Retention and permeation modelling: thermal effects

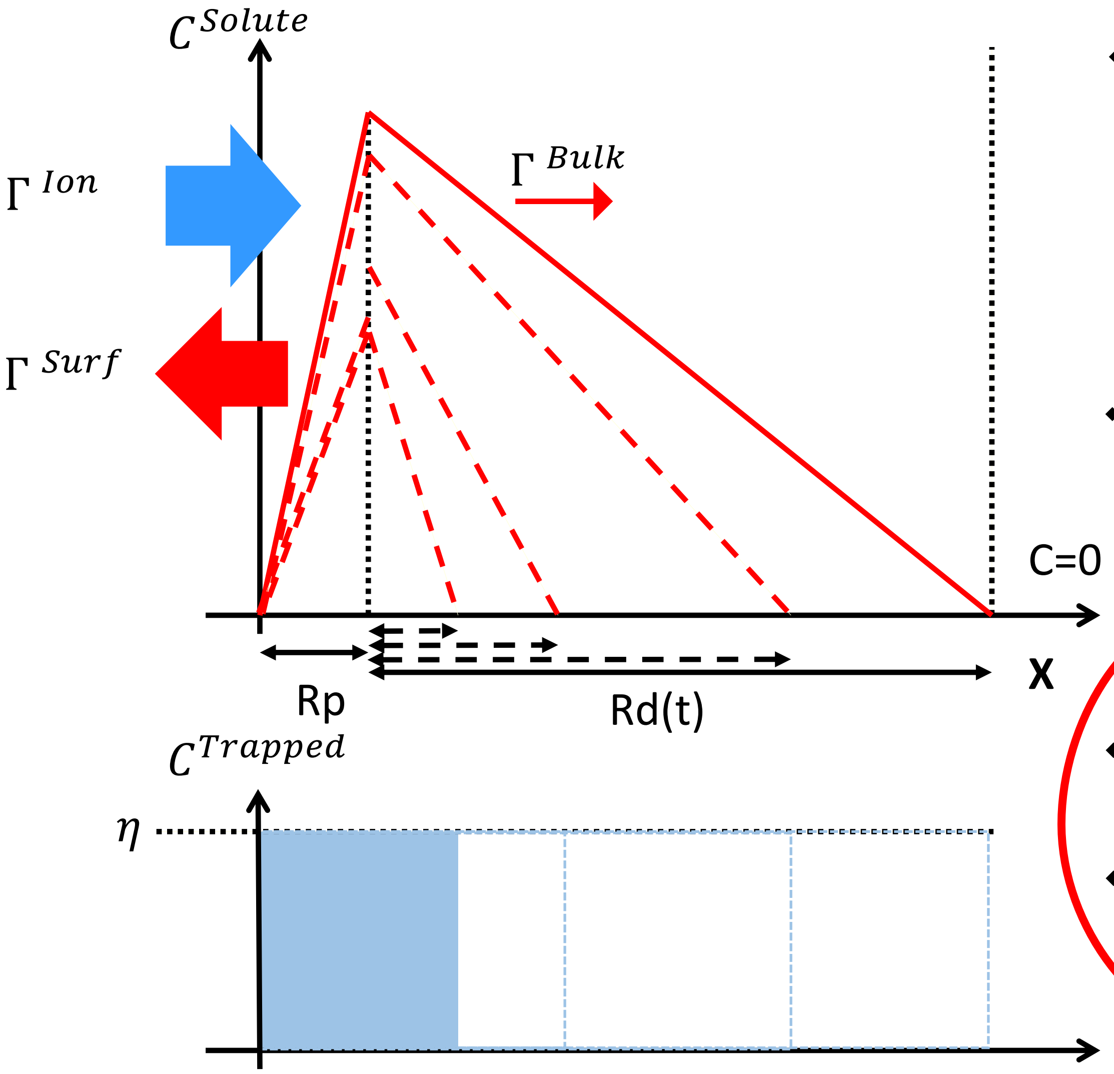
K. Schmid

Outline

- Why is the solute hydrogen important?
- Why can’t we directly measure the solute hydrogen?
- How to temperature gradients affect transport
- Modeling the expected effect of temperature gradients
- Possible caveats
- Summary

Why is the solute hydrogen important?

❖ **Retention of H in W is generally trap dominated:**



❖ low T ($< \Delta E_{Trap}/K_B$) trapping dominates transport
- Solute profile with moving absorbing boundary Rd(t)
- Decorating trap sites

❖ For all t flux balance at x = Rp

$$\Gamma^{Ion} = \Gamma^{Surf} + \Gamma^{Bulk}$$

→ C^{Solute} **~ 10^{-12} to 10^{-8} per W**

❖ Trap profile propagates with solute Rd(t)

❖ Maximum trapped concentration = η

$\eta\sim$ **10^{-7} to 10^{-2}**

- Γ^{Bulk} is the rate at which traps are decorated
- Γ^{Bulk} becomes permeation flux in equilibrium
- Γ^{Bulk} is determined by solute hydrogen dynamics
- Assuming diffusive transport:

$$\Gamma^{Bulk} = -D\rho\frac{\partial C_{SOL}}{\partial x}$$

$$\boldsymbol{C_{SOL}(x,t)} = ?$$

Why can't we directly measure the solute hydrogen?

