MODELLING OF IG-SCC MECHANISM AT LWR CONDITIONS THROUGH COUPLING OF A POTENTIAL-BASED COHESIVE MODEL AND FICK’S SECOND LAW

M. Sedlak¹, B. Alfredsson², P. Efsing³

¹ Royal Institute of Technology, KTH, Teknikringen 8, 100 44, Stockholm, Sweden
² Royal Institute of Technology, KTH, Teknikringen 8, 100 44, Stockholm, Sweden
³ Royal Institute of Technology, KTH, Teknikringen 8, 100 44, Stockholm, Sweden

ABSTRACT

A fracture mechanic and diffusion model was coupled to simulate the behavior of Intergranular Stress Corrosion Cracking (IG-SCC). To ensure correct physical behavior some assumptions were made, the ion travel, the non-reversible adsorption, the oxide growth dependencies and the diffusion dependency on damage. The model was implemented in a user subroutine in ABAQUS using a cohesive element formulation and an extra adsorption term in Fick’s second law. The coupling was achieved by assuming proportionality between the total adsorption and fracture energy. The physical assumption were verified on a DCB model.

Keywords: Intergranular Stress Corrosion Cracking, Finite Element Model, Fracture Mechanics, Diffusion

1. INTRODUCTION

The current trend among many operators of Nuclear Power Plants is to operate the plants beyond the originally designed lifetime. The extended service time makes it increasingly important to understand the ageing processes of materials in for instance LWR (Light Water Reactor) conditions. IG-SCC (Intergranular Stress Corrosion Cracking) plays an important role as one of the most commonly recognized degradation phenomena. IG-SCC is well-known and has been researched for a long time but due to its complicated nature the damage mechanism behind it is still not completely understood. In particular a coupled fracture mechanic and corrosion model is still not complete, but there exists some models regarding the subject. A model by T. Couvant et al. [1], involving coupling between fracture mechanics and diffusion of oxide. There also exists a model with crack tip mechanics and oxidation kinetics at crack tip by T. Shoji et al. [2]. Earlier research on IG-SCC in LWR conditions mostly focused on identifying the material and corrosion behavior through experiments and parameter fitting equations. This study is based on a multi-physics model, created to emulate the slip-oxidation mechanisms of IG-SCC in LWR conditions, introduced by Ford and Andresen in many of their publications e.g. [3] and [4]. The assumed mechanism is that exposure to water allows the ions to penetrate along grain boundaries. The rate of penetration is governed by strain, time and ion concentration. The ions are adsorbed at virgin material creating an oxide that weakens the grain boundaries mechanical strength. The boundaries will eventually crack due to the applied stress leaving new virgin material exposed. This process will repeat itself and cracks will grow continuously. The key physical assumptions for the model are:

1. Longer travel distances and smaller gap size makes it more difficult for the ions to reach the crack tip, than for shorter cracks with larger gap size.
2. The oxidation process is non-reversible, ions that are absorbed by the oxide can not go back into the solution.
3. Oxide kinetics is dependent on the amount of the concentration of ions and the strain level. The oxide has a maximum adsorption velocity of ions and a minimum (zero velocity) when no ions
are present. When the strain on the oxide is zero the oxide will grow at the minimum limit, but the crack will not advance.

4. When the oxide is completely damaged, the diffusivity of the ions will reach a maximum limit.

The computational model is solved using a commercial FEM-software (ABAQUS) where the multi-physics problem is introduced into a user subroutine *UEL as a FE cohesive element formulation. The element couples the fracture mechanics (modeled by cohesive law, introduced by Barenblatt [5] and Dugdale [6]) and the oxidation process (by diffusion of ions and degradation of cohesive law). The model outline, see figure 1, is a single crack at grain boundaries with multi-physics cohesive element placed at the grain boundaries, resulting in intergranular cracks only. At the crack mouth (left side of figure 1) the ions are constantly renewed and the boundary condition there is set to a constant concentration. The crack is initially concentration free but with time it will fill up due to diffusion of ions from the crack start. The diffusion process is achieved with Fick’s second law including an effective traction, ions concentration and damage dependent diffusivity parameter. When the ions travels throughout the crack they will be adsorbed along the way, but due to the low stress field along the crack compared to the crack tip, the concentration loss will be low but essential. The crack tip will adsorb more ions due to the higher stress field and the adsorbed ions will create an oxide and decrease the fracture properties in the cohesive element. The fracture mechanics part is solved using the modified version of the potential-based Xu and Needleman traction separation law by van der Bosch et al. [7].

