

The general equation for hydrogen permeation through a membrane, one-dimensional case.

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} + f(u) \quad (0.1)$$

$$\Gamma_{in}(t) + D \frac{\partial u}{\partial x} \Big|_{x=0} - k_u u^2(0, t) = 0 \quad (0.2)$$

$$- D \frac{\partial u}{\partial x} \Big|_{x=L} - k_d u^2(L, t) = 0 \quad (0.3)$$

Here u is the concentration, t - time, x - coordinate, D - diffusion coefficient, k_u and k_d - are hydrogen recombination coefficients on the upstream and downstream sides, respectively. The function $f(u)$ may express the contribution of hydrogen traps. The $\Gamma_{in}(t)$ is the incident atomic hydrogen flux. Now we can take the system from previous chapter. The matrix in the non-boundary points is same as in equation ???. But we have to reevaluate the boundary coefficients according to our boundary condition 0.2.

$$\Gamma_{inc}^n - k_u U_0^{n2} + D \frac{U_1^n - U_0^n}{\Delta x} = 0, \quad (0.4)$$

$$k_d U_{J-1}^{n2} + D \frac{U_{J-1}^n - U_{J-2}^n}{\Delta x} = 0 \quad (0.5)$$

By solving both quadratic equations for U_0^n and U_{J-1}^n , we can evaluate their values based on the calculated concentration from the previous time layer:

$$U_0^{n+1} = -\frac{D}{2k_u \Delta x} + \frac{1}{2} \sqrt{\left(\frac{D}{k_u \Delta x}\right)^2 + \frac{4DU_1^n}{k_u \Delta x} + \frac{4\Gamma_{inc}^n}{k_u}} \quad (0.6)$$

$$U_{J-1}^{n+1} = -\frac{D}{2k_d \Delta x} + \frac{1}{2} \sqrt{\left(\frac{D}{k_d \Delta x}\right)^2 + \frac{4DU_{J-2}^n}{k_d \Delta x}} \quad (0.7)$$