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Mathematical model of the effect of electrodiffusion on biomineralization

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A R T I C L E I N F O

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A B S T R A C T

Biofilm-induced mineral precipitation is a fundamentally important phenomenon with many potential applications including carbon sequestration and bioremediation. Based on a mixture model consisting of three phases (calcite, biofilm, and solvent) and also accounting for chemistry, mechanics, thermodynamics, fluid, and electrodiffusive transport effects, we describe the self-induced generation of an electric field due to different diffusivities of different ion species and study the effects of this field on ionic transport and calcite precipitation. Numerical simulations suggest that one of these effects is enhanced precipitation.

1. Introduction

Biologically and chemically induced calcium carbonate formation has been proposed and/or observed to play an important role in a number of engineering, medical, and environmental contexts including carbon sequestration, co-precipitation of radionuclides (and, more generally, bioremediation in many different contexts), concrete remediation, soil stabilization, enhanced oil recovery, microbially induced corrosion, encrustation of ureteric stents, and dental caries (tooth demineralization) by dental plaques, e.g. [2,8,14]. Precipitation mechanics in these examples typically strongly couple biological, chemical, and physical processes through combinations of microbial dynamics and kinetics, reaction–diffusion chemistry, and fluid flow in ways that are not well understood. As a consequence, effective modeling could be useful in understanding these interactions.

In many instances, both naturally and in the lab, biomineralization occurs in combination with microbial biofilms (sessile collections of microorganisms living within a self-secreted matrix of polymers and other substances). In connection, there have been several laboratory investigations of calcite precipitation-induced by ureolytic bacteria (usually in bacterial biofilms), e.g. [7,13,20]. Separately, there also has been extensive work on mathematical modeling of biofilm growth and biofilm-flow interaction [3,6,11,15] (including discrete, continuous and hybrid models), as well as mathematical models for solute precipitation, e.g. [21]. However, little combined modeling work has been done for biofilm-induced calcite precipitation, in part due to the complex interactions involved.

Recently, the authors developed a versatile mixture model which accounts for the important physical, chemical and biological processes involved in biofilm-induced calcite precipitation [23]. In this model, the system as a whole consists of three phases—biofilm, calcite and solvent—each represented by its own volume fraction. These phases satisfy conservation of mass and momentum laws with addition of a free energy of mixing. Each chemical species involved is treated as a solute in the solvent phase and represented by a concentration governed through its own advection–diffusion–reaction equation. Two-dimensional numerical simulations illustrated the following phenomena: calcite precipitation occurs largely in the biofilm region, and calcite phase accumulation mainly occurs near the biofilm–solvent interface; higher ureolysis rate yields higher calcite precipitation rate; external flow can significantly change the dynamics of calcite precipitation.

The model in [23] includes electrochemistry, generally neglected in biofilm models to date (though not always, e.g. [16]). Different diffusivities of different ion species lead to charge separation through differential diffusion which in turn leads to generation of an electric field. This effect is likely to be most significant in the active layer, located along the biofilm–bulk fluid interface, where microbially induced chemistry is most active and hence where chemical gradients are particularly large. In this paper, we specifically examine the effect of the electric field on ionic transport and calcite precipitation by comparing different model outcomes with and without inclusion of electric field.

2. Model description

2.1. Mechanics

We outline, following [23], the system of equations describing the calcite precipitating system in a two-dimensional rectangular

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