HMR–CHEM–4 — Prebiotic Networks and the Thermodynamic Threshold of Life: A ChronoChemical Solution (High-Fidelity Models)

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Symbol for the body of work: HMR

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Abstract. We elevate prebiotic models to high-fidelity chemical physics: reactive transport in hydrothermal gradients (advection–diffusion–reaction with Poisson–Nernst–Planck electrochemistry), mineral surface templating (heterogeneous kinetics with curvature-weighted coherence), and amphiphilic vesicles (Helfrich membrane mechanics, permeability, and growth–division kinematics). Building on the ChronoChemistry ledger $C[\rho, \mathbf{R}] - D[\rho, \mathbf{R}]$ and network action $\mathcal{A}$, we derive explicit, dimensionless *threshold inequalities* (in Peclet, Damkohler, and membrane numbers) for the onset of persistent cycles (molecular memory) and self-maintenance (proto-metabolism). Bounded diagrams depict flux landscapes, templated surfaces, vesicle morphodynamics, and gradient-driven circulation. The result is a quantitative *thermodynamic threshold of life* connecting field-resolvable parameters to cycle persistence and division.

Keywords: ChronoChemistry, reactive transport, Poisson–Nernst–Planck, templating, Helfrich membrane, vesicles, Damkohler, Peclet, large deviation, proto-metabolism.
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1. Introduction

HMR–CHEM–2 established bonding and resonance as stationarity of a coherence action; *HMR–CHEM–3* lifted the action to reaction networks. Here we model three prebiotic engines at *high fidelity*: (i) hydrothermal porous media with reactive transport and electrochemistry; (ii) mineral templating with heterogeneous kinetics and curvature-coupled coherence; (iii) amphiphilic vesicles governed by Helfrich elasticity with permeability and growth. We quantify *thresholds* where cycle affinity outcompetes dissipation and compartments persist long enough to couple cycles—i.e., the thermodynamic boundary where chemistry becomes metabolism.

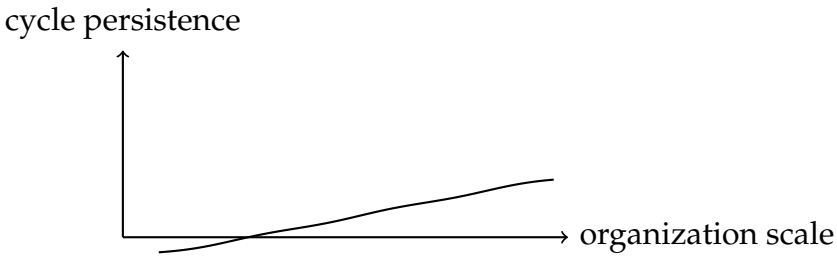

Diagram 1: thresholds—porous gradients, templating, vesicles

2. Framework: Reactive Transport, Surfaces, and Membranes

2.1 Hydrothermal reactive transport (ADR + PNP)

Let $c_i(\mathbf{x}, t)$ be species concentrations, ϕ electric potential, $\mathbf{u}$ Darcy velocity.

$$\partial_t c_i + \nabla\cdot\left(-D_i\nabla c_i - z_i u_T c_i \nabla\phi + \mathbf{u}\, c_i\right) = R_i(c) \quad \text{(ADR+electromigration)}, \tag{1}$$

$$-\nabla\cdot(\epsilon\nabla\phi) = \sum_i z_i e\, c_i \quad \text{(Poisson)}. \tag{2}$$

Here D_i diffusivities, z_i valences, $u_T = D_i/(k_B T/e)$ thermal mobility, ϵ permittivity. The fluid field satisfies Darcy–Brinkman or Stokes in pores; for steady, incompressible flow, $\nabla\cdot\mathbf{u} = 0$.

