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NUMERICAL ANALYSIS OF A MIXED FINITE ELEMENT APPROXIMATION OF A COUPLED SYSTEM MODELING BIOFILM GROWTH IN POROUS MEDIA WITH SIMULATIONS

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Abstract. In this paper, we consider mixed finite element approximation of a coupled system of nonlinear parabolic advection-diffusion-reaction variational (in)equalities modeling biofilm growth and nutrient utilization in porous media at pore-scale. We study well-posedness of the discrete system and derive an optimal error estimate of first order. Our theoretical estimates extend the work on a scalar degenerate parabolic problem by Arbogast et al, 1997 [4] to a variational inequality; we also apply it to a system. We also verify our theoretical convergence results with simulations of realistic scenarios.

Key words. Parabolic variational inequality, nonlinear coupled system, mixed finite element method, error estimates, biofilm–nutrient model, porous media.

1. Introduction

Biofilms play an important role in a variety of scientific and engineering applications including microbial enhanced oil recovery (MEOR) [26], CO_2 sequestration [29, 17], bioremediation engineering [30], and so on.

Biofilm growth in porous media is affected by the ambient fluid flow and nutrient availability. It is also subject to a volume constraint. In this paper we consider a model proposed in [35] which is a coupled system involving a nonlinear parabolic variational inequality (PVI) equipped with a new nonlinear diffusivity term and subject to Neumann boundary conditions assuming the system is isolated. The model of the biofilm growth is discussed in detail in Sec. 2. We are particularly interested in simulating this model on voxel grids at the pore-scale, i.e., grids corresponding to the x-ray tomography images of porous media at the pore-scale.

We approximate the model with mixed finite element method (MFEM). We believe this choice is better for the problem than the finite element method (FEM) we considered in our earlier work in [1], because of the conservative property of MFEM and its natural way of handling Neumann boundary conditions. (We remark that MFEM works also very well theoretically and computationally when Dirichlet condition is imposed unlike FEM that we succeeded in [1] in deriving an error estimate with Dirichlet conditions only.) Moreover, the implementation of MFEM with the lowest order of Raviart Thomas elements on rectangles and cubes $RT_{[0]}$ as cell centered finite difference method (CCFD) is very easy to implement and to use for voxel grids. We recall that CCFD is equivalent to this mixed FE up to quadrature order of $O(h^2)$ for smooth solutions [34, 40] where the later is more convenient to implement in practice.

MFEM has been studied extensively in literature including the theory developed in [11, 8]. However, most of the work is devoted to either unconstrained problems

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such as [13, 4, 23], etc, or constrained stationary problem as in [12]. Semi-discrete mixed finite element approximation for unconstrained parabolic problem was considered in [13] for the linear case and in [23] for the nonlinear case.

There are several challenges in analysing the biofilm–nutrient model considered in this paper. One of challenges is the fact that PVI lacks of regularity. In particular, the second derivative in time of the solution $u_{tt} \notin L^2$ [22, 6]. Johnson in his paper [22] overcomes this challenge by setting some realistic assumptions on the domain and derives the error estimate of the finite element approximation of his problem using summation by parts. We implemented Johnson's approach in our previous work [1] with the finite element approximation of a simple model of biofilm–nutrient dynamic proposed in [32]. However, there are some major differences between the problem in [1] and the problem considered here in this work. In [1] we considered a quasi-linear PVI, where the diffusivity depends only on the spatial variable with no advection term and the boundary conditions are of Dirichlet type. In contrast, the problem in this paper has nonlinear diffusivity and an advection term with Neumann boundary conditions. Johnson's technique used in [22] does not work with MFEM. Therefore, we implement time integration approach used in [4].

Another difficulty is the nonlinearity involved in both the diffusivity and the reaction terms. Woodward and Dawson [41] deal with the nonlinearity using the expanded mixed finite element method which introduces a new variable, and then solves the problem in three unknowns (the primary unknown, its flux, and the new variable). However, as it is described in [33], "the expanded mixed finite element method is not equivalent with the standard mixed finite element method and their results cannot be simply transferred to our method MFEM". Arbogast et al. [4] consider an unconstrained nonlinear parabolic problem, where the nonlinearity is in the reaction term and under time derivative; the diffusivity is nonlinear if the change of variable is used. To derive the error estimate, they use the weighted projection on the approximated space which depends on the diffusivity beside the time integration technique. When we implement this approach to our problem, we need to assume some regularities on the solution which we do not guarantee that they are realistic ones. Therefore, to deal with the nonlinear diffusivity, we first linearize our problem using Kirchhoff transformation as in [33], and then we implement the approach used in [4]. We would like to emphasize here that the works in [4] and [33] are on scalar unconstrained problems whereas our problem is a constrained coupled nonlinear system.
Moreover, there are some studies in literature that regularize the PVI first using Lagrange multipliers then approximate it with finite element method as in [21, 28, 31]. In this paper we keep the PVI formulation in the theoretical analysis, yet use the Lagrange multiplier in computations.

1.1. Outline. Below we set up the notation. In Sec. 2 we provide details of the model. The paper is next broken into two parts: the first deals with the scalar PVI involving nonlinear diffusivity, and the second next deals with the additional challenges due to the coupled nature of the system. In Sec. 3 we provide mathematical details and formulate assumptions on the scalar PVI involving a nonlinear diffusivity. In Sec. 4 we provide details of the discretization and prove well-posedness of the discrete system. In Sec. 5 we prove the result on the convergence of MFEM approximation to this scalar problem. In Sec. 6 we provide the analyses for the full coupled system, and in Sec. 7 we provide examples in $d = 1$ and $d = 2$.

The theoretical results we prove require various assumptions which are specific to the result. In particular, the well-posedness in Sec. 4 and Sec. 6 are derived under