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


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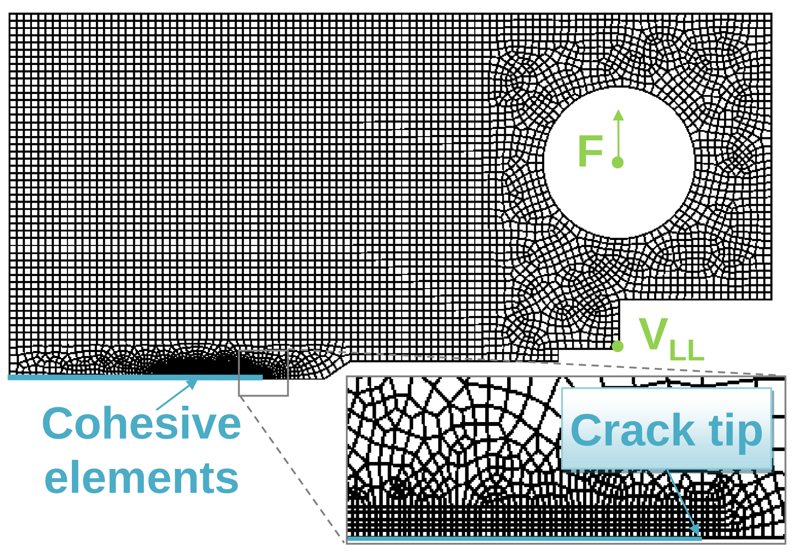
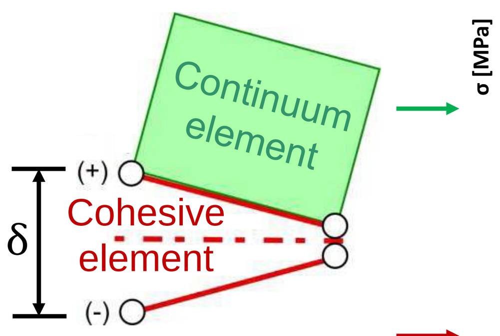
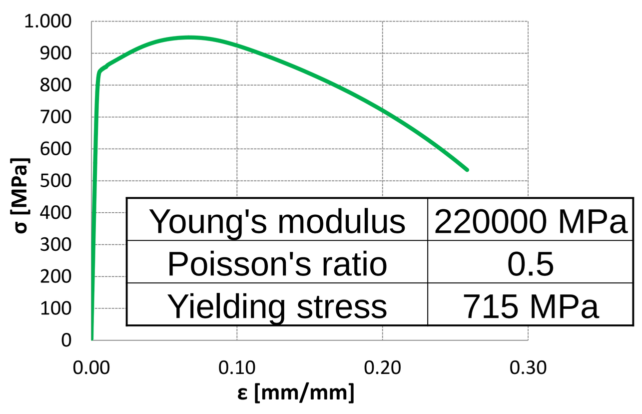
## Finite Element Cohesive Model



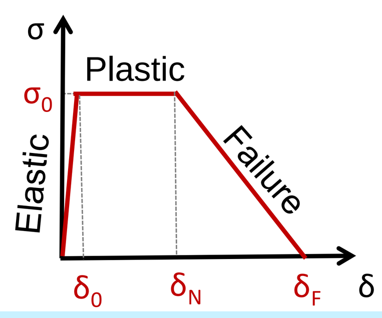

**AIM: development of numerical model to study hydrogen embrittlement effect on mechanical properties of steels and sensitivity analysis of the parameters**

