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ERROR ESTIMATES FOR SEMI-DISCRETE FINITE ELEMENT APPROXIMATIONS FOR A MOVING BOUNDARY PROBLEM CAPTURING THE PENETRATION OF DIFFUSANTS INTO RUBBER

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Abstract. We consider a moving boundary problem with kinetic condition that describes the diffusion of solvent into rubber and study semi-discrete finite element approximations of the corresponding weak solutions. We report on both *a priori* and *a posteriori* error estimates for the mass concentration of the diffusants, and respectively, for the *a priori unknown* position of the moving boundary. Our working techniques include integral and energy-based estimates for a nonlinear parabolic problem posed in a transformed fixed domain combined with a suitable use of the interpolation-trace inequality to handle the interface terms. Numerical illustrations of our FEM approximations are within the experimental range and show good agreement with our theoretical investigation. This work is a preliminary investigation necessary before extending the current moving boundary modeling to account explicitly for the mechanics of hyperelastic rods to capture a directional swelling of the underlying elastomer.

Key words. Moving boundary problem, finite element method, method of lines, *a priori* error estimate, *a posteriori* error estimate, diffusion of chemicals into rubber.

1. Introduction

Sharp interfaces moving in an *a priori* unknown way inside materials play a key role in a number of study cases in science and technology, including in the forecast of the durability of cementitious-based materials (cf. e.g. [24, 5, 11, 26]), large-time behavior of chemical species from the environment slowly penetrating by diffusion and swelling rubber-based materials (cf. e.g. [25, 27, 1]), to controlling phase transitions like melting and freezing or solid-solid changes in concrete (cf. e.g. [10, 29, 21]), to mention but a few. Due to the inherent non-linearity of such moving boundary problems, analytical representations of solutions are often either unavailable or not computable. Hence, one has to rely on direct computational approaches to get insight for instance in the behavior of large times of such moving sharp interfaces, as this usually defines the lifetime of the material under investigation.

In the framework of this paper, we study a semi-discrete finite element approximation of weak solutions to a one dimensional moving boundary problem that models the diffusion of solvent into rubber (see Section 2). This is a follow-up study of our recent work [1], where we proposed a finite element approximation of solutions to a moving boundary problem which we used to recover experimental data. Now, we explore the quality of our approximation scheme. Specifically, we report on both *a priori* and *a posteriori* error estimates for the mass concentration of the diffusants, and respectively, for the position of the moving boundary. Our working techniques include integral and energy-based estimates for the corresponding nonlinear parabolic problem posed in a transformed fixed domain, combined with a suitable use of the interpolation-trace inequality to handle the interface terms. At

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the technical level, we were very much inspired by the references: [6, 32, 30, 28], and [5]. It is worth noting that similar work has been done in related contexts. For instance, in [24], the authors show the convergence of a numerical scheme obtained by combining an Euler discretization in time with a Scharfetter-Gummel discretization in space for a concrete carbonation model with moving boundary reformulated for a fixed space domain. In [26], A. Zurek studies the long time regime of the moving interface driving the concrete carbonation reaction model by tailoring an implicit in time and finite volume in space scheme. He proves that the approximate free boundary increases in time with $\sqrt{t}$-law as theoretically predicted in [31]. In [23], one develops an adaptive moving mesh method for the numerical solution of an enthalpy formulation of a class of heat-conduction problems with phase change. The main aim of [22] is to provide a comparison of several numerical methods including displacing level sets, moving grids, and diffusing phase fields to address two well-known Stefan problems arising as best formulations for phase transformations like melting of a pure phase and diffusional solid-state phase changes in binary systems.

To handle our problem, we decided to use the finite element method as this fits best to the regularity of the (weak) solutions to our moving boundary problem. Mind though that other discretization methods are likely to be applicable as well. As our work is purely in 1D and no expensive computations are expected, and as, on top of this, we wish to rely on open source facilities, we chose Python for the implementation work.

We present here a preliminary investigation of this class of problems. This is necessary before extending the current moving boundary modeling to account explicitly for the mechanics of hyperelastic rods to capture a directional swelling of the underlying elastomer. In this spirit, a natural next step would be to perform the numerical analysis of a two-scale finite element approximation of the setup described in [25].

The outline of this study is as follows: We formulate our moving boundary problem in Section 2. The discussion of the setting of the model equations is based on [1]. We collect in Section 3 our basic assumptions on parameters and model components, as well as notations and existing preliminary results. Section 4 contains the fixed domain transformation of our problem and the definition of our concept of weak solutions which is then the subject of error approximation estimates investigated here. Benefiting of the mathematical analysis done for our problem in [3, 4], we are able to prove the global existence of weak solutions to the semi-discrete problem and obtain the needed uniform boundedness results to produce convergent numerical schemes. As main result, we obtain *a priori* and *a posteriori* error estimates as listed in Section 5. A couple of numerical experiments are discussed in Section 6. Essentially, they support numerically the available experimental results. Finally, a brief conclusion of this work is outlined in Section 7.

2. Model equations

We consider a thin slab of a dense rubber, denoted by Ω of vertical length $L > 0$, placed in contact with a diffusant reservoir. When the diffusant concentration at the bottom face of the rubber exceeds some threshold, the diffusant moves into the rubber creating a sharp interface that separates the rubber Ω into two parts, the diffusant free region and diffusant-penetrated region. Our region of interest is the diffusant-penetrated part where the diffusant's flux is assumed to satisfy Fick's