2. STRUCTURAL MODEL

The model is based on the coupling between the equilibrium equation and the diffusion equation (Fick’s second law). This coupling is inserted into a FE cohesive element. ABAQUS uses a Newton-Raphson iteration scheme, therefore both the force vector in and the linearization of the force vector needs to be defined. To accomplish this cohesive element force vector and its linearization has to be identified along with diffusion equations concentration vector-, mass-, adsorption- and diffusivity matrix. Starting with the equilibrium equation, the cohesive element force vector is

\[ \rho_c \dot{\mathbf{u}} = \text{div}\mathbf{\sigma} + \rho_c \mathbf{b} \]

with \( \mathbf{u} \) as displacement, \( \mathbf{\sigma} \) as Cachy stress, \( \rho_c \) as density in the current configuration (\( \rho \) is defined in the reference configuration) and \( \mathbf{b} \) as the body force. After applying the weighted integral, switching to the current configuration and further manipulations, the principle of virtual work gives

\[ \int_{\Omega_0} \mathbf{\delta u} \cdot \dot{\mathbf{u}} \rho dV + \int_{\Omega_0} \mathbf{\delta E} : \mathbf{S} dV + \int_{\partial \Omega_0^+} \mathbf{\delta \Delta} \cdot \mathbf{T}_{cz} dS = \int_{\Omega_0} \mathbf{\delta u} \cdot \mathbf{b} \rho dV + \int_{\partial \Omega_0^+} \mathbf{\delta u} \cdot \mathbf{T}_{ext} dS \]

where \( \mathbf{\delta E} \) is the virtual strain, \( \mathbf{\delta \Delta} \) is the virtual separation, \( \mathbf{T}_{ext} \) is the external traction and \( \mathbf{T}_{coh} \) is the cohesive traction.

2.1 Internal virtual work of the cohesive element

The cohesive zones is a two surface interface where the separation is defined by the vector \( \mathbf{\delta \Delta} = \mathbf{\delta u}^+ - \mathbf{\delta u}^- \). Starting in the current configuration according to figure 2 the work can be written as

\[ \delta \Pi_{int} = -\int_{\partial \Omega_0^+} \mathbf{\delta u}^+ \cdot \mathbf{t}_{cz}^+ ds - \int_{\partial \Omega_0^-} \mathbf{\delta u}^- \cdot \mathbf{t}_{cz}^- ds, \]

where \( \mathbf{t}_{cz}^+ \) is the traction in the current configuration working at the upper, positive surface and \( \mathbf{t}_{cz}^- \) is working on the lower negative surface. Note that the positive separation vector is defined in opposite direction to the positive cohesive traction hence the negative signs in equation 3. The negative sign for the
cohesive work on the negative surface is due to the separation vectors definition. Next the previous
equation will be discretized by applying the shape functions \( N \) and using Galerkin’s method as
\[
\delta u^+ \approx N, \quad \delta u^- \approx N
\]
equation 3 becomes
\[
\partial \Pi^e_{int} = (\delta u^e)^T \left[ \int_{\partial \Omega^e \times c^e} N^T T^e \, ds + \int_{\partial \Omega^e \times c^e} N^T T^e \, ds \right]
\]
Next, a change into the reference configuration is performed \( tds = TdS \), so it can be related to equation
2. Knowing both crack surfaces are equal \( d\Omega_0 = d\Omega_0^+ = d\Omega_0^- \) and the equilibrium condition
\[
T_{cz} = -T_{cz}^+ = T_{cz}^-,
\]
\[
\partial \Pi^e_{int} = (\delta u^e)^T \left[ \int_{\partial \Omega_0^e \times c^e} (N^T_\Omega - N^T_\Omega^-) T^e \, ds \right]
\]
The element force vector is derived with the simplification of a common separation shape function
defined as \( (N\Phi)^T = N^T_\Omega - N^T_\Omega^- \) giving,
\[
f^e_c = \int_{\partial \Omega_0^e \times c^e} (N\Phi)^T T_c \, ds \quad \text{where} \quad \Phi = \begin{bmatrix} 0_{2x2} & I_{2x2} \\ -I_{2x4} & I_{2x2} \end{bmatrix}
\]
In equation 7 \( I_{m,n} \) is the identity matrix with \( m \) rows and \( n \) columns.