- **Depth profiles always are a measure of** $C_{SOL}+C_{Trapped} \sim C_{Trapped}$, $C_{SOL} \ll C_{Trapped}$

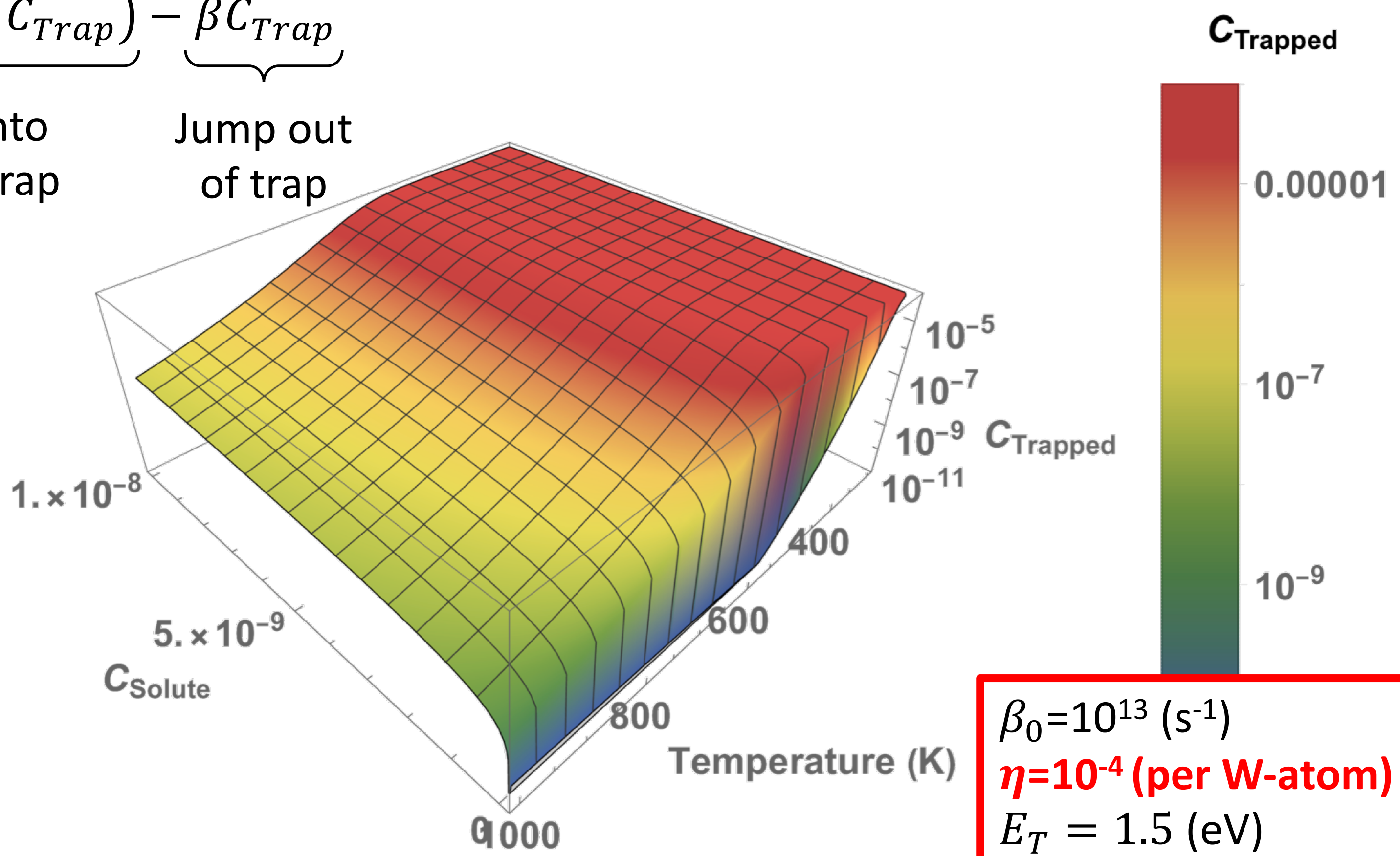
  - In equilibrium $\frac{\partial C_{Trap}}{\partial t} = 0 = \underbrace{\alpha\, C_{SOL}(\eta - C_{Trap})}_{\text{Jump into empty trap}} - \underbrace{\beta C_{Trap}}_{\text{Jump out of trap}}$

$$C_{Trap} = \frac{\eta}{1 + \frac{1}{C_{SOL}} \frac{\beta(T)}{\alpha(T)}}$$

$\beta(T)$ = Arrhenius de-trapping term = $\beta_0 e^{-E_T/K_B T}$

$\alpha(T)$=Arrhenius trapping term= $\alpha_0 e^{-E_D/K_B T}$

η=Concentration of trap sites



As soon as C_{SOL} != 0
$C_{Trap}(C_{SOL}, T) \sim C_{Trap}(T)$
$C_{Trap} \not\propto C_{SOL}$

You can't derive C_{SOL} from C_{Trap}

β_0=10^{13} (s^{-1})
η=10^{-4} (per W-atom)
E_T = 1.5 (eV)
E_D=0.25 (eV)
α_0= 7.4×10^{12} (s^{-1})

