

Sensitivity analysis of cohesive zone model parameters to simulate hydrogen embrittlement effect

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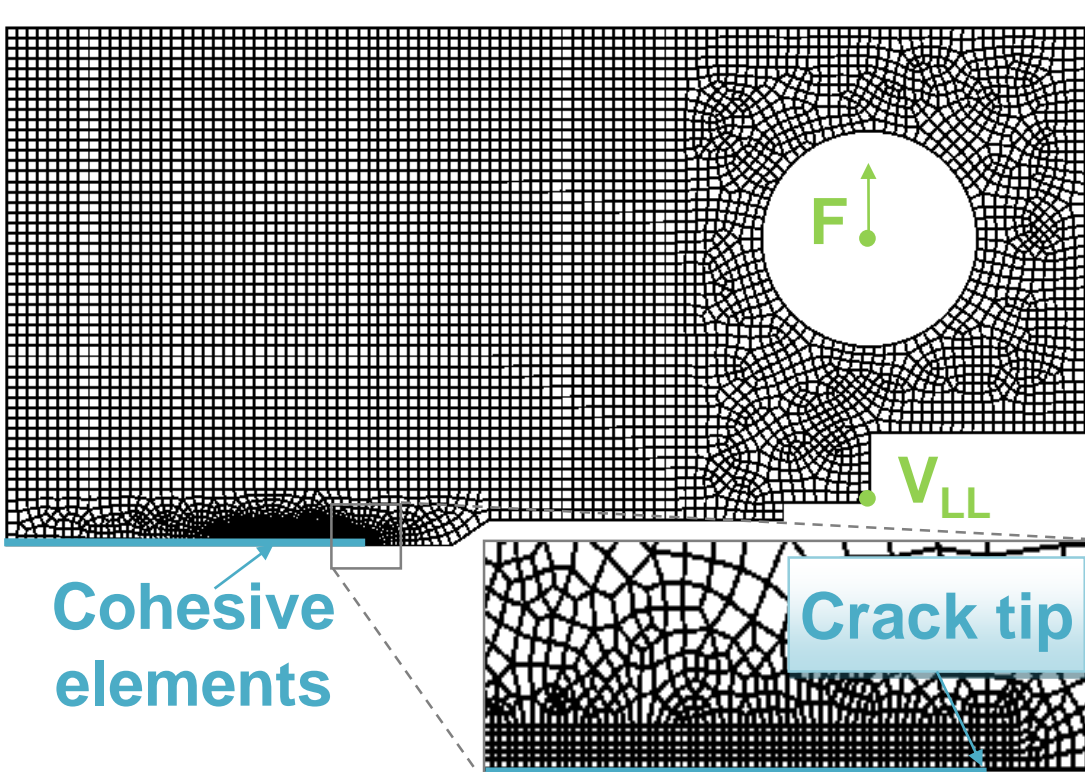
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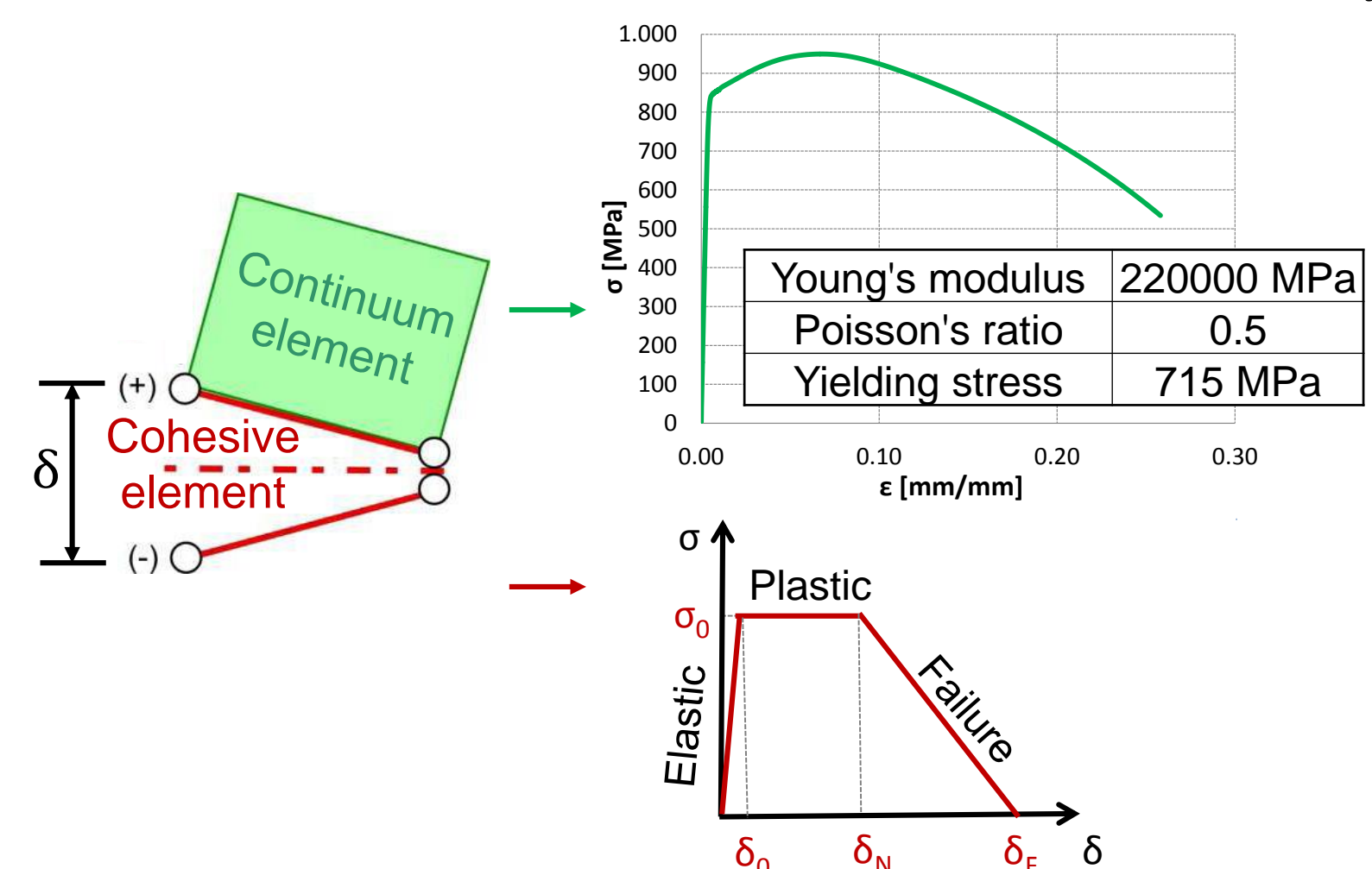


