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JUSTIFICATION OF NON-DIMENSIONAL SCHEMES AND IDENTIFICATION OF PARAMETERS ON MODELLING ELECTROKINETIC TRANSPORT PHENOMENA IN MICROCHANNELS

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INTRODUCTION

The electrokinetic transport phenomena are to be numerically studied based on cross-linked microchannel networks, which have been commonly employed for on-chip capillary electrophoresis applications. Applied potential field, flow field and concentration field should be solved to predict the species transport process under electrokinetic flows. Together with the well-designed channel geometry, a detailed physical model was firstly formulated through a series of governing equations and corresponding boundary/initial conditions, which was briefly re-presented from our previous publications. The emphasis of current work was to justify the simplest non-dimensional scheme and identify the most beneficial parameters so that an effective and simplified non-dimensional model was developed for numerical studies.

NOMENCLATURE

c	Species concentration
D	Species diffusion coefficient
l, w	Microchannel length and width
$\mathrm{Re}\,Sc$	Reynolds-Schmidt number
v	Velocity
μ_{eo}, μ_{ep}	Electroosmotic or electrophoretic mobility
ν	Kinematic viscosity
ϕ	Applied electrical potential

PHYSICAL PROBLEM FORMULATION

As shown in Fig-1, two perpendicular channels connecting four reservoirs are arranged in a microfluid chip. Analytes are injected horizontally and then separated in the vertical microchannel through a generated sample plug in the intersection. The whole process is initiated and controlled by the applied potential field settled by electrodes in reservoirs.

$$\nabla^2\phi = 0$$

The resulting flow field is determined by the continuity and simplified momentum equation,

$$\vec{\nabla}\cdot\vec{v} = 0; \qquad -\tfrac{1}{\rho}\vec{\nabla}p + \upsilon\nabla^2\vec{v} = 0$$

Due to the employed laminar flow with pretty low Reynolds numbers, the transient and convection term in momentum equation are ignored here. Meanwhile, the difference of velocity (parallel to channel wall) only exists in the very thin electrical double layer, and therefore a slip-wall boundary condition, $\vec{v}_l = \mu_{eo}\vec{E}_l$, is applied to replace the electrical drag force. As for the unsteady species transport, it is described by

$$\partial c_i/\partial t + \left[\left(\vec{v} + \vec{v}_{epi}\right)\cdot\vec{\nabla}\right]c_i = D_i\nabla^2 c_i$$

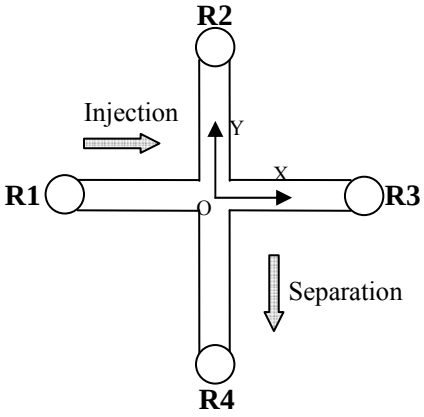

Fig-1. Schematic diagram of the cross-linked microchannel

NON-DIMENSIONALIZATION

In Tab-1, various reference values and scaling parameters are proposed for variable non-dimensionalization, and then investigated by comparing the resulting equation arrangements and pop-up controlling parameters. After applying them, the governing equations for a 2-D expansion will be,

$$\frac{\Delta\phi_r}{{\Delta x_r}^2}\left(\frac{\partial^2\phi^*}{\partial {x^*}^2} + \frac{\partial^2\phi^*}{\partial {y^*}^2}\right) = 0$$

$$\frac{\Delta u_r}{\Delta x_r}\left(\frac{\partial u^*}{\partial x^*} + \frac{\partial v^*}{\partial y^*}\right) = 0$$

$$\frac{\partial^2 u^*}{\partial x^{*2}}+\frac{\partial^2 u^*}{\partial y^{*2}}=\frac{\Delta p_r \Delta x_r}{\mu \Delta u_r}\frac{\partial p^*}{\partial x^*},\quad \frac{\partial^2 v^*}{\partial x^{*2}}+\frac{\partial^2 v^*}{\partial y^{*2}}=\frac{\Delta p_r \Delta x_r}{\mu \Delta u_r}\frac{\partial p^*}{\partial y^*}$$

$$\frac{\Delta x_r/\Delta u_r}{\Delta t_r}\frac{\partial c_i^*}{\partial t^*}+\left(u^*+u_{epi}^*\right)\frac{\partial c_i^*}{\partial x^*}+\left(v^*+v_{epi}^*\right)\frac{\partial c_i^*}{\partial y^*}=\frac{D_i}{\Delta u_r \Delta x_r}\left(\frac{\partial^2 c_i^*}{\partial x^{*2}}+\frac{\partial^2 c_i^*}{\partial y^{*2}}\right)$$

Accordingly, the local slip-wall velocity boundary condition and individual electrophoretic velocity are,

$$u_{local}^*=\frac{-\mu_{eo}\partial\phi/\partial x}{\Delta u_r}=-\frac{\mu_{eo}\Delta\phi_r}{\Delta u_r \Delta x_r}\frac{\partial\phi^*}{\partial x^*}$$

$$u_{epi-local}^*=\frac{-\mu_{epi}\partial\phi/\partial x}{\Delta u_r}=-\frac{\mu_{epi}\Delta\phi_r}{\Delta u_r \Delta x_r}\frac{\partial\phi^*}{\partial x^*}$$

