

Notes on the numerical implementation of a coupled theory of the chemo-mechanics of PEG-DA hydrogels in FEniCS

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1 Governing partial differential equations and boundary conditions

1. The governing partial differential equation for the mechanical problem in the absence of body forces and neglect of inertia is the force balance

$$\text{Div} \mathbf{T}_R = \mathbf{0} \quad \forall \mathbf{X} \in B, \quad (1.1)$$

where the Piola stress $\mathbf{T}_R \in B$ is given by

$$\mathbf{T}_R = G(\mathbf{F} - \mathbf{F}^{-\top}) + (1 + \Omega c_R) K \ln \left(\frac{J}{1 + \Omega c_R} \right) \mathbf{F}^{-\top}. \quad (1.2)$$

With $\partial B_{\mathbf{u}}$ and $\partial B_{\mathbf{t}_R}$ denoting complementary subsurfaces of the boundary ∂B of the body B , we consider a pair of possible boundary conditions:

$$\begin{aligned} \mathbf{u} &= \bar{\mathbf{u}} \quad \text{on } \partial B_{\mathbf{u}}, \\ \mathbf{T}_R \mathbf{n}_R &= \bar{\mathbf{t}}_R \quad \text{on } \partial B_{\mathbf{t}_R}. \end{aligned} \quad (1.3)$$

In the boundary conditions above $\bar{\mathbf{u}}$ and $\bar{\mathbf{t}}_R$ are prescribed displacement and tractions, both functions of (\mathbf{X}, t) .

2. The governing partial differential equation for mass balance is

$$\dot{c}_R + \text{Div} \mathbf{j}_R = 0, \quad (1.4)$$

where the referential mass flux \mathbf{j}_R is given by

$$\mathbf{j}_R = -M \nabla \mu, \quad (1.5)$$

with chemical potential

$$\begin{aligned} \mu &= R\vartheta \left(\ln \left(1 - \frac{1}{1 + \Omega c_R} \right) + \frac{1}{1 + \Omega c_R} + \frac{\chi}{(1 + \Omega c_R)^2} \right) - \Omega K \ln \left(\frac{J}{1 + \Omega c_R} \right), \quad \text{where} \\ \chi &= \chi_0 + \beta p, \quad \text{with} \quad p = -\frac{1}{3} \text{tr} \mathbf{T}, \end{aligned} \quad (1.6)$$

and \mathbf{M} the mobility tensor. Here, because of the constitutive assumptions made in Section 3 of Stewart et al. (2022), we have¹

$$\begin{aligned}\mathbf{M} &= \mathbf{C}^{-1} \left(\frac{Dc_R}{R\vartheta} \right), \quad \text{where} \\ D &= D_0 \exp \left(-\alpha \frac{\phi}{1-\phi} \right) + \gamma, \quad \text{with} \quad \phi = \frac{1}{1 + \Omega c_R}.\end{aligned}\tag{1.7}$$

With ∂B_μ and ∂B_{j_R} denoting complementary subsurfaces of ∂B , we consider a pair of possible boundary conditions:

$$\begin{aligned}\mu &= \bar{\mu} \quad \text{on } \partial B_\mu, \\ \mathbf{j}_R \cdot \mathbf{n}_R &= \bar{j} \quad \text{on } \partial B_{j_R}.\end{aligned}\tag{1.8}$$

In the boundary conditions above $\bar{\mu}$ and \bar{j} are *prescribed* chemical potential and normal species flux which are a function of (\mathbf{X}, t) .

Standard initial conditions involve the specifications

$$\mathbf{u}(\mathbf{X}, 0) = \mathbf{u}_0(\mathbf{X}), \quad \mu(\mathbf{X}, 0) = \mu_0(\mathbf{X}), \quad \text{and} \quad c_R(\mathbf{X}, 0) = c_{R0}(\mathbf{X}), \quad \text{on } B,\tag{1.9}$$

with \mathbf{u}_0 , μ_0 and c_{R0} prescribed functions of $\mathbf{X} \in B$.

