Optimisation of Diffusion Driven Degradation Processes

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Nature strives for optimal processes in order to prevent early damage or failure, for example bones which regulate the tissue in high stress areas or the optimal shape of trees. Many materials in nature are highly complex as they are designed for long duration. Taking nature itself as a role model means taking its complexity into account, especially when considering materials which suffer from chemical attacks and the degradation of materials. From this point of view, we create an algorithm which considers degradation processes triggered by chemical substances which depend on diffusion conditions in a finite element (FE) framework. In addition, we perform design optimisation with stress restrictions by taking evolutionary processes as a role model.

1 Numerical approach

The numerical approach is divided into two parts, a structural analysis with a continuum mechanical model and a structural optimisation framework. For structural analysis, we focus on coupled aspects between mechanics, diffusion and mass resorption. With a thermodynamically consistent formulation of a single-phase open system we evaluate the constitutive equations for the stresses, mass sink and the evolution of degradation. The diffusion is a gradient-based formulation of nutrient motion in analogy to Fick’s law. Thus, chemical reactions of specific nutrients trigger degradation processes leading to large deformations. The continuum mechanical theory is embedded in an FE-framework. An enhanced kinematic concept allows the decomposition of degradation and elastic deformations and, furthermore, enables the separation of degradation deformation, geometry and physics, see e.g. [1]. The coupled problem is embedded in a structural optimisation framework. For the sake of simplicity, we apply a Matlab optimisation toolbox as a solver. This combination allows full access to the power of Matlab, thus using the introduced FE-model. A general outline is plotted in Fig. 1. The entire computation runs in a Matlab framework, which includes a connection to the open software gmsh for mesh creation on the one hand, and an interface to a Fortran code using MEX-file interfaces on the other hand.

2 Structural analysis

The coupled diffusion and degradation approach in a permeable structure allows a gradient-based flow of concentrations. In analogy to degradation in a living structure we refer to a volumetric approach, see [4]. We apply a multiplicative decomposition of the deformation gradient into an elastic part $F_X^e$ and a degradation part $F_X^g$, see [2,3,5]. Assuming an isotropic degradation approach leads to the following description for the degradation deformation gradient $F_X^g$, i.e.

$$ F_X = F_X^e F_X^g \quad \text{with} \quad F_X^g = \nu X_g. $$

Based on a special kinematic approach, which separates the geometry, deformation and degradation aspects, allows the following kinematic restriction for the stretch ration $\nu$

$$ \nu = \sqrt{\frac{\rho_0}{\rho_0^*}} \quad \text{with} \quad \rho_0 = \rho_0^* \pm \int_{t_0}^t R_0 \, dt \quad \text{and} \quad R_0 = M_{\gamma} \, c_{\gamma}, $$

wherein $\rho_0^*$ is the resulting density in the reference configuration, which is affected by a sink term $R_0$ and depending on the initial density $\rho_0^*$. From the constitutive evaluation we get a connection between the mass sink term $R_0$ and the chemical impact of concentrations $c_{\gamma}$. The concentrations are the trigger for material degradation depending on the relevant chemical

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interaction. The velocity $x'_{c\gamma}$ of the concentration $c_{\gamma}$, is calculated in analogy to Fick’s law, assuming that the velocity moves from regions of high concentrations to regions of low concentrations with

$$x'_{c\gamma} = D_{\gamma} \nabla c_{\gamma}. \tag{3}$$

A numerical approximation, the FEM, is applied in order to solve the system of partial differential equations. This approach is used to solve for the set of degrees of freedom, including the displacement and the concentration based on the balance of momentum and the balance of mass for concentrations. This set of unknown quantities is determined via the Galerkin procedure. In order to solve the time dependent non-linear problem, we apply the implicit Newmark scheme. With quadratic ansatz functions for the FEM approach we obtain a stable numerical evaluation.

### 3 Structural optimisation

The optimisation problem follows as:

$$\begin{align*}
\min \ J(s) \quad \text{subject to} & : \ A s \leq b \\
& : s^u \leq s \leq s^o \\
& \text{with : } J(s_1, s_2) = (a, b) - (s_1, s_2) \quad \text{objective function.}
\end{align*}$$

Therein, $s$ is the design and $J(s)$ is the objective function. The linear constraint is evaluated from a linearised form of the von Mises stress $\sigma_{\text{VM}}$. In this example, the objective function $J(s)$ is the area of the structure aiming a reduction of material using the parameters of the hole as the design parameters $s_1$, $s_2$. With the side condition of a maximum value of the von Mises stress $\sigma_{\text{VM}} \leq \sigma_{\text{VM}}^{\text{max}}$, a tolerance for the design parameters $[s_1, s_2]_{\text{min}} \leq [s_1, s_2] \leq [s_1, s_2]_{\text{max}}$ and the gradients of the objective function, we apply a Matlab optimisation toolbox as a solver, creating new design parameters.

### 4 Numerical example

In this example we focus on a structure with a hole. We consider a concentration inflow from the left to the outflow on the right side of the structure, wherein the inflow condition increases in dependence of the time. The computation runs over 50 time steps with a time step size of 0.1 seconds. The time depending impact of the flowing concentration is plotted in the diagram of Fig. 3. The determinant of the degradation gradient $F_X$ decreases caused by the degradation process, triggered by the concentrations. The optimisation algorithm enables a design reduction, thus holding the side conditions.

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