Finite Element Cohesive Model



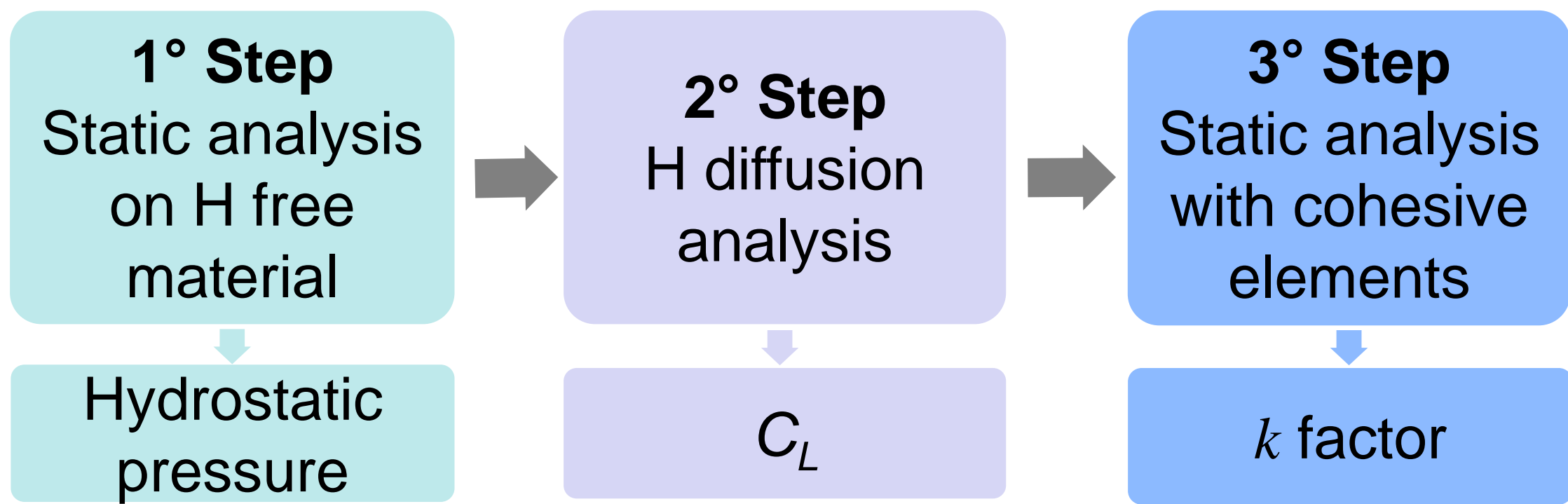
AIM: development of numerical model to study hydrogen embrittlement effect on mechanical properties of steels and sensitivity analysis of the parameters

- 2D model of CT specimen for fracture toughness test
- AISI 4130 high-strength low carbon steel used for hydrogen storage vessels



Mechanical parameters
Tensile test

TSL
Phenomenological law



C_T : hydrogen traps concentration
 $C_{tot} = (C_L + C_T) =$ total hydrogen concentration
 θ : hydrogen coverage
 Δg_b^0 : variation of Gibbs energy
 k : factor used to decrease TSL