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



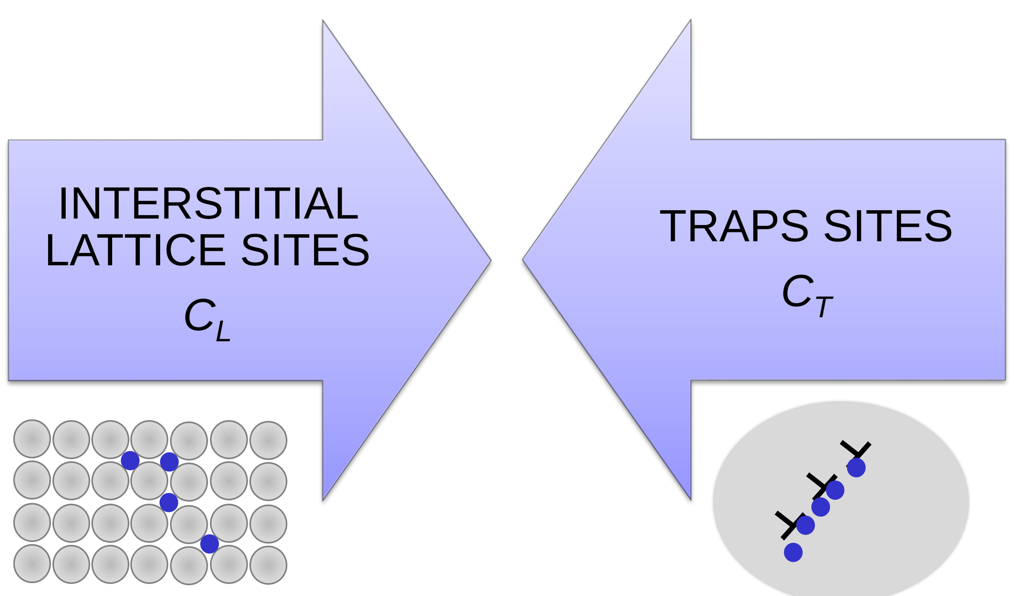




**Mechanical parameters**
Tensile test




**TSL**
Phenomenological law

### HYDROGEN CONCENTRATION




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

**1° Step** Static analysis on H free material → Hydrostatic pressure

**2° Step** H diffusion analysis → $C_L$

**3° Step** Static analysis with cohesive elements → $k$ factor

$C_T$ : hydrogen traps concentration

$Ctot = (C_L + C_T)$ = total hydrogen concentration

$\theta$ : hydrogen coverage

$\Delta g_b^0$ : variation of Gibbs energy

$k$ : factor used to decrease TSL

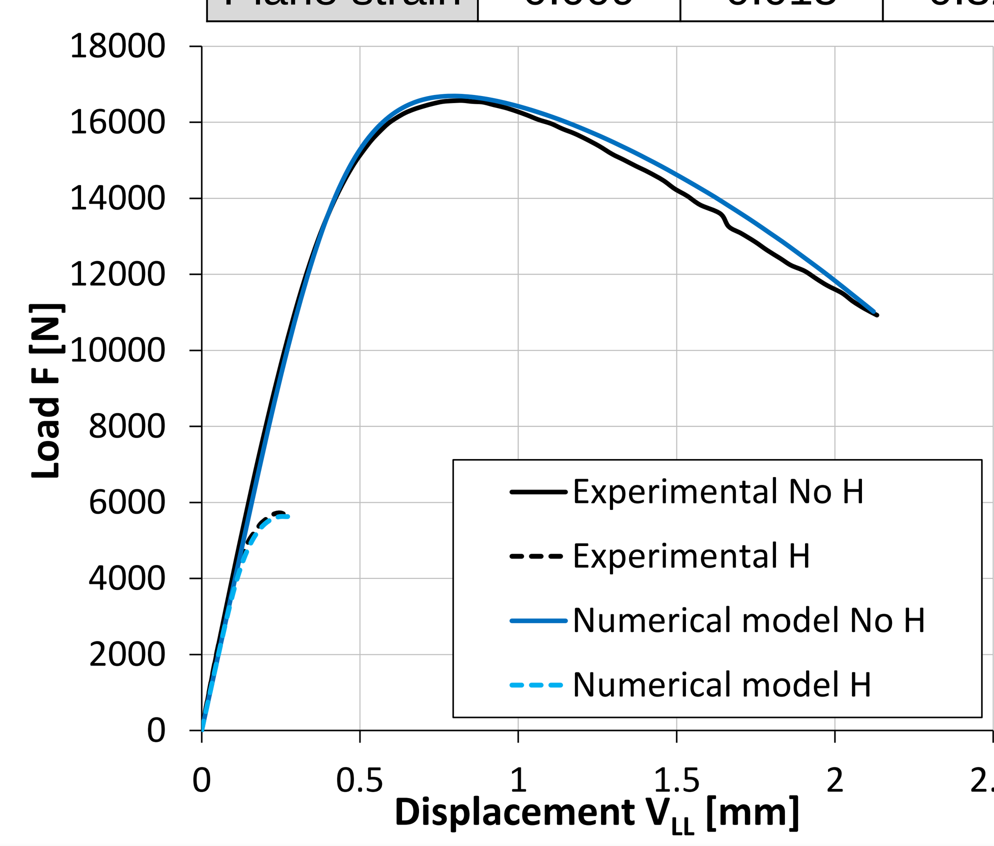
$$C_T = (49.0 \cdot \varepsilon_p + 0.1) \cdot C_L$$

