



Establishment of a finite element model for extracting chemical reaction kinetics in a micro-flow injection system with high throughput sampling



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ABSTRACT

Numerical simulation can provide valuable insights for complex microfluidic phenomena coupling mixing and diffusion processes. Herein, a novel finite element model (FEM) has been established to extract chemical reaction kinetics in a microfluidic flow injection analysis (micro-FIA) system using high throughput sample introduction. To reduce the computation burden, the finite element mesh generation is performed with different scales based on the different geometric sizes of micro-FIA. In order to study the contribution of chemical reaction kinetics under non-equilibrium condition, a pseudo-first-order chemical kinetics equation is adopted in the numerical simulations. The effect of reactants diffusion on reaction products is evaluated, and the results demonstrate that the Taylor dispersion plays a determining role in the micro-FIA system. In addition, the effects of flow velocity and injection volume on the reaction product are also simulated. The simulated results agree well with the ones from experiments. Although gravity driven flow is used to the numerical model in the present study, the FEM model also can be applied into the systems with other driving forces such as pressure. Therefore, the established FEM model will facilitate the understanding of reaction mechanism in micro-FIA systems and help us to optimize the manifold of micro-FIA systems.

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1. Introduction

Flow injection analysis (FIA) has been widely applied in analytical chemistry since it was introduced in 1975 [1]. Contrary to the conventional concept that chemical analysis relies on steady-state reactions, FIA provides a new way to exploit both physical and chemical processes under non-equilibrium conditions with reproducible operation timing. In addition, FIA can easily achieve automated operation with inexpensive instruments, which effectively makes it as a useful approach in practical applications. FIA has undergone one great development with three main generations including FIA (the first generation), sequential injection analysis (SIA, the second generation) [2] and bead-injection (BI)-lab-on-valve (LOV) [3] (the third generation). The main driving force of these progresses is to miniaturize the manifolds for reducing the consumption of samples

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and reagents in FIA systems. Recently, with the development of micro-total analysis system (μ TAS), an advanced generation of micro-FIA systems has been proposed to integrate the complex chemical manipulations and detection. In the early stage of the micro-FIA system, continuous flow model was usually used for bio-analysis [4], synthesis [5,6], sample purification [7] and extraction [8]. However, these devices encountered main disadvantages of significant consumption of reagents and cross-contamination. In order to overcome these problems, zone injection model using micro-pump and micro-valve has been proposed and soon became the main format in micro-FIA system [9–12]. Verpoorte and her coworkers [9] fabricated a micro-valve for sample injection and integrated both electrochemical and photometric detectors in a silica microchip for analyzing phosphate ions. Because of the difficulty in micro-valve fabrication, external pumps and injection valves instead of micro-valve fabricated on microchip were proposed. The established micro-FIA system with two external injection pumps was verified using numerical simulations [13]. Such system could also be used to determine antioxidant [14]. In this case, the injected sample volume is still very large, and the zone injection cannot be effectively achieved using the external pumps. In 1992, Manz's group [15] made a great progress in realizing non-valve sample injection in microchips using an electroosmotic

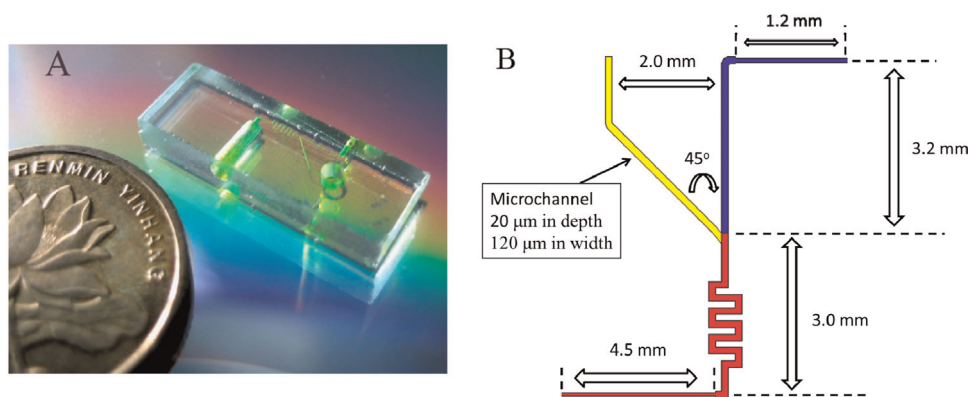


Fig. 1. Photograph of the chip used in a micro-FIA system driven by the gravity (A) and the fracture of simulation domain used in the numerical model (B). The outlet channel for controlling the difference in liquid levels is not included. The yellow and blue regions represent the sub-domains 1 and 2, respectively. These two regions are only used for introduction of reagent and sample, respectively. The red region is the sub-domain 3, where sample and reagent get mixed and then reaction starts. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

pump. However, the long-time stability of the whole system should be improved due to the Joule heat effect. This problem can be overcome simply by using the gravity driving force instead of the electroosmotic pump. We showed that gravity driven micro-FIA system could realize the zone sample injection (Fig. 1A) [16]. In this system, nanoliter sample injection and high-throughput analysis can be achieved easily.