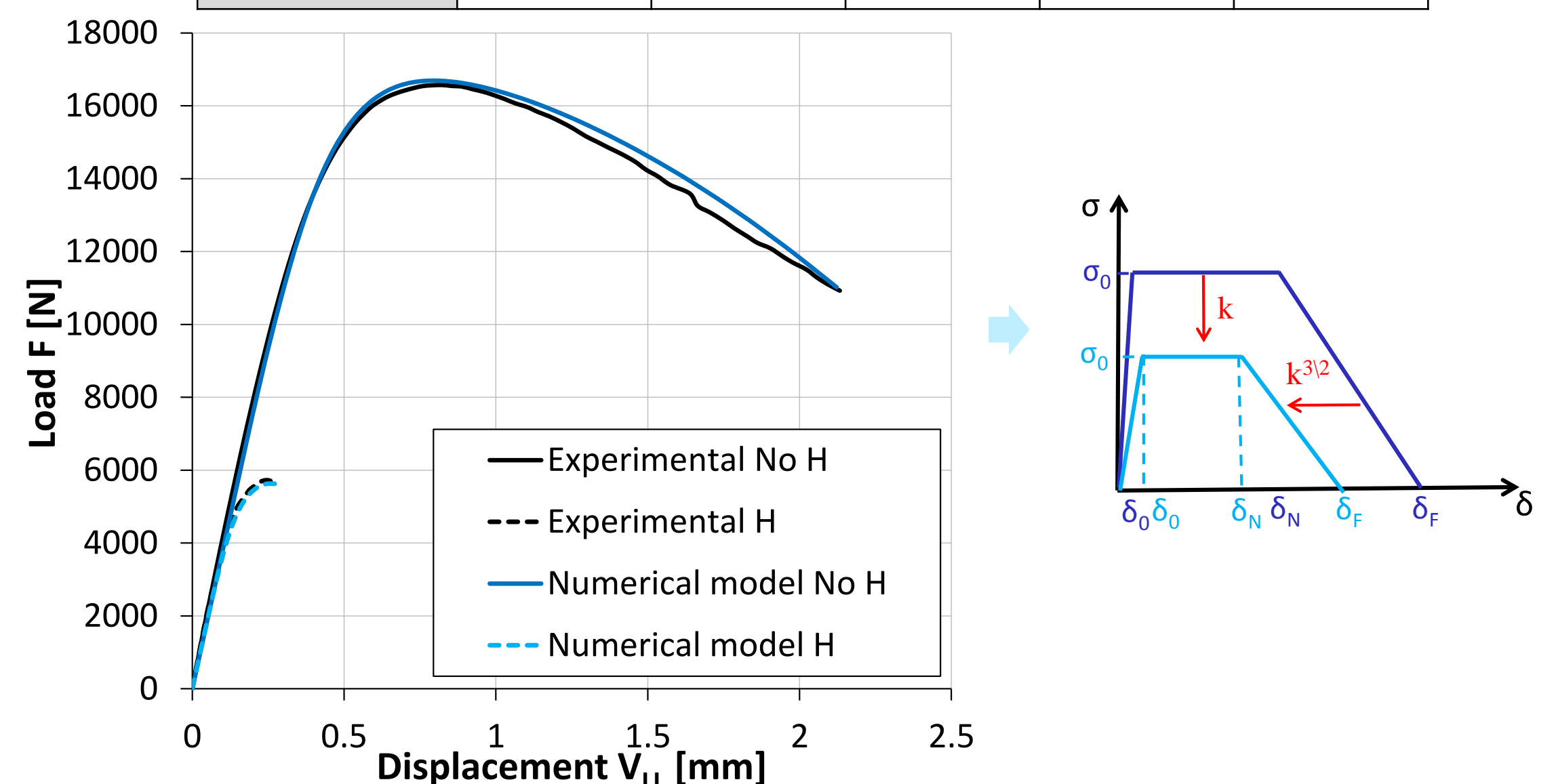
$$C_T = (49.0 \cdot \varepsilon_p + 0.1) \cdot C_L$$