### 2.2 The cohesive stiffness matrix
To obtain the element tangent stiffness matrix the cohesive force vector is differentiated with respect to
the element displacement
\[
K = \frac{\partial f^e_c}{\partial d^e} = \int_{\partial \Omega_0^e \times c^e} (N\Phi)^T \frac{\partial T_c}{\partial d^e} \, ds.
\]
The traction vector is split into a rotational part \( Q(n) \) and a local traction part \( T^{mid} \),
\[
T_c = Q(n)T^{mid}
\]
The rotational part \( Q(n) \) is a function of the normal belonging to the middle surface of the element. The
local traction \( T^{mid} \) is obtained through a traction separation law. Equation 9 inserted into equation 8 will
render into the tangential stiffness matrix
\[
K^e = \int_{\partial \Omega_0^e \times c^e} (N\Phi)^T Q(n) \frac{\partial T^{mid}}{\partial d^e} \, ds + \int_{\partial \Omega_0^e \times c^e} (N\Phi)^T \frac{\partial Q(n)}{\partial d^e} T^{mid} \, ds
\]
where the first integral is the material stiffness and the second integral is the geometrical stiffness.

### 2.3 Finite element implementation
The cohesive element is constructed from two linear line elements. The two line elements lie together in
the unstressed state (zero thickness) and as they are separated the traction force will force them together,
see figure 3. The physical coordinate system is mapped to the natural with the shape functions,
\[ N_1(\xi) = \frac{1}{2} (1 - \xi), \quad N_2(\xi) = \frac{1}{2} (1 + \xi) \]  

where \( \xi \) is the coordinate in the natural coordinate system. The separation distance \( \Delta u \) is calculated by taking the displacement difference between the top and bottom nodes, in both \( x \) and \( y \) direction. In matrix form the nodal separation distance can be calculated as,

\[ \Delta u_N = \Phi d_N \]

where \( \Phi \) was defined in equation 7 and the nodal displacement is defined as,

\[ d_N = (d_{1x}, d_{1y}, d_{2x}, d_{2y}, d_{3x}, d_{3y}, d_{4x}, d_{4y})^T \]

Using the shape functions in equation 11, the nodal separation distances can be mapped to the natural coordinate system giving a continuous separation distance through the element,

\[ \Delta u(\xi) = \begin{pmatrix} \Delta u_x(\xi) \\ \Delta u_y(\xi) \end{pmatrix} = \begin{pmatrix} N_1(\xi) & 0 \\ 0 & N_2(\xi) \end{pmatrix} \Delta u_N \]

To distinguish between the tangential and normal separation applied to the cohesive element in large displacement a mid-element coordinate system is specified. This coordinate system is defined at the middle plane in the cohesive element and the origin is at the middle, see figure 4. The mid-plane is computed by linear interpolation between top and bottom nodes as

\[ d_{N}^{\text{mid}} = \frac{1}{2} \begin{bmatrix} I_{4 \times 4} & 0_{2 \times 2} \\ I_{2 \times 2} & 0_{2 \times 2} \end{bmatrix} (X_N + d_N) \]

where \( X_N \) are the coordinates in the initial configuration. To make the mid-plane continuous the shape functions are used in equation 15 giving

\[ d_{\text{mid}}(\xi) = N d_{N}^{\text{mid}} \]

The tangential and normal directions to the mid-plane are obtained by differentiation the mid-plane positions in the natural coordinate system. After normalizing the mid-plane direction vectors, they will be used as a transformation matrix to move between the global and the mid-plane coordinates. Starting with the vector in the \( 1 \)-direction located at the mid-plane

\[ e_1 = \frac{\partial d_{\text{mid}}(\xi)}{\partial \xi} = \frac{\partial N(\xi)}{\partial \xi} d_{N}^{\text{mid}} \]

