

COMPUTATIONAL MODELING FOR HYDROGEN TECHNOLOGIES

ANDRES DÍAZ^{*}, TIM HAGEMAN[†]
AND EMILIO MARTÍNEZ-PAÑEDA[†]

^{*} University of Burgos
Escuela Politécnica Superior, 09006 Burgos
adportugal@ubu.es

[†] University of Oxford
Department of Engineering Science, Oxford OX1 3PJ, UK
tim.hageman@eng.ox.ac.uk ; emilio.martinez-paneda@eng.ox.ac.uk ;
<https://mechmat.web.ox.ac.uk/>

ABSTRACT

Hydrogen has been hailed as the energy vector of the future. It can decarbonise many applications and sectors, including some that are known to be particularly difficult to decarbonise, such as steelmaking or aviation. However, this comes with significant safety challenges due to the flammability of hydrogen and its ability to embrittle metals. For example, the deployment of a hydrogen energy infrastructure is compromised by the fact that hydrogen can reduce the fracture toughness, ductility and fatigue crack growth resistance of metals by orders of magnitude [1]. Models are urgently needed to map regimes of operation, assess the efficiency of hydrogen decarbonisation across sectors and enable a safe deployment of a hydrogen energy infrastructure.

This mini-symposium is aimed at bringing together computational solid and fluid mechanicians working in hydrogen technologies. This includes scientists working in the areas of: (i) hydrogen embrittlement, (ii) electrolysis, and (iii) hydrogen combustion. From the development of multi-physics (deformation-diffusion-fracture) models for predicting hydrogen-assisted fracture [2] to recent progress in understanding and simulating hydrogen combustion.

REFERENCES

- [1] Chen, Y.S., Huang, C., Liu, P.Y., Yen, H.W., Niu, R., Burr, P., Moore, K.L., Martínez-Pañeda, E., Atrens, A. and Cairney, J.M., “Hydrogen trapping and embrittlement in metals—a review”. *International Journal of Hydrogen Energy* 136, pp. 789-821 (2025)
- [2] Hageman, T. and Martínez-Pañeda, E., “A phase field-based framework for electro-chemo-mechanical fracture: Crack-contained electrolytes, chemical reactions and stabilisation”. *Computer Methods in Applied Mechanics and Engineering* 415, 116235 (2023)