How to temperature gradients affect transport

- $\Gamma^{\,Bulk} = -D\rho \frac{\partial C_{SOL}}{\partial x}$ is just a special case of general transport equation $\Gamma^{\,Material} = \sum_j M_j \nabla \Phi_j$

  $\nabla\Phi_j$=Gradients in energy (e.g. Electrical/Chemical potential, Pressure, Temperature…)
  M_j=Transport coefficient (mobility of transported species)

"Forces relax over time by random particle movement"

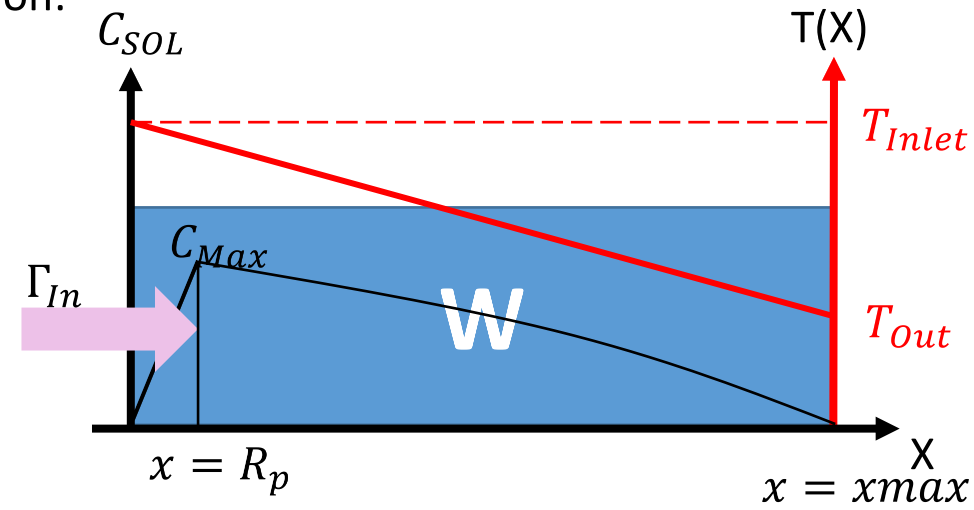
- Including $\nabla\Phi_j = \nabla T$ and ∇C_{SOL} yields the following material flux equation:

  (Following G. R. Longhurst, J. Nucl. Mat. 131 (1985) p. 61)

$$\Gamma^{\,Bulk} = -D(T)\left(\nabla C_{SOL} + C_{SOL} * \frac{Q(T)}{K_B T^2}\nabla T\right)$$

$Q(T) = Q_0 + Q_T\, T$ = **Soret coefficient**

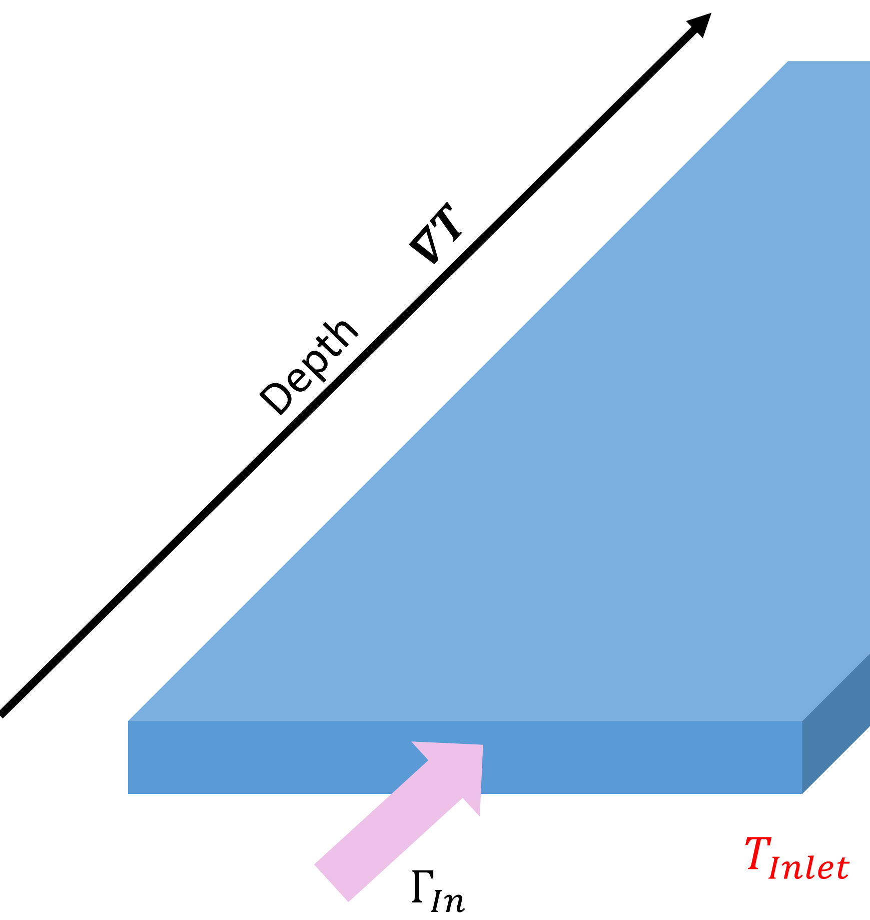
→ Soret effect is important if $\nabla C_{SOL} \sim C_{SOL} * \frac{Q(T)}{K_B T^2}\nabla T$

