Diffusion-induced instabilities in soft solid sheets

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part I: de-hydration induced instabilities

Figure 1:
Water evaporates both from walls and cavity

Water

Air

Water

Water evaporates both from walls and cavity

Standard buckling

De-hydration buckling

\[ p_i = 0 \]

\[ p_e = 0 \]

\[ V_c = \bar{V}_c \]

\[ V_c^{\text{free}} \]
standard vs de-hydration buckling

**standard instability**

- $p_i = 0$
- $V_c$ free
- $p_e \neq 0$

**de-hydration instability**

- $p_i \neq 0$
- $V_c = \bar{V}_c$
- $p_e = 0$

Water evaporates both from walls and cavity.

Figure 1:

- **a)**
- **b)**

**balance equations**

\[
\text{div} \mathbf{S}_d = 0 \quad \mathbf{S}_d = \dot{\mathbf{S}}_d - p \mathbf{F}^*_d
\]

in \( \mathcal{B}_d \)

\[
\dot{c} = -\text{div} \mathbf{h}_d \quad \mathbf{h}_d = M \nabla (\hat{\mu} + \Omega p)
\]

The constitutive eqns for stress and chemical potential come from Flory-Rehner thermodynamics.

**local VC**

**incompressibility effect**

\[
dV_d = J_d dV_d = dV_d + \Omega \ c_d \ dV_d
\]

\[
J_d := \det \mathbf{F}_d = \det (\mathbf{I} + \nabla \mathbf{u}_d) = 1 + \Omega c_d =: \hat{J}_d(c_d)
\]
The evolution problem rewrites as follows: solve for constraint (volume formula): 

\[ \mu_i = \Omega p_i(t) \quad \text{and} \quad p_i = p_i(t) \]

The following balance equations on the boundary flux and \( \nabla \) \( \mu \):

\[ v_w(t) = v_{wo} - v^i_w(t) \]

\[ v_{wo} = v_{co} = v_c(0) = \frac{1}{3} \int_{\partial C_d} (X_d + u_o) \cdot \mathbf{F}^* d \mathbf{m} dA_d \]

\[ v^i_w(t) = \int_{\partial C_d} q_s dA_d = - \int_{\partial C_d} \mathbf{h}_d \cdot \mathbf{m} dA_d, \quad v^i_w(0) = 0 \]

\[ v_c(t) = \int_{C_t} dv = \frac{1}{3} \int_{\partial C_t} x \cdot \mathbf{n} dA = \frac{1}{3} \int_{\partial C_d} (X_d + u_d) \cdot \mathbf{F}^* d \mathbf{m} dA_d \]

**Boundary conditions**

\( \mathbf{S}_d \mathbf{m} = \mathbf{t} \quad \text{and} \quad \mu = \mu_e \)

**Boundary pressure**

chemical potential of the environment

**Chemical potential of the environment**

\( \mu_e = \mu_w \)

\( \mu_i = \mu_w \)

\( p_i = p_{atm} \simeq 0 \)

\( p_e = p_{atm} \simeq 0 \)

Water evaporation both from walls and cavity
a first glance at mechanical instabilities
a first glance at mechanical instabilities/2
**purely mechanical model based on 3D Wesolowski model for the spherical shell (Arch.Mech.Stosow.19(1), 1967)**

- liquid diffusion is frozen at the onset of instability (red circle) which occurs instantaneously with respect to the diffusion time
- deformations are purely radial

\[
\begin{align*}
    r &= r(R), \quad \theta = \Theta, \quad \phi = \Phi \quad \text{and} \quad r^2 r' = J_o R^2 \\
    r_c &= \left(\frac{3v_c}{4\pi}\right)^{1/3}
\end{align*}
\]
the 0-chemo-mechanical solution

bulk equations

\[ J_0 = 1 + \Omega c_0 \]
\[ r^2 r' = R^2 J_0 \]
\[ \text{div } S_0 = 0 \]
\[ \text{div } h_0 = 0 \]
\[ p_0' R + 2 G_d Q_0 (-1 + J_0 Q_0^3)^2 - G_d Q_0^4 J_0' R = 0 \]
\[ Q_0(R) = R/r(R) \]

boundary conditions

\[ S_{0RR}(R_d) = 0 \]
\[ \mu(R_d) = \mu_e \]
\[ \mu(R_c) + \Omega Q_0^2(R_c) S_{0RR}(R_c) = 0 \]

\[ \beta := \frac{v_c}{v_{co}} \]

