SIMULATION OF REACTIVE FLOW IN POROUS MEDIA WITH VARIABLE POROSITY AS APPEARS WHEN MODELLING CONCRETE CARBONATION

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Reinforced concrete is a widely used material in buildings, bridges or dams. Concrete has a porous structure, with fine pores encountered at a micro-metre scale. These pores are filled by water and air, and various reactions are taking place within. One of the most important processes is concrete carbonation, as it may affect the durability of reinforced concrete.

The carbonation reaction is

$$CO_2(g \to aq) + Ca(OH)_2(s \to aq) \to CaCO_3(aq \to s) + H_2O, \qquad (1)$$
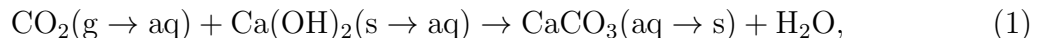
where $Ca(OH)_2$ is the calcium hydroxide and $CaCO_3$ is the calcium carbonate. To understand this process inside concrete, reliable mathematical models are required. Such models should include: saturated/unsaturated flow in concrete, diffusive, convective and reactive transport of CO_2, $Ca(OH)_2$ and $CaCO_3$, dissolution of CO_2 from the air phase (g) to liquid phase (aq), dissolution of $Ca(OH)_2$ from the solid phase (s) to liquid phase and precipitation of $CaCO_3$ from the liquid phase to solid phase. Due to the production of water in (1), the flow and transport equations are now fully coupled. Moreover, at the scale of pores, the dissolution of $Ca(OH)_2$ and precipitation of $CaCO_3$ lead to changes in the pore structure, and consequently to an evolving microstructure. These processes are encountered at the pore scale. However, the main interest is in the averaged behaviour of the system at a larger (macro) scale, where the evolving microstructure is reflected in a variable porosity. This gives an additional coupling between the flow and transport equations, and makes the design of robust numerical schemes for such complex problems very difficult.

The major challenges are to derive an effective model for the evolution of the porosity and to design robust and efficiently numerical schemes for the resulting model, which consists of coupled partial and differential equations. Especially, the numerical model should be able to treat possible pore clogging due to precipitation.

This work builds on the model proposed in [1], which includes a generic equation (ordinary differential equation) for the variation of the porosity, based on a volume balance. Further, a mass conservative discretization scheme is analyzed. In this work, an effective, macro-scale model is derived by means of upscaling techniques. This involves a two scale formal homogenisation approach. To account for the evolving microstructure, and for deriving the effective model, ideas in [2, 3, 4, 5] are followed. There the precipitate is viewed as a layer of unknown thickness, and the interface between the precipitate and the void space in the pores is a free boundary. For the resulting model, two scale asymptotic expansion methods are applied.

The numerical scheme for the computational (upscaled) model is based on the mixed finite element method for the spatial discretization, backward Euler for the temporal dis-cretization and Newton's method for the linearization, see [1] for details. The convergence of the scheme is rigorously analysed and error estimates will be presented. Finally, some numerical studies will be discussed.

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