Up to now, numerous mathematical models have been established to study the mechanism of mass transport in traditional FIA [17–24]. The “black” box method was first adopted to address mass transport in the complicated FIA systems. The regression equations [17–20] and artificial neural networks [21] are two typical representations. These methods can be used to predict reactions in FIA, however, they meet the main drawback of the requirement of a larger number of experimental data. Therefore, this “black” box method has been replaced by the analytical method in the recent years. On the basis of the mathematical descriptions of the flow pattern, mass-transport and chemical reaction kinetics, the analytical method allows deep insights into the process of FIA systems. For example, the dispersion of sample and chemical reaction kinetics can be successfully described by using the analytical methods [22–24].

With the development of photolithographic techniques, fabrication of microchip with smaller size has become feasible. It has been reported that miniaturization of the FIA systems will induce complicated mass transport behavior, i.e., the molecular diffusion will become the predominant factor in determining the chemical reaction kinetics as scaling down the dimension. Therefore, study of the interactions among diffusion, convection and chemical reaction kinetics will help us to have a comprehensive understanding of the chemical reactions in the micro-FIA systems and design appropriate micro-FIA system. In this work, a finite element model (FEM) is established to extract chemical reaction kinetics in a micro-FIA system using high throughput sample introduction. The effects of reactants diffusion, the flow velocity and injection volume on the reaction product have been simulated. The good agreement between the simulated and the experimental results demonstrates the effectiveness of the established simulation method.

2. Theory and numerical method

In the current study, the physical model for the microchip with gravity driven flow can be established by using the following equations. Firstly, the mass and momentum transports in the gravity driven flow are governed by the Navier–Stokes equation.

$$\rho \frac{\partial u}{\partial t} - \nabla \cdot \eta (\nabla u + (\nabla u)^T) + \rho u \cdot \nabla u + \nabla p = f \quad (1)$$

$$\nabla \cdot u = 0 \quad (2)$$

where, ρ is the density of fluid, η is the dynamic viscosity of fluid, and f is the body force of fluid; u is the velocity of the fluid; p is the pressure of fluid.

Since the inertial forces of the fluid are small compared to viscosity forces, $\rho u \cdot \nabla u$ can be set as zero. Furthermore, there are no applied pressure gradients, thus, Eq. (1) can be simplified into the Stokes equation.

$$\rho \frac{\partial u}{\partial t} - \nabla \cdot \eta (\nabla u + (\nabla u)^T) = f \quad (3)$$

where, f is the body force of fluid and set as $f = \rho g$.

The diffusion and convection equation accounts for the mass transport and reaction in micro-FIA system by combining with the term of chemical reaction kinetics.

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i + c_i u) = R_i \quad (4)$$

where, c_i and D_i denote the concentration and diffusion coefficient of species i , respectively; R denotes the reaction term, which is formulated by

$$R = k c_1 c_3 \quad (5)$$

where, k is the reaction rate constant, c_1 and c_3 denote the concentrations of reaction reagent and sample, respectively. Considering that the concentration of reagent (c_1) is larger than the concentration of sample (c_3), the whole chemical reaction can be simplified into a pseudo-first-order reaction. Therefore, the reaction term R can be rewritten into $R = k' c_3$ (where $k' = k c_1$).

Based on Eqs. (2)–(5), the FEM model for describing the micro-FIA system is established. The whole computation domain is divided into 3 sub-domains as shown in Fig. 1B, the yellow and blue regions represent the sub-domains 1 and 2, respectively. These two regions are only used for introduction of reagent and sample. The red region is the sub-domain 3, where sample and reagent get mixed and then reaction starts. Therefore, due to no reaction in the sub-domains 1 and 2, the reaction term in Eq. (4) is not considered. The boundary and initial conditions for the FEM model are listed in Table 1.

The scales of our computation domain (Fig. 1B) are identical to the ones in experiments reported recently [16]. The injection volume of sample can be simulated by controlling the width of sample plug in numerical model. Therefore, autosample system is not necessary to be included in our numerical model.

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