Where the external chemical potential suddenly drops to its plateau value and the pressure rises at nearly constant cavity volume the static solution cannot reproduce the numerical values.
the incremental chemo-mechanical problem

div \textbf{S}_1 = 0 \quad \text{with} \quad \textbf{S}_1 = -J_0 p_1 \mathbf{F}_0^{-T} - J_1 p_0 \mathbf{F}_0^{-T} + J_0 p_0 \mathbf{F}_0^{-T} \mathbf{F}_1 \mathbf{F}_0^{-T} + G_d \mathbf{F}_1

div \textbf{h}_1 = 0 \quad \text{with} \quad \textbf{h}_1 = -M_0 \nabla \mu_1 - M_1 \nabla \mu_0

* the analysis of the global volume constraint shows that to first order the perturbation of the cavity volume vanishes for any incremental displacement field and the pressure fields of the enclosed liquid remains unchanged up to the first order
The system of ODEs which put together both the zeroth external potential: the first to find the critical value of ordinary differential equations. As described in § since the spherical configuration becomes unstable.

We recall that the ratio between the actual and the swollen volume enclosed by the spherical shell, (c) Critical volumes and bifurcation modes

In so doing, the system of six first-order linear equations (4.23) is complemented with the six first-order equations (4.26) which are the same used in the numerical variation through terms of the type (4.30). However, it can be proved that the perturbation of volume is determined by the variation through terms of the type (4.31) up to a multiplicative constant. To remove this indeterminacy, we consider higher order terms in the expansion.

The substitution of (4.32), (4.33) shows that to first order the perturbation of volume correction is completely unchanged up the first order and, hence, it must be that is, the cavity volume, is measured by the parameter (c).

The cavity volume perturbation due to the displacement field (2) at (1) we have the system of linear equations (2) with (2) as a new unknown variable, where (2) can be replaced by the two conditions (2)

Figure 31: Critical modes and critical profile mode corresponding to the solution of the first order incremental problem

\[ d \frac{\partial}{\partial r} \left( \frac{1}{\rho} \frac{\partial p}{\partial r} \right) + \frac{\partial}{\partial r} \left( \frac{1}{\rho} \frac{\partial p}{\partial r} \right) = 0 \]

\[ \rho \frac{\partial^2 u}{\partial r^2} + \frac{\partial^2 u}{\partial \theta^2} + \frac{1}{\rho} \frac{\partial p}{\partial r} = 0 \]

\[ \rho \frac{\partial^2 v}{\partial r^2} + \frac{\partial^2 v}{\partial \theta^2} + \frac{1}{\rho} \frac{\partial p}{\partial r} = 0 \]

\[ \rho \frac{\partial^2 \theta}{\partial r^2} + \frac{\partial^2 \theta}{\partial \theta^2} = 0 \]

\[ \rho \frac{\partial^2 \phi}{\partial r^2} + \frac{\partial^2 \phi}{\partial \theta^2} = 0 \]

\[ \rho \frac{\partial^2 \psi}{\partial r^2} + \frac{\partial^2 \psi}{\partial \theta^2} = 0 \]
the change of de-hydration across the thickness of the shell delivers a spontaneous curvature and a frustration which may be caught by 2D shell models

occurrence of cavitation instability is also interesting (and here is not considered, by assuming that adhesion energy density is infinite)

