffusion mixes on an unacceptably slow time-scale. In this paper we discuss the mathematical modelling of an annular magnetohydrodynamic (MHD) micromixer, prototypes of which are under development at the Irish National Microelectronics Research Centre [3]. The device consists of an annular channel (see Figure 1), with inner and outer walls acting as electrodes, and an electromagnet underneath, which provides a vertical magnetic field. A radial electric field is imposed by applying a potential difference across the inner and outer electrodes, and the resulting current density $\mathbf{j}$ combines with the magnetic field $\mathbf{B}$ to give an azimuthal Lorentz force $\mathbf{j} \times \mathbf{B}$ on the fluid [4].

The mixing action of this device in the absence of molecular diffusion was considered in [1]. In realistic applications, the actions of convection and diffusion are felt simultaneously, and the goal of this paper is to examine their effect upon the efficiency of the mixer. The discussion here is limited to two dimensions, where the idealized limit of infinite depth has been taken. Previous studies of MHD pumping in an annulus have been motivated by liquid-metal flows and their stability [4],
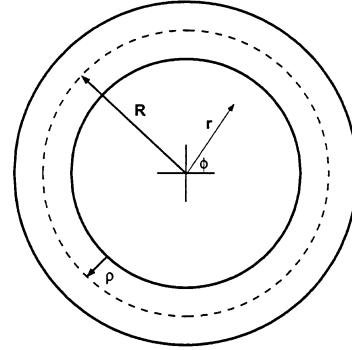

Figure 1: Annular geometry, showing the centre-line radius R, and the channel half-width ρ.

[5], but to our knowledge, this is the first investigation of the mixing effects in an annular geometry.

2 Notation and equations

The geometry of the annulus is shown in Figure 1. The radius of the center-line is R, and ρ represents the half-width of the channel, so the inner wall is located at $r = R - \rho$, and the outer wall at $r = R + \rho$. We describe the geometry using the nondimensional parameter

$$\gamma = \frac{\rho}{R}, \quad (1)$$

which may take values between zero and one. Note that the limit $\gamma \to 0$ corresponds to a locally straight channel, and γ approaches 1 as the annulus becomes a punctured disk.

The fluid velocity in the micromixer is found by solving the steady Navier-Stokes equations in the presence of the MHD body force [5]. In the two-dimensional case considered here, only the azimuthal velocity $v(r)$ is non-zero, and may be found explicitly by solving an ordinary differential equation [1]. In this paper we characterize the velocity by an average angular velocity ω. The mixing of a plug of solute into a surrounding solvent is governed by the convection-diffusion equation (assuming both fluid phases have similar density, viscosity, etc.) for the solute concentration $c(r, \phi, t)$:

$$\frac{\partial c}{\partial t} + \frac{v(r)}{r}\frac{\partial c}{\partial \phi} - \frac{\kappa}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) - \frac{\kappa}{r^2}\frac{\partial^2 c}{\partial \phi^2} = 0, \quad (2)$$

with no-flux boundary conditions at the walls. Here κ is the molecular diffusivity. In the following sections we examine solutions of (2) using analytical, asymptotic, and numerical methods.

The dimensionless parameter used to compare the importance of convection and diffusion in (2) is the Peclét number, which we define for our system as

$$Pe = \frac{\omega R \rho}{\kappa}. \tag{3}$$

Note that ωR is the characteristic linear velocity, while ρ is the smallest linear dimension in the system. Two natural groupings of parameters to give a dimensional time will be used in the sequel: the diffusion time R^2/κ, which measures the time for azimuthal mixing by diffusion in the absence of convection; and the convection time ω^{-1}, which is representative of the timescale of rotation of the fluid. The choice of appropriate time-scaling depends on whether diffusion or convection is dominant—we initially choose ω^{-1}, but will consider the alternative in the final section.

A completely mixed solute-solvent system has the initial concentration of solute spread evenly over the whole annulus. We define mixing efficiency using the timescale over which the concentration profile evolves to the uniform state. In order to measure the deviation from uniformity, we define an average over the annulus, so that the average concentration (for instance) is

$$\langle c \rangle = \frac{1}{4\pi R \rho} \int_{R-\rho}^{R+\rho} \int_0^{2\pi} c(r, \phi, t) r \, d\phi \, dr. \tag{4}$$

In fact, it is straightforward to show from the convection-diffusion equation that $\langle c \rangle$ is a constant; the total amount of solute is not changed over time, it is simply redistributed evenly over the annulus. In the following sections we adopt a simple initial concentration

$$c(r, \phi, 0) = 1 + \cos \phi, \tag{5}$$

for ease of asymptotic analysis. Numerical results [6] indicate that the asymptotic results remain valid for other initial conditions.