2 Weak forms of the governing partial differential equations

1. Mechanical problem:

Consider a test field $\mathbf{u}_{\text{test}}(\mathbf{X})$ on B which satisfies $\mathbf{u}_{\text{test}}(\mathbf{X}) = \mathbf{0}$ on $\partial B_{\mathbf{u}}$. If the balance equation $\text{Div } \mathbf{T}_R = \mathbf{0}$ on B and the traction condition $(\bar{\mathbf{t}}_R - \mathbf{T}_R \mathbf{n}_R) = \mathbf{0}$ on $\partial B_{\mathbf{t}_R}$ are satisfied, then clearly

$$\int_B (\text{Div } \mathbf{T}_R) \cdot \mathbf{u}_{\text{test}} dv_R + \int_{\partial B_{\mathbf{t}}} (\bar{\mathbf{t}}_R - \mathbf{T}_R \mathbf{n}_R) \cdot \mathbf{u}_{\text{test}} da_R = 0,\tag{2.1}$$

or equivalently

$$\int_B (\text{Div } \mathbf{T}_R) \cdot \mathbf{u}_{\text{test}} dv_R - \int_{\partial B_{\mathbf{t}}} \mathbf{T}_R \mathbf{n}_R \cdot \mathbf{u}_{\text{test}} da_R + \int_{\partial B_{\mathbf{t}}} \bar{\mathbf{t}}_R \cdot \mathbf{u}_{\text{test}} da_R = 0\tag{2.2}$$

holds for all admissible test functions \mathbf{u}_{test} . Thus, using $\mathbf{u}_{\text{test}} = \mathbf{0}$ on $\partial B_{\mathbf{u}}$ we may extend the first boundary integral in the equation above to the whole boundary ∂B , and we may rewrite this equation as

$$\int_{\partial B_{\mathbf{t}}} \bar{\mathbf{t}}_R \cdot \mathbf{u}_{\text{test}} da_R = \int_{\partial B} \mathbf{T}_R \mathbf{n}_R \cdot \mathbf{u}_{\text{test}} da_R - \int_B \text{Div } \mathbf{T}_R \cdot \mathbf{u}_{\text{test}} dv_R.\tag{2.3}$$

Next, by the divergence theorem

$$\int_{\partial B} \mathbf{T}_R \mathbf{n}_R \cdot \mathbf{u}_{\text{test}} da_R = \int_{\partial B} (\mathbf{T}_R^\top \mathbf{u}_{\text{test}}) \cdot \mathbf{n} da_R = \int_B \text{Div } \mathbf{T}_R \cdot \mathbf{u}_{\text{test}} dv_R + \int_B \mathbf{T}_R : \nabla \mathbf{u}_{\text{test}} dv_R,\tag{2.4}$$

use of which in (2.3) gives

$$\int_{\partial B_{\mathbf{t}}} \bar{\mathbf{t}}_R \cdot \mathbf{u}_{\text{test}} da_R = \int_B \mathbf{T}_R : \nabla \mathbf{u}_{\text{test}} dv_R.\tag{2.5}$$

¹We introduce a small numerical factor $\gamma = 3 \times 10^{-4}$ which prevents zero-valued diffusivity as $\phi \rightarrow 1$.

Hence, if the balance equation $\text{Div } \mathbf{T}_R = \mathbf{0}$ on B and the traction condition $(\bar{\mathbf{t}}_R - \mathbf{T}_R \mathbf{n}_R) = \mathbf{0}$ on $\partial B_{\mathbf{t}_R}$ are satisfied, then the weak form

$$\int_B \mathbf{T}_R : \nabla \mathbf{u}_{\text{test}} dv_R - \int_{\partial B_{\mathbf{t}}} \bar{\mathbf{t}}_R \cdot \mathbf{u}_{\text{test}} da_R = 0 \quad (2.6)$$

holds for all admissible test fields \mathbf{u}_{test} which vanish on $\partial B_{\mathbf{u}}$.