Tab-1. Non-dimensionalization of variables

General variable	$\boldsymbol{\theta}$	$\boldsymbol{\theta_r}$	$\boldsymbol{\Delta\theta_r}$	$\boldsymbol{\theta^*=\frac{\theta-\theta_r}{\Delta\theta_r}}$
Geometry $\boldsymbol{l_1\sim l_4, w_h, w_v}$	x	$x_r=0$	Δx_r	$x^*=x/\Delta x_r$
Potential $\boldsymbol{\phi_1\sim\phi_4}$	ϕ	ϕ_r	$\Delta\phi_r$	$\phi^*=\frac{\phi-\phi_r}{\Delta\phi_r}$
Flow	u	$u_r=0$	Δu_r	$u^*=u/\Delta u_r$
	p	$p_r=p_a$	Δp_r	$p^*=\frac{p-p_a}{\Delta p_r}$
Concentration $\boldsymbol{t_{inj}, t_{sep}}$ $\boldsymbol{\mu_{epi}}$, $\boldsymbol{D_i}$	c	$c_r=0$	$\Delta c_r=c_{orig}$	$c^*=\frac{c}{c_{orig}}$
	t	$t_r=0$	Δt_r	$t^*=t/\Delta t_r$

If we chose $\Delta p_r=\frac{\mu\Delta u_r}{\Delta x_r}$ and $\Delta t_r=\frac{\Delta x_r}{\Delta u_r}$, some coefficients in above equations will be kept as one no matter how the rest of scaling parameters are determined. As a result, the problem becomes to choose the three scaling parameters ($\Delta x_r, \Delta u_r and\ \Delta\phi_r$) to acquire the simplest non-dimensional equations with minimum number of controlling parameters. For the length scaling parameter, the vertical channel width w_v is found to be better than other options like horizontal channel width w_h or any channel length $l_1\sim l_4$. By doing so, a unique non-dimensional separation channel width is ensured for different scenarios, and the separation process in this channel is the most important issue people concerned.

As listed in Tab-2, three different velocity scaling parameters are proposed based on reference diffusivity, kinematic viscosity and electroosmotic velocity. A consistent time scaling parameter (i.e. the time consumption for this velocity scale to pass through a characteristic length) for each is developed accordingly. For these three schemes, there is no difference for the final whole set of equations and boundary/initial conditions except for two things. One is the coefficient of diffusion term in non-dimensional concentration equation, C_D, and the other is the coefficient (C_V) of the non-dimensional expression of slip-wall velocity boundaries, $u_{local}^*=-C_V l^*\partial\phi^*/\partial x^*$, and individual electrophoretic velocities, $u_{epi-local}^*=-C_V\mu_{epi}^* l^*\partial\phi^*/\partial x^*$. It can be seen that there is only one controlling parameter $ReSc_i$ for the choice of an electroosmotic velocity under a reference applied potential field strength, $E_{ref}=\Delta\phi_r/l$. Thus, this scheme is considered as the best and then adopted in practice.

Tab-2. Three scaling parameters and resulting coefficients

	$\boldsymbol{D_{ref}}$	$\boldsymbol{\nu}$	$\boldsymbol{v_{eo}}$
$\boldsymbol{\Delta u_r}$	$D_{ref}/\Delta x_r$	$\nu/\Delta x_r$	$\mu_{eo}E_{ref}$,
$\boldsymbol{\Delta t_r}$	$(\Delta x_r)^2/D_{ref}$	$(\Delta x_r)^2/\upsilon$	$\Delta x_r/(\mu_{eo}E_{ref})$
$\boldsymbol{C_D}$	D_i/D_{ref}	$1/Sc_i$	$1/(ReSc_i)$
$\boldsymbol{C_V}$	$ReSc_{ref}$	Re	1

Two options are available for the non-dimensionalization of the last applied potential by choosing ϕ_r and $\Delta\phi_r$. The first method is to use $\phi^*=\frac{\phi-\phi_{4s}}{\phi_{2s}-\phi_{4s}}$ (or $\phi^*=\frac{\phi-\phi_{3i}}{\phi_{1i}-\phi_{3i}}$) to non-dimensionalize both injection and separation. The second one is to apply $\phi^*=\frac{\phi-\phi_{3i}}{\phi_{1i}-\phi_{3i}}$ for injection and $\phi^*=\frac{\phi-\phi_{4s}}{\phi_{2s}-\phi_{4s}}$ for separation, respectively. It is found that the second scheme is better by producing one less parameter. Two new controlling parameters (ϕ_{1i}^*, ϕ_{3i}^*) appear in the first method, but only one ($Re_{inj}Sc_i$) shows up in the second scheme. Moreover, one unique solution will be achieved for potential and flow by avoiding duplicated simulations, and it will not bring any influence to the intermediate concentration distribution between injection and separation.

PARAMETERS IDENTIFICATION

In the final non-dimensional model, four groups of optimized controlling parameters are generated to formulate the problem, and they are geometry (channel length $l_1^*\sim l_4^*$ and width w_h^*), applied electrical potentials (individual side potentials, ϕ_{2i}^*, ϕ_{4i}^* and ϕ_{1s}^*, ϕ_{3s}^*), species-fluid properties (electrophoretic mobilities μ_{epi}^* and Reynolds-Schmidt number $ReSc_i$), and operational time (for injection t_{inj}^* and separation t_{sep}^*). All above parameters will be investigated and future employed to perform parametric studies.

In summary, an effective and optimized non-dimensional model was achieved for subsequent numerical analysis on electrokinetic transport phenomena in microchannels. People can benefit from the simple and tidy non-dimensional equations and boundary/initial conditions derived in this study. Meanwhile, the minimum number of controlling parameters ensures adequate simplification of the model, and a meaningful parameter $ReSc_i$ is obtained to understand the problem better.

REFERENCES

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