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Models for capturing the penetration of a diffusant concentration into rubber: Numerical analysis and simulation.

Abstract

Understanding the transport of di usants into rubber plays an important role in forecasting the material's durability. In this regard, we study di erent models, conduct numerical analysis, and present simulation results that predict the evolution of di usant penetration fronts. We employ a moving-boundary approach to model this phenomenon, utilizing a numerical scheme based on the Galerkin nite element method combined with the backward time discretization, to approximate the di usant pro le and the position of the penetration front. Both semi-discrete and fully discrete approximations are analyzed, demonstrating good agreement between numerical and theoretical convergence rates. Numerically approximated di usants penetration front recovers well the experimental data. We introduce a random walk algorithm as an alternative tool to the nite element method, showing comparable results to the nite element approximation. In a multi-dimensional scenario, we consider a strongly coupled elliptic-parabolic two-scale system with non-linear dispersion, describing the particle transport in a porous medium. We present two numerical schemes and compare them based on computational time and approximation errors. A precomputing strategy signi cantly improves computational e ciency.