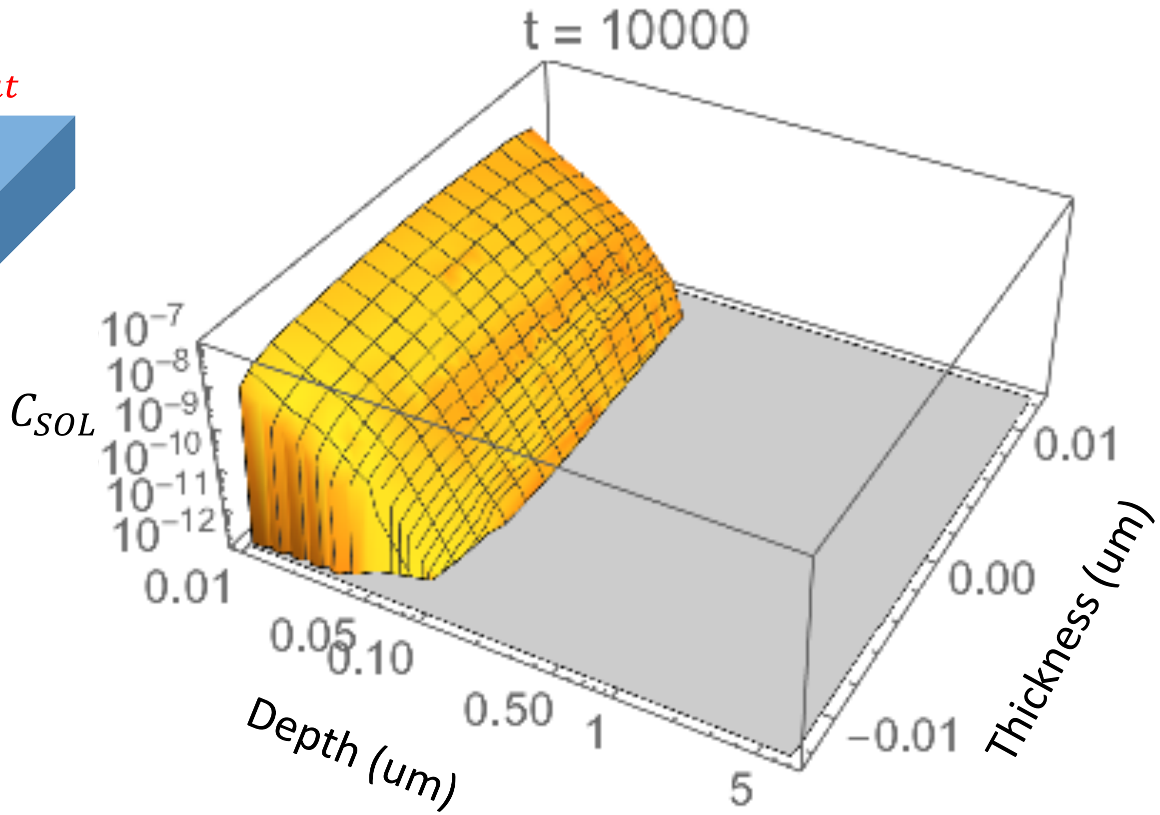


→ Soret effect dominates for high ∇T and low T
→ Soret effect becomes negligible at low C_{SOL}
→ Soret effect is strongest at the surface high T & high C_{SOL}

