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Diffusion-convection-reaction framework for coupled hydrogen transport in metals: implementation in Comsol and stabilization analysis

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Prediction of hydrogen distributions within metals and alloys is crucial in many applications requiring H_2 handling, storage or transport, as well as in aqueous environments where hydrogen can be electrochemically generated. Hydrogen embrittlement depends on the accumulation near the crack tip and thus transport modelling becomes necessary to simulate hydrogen assisted cracking.

In the present work, the most representative modelling updates since the seminar work of Sofronis & McMeeking (1989) [1] are discussed and implemented in a comprehensive and user-oriented Finite Element (FE) framework within the commercial software Comsol Multiphysics. Thermodynamic and mechanical theory behind all the implemented transport phenomena is presented, including kinetic and equilibrium trapping, multiple trapping, dislocation transport, stress-dependent hydrogen uptake and generalised entry flux in electrochemical charging. The numerical schemes for hydrogen transport and the corresponding implementation strategies found in literature are revisited. However, the focus is put here on the implementation in Comsol Multiphysics, which is validated and discussed taking results from literature as benchmarks. Diffusion-convection-reaction terms are derived from hydrogen transport theory and modelled through the *Transport of Diluted Species* module. Since hydrogen diffusion is drifted by hydrostatic stress and hydrogen trap density increases with plastic strain [2], the coupled nature of the crack tip simulation is discussed; it is found that a conservative flux can be modelled to avoid calculation of second-order derivatives of hydrostatic stress. In addition, staggered schemes give accurate enough results for the coupled mechanical-diffusion problem. Finally, the stability of the problem and the appearance of numerical oscillations are analysed for high convective or reaction terms in comparison to diffusive terms, i.e. evaluating non-dimensional Péclet and Damköhler numbers, affected respectively by the hydrostatic stress and the plastic strain rate. It has been found that for a zero-concentration initial condition some stabilization strategies are required to avoid numerical noise.

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