part II: the bar mechanism

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(under the supervision of D.P. Holmes)
In this Section we derive the equilibrium equations and the boundary conditions. We regard the bar as a stretchable and flexible rod belonging to the $(x, y)$-plane. This is represented by a parametric curve $\mathbf{r}(s)$, where $s$ denotes the arc-length and the referential arc-length. We denote with $\mathbf{e}_x, \mathbf{e}_y$ the unit vectors along, respectively, the $x$ and $y$-axes. We parametrize the tangent and the normal by $\mathbf{e}_x(s)$ and $\mathbf{e}_y(s)$ respectively, the $\mathbf{e}_x$-axis being $\mathbf{e}_x(s)$ and $\mathbf{e}_y(s)$ being the $\mathbf{e}_x$ and $\mathbf{e}_y$-axes.

In the plane of the curve, we introduce a Cartesian frame of reference $\{O, \mathbf{e}_x, \mathbf{e}_y\}$, with $O$ as the origin and $\mathbf{e}_x$ as the $x$-axis. This frame moves with the curve and is always orthogonal to $\mathbf{e}_y(s)$. The origin of the frame corresponds to the detachment point of the bar. The point $P(s)$ is the end of the bar when $s=S$.

The 3 phases of the bar mechanism:

1. **Compression phase**: The bar is stretched, with no curvatures. The end of the bar is fixed, and the force $F$ is applied.

2. **Buckling phase**: The bar buckles, and the force $F$ is applied. The bar maintains its shape and no new forces are applied.

3. **Catapult phase**: The bar is released, and the force $F$ is applied. The bar stretches and buckles, and the force $F$ is applied.

Investigations on Michael’s catapult
p, ud (\cos u = \frac{1}{\sqrt{2}}) = \frac{1}{2} (\cos 0 = 1), \quad \frac{1}{2} (\cos \pi = -1) +\quad \frac{1}{2} \quad \frac{1}{2}

\text{Investigations on Michael's catapult}

\frac{1}{2}

\begin{align*}
\mathcal{W}_f &= \int_0^{\bar{S}} \kappa (\theta' - c_o)^2 \, dS \\
\mathcal{W}_a &= \int_{\bar{S}}^{L/2} (\kappa c_o^2 - 2w) \, dS
\end{align*}

l_{ec} := \sqrt{\frac{\kappa}{w}}

\text{energy of the buckled region}

\text{energy of the adhered region}

\begin{align*}
\theta(0) &= 0 \quad \text{even symmetry} \\
\theta(\bar{S}) &= 0 \quad \text{continuity} \\
\kappa [\theta'(\bar{S})]^2 &= 2w \quad \text{transversality condition} \\
a &= \int_0^{\bar{S}} \cos \theta \, dS + \frac{L}{2} - \bar{S} \quad \text{global constraint}
\end{align*}

\[ W_{\text{buck}} = \frac{2\kappa}{l_{\text{ec}}^2} \left[ 2\bar{x} - a \left(2 + \frac{\epsilon}{1 - \cos \theta_0}\right)\right] + 2ac_0^2\kappa (1 + \epsilon) \]

\[ \frac{W}{\kappa/a} = 2\frac{2a^2}{l_{\text{ec}}^2} \left[(l_{\text{ec}}c_0)^2(1 + \epsilon) - \frac{\epsilon}{1 - \cos \theta_0}\right] \quad \text{VS} \quad W_{\text{co}} = 0 \]

- the pattern is not monotonic with \( l_{\text{ec}} \);
- to each value of \( l_{\text{ec}} \), it corresponds a value of \( c_0 \) which makes the catapult realizable;
- for \( c_0 = 0 \), we can't have the catapult mechanism as \( W \) never goes beyond the 0 energy level

work in progress: relate the change of de-hydration across the thickness of the beam to the spontaneous curvature, analyse the buckled problem and the role of the key parameters, study possible different catapult mechanisms
Research project:
Microencapsulation based on intelligent actively-remodeling bio polymer gels for controlled drug release
a joint project with Anne Bernheim Ben Gurion University at the Negev (Israel)

Research project:
Mathematics of active materials: from mechanobiology to smart devices