The mid-plane normalized direction vectors are defined as,

\[ \hat{e}_1 = \frac{e_1}{|e_1|} = \frac{1}{\left| \frac{\partial d_{\text{mid}}(\xi)}{\partial \xi} \right|} \left( \frac{\partial d_{\text{mid}}^{\text{mid}}(\xi)}{\partial \xi}, \frac{\partial d_{\text{mid}}^{\text{mid}}(\xi)}{\partial \xi} \right)^T \]

\[ \hat{e}_n = \frac{e_3 \times e_1}{|e_3 \times e_1|} = \frac{1}{\left| \frac{\partial d_{\text{mid}}(\xi)}{\partial \xi} \right|} \left( -\frac{\partial d_{\text{mid}}^{\text{mid}}(\xi)}{\partial \xi}, \frac{\partial d_{\text{mid}}^{\text{mid}}(\xi)}{\partial \xi} \right)^T \]
where the vector $\mathbf{e}_z = (0,0,1)$ is the vector thru the thickness. Finally the transformation between the physical coordinate system and the mid-plane system is defined as

$$\Delta \mathbf{u}^{\text{mid}} = \Theta^T \Delta \mathbf{u}, \quad T_{cz} = \Theta T^{\text{mid}}$$

where $\Theta_{2x2} = [\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_z]$.  

### 2.4 Stiffness and internal force

The internal force matrix of the element is defined in 2D as,

$$\mathbf{f}^e = \int_{A_e} \mathbf{N}^T \mathbf{T}_{cz} dA = W \int_{l_e} \mathbf{N}^T \mathbf{T}_{cz} dl$$

where $W$ is the cross-plane width and the separation shape functions $\mathbf{N} = \mathbf{N}\mathbf{\Phi}$. Equation 22 is then moved to the natural coordinate system and the tractions are transformed to the mid-plane with equation 21,

$$\mathbf{f}^e = W \int_{-1}^{1} \hat{\mathbf{N}}^T \mathbf{T}_{cz} \text{det} \mathbf{J} d\xi = W \int_{-1}^{1} \hat{\mathbf{N}}^T \Theta \mathbf{T}^{\text{mid}} \text{det} \mathbf{J} d\xi$$

where $\text{det} \mathbf{J}$ is the determinant of the Jacobian that will be constant due to the referential mapping. The determinant of the Jacobian is defined as

$$\text{det}(\mathbf{J}) = \sqrt{\left(\frac{\partial d_{x0}^{\text{mid}}(\xi)}{\partial \xi}\right)^2 + \left(\frac{\partial d_{t0}^{\text{mid}}(\xi)}{\partial \xi}\right)^2}$$

and

$$\left(\frac{\partial d_{x0}^{\text{mid}}(\xi)}{\partial \xi}\right)^2 = \frac{1}{2} \mathbf{N}_{\xi} \Psi \mathbf{X}_N \quad \text{where} \quad \Psi = \begin{bmatrix} I_{4x4} & 0_{2x2} & I_{2x2} \\ I_{2x2} & 0_{2x2} & 0_{2x2} \end{bmatrix}$$

The elemental algorithmic stiffness matrix was defined in equation 10. The geometrical stiffness is not considered due to the small rotations. The material stiffness is derived by obtaining a local stiffness term that can be expressed by the local separation $\Delta \mathbf{u}^{\text{mid}}$. The local separation can be obtained by inserting equations 13 and 12 into equation 21 giving

$$\Delta \mathbf{u}^{\text{mid}} = \mathbf{Q}^T (\mathbf{n}) \mathbf{N}\mathbf{\Phi} \mathbf{d}$$

Changing the material stiffness part in equation 10 to two-dimensions, applying the chain rule and mapping to natural coordinate gives

$$\mathbf{K}^e_{\text{material}} = \int_{-1}^{1} (\mathbf{N}\mathbf{\Phi})^T \mathbf{Q}(\mathbf{n}) \mathbf{D}_{\text{loc}} \mathbf{Q}^T (\mathbf{n})(\mathbf{N}\mathbf{\Phi}) \text{det}(\mathbf{J}) d\xi$$

where $\mathbf{D}_{\text{loc}}$ is the local matrix.

### 3. DIFFUSION MODEL

The diffusion model describes the transport of ions from the crack mouth to the crack tip. To obey assumption 1, Fick’s second law can be used because the cross area and length is influencing the diffusion. Longer travel distances will experience more concentration loss along the way and the
oxidation process in the crack tip will also create a concentration loss due to adsorption. This was modeled with the following PDE in one dimension,

\[
\frac{\partial c}{\partial t} = D(\eta_T) \frac{\partial^2 c}{\partial x^2} - h(c, \eta_T^{rev})
\]

where \( D(\eta_T) \) is the diffusivity as a function of irreversible normalized traction \( \eta_T \), \( c \) is the concentration of ions and \( h(c, \eta_T^{rev}) \) is the adsorption rate of the ions to the boundary. The physical assumption 4 is applied to the diffusivity as

\[
D(\eta_T) = (D_s - D_l)\eta_T + D_l
\]