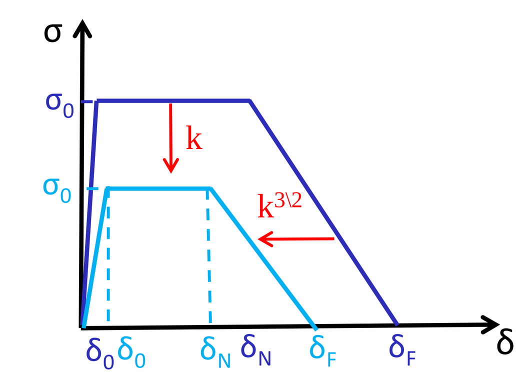
$$\theta = \frac{C_{tot}}{C_{tot} + \exp(-\Delta g_b^0 / RT)}$$

$$k = 1 - 1.04670\theta + 0.16870\theta^2$$


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

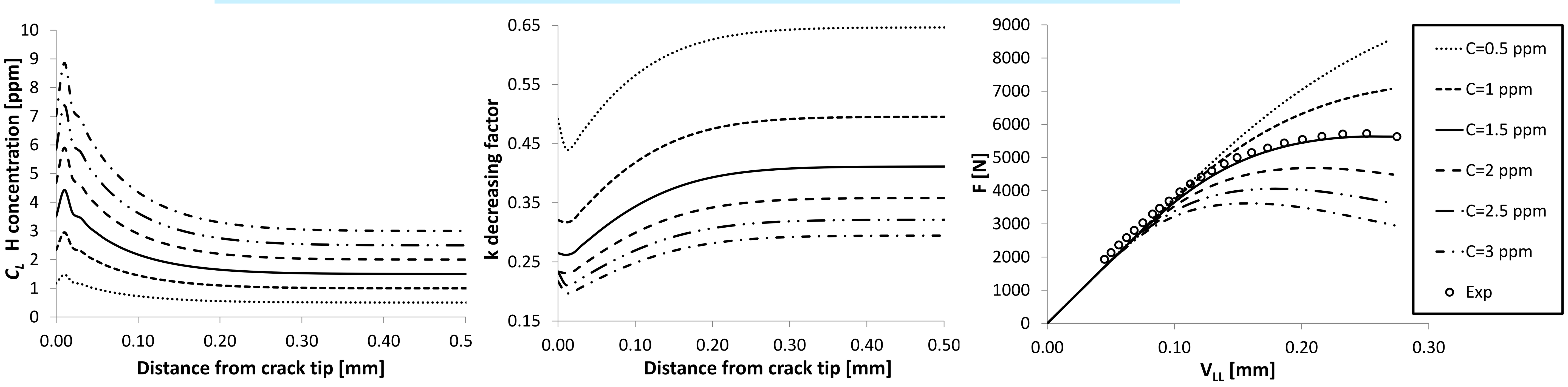

| Hydrogen free model | $\delta_0$ [mm] | $\delta_N$ [mm] | $\delta_F$ [mm] | $\sigma_0$ [MPa] | Area [N/mm] |
|---|---|---|---|---|---|
| Plane strain | 0.009 | 0.015 | 0.320 | 1260 | 205.4 |



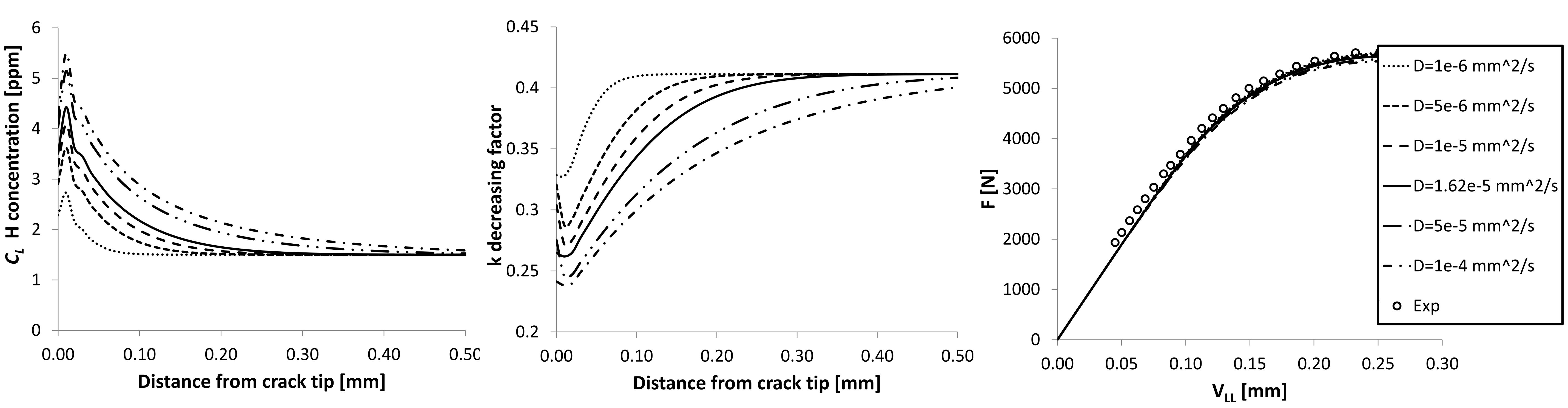

## Sensitivity analysis

### 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 = $1\cdot10^{-6}$ - $1\cdot10^{-4}$ [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.