$$\theta = \frac{C_{tot}}{C_{tot} + \exp(-\Delta g_b^0 / RT)}$$

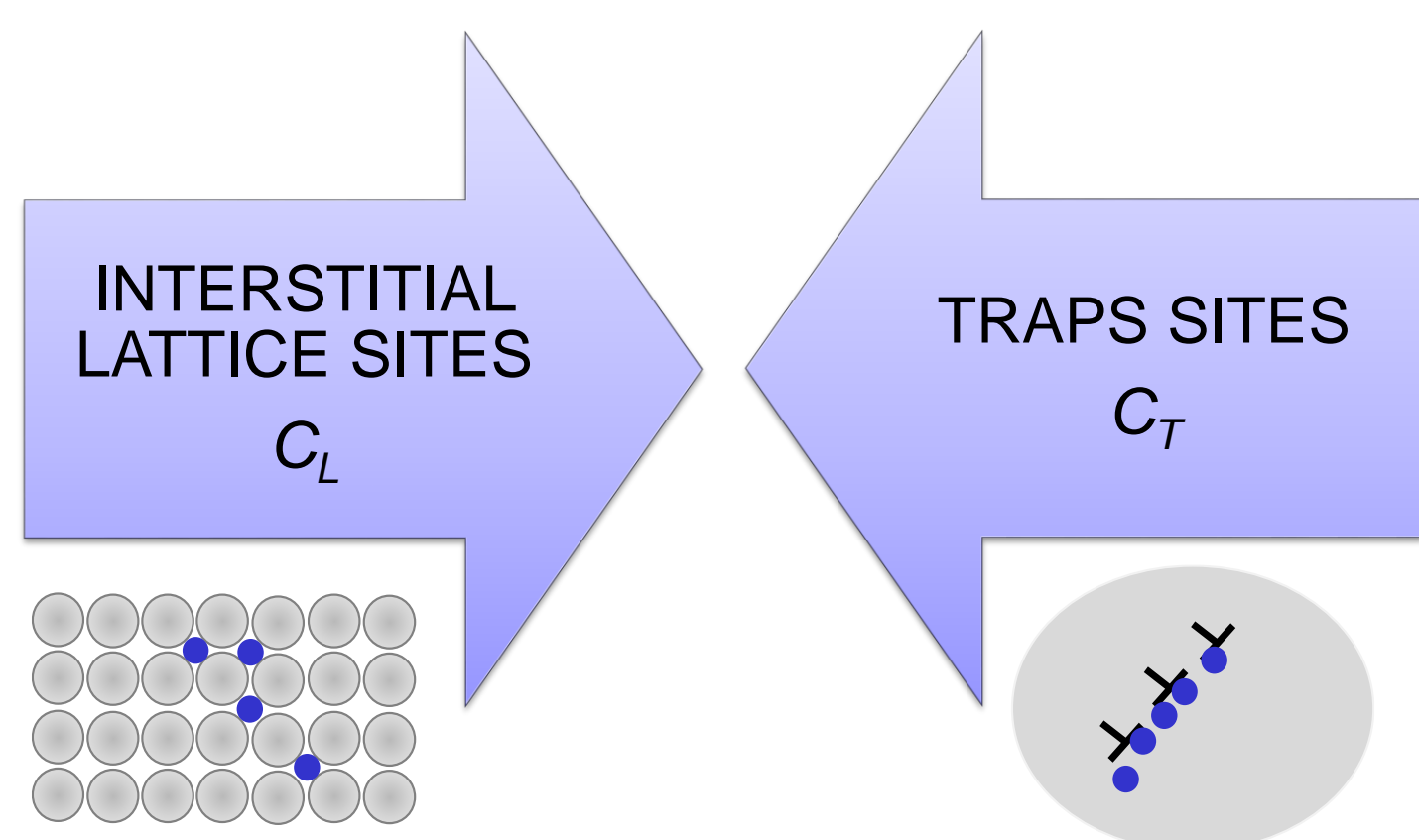
$$k = 1 - 1.0467\theta + 0.1687\theta^2$$

* 1) S. Serebrinsky et al. J. Mech. Phys. Solids 52 (2004)
 2) V. Olden et al. Int J Hydrogen Energy 37 (2011)

Hydrogen free model	δ_0 [mm]	δ_N [mm]	δ_F [mm]	σ_0 [MPa]	Area [N/mm]
Plane strain	0.009	0.015	0.320	1260	205.4