How to temperature gradients affect transport

- 2D example calculation, no trapping





- Out-diffusion through non loaded surfaces

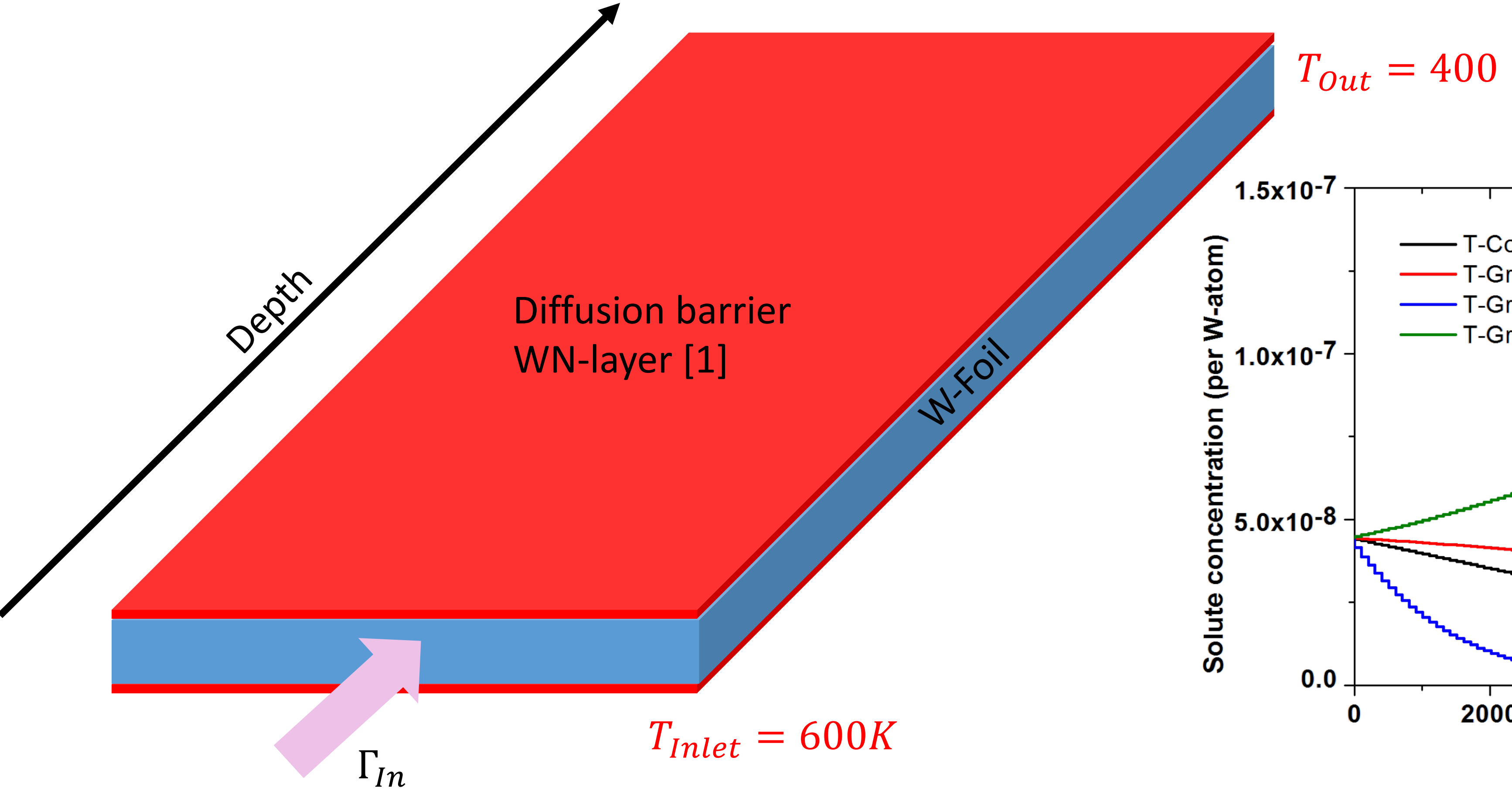
→ Profile "stops" at depth ≈ foil thickness