A *mixing measure* $m(t)$ is a positive function of time characterizing the deviation of the concentration at time t from its uniformly mixed state $c = \langle c \rangle$. Define $m(t)$ by

$$m(t) = \frac{\left\langle (c(r, \phi, t) - \langle c \rangle)^2 \right\rangle}{\left\langle (c(r, \phi, 0) - \langle c \rangle)^2 \right\rangle}, \tag{6}$$

so that $m(0) = 1$, and $m(t) \to 0$ as $t \to \infty$. The time T_M for $m(t)$ to decay from 1 to a specified value M is called the *mixing time*, and is defined by the condition

$$m(T_M) = M. \tag{7}$$

From the point of view of experimentalists and design engineers, it is desirable to have simple formulas relating the mixing time T_M to the Peclét number Pe and the geometry ratio γ of the micromixer. We proceed to obtain asymptotic approximations to the solution of (2), and hence scaling laws for the mixing times T_M.

3 Low Peclét numbers

When the Peclét number (3) is sufficiently small, diffusive effects completely dominate convective motion. The mixing time by diffusion alone may be calculated by solving the equation resulting from neglecting the convective term in (2). It is straightforward to find an infinite series solution by separating variables. Consequently, the mixing measure (6) in this case is

$$m(t) = \sum_{j=1}^{\infty} e^{-2\kappa \lambda_{1j} t} \frac{\left\langle F_1 \left(r \sqrt{\lambda_{1j}} \right) \right\rangle^2}{\left\langle F_1 \left(r \sqrt{\lambda_{1j}} \right)^2 \right\rangle}, \tag{8}$$

where F_1 denotes the first radial eigenfunction, and may be written in terms of Bessel functions. The form of $m(t)$ at large times t is dominated by the first term ($j = 1$) in this sum. Indeed, in the limit $\gamma \to 0$, we have

$$m(t) \sim \exp(-2\kappa \lambda_{11} t) \quad \text{as } t \to \infty, \tag{9}$$

with the eigenvalue given by

$$\lambda_{11} = \frac{1}{R^2} \left[1 + \frac{1}{3}\gamma^2 + O(\gamma^4) \right] \text{ for } \gamma \ll 1. \tag{10}$$

The asymptotic mixing time T_M as defined in (7) then follows from (9) and (10):

$$T_M \sim \frac{1}{2\kappa \lambda_{11}} \ln \left(\frac{1}{M} \right) \quad \text{as } M \to 0, \tag{11}$$

and so the nondimensional mixing time is

$$\omega T_M \approx \frac{Pe}{2\gamma} \ln \left(\frac{1}{M} \right) \left[1 - \frac{1}{3}\gamma^2 + \ldots \right] \quad \text{for } \gamma \ll 1. \tag{12}$$

4 Intermediate Peclét numbers

Taylor [7], [8] calculated the dispersion in a straight capillary due to convection, and his methods are readily adapted to find the Taylor dispersion in an annulus, see Nunge et al. [9]. An examination of the Peclét numbers for which Taylor's approximations are valid [6] leads us to conclude that for Pe in the range

$$7.2 \ll Pe \ll 15/\gamma, \tag{13}$$

the mixing measure has an exponential tail

$$m(t) \sim \exp(-2Dt) \quad \text{as } t \to \infty, \tag{14}$$

with Taylor dispersion coefficient D. The nondimensional mixing time can be shown to have the asymptotic form

$$\omega T_M \approx \frac{1}{\gamma Pe} \ln\left(\frac{1}{M}\right) \frac{105}{4} \left[1 - \frac{18165}{1576}\gamma^2 + \ldots\right] \text{ for } \gamma \ll 1. \tag{15}$$

5 Convection-dominated mixing

When the molecular diffusion term is small in comparison to the convective term, i.e., the limit of large Peclét number, a singularly-perturbed problem results. Regular perturbation methods fail to give approximations which are uniformly valid in time for such problems, and so we introduce multiple time scales. After some analysis [6], the mixing measure is calculated to leading order as

$$m(t) = \frac{\sqrt{\pi}}{2} F\left(\frac{6\omega^3 t^3}{\gamma Pe}\right), \tag{16}$$

where F is defined as the monotonic function

$$F(x) = x^{-1/2}\text{erf}(x^{1/2}). \tag{17}$$

The nondimensional mixing time corresponding to a mixing measure value of M is therefore

$$\omega T_M \approx \left[\frac{\gamma Pe}{6} F^{-1}\left(\frac{2M}{\sqrt{\pi}}\right)\right]^{1/3}, \tag{18}$$

and note in particular that this increases as $Pe^{1/3}$ when M and γ are fixed.

