SUPPORTING MATERIAL

Mechanochemical Symmetry Breaking in *Hydra* Aggregates

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PARAMETERS AND INITIAL CONDITIONS

In the following, we show the detailed parameter values we have used for presented simulations.

OMC model: Due to the reduced complexness of the used model (e.g., curved 2D surfaces instead of real 3D bodies) a direct parametrization by experimentally determined parameters was not possible. Instead, model parameters have been chosen such that simulated space and time scales fit to the experimental results, guided by the behavior of an aggregate of "ideal size". Especially, parametrization has been chosen such that symmetry breaking occurs after five oscillations where $t_{SB} = 21.4\,h$ is minimal for a size of $r = 138\,\mu m$ (1). By setting $v_{phys} = \epsilon_v\, v_{abs}$, we transformed temporal ($v = t$) and spatial ($v = \vec{X}$) abstract dimensionless quantities v_{abs} by a characteristic unit of measure ϵ_v into a physical reasonable variable v_{phys}. Concretely, we used $\epsilon_t = 173.97\,h$ for temporal and $\epsilon_X = 138\,\mu m$ for spacial scales. Most other variables we have kept dimensionless; especially we have used (as not otherwise stated): $\Delta C_{eff} = 30$, $\alpha = 1$, $\kappa_1 = 100$, $\lambda = 300$, $\xi = 500$, $\kappa_3 = 1$, $\beta = (1.25)^2$, $t_{heal} - t_{rupt} = 5\,min$, $L = 1$, $D_A = 27.5$, $C_A = 174$, $\tilde{D}_B = 5250$ and $C_B = 350$. As initial morphogen distribution we have always set Φ_A and Φ_B stochastically and uniformly distributed in the interval $[1.0, 1.1]$.

Turing model: We use $c_1(r_0) = 0.0004362997 r_0 - 0.0209382395$ and $u_{threshold} = e$. For every fit, we generated randomly an initial guess fulfilling the Turing conditions and use them for MATLABs built-in function `fmincon`. We assume that $D_u < D_v (< D_w)$ and use the transformation $\tilde{t} = D_u t$ to reduce the parameter space.

Curvature-increasing model: Based on the model presented in Mercker et al. (2), we have always used the parameters $L_X = 1.0$, $\kappa = 0.01$, $\gamma = 0.4$, $\delta = 1.0$ and $\beta = 1.0$, where ζ (respectively $\tilde{\zeta}$) and system size have been varied. For all simulations of this model we assumed as the initial tissue geometry a sphere as well as a stochastic distribution for the morphogen concentration Φ, uniformly distributed in the interval $[0, 0.05]$.

SOC model: In accordance with the model of Gamba et al. (3) we have used an average conservation level of $C = 0.95$. Furthermore, we have considered the $\nu \to 0$ limit as described by Jensen (4). All SOC simulations were started with an always newly generated stochastic distribution for the *Ks1*-promoting factor, uniformly distributed below the threshold value.

FITTING PARAMETERS

Here, we present parameters for analytical fitting curves used within different figures in the main manuscript.
Fig. 2E: grey solid line: $-0.234\,\Delta C_{eff} + 0.015$.
Fig. 2 F: grey solid line: $10.323\,(\tanh(0.0117\,r_0 - 1.680) + 0.747)$.
Fig. 4 C: grey dashed line: $64.646/(2.551\,s^{0.3} - 1)$.
Fig. 4 C: grey solid line: $20. + 34.285/(2s)$.
Fig. 4 E: grey solid line: linearly interpolated values as a guide to the eye.
Fig. 5 A-C: black solid line: experimental data given by $21.4+152.3(r_0/138-1)^2$ (taken from Soriano et al. (1)).
Fig. 5 A: Diffusion coefficients $D_u = 2724, D_v = 4723677$, entries of the Jacobian $f_u = 0.931, f_v = 1, g_u = -2f_u g_v, g_v = -158.276$.
Fig. 5 B: For simulation data we have used $\zeta = 8.0$ with temporal scaling $1.3\,t_c = t\,h$ and spacial scaling $189\,r_c = r\,\mu m$ (where v_c are the abstract dimensionless variables used within the model).
Fig. 5 C: For simulation data we have used the temporal scaling $(1/57)\,z = t\,h$, where z is the number of cascades.

CALCULUS OF VARIATIONS

To obtain the detailed dynamic tissue surface equations (eq. 7, main manuscript), we need to calculate normal variations (i.e., with respect to $\vec{X}\cdot\vec{n}$), in the following in the strong formulation denoted by $\frac{\delta^\perp}{\delta\vec{X}}\mathcal{F}[...]$, in the weak formulation by $\delta^\perp[...]$. For technical details and further definitions concerning this approach, we refer to Mercker et al. (5). Since variations of $\mathcal{F}_{bend}$ can be already found in Mercker et al. (5), here, we restrict our calculations to normal variations of $\mathcal{F}_{osm}$ and $\mathcal{F}_{comp}$, respectively.
Lemma 1: It holds:

$$\frac{\delta^\perp}{\delta\vec{X}}\big[\mathcal{F}_{osm}\big] = \kappa_1\Big(\int_\Omega d\vec{V} - V(t)\Big).$$