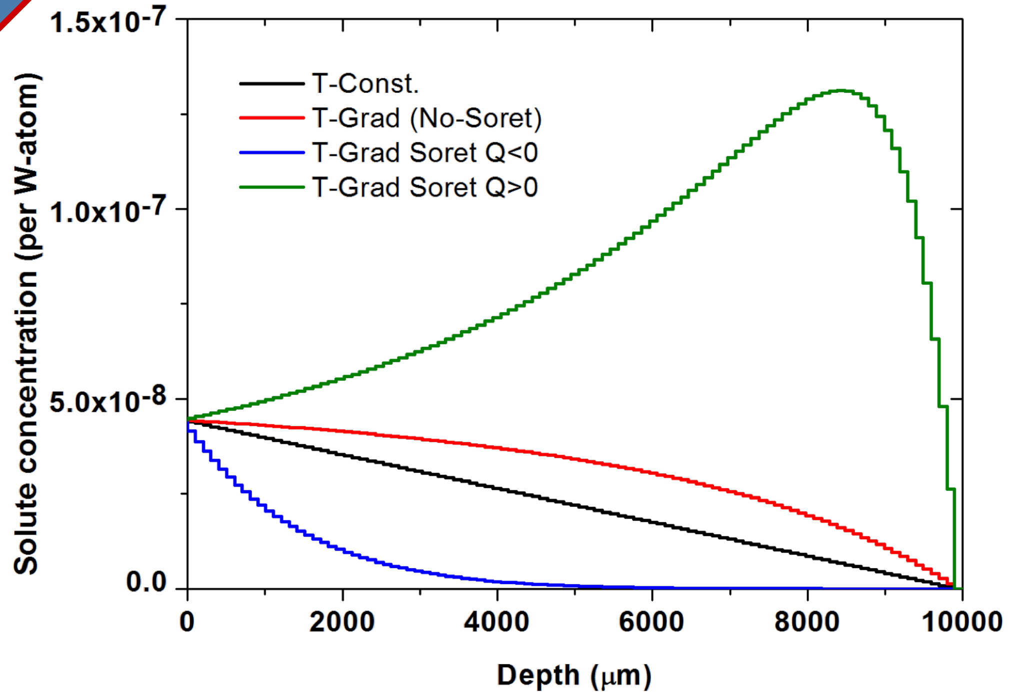
→ No permeation along T-gradient

→ <u>Need a diffusion barrier</u>

How to temperature gradients affect transport

❖ **2D example calculation, no trapping with diffusion barrier**





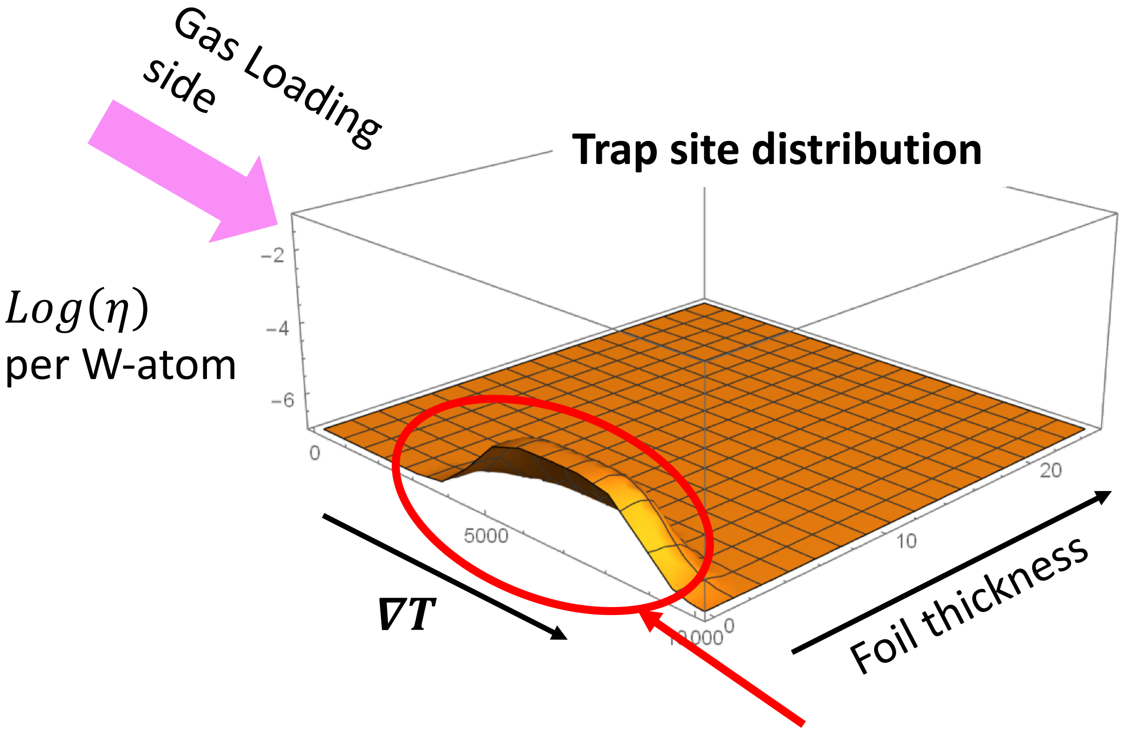
❖ **Soret effect increases Q >0 or decreases Q<0 transport**

→ **Deeper or shallower penetration of diffusion front**

[1] L.Gao recipe

Modeling the expected effect of temperature gradients

- **Simple 2D TESSIM type calculation**
  - Gas loading is modeled as a Dirichlet boundary condition from Sievert's law: ~4×10^{-8} D/W solute concentration
  - A single trap with 2eV de-trapping energy is assumed as the "permeation integration layer"
  - The W-nitride diffusion barrier is modeled as a Neumann boundary on top and bottom of W-layer



- **Equations solved:**

$$\partial_t C_{SOL} = \nabla\left(D(T)\left(\nabla C_{SOL} + C_{SOL} * \frac{Q(T)}{K_B T^2}\nabla T\right)\right) - \partial_t C_{Trap}$$

$$\frac{\partial C_{Trap}}{\partial t} = \alpha\, C_{SOL}(\eta - C_{Trap}) - \beta C_{Trap}$$

  - Soret coefficient $Q(T)$ for Fe

$$Q(T) = Q_0 + Q_T\, T = -0.728 + 5\times10^{-5}\mathrm{T}$$

→ **For T < 600K Q(T) is negative**

  - Temperature profile:

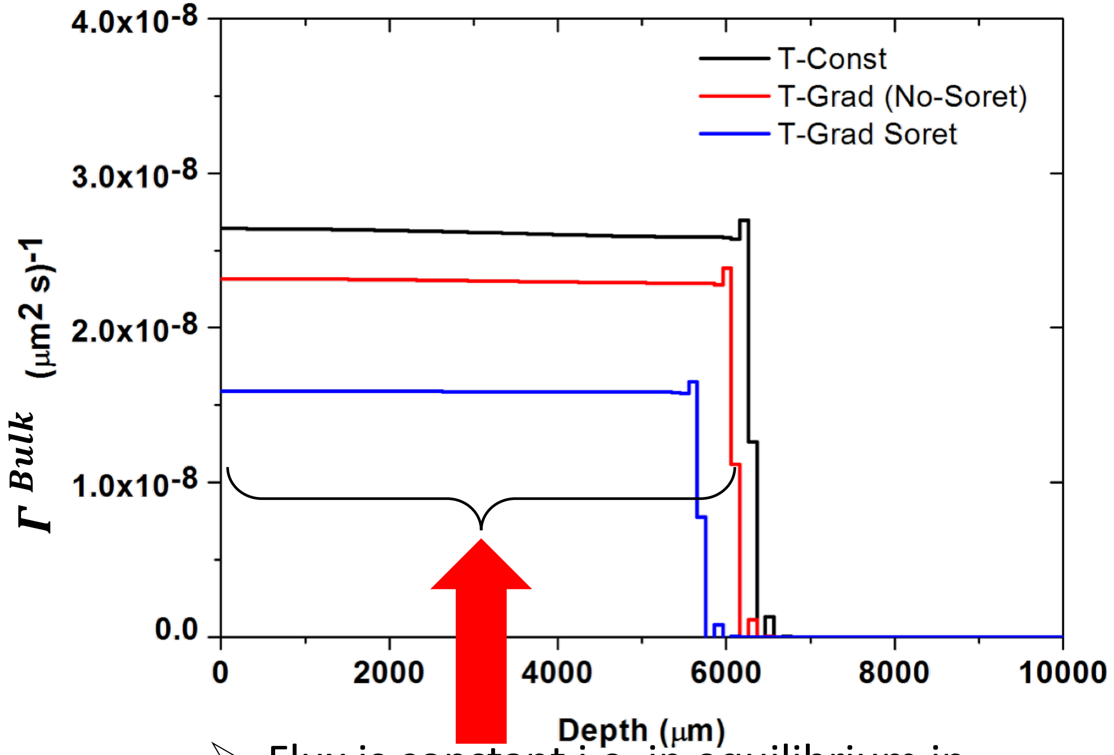
$$T(x) = T_0 + \nabla T * x = 600 - 0.006 * \mathrm{x}$$