2. Mass balance problem:

Next, consider a scalar test field $\mu_{\text{test}}(\mathbf{X})$ on B which satisfies $\mu_{\text{test}}(\mathbf{X}) = 0$ on ∂B_μ . If the balance equation

$$\dot{c}_R + \text{Div } \mathbf{j}_R = 0 \quad \text{on } B,$$

and the boundary condition $\mathbf{j}_R \cdot \mathbf{n} = \bar{j}$ on $\partial B_{\mathbf{j}_R}$ are satisfied, then

$$\int_B \dot{c}_R \mu_{\text{test}} dv_R + \int_B (\text{Div } \mathbf{j}_R) \mu_{\text{test}} dv_R + \int_{\partial B_{\mathbf{j}}} (\bar{j} - \mathbf{j}_R \cdot \mathbf{n}) \mu_{\text{test}} da_R = 0, \quad (2.7)$$

or equivalently

$$\int_B \dot{c}_R \mu_{\text{test}} dv_R + \int_B (\text{Div } \mathbf{j}_R) \mu_{\text{test}} dv_R - \int_{\partial B_{\mathbf{j}}} \mathbf{j}_R \cdot \mathbf{n}_R \mu_{\text{test}} da_R + \int_{\partial B_{\mathbf{j}}} \bar{j} \mu_{\text{test}} da_R = 0 \quad (2.8)$$

holds for all test fields μ_{test} . Thus, since $\mu_{\text{test}} = 0$ on ∂B_μ the first boundary integral in expression above may be extended to all of ∂B ,

$$\int_B \dot{c}_R \mu_{\text{test}} dv_R + \int_B (\text{Div } \mathbf{j}_R) \mu_{\text{test}} dv_R - \int_{\partial B} \mathbf{j}_R \cdot \mathbf{n}_R \mu_{\text{test}} da_R + \int_{\partial B_{\mathbf{j}}} \bar{j} \mu_{\text{test}} da_R = 0 \quad (2.9)$$

Next, by the divergence theorem

$$\int_{\partial B} \mathbf{j}_R \cdot \mathbf{n}_R \mu_{\text{test}} da_R = \int_{\partial B} (\mu_{\text{test}} \mathbf{j}_R) \cdot \mathbf{n} da_R = \int_B \mu_{\text{test}} \text{Div } \mathbf{j}_R dv_R + \int_B \mathbf{j}_R \cdot \nabla \mu_{\text{test}} dv_R. \quad (2.10)$$

Use of (2.10) in (2.9) gives the weak form

$$\int_B \dot{c}_R \mu_{\text{test}} dv_R - \int_B \mathbf{j}_R \cdot \nabla \mu_{\text{test}} dv_R + \int_{\partial B_{\mathbf{j}}} \bar{j} \mu_{\text{test}} da_R = 0. \quad (2.11)$$

We use a first-order finite difference approximation to write

$$\dot{c}_R = \frac{c_R - c_{R \text{ old}}}{\Delta t}, \quad (2.12)$$

so that the weak form (2.11) may be expressed as

$$\int_B \frac{c_R - c_{R \text{ old}}}{\Delta t} \mu_{\text{test}} dv_R - \int_B \mathbf{j}_R \cdot \nabla \mu_{\text{test}} dv_R + \int_{\partial B_{\mathbf{j}}} \bar{j} \mu_{\text{test}} da_R = 0. \quad (2.13)$$

Summarizing, the weak forms of the governing equations for the coupled problem are

$$\boxed{\begin{aligned} \int_B \mathbf{T}_R : \nabla \mathbf{u}_{\text{test}} dv_R - \int_{\partial B_t} \bar{\mathbf{t}}_R \cdot \mathbf{u}_{\text{test}} da_R &= 0, \\ \int_B \frac{c_R - c_{R,\text{old}}}{\Delta t} \mu_{\text{test}} dv_R - \int_B \mathbf{j}_R \cdot \nabla \mu_{\text{test}} dv_R + \int_{\partial B_j} \bar{j} \mu_{\text{test}} da_R &= 0, \end{aligned}} \quad (2.14)$$

for all vector-valued test functions $\mathbf{u}_{\text{test}}(\mathbf{X})$ which vanish on ∂B_u and all scalar test functions $\mu_{\text{test}}(\mathbf{X})$ which vanish on ∂B_μ .