where the diffusivity function \( D(\eta_T) \) has the requirement to change from the diffusivity of the species in the bulk material \( D_s \) to the diffusivity of the species in the liquid \( D_l \). A simple definition of \( h(c, \eta_T^{rev}) \) was made to meet assumption 3 on the adsorption kinetics

\[
h(c, \eta_T^{rev}) = \dot{h}_{max}(1 - \exp(-n_1(\eta_T^{rev})c))
\]

where \( \dot{h}_{max} \) is the maximum adsorption rate and \( n_1(\eta_T^{rev}) \) is a function depending on the reversible normalized traction, which is changing the angle of the exponential slope resulting in a different adsorption velocity at specific concentrations. Equation 30 insures the concentration to converge at zero if no concentration is added on the boundary, which ensures assumption 2. The function \( n_1 \) is defined as

\[
n_1(\eta_T^{rev}) = (m_{corr} - m_{corr})\eta_T^{rev} + m_{corr}
\]

where \( m_{corr} \) is a fitting parameter for the concentration loss in highly stressed environment and \( m_{corr} \) is in an unstressed environment. The boundary and initial conditions are

\[
c_s = c_s(x,t) \text{ on } \partial\Omega_s
\]

\[
s(x,0) = c_0(x)
\]

where the boundary condition surface \( \partial\Omega_s \) is defined at the crack mouth with the concentration value is constant due to the continuous exchange of new ions. The initial condition is set to zero concentration at all positions except for the boundary at the crack mouth, see figure 5.

### 3.1 Diffusion element formulation

Equation 28 is rewritten to weak form by applying the weighted integral and divergence theorem. The shape functions \( N_i \) and their derivatives \( B_i \) are used for the discretization of the diffusion equation giving the semi-discrete matrix system [8],

\[
M \frac{\partial e_c}{\partial t} + Ke_c = R
\]

where \( M \) is the element mass concentration matrix and \( K \) is the element diffusivity matrix. The \( R \) matrix will force the loss in concentration. Backward Euler iteration scheme is employed for the discretization of the concentration time differential giving the internal force vector and its stiffness as
\[ f_{\text{diff}}^e = [A \int \rho N^T \mathbf{d}x + \Delta t A \int_{x} \mathbf{D}(\eta_T) \mathbf{B}^T \mathbf{B} \mathbf{d}x] c_{e}^{\text{diff}} - \]
\[ A \int \rho N^T \mathbf{d}x \mathbf{c}_{\text{e}}' + p \int N^T h_{\text{max}}^{\text{diff}} (1 - \exp(-n_{\text{e}} N c_{\text{e}})) \mathbf{d}x \Delta t \]
\[ K_{\text{diff}}^e = A \int \rho N^T \mathbf{d}x + \Delta t A \int_{x} \mathbf{D}(\eta_T) \mathbf{B}^T \mathbf{B} \mathbf{d}x + \Delta t p \int N^T h_{\text{max}}^{\text{diff}} \exp(-n_{\text{e}} N c_{\text{e}}) (n_{\text{e}} N) \]

where \( A \) is the surface area, \( W \) is the cross section width and \( I \) is the identity matrix. The diffusion solution is only in one direction and therefore only two nodes in the cohesive element in figure 3 are necessary, in this case the two bottom nodes (1,2). Similar shape functions to the ones used in the cohesive element are implemented (equation 11) with their derivatives. The shape functions are inserted into the diffusion internal force vector \( f_{\text{diff}}^e \) and its stiffness \( K_{\text{diff}}^e \), equation 35 and 36.

### 3.2 Grain boundary degradation by ions

The degradation of the material is implemented by changing the parameters inside the Traction Separation Law TSL (relation between separation and traction) in the cohesive element. The amount of degrading is coupled to the amount of ions adsorbed at the cohesive element. The traction separation law defines the amount of traction needed to separate the cohesive element. There exist a vast amount of different TSL, the one used here is a modified Xu and Needleman TSL from van der Bosch et al. [7]. The modified Xu and Needleman TSL is an intrinsic model which is normally used in implicit solutions. Differentiating the potential gives the traction separation law, see figure 6.