Proof: Using the product rule as well as $\frac{\delta^\perp}{\delta\vec{X}}[c\int_\Omega d\vec{V}] = c$ for any constant c (6, 7) yields

$$\frac{\delta^\perp}{\delta\vec{X}}\big[\mathcal{F}_{osm}\big] = \kappa_1\Big(\int_\Omega d\vec{V} - V(t)\Big)\frac{\delta^\perp}{\delta\vec{X}}\Big[\int_\Omega d\vec{V}\Big] = \kappa_1\Big(\int_\Omega d\vec{V} - V(t)\Big). \quad \square$$

Lemma 2: It holds:

$$\frac{\delta^{\perp}}{\delta \vec{X}}[\mathcal{F}_{comp}] = \sqrt{g} H \kappa_2 (\sqrt{g} - \sqrt{g_0})/\sqrt{g_0}.$$

Proof: Using the product rule as well as $\delta^{\perp}[\sqrt{g}] = H\sqrt{g}\psi$ with test function ψ (7) yields

$$\delta^{\perp}[\mathcal{F}_{comp}] = \int_{S^2} \kappa_2 (\sqrt{g} - \sqrt{g_0})/\sqrt{g_0}\, \delta^{\perp}[\sqrt{g}]\, d\vec{s}. \quad \Box$$

TURING CONDITIONS

Here, we describe the conditions for the entries of 2×2 and 3×3 matrices leading to diffusion-driven instability. We denote the eigenvalues of the Laplacien by $\mu_\ell(r_0) = \ell(\ell+1)/r_0^2$.

The matrix $J = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}$ has eigenvalues with negative real parts iff $\operatorname{tr} J < 0$ and $\det J > 0$. The matrix $J_\ell(r_0)$ may have positive eigenvalues if $f_u > 0$ or $g_v > 0$ holds. For suitable diffusion coefficients this leads for a certain range of r_0 to

$$\det J_\ell^2(r_0) = \det J - (f_u D_v + g_v D_u)\mu_\ell(r_0) + D_u D_v \mu_\ell^2(r_0) < 0.$$

For the 3×3 matrix $J = \begin{pmatrix} f_u & f_v & f_w \\ g_u & g_v & g_w \\ h_u & h_v & h_w \end{pmatrix}$, we define

$$\Sigma J := \det\begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} + \det\begin{pmatrix} f_u & f_w \\ h_u & h_w \end{pmatrix} + \det\begin{pmatrix} g_v & g_w \\ h_v & h_w \end{pmatrix}.$$

J has eigenvalues with negative real parts, if and only if it holds (8)

$$\operatorname{tr} J < 0, \det J < 0 \quad \text{and} \quad \operatorname{tr} J \cdot \Sigma J - \det J < 0.$$

$J_\ell(r_0)$ may have eigenvalues with positive real parts if at least one of the conditions

$$f_u < 0, g_v < 0, h_w < 0, \det\begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} > 0, \det\begin{pmatrix} f_u & f_w \\ h_u & h_w \end{pmatrix} > 0 \text{ and } \det\begin{pmatrix} g_v & g_w \\ h_v & h_w \end{pmatrix} > 0$$

is violated. For suitable choices of the diffusion coefficients this leads for a certain range of r_0 to

$$\begin{aligned} \det J_\ell(r_0) = {} & \det J - \mu_\ell(r_0)\left(D_u \det\begin{pmatrix} g_v & g_w \\ h_v & h_w \end{pmatrix} + D_v \det\begin{pmatrix} f_u & f_w \\ h_u & h_w \end{pmatrix} + D_w \det\begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}\right) \\ & + \mu_\ell^2(r_0)\left(f_u D_v D_w + g_v D_u D_w + h_w D_u D_v\right) - \mu_\ell^3(r_0) D_u D_v D_w > 0 \end{aligned}$$

or to

$$
\begin{aligned}
&\operatorname{tr} J_\ell(r_0) \cdot \Sigma J_\ell(r_0) - \det J_\ell(r_0) = (\operatorname{tr} J \cdot \Sigma J - \det J) \\
&- \mu_\ell(r_0)\Big((D_u{+}D_v)\det\begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} + (D_u{+}D_w)\det\begin{pmatrix} f_u & f_w \\ h_u & h_w \end{pmatrix} \\
&\qquad + (D_v{+}D_w)\det\begin{pmatrix} g_v & g_w \\ h_v & h_w \end{pmatrix} \\
&\qquad + (f_u + g_v + h_w)\big(f_u(D_v + D_w) + g_v(D_u + D_w) + h_w(D_u + D_v)\big)\Big) \\
&+ \mu_\ell^2(r_0)\Big(2(f_u{+}g_v{+}h_w)(D_uD_v{+}D_uD_w{+}D_vD_w) \\
&\qquad + f_u(D_v^2{+}D_w^2){+}g_v(D_u^2{+}D_w^2){+}h_w(D_u^2{+}D_v^2)\Big) \\
&- \mu_\ell^3(r_0)\Big(D_u^2(D_v{+}D_w){+}D_v^2(D_u{+}D_w){+}D_w^2(D_u{+}D_v){+}2D_uD_vD_w\Big) > 0.
\end{aligned}
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Supporting References

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