Remarks:

1. As phrased above, the basic degrees of freedom in the boundary value problem are the displacement field and the chemical potential,

$$\{\mathbf{u}, \mu\}.$$

However, as is clear from (2.14)₂, we also need knowledge of the species concentration c_R to obtain a solution. Given (\mathbf{u}, μ) the concentration c_R may be calculated from the expression for the chemical potential

$$\mu = R\vartheta \left(\ln \left(1 - \frac{1}{1 + \Omega c_R} \right) + \frac{1}{1 + \Omega c_R} + \frac{\chi}{(1 + \Omega c_R)^2} \right) - \Omega K \ln \left(\frac{J}{1 + \Omega c_R} \right), \quad (2.15)$$

which, with $J = J(\mathbf{u})$ and μ known, may be written as an implicit equation for c_R ,

$$\frac{\mu}{R\vartheta} - R\vartheta \left(\ln \left(1 - \frac{1}{1 + \Omega c_R} \right) + \frac{1}{1 + \Omega c_R} + \frac{\chi}{(1 + \Omega c_R)^2} \right) + \frac{\Omega K}{R\vartheta} \ln \left(\frac{J}{1 + \Omega c_R} \right) = 0 \quad (2.16)$$

On account of the inability of the FEniCS framework to solve nonlinear equations at the Gauss-point level, we consider solving equation (2.16) in a *weak sense* by introducing a test function c_{test} ,

$$\int_B \left[\frac{\mu}{R\vartheta} - R\vartheta \left(\ln \left(1 - \frac{1}{1 + \Omega c_R} \right) + \frac{1}{1 + \Omega c_R} + \frac{\chi}{(1 + \Omega c_R)^2} \right) + \frac{\Omega K}{R\vartheta} \ln \left(\frac{J}{1 + \Omega c_R} \right) \right] c_{\text{test}} dv_R = 0. \quad (2.17)$$

2. Summarizing, the complete set of weak forms of the coupled problem are

$$\begin{aligned} \int_B \mathbf{T}_R : \nabla \mathbf{u}_{\text{test}} dv_R - \int_{\partial B_t} \bar{\mathbf{t}}_R \cdot \mathbf{u}_{\text{test}} da_R &= 0, \\ \int_B \frac{c_R - c_{R,\text{old}}}{\Delta t} \mu_{\text{test}} dv_R - \int_B \mathbf{j}_R \cdot \nabla \mu_{\text{test}} dv_R + \int_{\partial B_j} \bar{j} \mu_{\text{test}} da_R &= 0, \\ \int_B \left[\frac{\mu}{R\vartheta} - \left(\ln \left(1 - \frac{1}{1 + \Omega c_R} \right) + \frac{1}{1 + \Omega c_R} + \frac{\chi}{(1 + \Omega c_R)^2} \right) + \frac{\Omega K}{R\vartheta} \ln \left(\frac{J}{1 + \Omega c_R} \right) \right] c_{\text{test}} dv_R &= 0. \end{aligned} \quad (2.18)$$

3 Normalization

Since we plan to solve all the governing equations related to multiple physical fields simultaneously, it is beneficial to rewrite the three residuals so that they have approximately the same magnitudes, and to use degrees of freedom which take on values on the order of unity. To this end:

1. The species concentration c_{R} mol/m³ is normalized by the molar volume Ω [m³/mol] as

$$\hat{c} \stackrel{\text{def}}{=} \Omega c_{\text{R}}. \quad (3.1)$$

2. The chemical potential μ [J/mol] is normalized by $R\vartheta$ [J/mol],

$$\hat{\mu} = \frac{\mu}{R\vartheta}. \quad (3.2)$$

3. Recall the mass balance equation:

$$\dot{c}_{\text{R}} + \text{Div} \mathbf{j}_{\text{R}} = 0.$$

This may be written as,

$$\frac{1}{\Omega} \dot{\hat{c}} + \text{Div} \mathbf{j}_{\text{R}} = 0.$$

4. Next, the species flux \mathbf{j}_{R} is given by the constitutive equation,

$$\mathbf{j}_{\text{R}} = -\mathbf{M} \nabla \mu \quad \text{with} \quad \mathbf{M} = \mathbf{C}^{-1} \left(\frac{D c_{\text{R}}}{R\vartheta} \right). \quad (3.3)$$