\[ T_{n}^{\text{mid}} = \phi_{n} \exp \left( - \frac{\Delta u_{n}^{\text{mid}}}{\delta_{n}} \right) \left[ \frac{\Delta u_{n}^{\text{mid}}}{\delta_{n}} \exp \left( - \frac{(\Delta u_{n}^{\text{mid}})^2}{\delta_{n}^2} \right) \right] \]
\[ T_{1}^{\text{mid}} = 2 \left( \frac{\phi_{n} \Delta u_{1}^{\text{mid}}}{\delta_{1}^2} \right) \left[ 1 + \frac{\Delta u_{1}^{\text{mid}}}{\delta_{1}^2} \right] \exp \left( - \frac{\Delta u_{1}^{\text{mid}}}{\delta_{1}^2} \right) \exp \left( - \frac{(\Delta u_{1}^{\text{mid}})^2}{\delta_{1}^2} \right) \]

### 3.3 Degradation implementation

The oxide fracture properties are obtained by changing the TSL of the cohesive element and the amount of oxidation is linked to the amount of ions adsorbed at the surface

\[ \phi_{n} \propto \int h(c)dt = c_{n}^{\text{ad}} \]
\[ \phi_{1} \propto \int h(c)dt = c_{1}^{\text{ad}} \]

The proportion between the fracture energy and the amount of ions is assumed to be linear using \( k_{e}^{\phi} \) and subtracting it from the initial energy \( \phi_{e}^{\text{ini}} \) as

\[ \phi_{n} = \phi_{n}^{\text{ini}} - k_{n}^{\phi} c_{n}^{\text{ad}} \]
\[ \phi_{1} = \phi_{1}^{\text{ini}} - k_{1}^{\phi} c_{1}^{\text{ad}} \]

with the oxide fracture energy as a minimum limit and the initial energy as a maximum limit \( \phi_{e}^{\text{ini}}, \phi_{e}^{\text{ini}} \), see figure 7. The decrease in fracture energy is also irreversible (requirement for assumption 2 in the
introduction) due to the always positive concentration in equation 30. Two history parameters are defined, both of them are effective parameters of the traction in normal and tangential direction. Now, $\eta_{T}$ is defined as

$$\eta_{T} = \frac{T_{\text{eff}}}{T_{\text{ini}}} = \frac{\sqrt{T_{n,\text{max}}^2 + T_{t,\text{max}}^2}}{\sqrt{T_{n,\text{ini}}^2 + T_{t,\text{ini}}^2}}$$

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It is a dimensionless traction and is used to determine the diffusivity in the material. The maximum effective traction $T_{\text{max}}^{\text{eff}}(\Delta_{\text{max}})$ is dependent on the maximum separation $\Delta_{\text{max}}$ and therefore it will not change during unloading and reloading. The next parameter is also a normalized traction

$$\eta_{T}^{\text{rev}} = \frac{T_{\text{eff}}}{T_{\text{ini}}} = \frac{\sqrt{T_{n}^2 + T_{t}^2}}{\sqrt{T_{n,\text{ini}}^2 + T_{t,\text{ini}}^2}}$$

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but this one is dependent on the current separation $\Delta_{\text{eff}}$ and will thereby change during unloading and reloading.

4. MODEL SIMULATION

The cohesive element that contains the multi-physics model was written in FORTRAN and implemented in ABAQUS using its subroutine *UEL. A DCB model was used to verify the assumptions stated in the introduction and the internal parameters in the multi-physics model were studied showing different behavior of the processes.

4.1 Applications to DCB specimen

The double cantilever beam (DCB) in figure 8 is used to test the multi-physics cohesive elements. The DCB is constrained at one bottom node and a constant force, which does not rotate with the current configuration, is applied to the upper left node. The geometric dimension for the DCB model is $a = 5\, \mu m$, $L = 10\, \mu m$ and $b = 2\, \mu m$. The fracture energy used is $\phi = 0.002\, J/\mu m^2$ and the maximum stress is $T_{n,\text{ini}} = 0.2\, \text{GPa}$ for normal direction and $T_{t,\text{ini}} = 0.2\, \text{GPa}$ for the tangential direction. The elements used around the cohesive elements are ordinary elastic elements with the elastic modulus $E = 200\, \text{GPa}$ and the Poisson’s ratio $\nu = 0.3$. The energy for the oxide material is reduced to half of the initial traction and a tenth of the fracture energy. The diffusivity is set to zero in solid $D_s$ and in liquid $D_l = 10^4\, \mu m^2/s$. The contour plots shown in figures 9 and 10 are showing the mesh and the typical distribution of the von Mises stresses and ion concentrations. At the starting time the DCB is exposed to initial bending giving the high oxide and crack tip velocities in figure 11. At the end of the time the crack has reached a critical level and the crack will continue without the oxidation process, this means that only the middle interval in the plots is interesting. The crack tip position and oxide start position is growing slower with time, see figure 12, due to the increasing crack length, this is because the ion concentration is decreased from the concentration loss at the crack sides, this verifies assumption 1. The thickness of the oxide is kept constant during the middle interval, this can be seen by the same oxide and crack tip velocities, shown in figure 11. To verify assumption 3 the stress and ion concentration at the boundary was varied showing that higher ion concentration and higher stress concentration gives a higher oxide thickness and higher crack tip velocity, see figures 13 and 14 for oxide thickness and figures 15 and 16 for crack velocity. Assumption 2 is verified by including an extra cycle where the concentration boundary is set to zero after 4000 s, see figure 17. The ions become depleted and the crack tip position and the oxide goes to rest.
CONCLUSIONS
The solutions and verification on the physical assumption were,