Dimensionless groups. For a feature length L and speed U,

$$\mathrm{Pe} = \frac{UL}{D}, \qquad \mathrm{Da} = \frac{kL}{U} \quad (\text{or } kL^2/D \text{ in diffusion-limited}), \qquad \Lambda = \frac{e\Delta\phi}{k_B T}.$$

Large Pe concentrates along streamlines; large Da drives strong conversion; Λ controls electrostatic bias.

2.2 Mineral templating (heterogeneous kinetics)

On a templating surface Γ,

$$-D_i\,\mathbf{n}\cdot\nabla c_i = J_i^{\Gamma} = k_i^{\mathrm{ads}} c_i - k_i^{\mathrm{des}}\theta_i \quad \text{on } \Gamma, \tag{3}$$

$$\partial_t \theta_i = k_i^{\mathrm{ads}} c_i - (k_i^{\mathrm{des}} + k_i^{\mathrm{rxn}})\theta_i + \sum_{j\neq i} k_{ji}^{\mathrm{swap}}\theta_j, \tag{4}$$

with coverage $\theta_i \in [0,1]$, reaction k_i^{rxn} on surface. A *curvature-weighted coherence* factor $\kappa(\mathcal{H})$ multiplies surface rates to encode local geometric stabilization: $k^{\mathrm{rxn}} \to \kappa(\mathcal{H})k^{\mathrm{rxn}}$, where $\mathcal{H}$ is mean curvature (higher curvature can stabilize transition states by orientational confinement).

2.3 Amphiphilic vesicles (Helfrich–Canham–Evans)

Membrane energy

$$E_m = \int_{\Sigma} \Big(\frac{\kappa_b}{2}(2H - c_0)^2 + \bar{\kappa}\,K\Big)\,\mathrm{d}A + \lambda_A(A - A_0) + \lambda_V(V - V_0),$$

with bending modulus κ_b, spontaneous curvature c_0, Gaussian curvature K, area/volume constraints via multipliers λ_A, λ_V. Growth from lipid influx J_ℓ: $\dot{A} = \alpha_\ell J_\ell$; solute permeation P_s gives $\dot{V} = \sum_s P_s(c_s^{\mathrm{out}} - c_s^{\mathrm{in}})A$. Division can be triggered by reaching a necking instability set by local H and tension.

Membrane numbers. Define a *membrane Peclet* $\mathrm{Pe}_m = \frac{U_m R}{D_m}$ and a *leakage number* $\mathrm{Le} = \frac{\sigma_D}{\sigma_C}$ with surface coherence σ_C and dissipation σ_D (see Thm. **??**).

3. Action Principles and Thresholds

3.1 Network action with transport coupling

Let $x(t)$ be bulk concentrations sampled along a streamline γ in the porous domain, with reaction fluxes $J(x)$ and transport operator $\mathcal{T}$ (ADR+PNP linearization). Define

$$\mathcal{A}[x,\Lambda] = \int_0^T \Big(\Phi_C(x) - \Phi_D(x) + \Lambda^{\top}(\dot{x} - SJ(x) - \mathcal{T}x)\Big)\,\mathrm{d}t,$$

where Φ_C, Φ_D are coherence/dissipation reductions from molecular functionals (CHEM–2). Stationarity gives Euler–Lagrange kinetics with transport; the minimum-action path yields large-deviation rates $k \sim Ae^{-S^*/\hbar_{\mathrm{eff}}}$.

3.2 Hydrothermal cycle threshold

Theorem 1 (Gradient-driven cycle). Consider a single dominant cycle $\mathcal{C}$ embedded in ADR+PNP transport with cycle affinity $\mathcal{A}_{\mathcal{C}}$, effective dispersion D_{eff}, and advection U over length L. Define

$$\Xi_{\text{HT}} \;=\; \mathcal{A}_{\mathcal{C}} \;-\; \underbrace{\left(\frac{L^2}{D_{\text{eff}}\,T_{\text{mix}}} + \beta\,\Lambda^2\right)}_{\text{transport + electrostatic losses}} \;-\; \gamma\,\text{Da}^{-1}.$$