6 Numerical simulations

To check the asymptotic results derived in previous sections, and to extend to cases with initial conditions other than the simple form (5), we solve the convection-diffusion equation (2) numerically. Logarithmic plots of $m(t)$ as a function of time at various Pe values are shown in Figure 3 for $\gamma = 0.05$. For comparison we plot also the asymptotic forms of $m(t)$, using (9) in the diffusive regime, (14) in the Taylor regime, and (16) in the convective regime. The asymptotic formulas fit the numerical results well, even at early times. Note that the straight-line asymptotes at very large times for the high-Pe case are not reproduced by the multiple-time solution—this is apparently due to the neglect of the boundary conditions in our analysis, and the subsequent importance of boundary layers at the inner and outer walls.

From the numerical solution for $m(t)$, it is straightforward to calculate the mixing times T_M required for the measure to decay from its initial value of 1 to the value M. We choose three values of M for comparison with the asymptotic predictions: $M = 0.3, 0.1,$ and
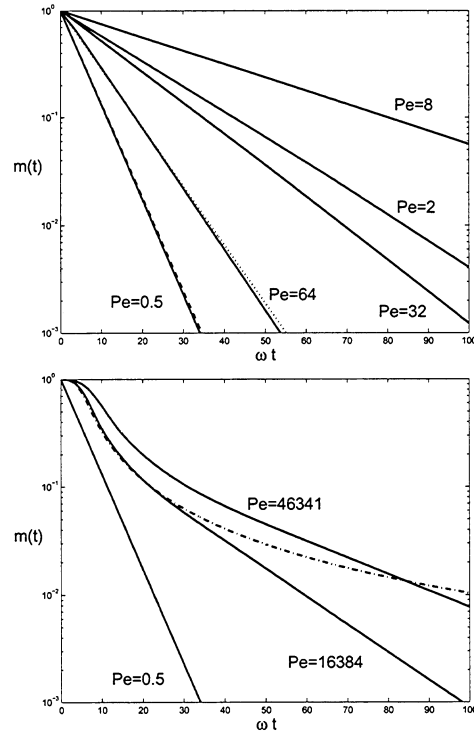
Figure 2: Mixing measure $m(t)$ as a function of nondimensional time, calculated in numerical simulations with $\gamma = 0.05$ and various Peclét numbers as shown. Asymptotic predictions are also shown for: $Pe = 0.5$ (dashed) using (9); $Pe = 64$ (dotted) using (14); and $Pe = 16384$ (dot-dash) using (16).

0.01, and investigate a wide range of Peclét numbers. The numerical values of nondimensional times ωT_M are plotted in Figure 4 along with the straight lines corresponding to the formulas (12), (15), and (18). Note the excellent agreement with predictions, except for the lowest value of M, when the multiple scale solution no longer accurately describes the time evolution of $m(t)$. We have also shown in [6] that the asymptotic predictions remain valid when γ is a sizable fraction of unity, and for different initial conditions than (5).

The nondimensional time ωT_M used in Figure 3 may be replaced by the alternative nondimensionalization, i.e., the diffusion time $\kappa T_M/R^2$. The timescales are related by

