

# A COMSOL framework for predicting hydrogen embrittlement: List of models

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March 21, 2025

COMSOL models provided with the following papers:

A. Díaz, J.M. Alegre, I.I. Cuesta, E. Martínez-Pañeda. [A COMSOL framework for predicting hydrogen embrittlement, Part I: coupled hydrogen transport](#). Engineering Fracture Mechanics 319, 111007 (2025)

A. Díaz, J.M. Alegre, I.I. Cuesta, E. Martínez-Pañeda. [A COMSOL framework for predicting hydrogen embrittlement, Part II: phase field fracture](#). Engineering Fracture Mechanics 319, 111008 (2025)

## 1 Part I: Coupled hydrogen transport

1. [Krom\\_HTransport.mph](#): Stress-assisted diffusion with trapping and plastic strain rate effects. Validated with Krom et al. [1].
2. [DiLeo\\_Chemical\\_based.mph](#): Governing equation based on chemical potential. Validated with Di Leo and Anand [2].
3. [DiLeo\\_Chemical\\_based\\_TransportSolids.mph](#): Governing equation based on chemical potential and solved in a material frame. Validated with Di Leo and Anand [2].
4. [Dadfarnia\\_Dislocation\\_Transport.mph](#): Hydrogen transport by dislocations. Validated with Dadfarnia et al. [3].
5. [TDS\\_2traps\\_Legrand\\_McNabb-Foster.mph](#): Thermal Desorption Spectroscopy (TDS) with 2 traps and kinetic trapping-detrapping. Validated with Legrand et al. [4].
6. [Kotake\\_Softening.mph](#): Influence of hydrogen-induced softening. Validated with Kotake et al. [5].
7. [Martinez-Paneda\\_McNabb-Foster.mph](#): Kinetic trapping (McNabb-Foster's formulation) for hydrogen transport. Validated with Martínez-Pañeda et al. [6].
8. [Martinez-Paneda\\_Electrochemical\\_Uptake.mph](#): Generalised boundary conditions for electrochemical hydrogen uptake. Validated with Martínez-Pañeda et al. [6].

## 2 Part II: Phase field fracture

1. [Elastic\\_HPF.mph](#): Single-edge cracked plate with an elastic-brittle phase field model to capture hydrogen embrittlement. Validated with Cui et al [7].
2. [HPF\\_BoundaryLayer\\_Multitrap.mph](#): Boundary layer with a ductile phase field model to capture hydrogen embrittlement influenced by multiple traps.

## References

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- [4] E. Legrand, A. Oudriss, C. Savall, J. Bouhattate, and X. Feaugas, “Towards a better understanding of hydrogen measurements obtained by thermal desorption spectroscopy using FEM modeling,” *International Journal of Hydrogen Energy*, vol. 40, pp. 2871–2881, 2 2015.
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- [7] C. Cui, R. Ma, and E. Martínez-Pañeda, “A generalised, multi-phase-field theory for dissolution-driven stress corrosion cracking and hydrogen embrittlement,” *Journal of the Mechanics and Physics of Solids*, vol. 166, p. 104951, 9 2022.