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Full simulation of electrolyte and metals including boundary interactions

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Many high-strength metals are susceptible to hydrogen embrittlement [1]. One source of this absorbed hydrogen is contact with electrolytes such as water [2]. This contact causes hydrogen ions to be absorbed and causes corrosion, both of which alter the local pH and electric potential. However, when simulating the diffusion into the metal, this contact with an electrolyte is commonly simplified to directly imposing a hydrogen concentration or inflow [3, 4], neglecting these changes in environment.

A finite element scheme is presented which directly simulates the electrolyte and its reactions at the metal surface, allowing an accurate prediction of the actual hydrogen absorbed into the metal. This scheme is compared to results using the simplified boundary conditions showcasing the large influence of these simplifications on the hydrogen diffusion within the metal.

However, fully simulating the electrolyte is computationally costly when only interested in the absorbed hydrogen. To remedy this an additional formulation is presented which incorporates the diffusion within the electrolyte in a two-scale approach: Fully resolving the absorbed hydrogen and displacements in the metal, while approximating the electrolyte as a one-dimensional diffusion problem at each integration point on the boundaries. This scheme allows the changes in electrolyte concentrations to be approximated in the finite element formulation, while not adding additional degrees of freedom to the overall formulation.

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