Using the normalized variables $\hat{\mu}$ and \hat{c} we may rewrite it as follows:

$$\mathbf{j}_{\text{R}} = -\mathbf{M} \nabla \hat{\mu} \times R\vartheta \quad \text{with} \quad \mathbf{M} = \mathbf{C}^{-1} \left(\frac{D \hat{c}}{\Omega R\vartheta} \right), \quad (3.4)$$

where D is given by

$$D = D_0 \exp \left(-\alpha \frac{\phi}{1 - \phi} \right) + \gamma, \quad \text{with} \quad \phi = \frac{1}{1 + \hat{c}}. \quad (3.5)$$

5. Finally we choose to normalize the stress with the shear modulus G :

$$\hat{\mathbf{T}}_{\text{R}} \stackrel{\text{def}}{=} \frac{\mathbf{T}_{\text{R}}}{G} = (\mathbf{F} - \mathbf{F}^{-\top}) + (1 + \hat{c}) \frac{K}{G} \ln \left(\frac{J}{1 + \hat{c}} \right) \mathbf{F}^{-\top}. \quad (3.6)$$

6. Summarizing the normalized governing equations may then be expressed as

$$\begin{aligned} \text{Div} \hat{\mathbf{T}}_{\text{R}} &= 0 \\ \dot{\hat{c}} \Omega^{-1} + \text{Div} \mathbf{j}_{\text{R}} &= 0. \end{aligned} \quad (3.7)$$

With the normalizations introduced above and the normalized parameters denoted by $\{\bullet\}$, the weak forms of the coupled problem may be written as

$$\begin{aligned} \int_{\text{B}} \hat{\mathbf{T}}_{\text{R}} : \nabla \mathbf{u}_{\text{test}} dv_{\text{R}} - \int_{\partial \text{B}_{\text{t}}} \bar{\mathbf{t}}_{\text{R}} \cdot \mathbf{u}_{\text{test}} da_{\text{R}} &= 0, \\ \int_{\text{B}} \frac{\hat{c} - \hat{c}_{\text{old}}}{\Delta t} \hat{\mu}_{\text{test}} dv_{\text{R}} - \int_{\text{B}} \Omega \mathbf{j}_{\text{R}} \cdot \nabla \hat{\mu}_{\text{test}} dv_{\text{R}} + \int_{\partial \text{B}_{\text{j}}} \Omega \bar{j} \hat{\mu}_{\text{test}} da_{\text{R}} &= 0, \\ \int_{\text{B}} \left[\hat{\mu} - \left(\ln \left(1 - \frac{1}{1 + \hat{c}} \right) + \frac{1}{1 + \hat{c}} + \frac{\chi}{(1 + \hat{c})^2} \right) + \frac{\Omega K}{R\vartheta} \ln \left(\frac{J}{1 + \hat{c}} \right) \right] \hat{c}_{\text{test}} &= 0. \end{aligned} \quad (3.8)$$

Remark. Note that in writing the weak form of the mass balance above we have multiplied through by Ω , which we found helps keep the residuals on a similar order of magnitude and aids numerical convergence.

4 Solution procedure in the FEniCS code

In brief, in FEniCS, we use the following degrees of freedom

$$\{\mathbf{u}, \hat{\mu}, \hat{c}\}, \quad (4.1)$$

as well as their known values from the previous step

$$\{\mathbf{u}_{\text{old}}, \hat{\mu}_{\text{old}}, \hat{c}_{\text{old}}\}, \quad (4.2)$$

to calculate the *residuals* which correspond to the weak forms of the governing equations, viz.