If $\Xi_{\text{HT}} > 0$, then persistent circulation along $\mathcal{C}$ is exponentially favored (cycle survives mixing and electrostatic dissipation). □

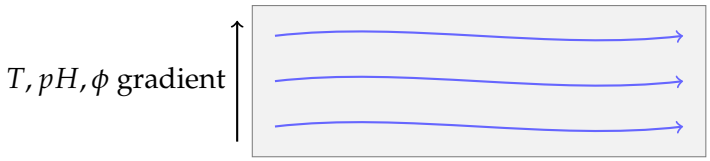

Diagram 2: gradient-driven streamlines in porous rock

3.3 Templating threshold

Theorem 2 (Curvature-coherence templating). Let a surface domain Γ with mean curvature H impose a rate multiplier $\kappa(\mathcal{H}) = 1 + \eta H^2$ on productive steps. Define a *templating number*

$$\text{Te} \;=\; \frac{\displaystyle\int_\Gamma \kappa(\mathcal{H})\,k^{\text{rxn}}\,\theta\,\mathrm{d}A}{\displaystyle\int_\Gamma k^{\text{des}}\,\theta\,\mathrm{d}A + J_{\text{loss}}}.$$

If $\text{Te} > 1$, templating lowers the action S^* enough to flip the network from transient to persistent cycling. □

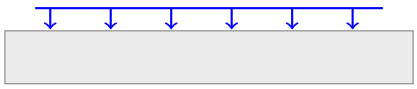

Diagram 3: curvature-weighted adsorption/reaction

3.4 Vesicle threshold

Theorem 3 (Compartment persistence). For a vesicle of radius R, surface coherence σ_C, dissipation σ_D, and bending modulus κ_b,

$$4\pi R^2(\sigma_C - \sigma_D) \;>\; 8\pi\kappa_b \quad \Longrightarrow \quad \text{stable compartment with net growth.} \tag{5}$$

In terms of $\mathrm{Le} = \sigma_D/\sigma_C$, the condition is $(1 - \mathrm{Le})R^2 > 2\kappa_b/\sigma_C$. □ Growth–division requires, in addition, a necking mode H_{neck} crossing a critical curvature set by tension; permeability and osmotic flows determine the division timescale.

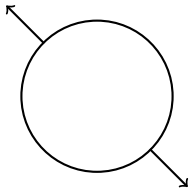

Diagram 4: growth + leakage balance on a vesicle

4. Quantified Handoff: The Thermodynamic Threshold of Life

Definition (Threshold). Fix environmental parameters $T, P, \Delta\phi$, feed composition, permeability set. The *thermodynamic threshold of life* is the boundary in parameter space where there exists a set of cycles $\{\mathcal{C}_k\}$ and a compartment geometry s.t.

$$\exists\,\{\mathcal{C}_k\},\ \text{compartment}: \quad \min_k\ \Xi^{(k)}_{\mathrm{HT}}(\mathrm{Pe}, \mathrm{Da}, \Lambda) \;>\; 0, \quad \mathrm{Te} > 1, \quad \text{and} \quad (5)\ \text{holds.}$$

Inside this region, the network exhibits persistent cycles and self-maintenance; outside, it relaxes to equilibrium.

Corollary (Design principle). Optimizing $(\mathrm{Pe}, \mathrm{Da}, \Lambda)$ by pore geometry, feed rate, and gradients; engineering curvature patterns on templates; and tuning $(\sigma_C, \sigma_D, \kappa_b)$ of vesicles jointly expands the feasible region—predicting concrete laboratory targets.