$$\frac{\kappa T_M}{R^2} = \frac{\gamma}{Pe}\omega T_M, \tag{19}$$

and so the data of Figure 3 is easily recast in terms of the diffusion time, see Figure 4. Figure 4 is especially of interest to experimentalists working with a particular solute and solvent (so that κ is fixed) while varying the rate of rotation velocity ω of the micromixer to change Pe. The mixing time is seen to decrease from the diffusion time through the Taylor regime (at a rate
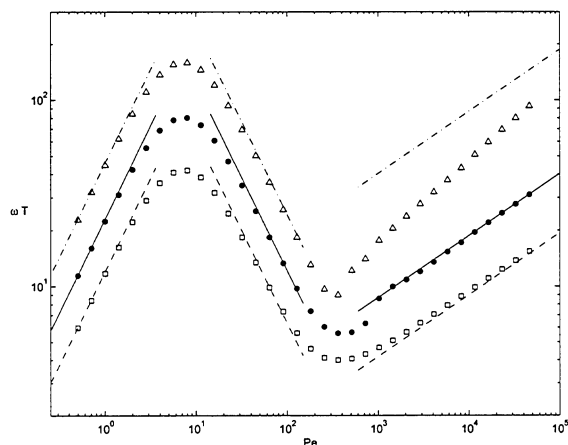
Figure 3: Nondimensional mixing times ωT_M as a function of Peclét number, for $\gamma = 0.05$. Asymptotic results are shown as lines, and numerical results as symbols for values of the mixing measure: $M = 0.3$ (dashed line; squares), $M = 0.1$ (solid line, points), and $M = 0.01$ (dot-dash line, triangles)
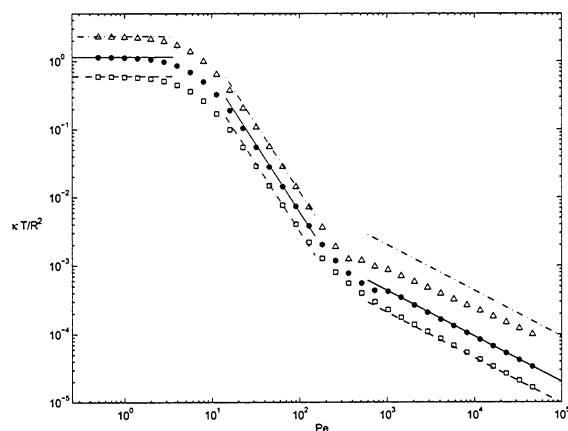

Figure 4: Mixing times nondimensionalized by the diffusion time, $\kappa T/R^2$, as a function of Peclét number, for $\gamma = 0.05$. See Figure 3 for legend.

proportional to Pe^{-2}), and then continue to decrease at a slower rate beyond the Taylor regime. The slower rate corresponds to a $Pe^{-2/3}$ scaling when (16) is valid, i.e., for $M \geq 0.1$, but is closer to $Pe^{-1/2}$ for very small values of M. This is again a consequence of the failure of the multiple-scale method to account for the very long time scales where boundary layer effects become non-negligible.

From our analysis of the limits of validity of the Taylor dispersion description we can estimate the end of the Taylor regime as $15\gamma^{-1}$ for small γ. Of interest to the micromixer designer is the influence of the geometry ratio γ: as the mixing time decreases as Pe^{-2} until $Pe \approx 15\gamma^{-1}$, it is desirable to decrease γ as much as possible in order to achieve faster mixing at lower velocities (i.e., lower power inputs in electric and magnetic fields). Of course smaller γ may imply lower volumes of fluid in the mixer, and due consideration must be given to the loading and unloading times of the fluids.

REFERENCES

[1] J. P. Gleeson and J. West, "Magnetohydrodynamic Micromixing," *Proceedings of the Fifth International Conference on Modeling and Simulation of Microsystems 2002,"* 318, (2002).

[2] I. Meisel and P. Ehrhard, "Simulation of electrically excited flows in microchannels for mixing application," *Proceedings of the Fifth International Conference on Modeling and Simulation of Microsystems 2002,"* 62, (2002).

[3] J. West et al., "Application of magnetohydrodynamic actuation to continuous flow chemistry," *Lab on a Chip,* to appear.

[4] P. Tabeling and J. P. Chabrerie, "Magnetohydrodynamic Taylor vortex flow under a transverse pressure gradient," *Phys. Fluids* **24**, 406, (1981).

[5] M-H. Chang and C-K. Chen, "Hydromagnetic stability of current-induced flow in a small gap between concentric cylinders ," *J. Fluids Eng.* **121**, 548, (1999).

[6] J. P. Gleeson et al. , "Modelling Annular Micromixers," in preparation.

[7] G. I. Taylor, "Dispersion of soluble matter in solvent flowing slowly through a tube," *Proc. Roy. Soc. Lond.* **A219**, 136, (1954).

[8] R. F. Probstein, *Physiochemical Hydrodynamics,* 2nd ed, Wiley, New York (1994).

[9] R. J. Nunge, T.-S. Lin and W. N. Gill, "Laminar dispersion in curved tubes and channels," *J. Fluid Mech.* **51**, 363 (1972).