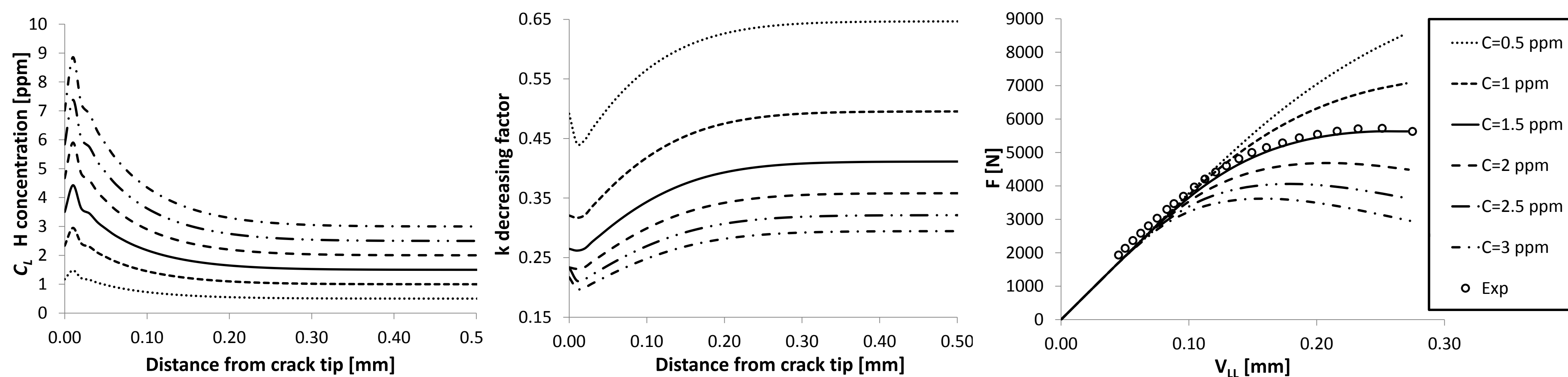
HYDROGEN CONCENTRATION



- Interstitial lattice sites concentration \rightarrow follows the hydrostatic stress field
- Trap sites concentration (inclusions, second phases, grain boundaries) \rightarrow associated with plastic strain, dislocations

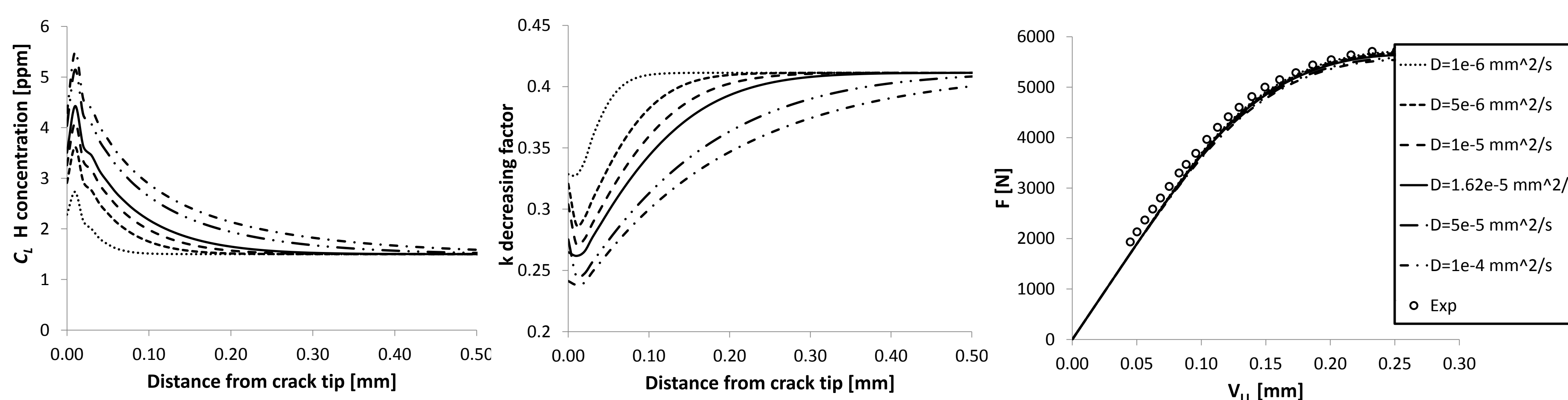
Sensitivity analysis

Variation of INITIAL CONCENTRATION $C = 0.5 - 3$ ppm



- Curves of C_L are shifted upwards with the increase of H content, both near and far from the crack tip.
- This has a direct influence on k and F plots. With the increase of applied displacement, the resulting F at the grips is higher or lower depending on C .
- The increase of C has not a symmetrical effect on the plots

Variation of DIFFUSION COEFFICIENT $D = 1 \cdot 10^{-6} - 1 \cdot 10^{-4}$ [mm²/s]



- Increasing the diffusivity, more hydrogen is recalled at the crack tip region, reaching extremely high values.
- Opposite trend for k : moving far away from the tip, the effect of D on k becomes negligible.
- No effect on F - V_{LL} plot since the model is not coupled (mass diffusion and stress analyses).

Conclusions

- A cohesive model to reproduce the fracture mechanical behavior of a steel operating in hydrogen contaminated environment was developed with three steps of simulations
- A sensitivity analysis of the model was carried out varying the initial concentration and the diffusion coefficient according to literature values
- Both a comparison of the values used in the model with literature data and a critical discussion of the results obtained by the sensitivity analysis were presented.