$$\begin{aligned} R_{\mathbf{u}} &= \int_{\mathbf{B}} \hat{\mathbf{T}}_{\mathbf{R}} : \nabla \mathbf{u}_{\text{test}} \, dv_{\mathbf{R}} - \int_{\partial \mathbf{B}_{\mathbf{t}}} \bar{\mathbf{t}}_{\mathbf{R}} \cdot \mathbf{u}_{\text{test}} \, da_{\mathbf{R}}, \\ R_{\hat{\mu}} &= \int_{\mathbf{B}} \left(\frac{\hat{c} - \hat{c}_{\text{old}}}{\Delta t} \right) \hat{\mu}_{\text{test}} \, dv_{\mathbf{R}} - \int_{\mathbf{B}} \Omega \mathbf{j}_{\mathbf{R}} \cdot \nabla \hat{\mu}_{\text{test}} \, dv_{\mathbf{R}} + \int_{\partial \mathbf{B}_{\mathbf{j}}} \Omega \bar{j} \hat{\mu}_{\text{test}} \, da_{\mathbf{R}}, \\ R_{\hat{c}} &= \int_{\mathbf{B}} \left[\hat{\mu} - \left(\ln \left(1 - \frac{1}{1 + \hat{c}} \right) + \frac{1}{1 + \hat{c}} + \frac{\chi}{(1 + \hat{c})^2} \right) + \frac{\Omega K}{R\vartheta} \ln \left(\frac{\hat{J}}{1 + \hat{c}} \right) \right] \hat{c}_{\text{test}} \, da_{\mathbf{R}}. \end{aligned} \quad (4.3)$$

FEniCS then automatically differentiates these residuals with respect to the separate degrees of freedom to obtain *tangents*. At each step in time, FEniCS uses the residuals and tangents in a global Newton-Raphson solver to determine current values of the degrees of freedom $\{\mathbf{u}, \hat{\mu}, \hat{c}\}$ for which the residuals are zero,² and which therefore satisfy the governing equations as well as the initial and boundary conditions (in a weak sense).

Remark. A mixed finite element method is utilized to solve for the displacement \mathbf{u} , chemical potential $\hat{\mu}$, and the concentration field \hat{c} , concurrently. To avoid numerical instabilities the basis functions for the displacement are taken as Lagrange quadratic, while those of the chemical potential are one-order lower, Lagrange linear. The field \hat{c} is also interpolated as a linear Lagrange field.

²To within some small numerical tolerance.

4.1 Algorithm for calculation of the residuals

The algorithm we follow in our code to calculate the residuals in (4.3) is summarized below.

1. Begin the step with known values of

$$\{\mathbf{u}_{\text{old}}, \hat{\mu}_{\text{old}}, \hat{c}_{\text{old}}\}, \quad (4.4)$$

where for the first step these quantities are given by the initial conditions for \mathbf{u} , $\hat{\mu}$ and \hat{c}_0 .

2. Calculate necessary kinematical quantities for the current step as,

$$\begin{aligned} \mathbf{F} &= \mathbf{1} + \nabla \mathbf{u}, \\ J &= \det \mathbf{F}, \\ \mathbf{C}^{-1} &= (\mathbf{F}^\top \mathbf{F})^{-1}. \end{aligned} \quad (4.5)$$

3. Calculate J^e ,

$$J^e = \frac{J}{1 + \hat{c}}. \quad (4.6)$$

4. Calculate the Piola stress,

$$\hat{\mathbf{T}}_{\mathbf{R}} = (\mathbf{F} - \mathbf{F}^{-\top}) + (1 + \hat{c}) \frac{K}{G} \ln(J^e) \mathbf{F}^{-\top}, \quad (4.7)$$

and associated pressure for the pressure-dependence of χ ,

$$p = -\frac{1}{3} \operatorname{tr} \left(G J^{-1} \hat{\mathbf{T}}_{\mathbf{R}} \mathbf{F}^\top \right). \quad (4.8)$$

5. Calculate the species flux,

$$\mathbf{j}_{\mathbf{R}} = -\mathbf{M} \nabla \hat{\mu} \times R \vartheta \quad \text{with} \quad \mathbf{M} = \mathbf{C}^{-1} \left(\frac{D \hat{c}}{\Omega R \vartheta} \right), \quad (4.9)$$

where D is given by

$$D = D_0 \exp \left(-\alpha \frac{\phi}{1 - \phi} \right) + \gamma, \quad \text{with} \quad \phi = \frac{1}{1 + \hat{c}}. \quad (4.10)$$