1. By implementing Fick’s second law an influences of ion travel distance was included, see equation 28. In figure 12 the crack tip velocity is decreased in time, this is a result from the ion travels distance.
2. The non-reversible process of the ion adsorption is implemented with equation 30 and verified in figure 17, where both the crack tip and oxide is set to rest when the concentration at the concentration BC is set to zero.
3. Variation of stress and ion concentration at the boundary changes the oxide thickness and crack tip velocity. This was shown in figure 13, 14, 15 and 16. Both ion increase and stress increase gave thicker oxides and increased crack tip velocities.
4. In equation 29 the diffusivity $D(\eta_r)$ is a linear function of the irreversible damage, equation 41. During softening the traction $T_{\text{eff}}$ in equation 41 will decrease and the diffusivity will increase linearly to $D_f$. So a completely damage element will have the diffusivity $D_f$.

The previous list concludes that all physical assumption where verified except the gap size influence, which is not verified but implemented through Fick’s law. Due to the lack of a chemistry implementation, the model becomes strongly dependent on the crack length, this can be solved with more chemistry approach instead of a diffusion model.

REFERENCES
NOMENCLATURE

Figure 1: Schematic figure of the bulk material undergoing constant loading and diffusion of ions into the crack.
Figure 2: Body with a cohesive zone. The influence of is illustrated in the left part of the figure.

Figure 3: The top left part of the figure is showing the cohesive element in the physical coordinate system and the bottom right part is in the natural coordinate system.
Figure 4: The dark area inside the cohesive element is the mid-plane; the $e_1$ and the $e_n$ are the tangential and normal directions to the mid plane. The separation in the x and y directions are defined.

Figure 5: Schematic figure of ions passing through the crack from the mouth to the crack tip by diffusion. The red elements represent failed elements while the blue elements are not failed (with different diffusivity). At a higher stress more ions will be adsorbed and creating a thicker oxide.
Figure 6: The traction separation is presented in the left and right part of the figure for the normal and tangential direction, respectively.

Figure 7: Influence of oxidation on a specific point on the TSL. The smaller exponential curve is the TSL for the oxide and the greater curve is the TSL for the virgin material. Note that the irreversibility makes it impossible for the specific point to go back in the same TSL, instead it moves linearly back to the origin.
Figure 8: The DCB model, showing the locations for boundary conditions and loads.

Figure 9: von Mises stresses.
Figure 10: The DCB model with the concentration after 4000 s. Notice that the concentration is plotted at the the elastic elements underneath the cohesive elements.

Figure 11: The velocity of the crack tip and the oxide start. The velocities are obtained from a polynomial fit of the smoothened displacement.
Figure 12: The crack tip and the oxide start position. The space between the two curves is the oxide thickness. Due to the coarse mesh a smoothening algorithm has been used to clarify the results.

Figure 13: The influence on the oxide thickness under stress variation.
Figure 14: The influence on the oxide thickness under ion variation.

Figure 15: The influence on the crack tip velocity under stress variation. The oscillation of the blue curve is due to the combination of a coarse mesh and a low crack tip velocity. This then creates oscillations when smoothening and polynomial fit is used to obtain the velocity.
Figure 16: The crack tip velocity at ion variation. The higher crack tip velocity at the end of the green curve is because the specimen exceeded the critical fracture strength.

Figure 17: The crack tip position when the concentration BC is set to zero at 4000 s. Both the crack tip and oxide stops to grow.