(= 6K/mm)

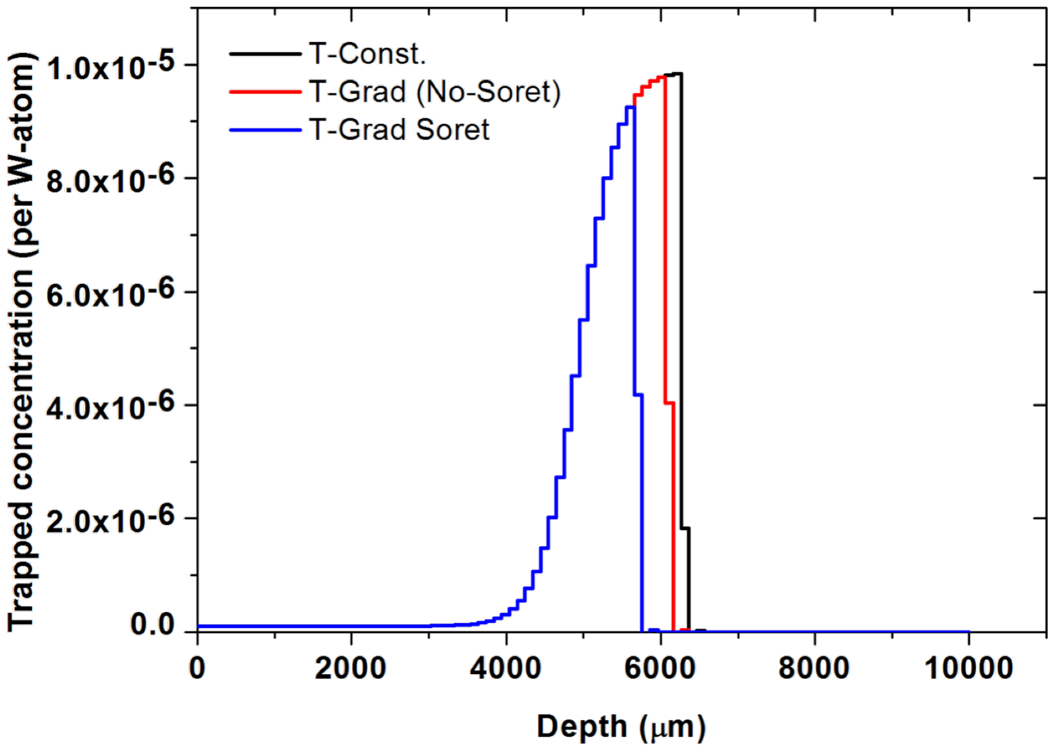
Modeling the expected effect of temperature gradients

- Simple 2D TESSIM type calculation: 6 K/mm, Q(T) for Fe < 0

$$\Gamma^{\,Bulk} = -D(T)\left(\nabla C_{SOL} + C_{SOL} * \frac{Q(T)}{K_B T^2}\nabla T\right)$$



Trapped D depth profile



- Flux is constant i.e. in equilibrium in front of trap filling front
- Negative Q(T) slows down bulk flux