6. Use the quantities from steps 1-5 to compute the residuals as

$$\begin{aligned} R_{\mathbf{u}} &= \int_{\mathbf{B}} \hat{\mathbf{T}}_{\mathbf{R}} : \nabla \mathbf{u}_{\text{test}} dv_{\mathbf{R}} - \int_{\partial \mathbf{B}_{\mathbf{t}}} \bar{\mathbf{t}}_{\mathbf{R}} \cdot \mathbf{u}_{\text{test}} da_{\mathbf{R}}, \\ R_{\hat{\mu}} &= \int_{\mathbf{B}} \left(\frac{\hat{c} - \hat{c}_{\text{old}}}{\Delta t} \right) \hat{\mu}_{\text{test}} dv_{\mathbf{R}} - \int_{\mathbf{B}} \Omega \mathbf{j}_{\mathbf{R}} \cdot \nabla \hat{\mu}_{\text{test}} dv_{\mathbf{R}} + \int_{\partial \mathbf{B}_{\mathbf{j}}} \Omega \bar{j} \hat{\mu}_{\text{test}} da_{\mathbf{R}}, \\ R_{\hat{c}} &= \int_{\mathbf{B}} \left[\hat{\mu} - \left(\ln \left(1 - \frac{1}{1 + \hat{c}} \right) + \frac{1}{1 + \hat{c}} + \frac{\chi}{(1 + \hat{c})^2} \right) + \frac{\Omega K}{R \vartheta} \ln \left(\frac{\hat{j}}{1 + \hat{c}} \right) \right] \hat{c}_{\text{test}} da_{\mathbf{R}}, \end{aligned} \quad (4.11)$$

7. FEniCS solves for the current values of $\{\mathbf{u}, \hat{\mu}, \hat{c}\}$.

8. Set these current values as the “old” values for the next step in time,

$$\{\mathbf{u}, \hat{\mu}, \hat{c}\} \implies \{\mathbf{u}_{\text{old}}, \hat{\mu}_{\text{old}}, \hat{c}_{\text{old}}\}. \quad (4.12)$$

9. Repeat steps 1-8 for desired number of steps in time.

5 Unit system and material parameters

Our numerical implementation uses the SI (mm) unit system listed below. For reference, we also include quantities in the more standard SI (m) unit system.

Quantity	SI (m)	SI (mm)
Length	m	mm
Mass	kg	tonne (10^3 kg)
Time	s	s
Force	N	N
Energy	J	mJ (10^{-3} J)
Mass Density	kg/m ³	tonne/mm ³
Amount of substance	mol	mol
c_R , species concentration	mol/m ³	mol/mm ³
μ , Chemical potential	J/mol	mJ/mol
G and K , Stress	Pa	MPa (N/mm ²)
Ω , molar volume	m ³ /mol	mm ³ /mol
D species Diffusivity	m ² /s	mm ² /s
Gas Constant R	8.3145 J/(mol K)	8.3145×10^3 mJ/(mol K)
Temperature	K	K

The values of the material parameters used for modeling the PEG-DA hydrogel are listed below in both the SI(m) and SI(mm) unit systems.

Quantity	Value SI (m)	Value SI (mm)
G Shear modulus	1×10^6 Pa	1 MPa
K , Bulk modulus	1×10^8 Pa	100 MPa
Ω , Molar volume of water	1.8×10^{-5} m ³ /mol	1.8×10^4 mm ³ /mol
D_0 , Solvent diffusivity when $\phi = 0$	2.0×10^{-6} m ² /s	2 mm ² /s
α , Yasuda form shape parameter	7.7	7.7
χ_0 , Zero-pressure Flory-Huggins parameter	0.52	0.52
β , Flory-Huggins pressure-dependence parameter	1.9×10^{-7} Pa ⁻¹	1.9×10^{-1} MPa ⁻¹
ϕ_0 , Initial polymer volume fraction	0.999	0.999
Gas Constant R	8.3145 J/(mol K)	8.3145×10^3 mJ/(mol K)
Temperature ϑ	298 K	298 K

References

E. M. Stewart, S. Narayan, and L. Anand. On modeling the infiltration of water in a PEG-DA hydrogel and the resulting swelling under unconstrained and mechanically-constrained conditions. *Extreme Mechanics Letters*, 54:101775, July 2022.