Journal of Computational Physics 276 (2014) 563–595

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A conservative, positivity preserving scheme for reactive solute transport problems in moving domains

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ARTICLE INFO

Article history:
Received 16 April 2014
Received in revised form 2 July 2014
Accepted 29 July 2014
Available online 5 August 2014

Keywords:
Reactive transport
Flux corrected transport
Arbitrary Lagrangian–Eulerian methods
Convection dominated flow

ABSTRACT

We study the mathematical models and numerical schemes for reactive transport of a soluble substance in deformable media. The medium is a channel with compliant adsorbing walls. The solutes are dissolved in the fluid flowing through the channel. The fluid, which carries the solutes, is viscous and incompressible. The reactive process is described as a general physico-chemical process taking place on the compliant channel wall. The problem is modeled by a convection–diffusion adsorption–desorption equation in moving domains. We present a conservative, positivity preserving, high resolution ALE-FCT scheme for this problem in the presence of dominant transport processes and wall reactions on the moving wall. A Patankar type time discretization is presented, which provides conservative treatment of nonlinear reactive terms. We establish CFL-type constraints on the time step, and show the mass conservation of the time discretization scheme. Numerical simulations are performed to show validity of the schemes against effective models under various scenarios including linear adsorption–desorption, irreversible wall reaction, infinite adsorption kinetics, and nonlinear Langmuir kinetics. The grid convergence of the numerical scheme is studied for the case of fixed meshes and moving meshes in fixed domains. Finally, we simulate reactive transport in moving domains under linear and nonlinear chemical reactions at the wall, and show that the motion of the compliant channel wall enhances adsorption of the solute from the fluid to the channel wall. Consequences of this result are significant in the area of, e.g., nanoparticle cancer drug delivery. Our result shows that periodic excitation of the cancerous tissue using, e.g., ultrasound, may enhance adsorption of cancer drugs carried by nanoparticles via the human vasculature.

1. Introduction

The reactive transport of chemical solutes in deformable media is an important problem with wide-spread engineering and biological applications. These applications include the transport of dissolved solutes in blood vessels [56], chemical transport in reactors, chromatographic separation [1,6,48,53], and the transport of solutes in petroleum recovery [30]. Reactive transport is usually studied under three different flow regimes, which are *diffusion dominated flow*, *convection dominated flow*, and *chaotic advection* [1,53]. For the first flow regime, diffusion is more influential than convection in the overall flow of the solutes. In the second regime, the convection is more influential than diffusion, giving rise to the so called Taylor

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http://dx.doi.org/10.1016/j.jcp.2014.07.049
0021-9991/

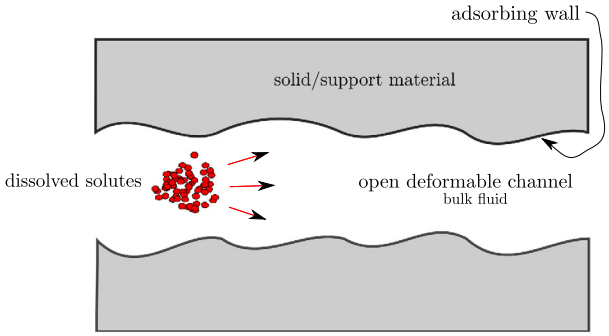

Fig. 1. Reactive transport phenomena in a narrow deformable channel with active adsorbing walls. The chemical solutes are dissolved in a solvent flowing under a pressure gradient, and undergoing (Taylor) dispersion in the cylindrical channel. Upon reaching the channel walls they are adsorbed due to their affinity to the wall. The solid/supporting material has zero porosity. Compliancy of the wall is due to the normal stress exerted by the fluid onto the compliant channel wall.

dispersion effects. An example of this is Taylor dispersion-mediated mixing [1]. In the third flow regime, turbulent mixing is observed. In this paper we concern ourselves with flow characterized by dominant convection, typically associated with Taylor dispersion. This is the case mathematically defined by moderate to large Péclet numbers $Pe \gg 1$.

Our study concerns chemical solutes that are dissolved in a viscous incompressible fluid flowing in a channel with moving walls. The fluid flow is modeled by the Navier–Stokes equations. The location of the moving boundary is calculated using a fluid–structure interaction (FSI) solver, previously developed in [10,29]. For the problem studied in this manuscript, the location of the moving boundary and the fluid flow are given, and are obtained using an FSI solver. For more details on mathematical models, analysis and numerical schemes for incompressible fluid flow in compliant domains please see [10,11,15–19,29,33,46], and the references therein.

The solute species are assumed to have no effect on the flow character of the fluid, and can thus be treated as trace particles. Solute dynamics in the bulk fluid are described by a convection–diffusion equation in a moving domain with the convection flux defined by the (given) fluid velocity. The reactive process is described as a general physico-chemical process taking place on the compliant channel wall. The reaction process may consist of adsorption–desorption, multi-stage reactions, or catalyzed wall reactions. Common examples of such physico-chemical models are the linear Henry's law, Langmuir adsorption, Freundlich adsorption, Langmuir–Freundlich adsorption and Langmuir–Hinshelwood catalytic reactions among many others [31,54]. Our model extends the reactive transport models for various reaction systems in a fixed cylindrical channel, studied in [6,20–22,41–43,45,53], to the reactive transport models in channels with moving walls. More complex fixed channel geometries are considered in [9,47]. Notable examples of reactive transport with moving domains can be found in [27,34]. In [34], the reactive process affects the wall deformation by precipitation and dissolution of solutes on the wall. This leads to a coupled fluid flow and solute transport problem in which the fluid profile and wall deformation is constantly updated. In [27], erosion of a solid domain resembling a stent embedded in arterial wall is considered. The solute transport problem involves the reaction of drug solutes on the boundary of the stent.

For Taylor dispersion and for other convection dominated flows, numerical schemes for solute transport may lead to undesirable numerical artefacts. These are usually shown by oscillations in the profile of the numerical solution (solute concentration). Therefore, such schemes require stabilization to deal with oscillations that occur in the numerical solution. In the finite element context, stabilization methods of FCT type were studied by Löhner et al. in [38,39]. Recently there have been studies for various *fixed domain problems* in [35–37,44] and [32]. In [32], a comparative study of various stabilization schemes, including FCT was done. The FCT type of schemes emerges as the most superior and efficient. In moving domains, upwinding has been applied to convection–diffusion problems by Badia et al. in [4], and Boiarkine et al. in [8]. In both of those papers the finite element discretization in arbitrary Lagrangian–Eulerian (ALE) framework is used. The work of Badia et al. uses the orthogonal subgrid scale type stabilization, while the work of Boiarkine et al. constructs an FCT type of stabilization. In this paper, we extend the FCT type design under the ALE framework to general reactive transport problems. Additionally, we introduce a linearization technique for treating nonlinear reaction terms in a conservative way following the Patankar linearization techniques, proposed in [12–14] and [28]. This linearization is designed such that second order time discretization is achieved, and the fully discrete scheme is mass conservative. Furthermore, our second-order time discretization will ensure that the geometric conservation law (GCL) is satisfied.

To validate the numerical scheme, we consider first the transport in fixed channels with fixed and moving meshes. The tests include reactive processes such as irreversible reactions, linear adsorption–desorption, infinite adsorption, and nonlinear adsorption processes. The numerical results of our scheme are compared to the solutions of effective models considered in [21,23,53], showing excellent agreement.

We then consider grid convergence on fixed and moving meshes for the scheme under the linear and nonlinear chemical reactions, mentioned above. The moving mesh error is studied to show that the solution is "mesh independent" up to a certain tolerance, showing excellent mesh independence property.