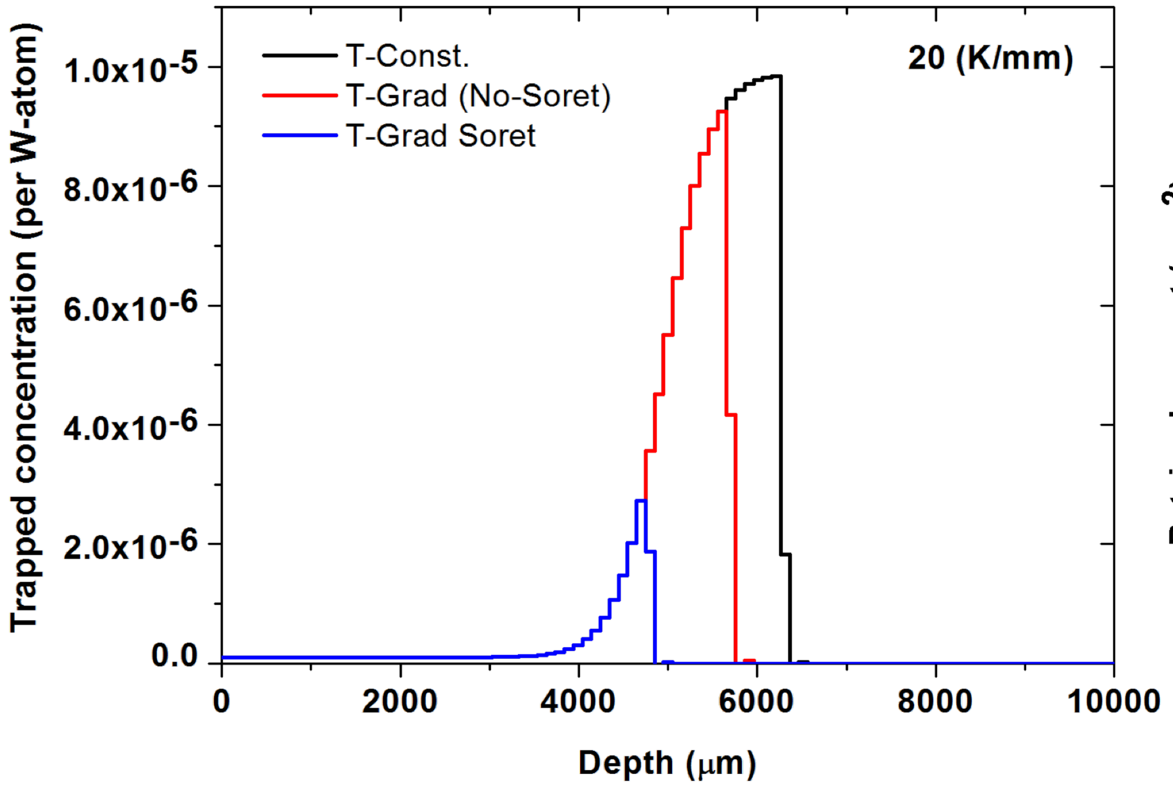
- Less traps are filled

→ At 6 K/mm using Q(T) for Fe the Soret effect is not large

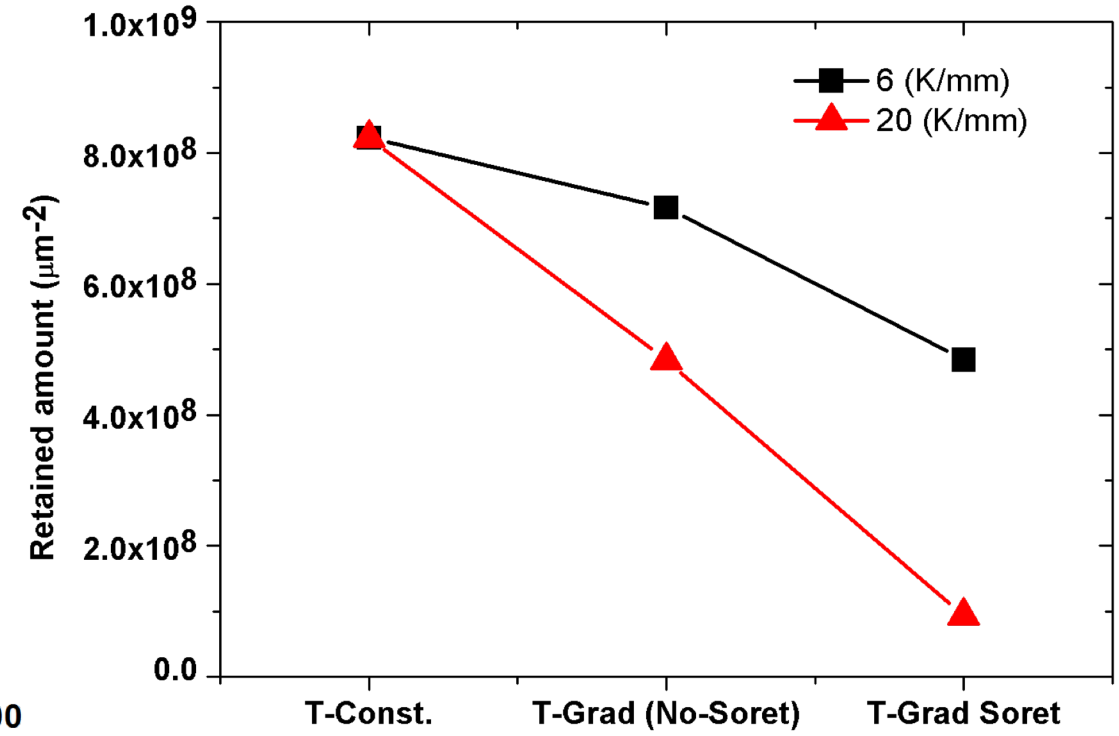
Modeling the expected effect of temperature gradients

❖ **Simple 2D TESSIM type calculation: 20 K/mm, Q(T) for Fe < 0**

Trapped D depth profile



Total retained amount



➢ **Stronger DEMO first wall like gradient shows significant impact on bulk transport**

Conclusions

- The transport of hydrogen in W is limited by trapping, but is carried by the solute hydrogen population

- The solute hydrogen profile is shadowed by the trapped profile
- There is no proportionality between trapped and solute depth profiles
  - A direct measurement is impossible

- Depending on sign of Soret coefficient ∇T can speed up or slow down permeation

- Soret effect probably only important for very strong ∇T > 10K/mm

- Implementation of Soret effect in TESSIM-X is straight forward
  - The real problem is to measure the Soret coefficient…