5. Visual Landscapes (bounded)

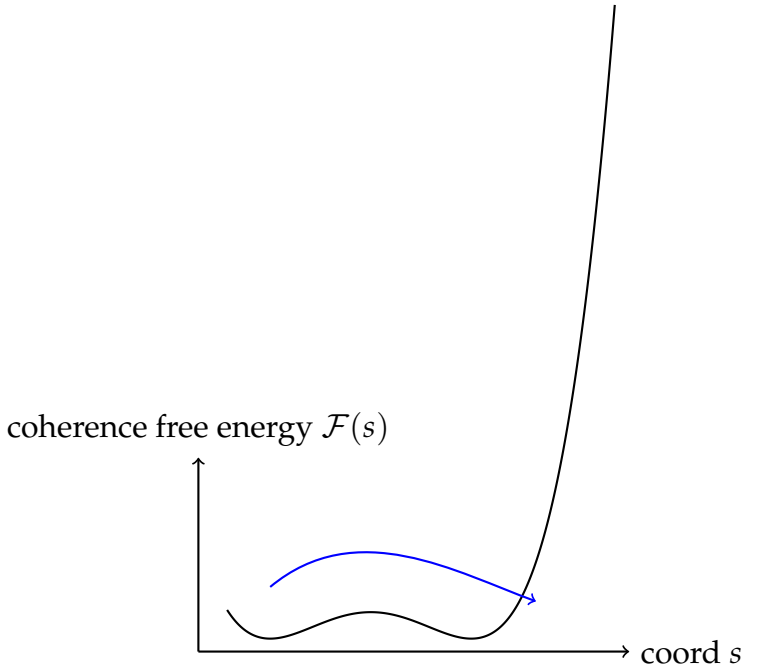

Diagram 5: minimum-action circulation between wells

6. Consequences and Predictions

- **C1. Pore geometry windows.** There exist optimal Pe, Da bands where cycle affinity beats transport loss; mapable via microfluidic porous analogs.
- **C2. Curvature patterning.** Surfaces with tuned $H(\mathbf{x})$ (nano-ridged clays, Fe–S clusters) raise Te and selectively amplify productive pathways.
- **C3. Vesicle materials.** Compositions increasing σ_C (ordered packing) and lowering σ_D (reduced leakage) reduce the minimal R for persistence; predict growth–division periods.
- **C4. Gradient coupling.** Electrochemical potential Λ couples to selective transport; cycle bias scales with Λ^2 at low field—test via imposed potentials across rock membranes.
- **C5. Unified protocol.** Use NEB/string to obtain $\mathcal{F}(s)$, compute S^*, compare to inequalities above to forecast persistence/division regions before experimentation.

7. Discussion

The high-fidelity view unifies fluid mechanics, electrochemistry, surface science, and membrane mechanics under the ChronoChemistry action. Hydrothermal porous media act as gradient engines; mineral templates as curvature-coherence amplifiers; vesicles as dynamic, selectively leaky reactors. The threshold of life is thus not a slogan but a calculable region in $(\mathrm{Pe}, \mathrm{Da}, \Lambda, \sigma_C, \sigma_D, \kappa_b)$. Crossing it predicts *molecular memory* and *self-maintenance*—the hallmarks of proto-metabolism.

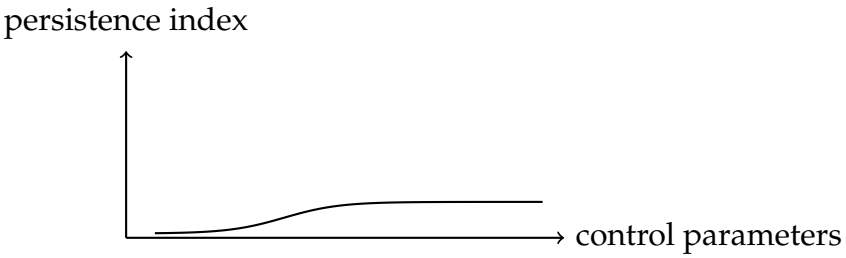

Diagram 6: crossing the thermodynamic threshold

8. References

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9. Conclusion

By embedding ADR+PNP transport, heterogeneous surface kinetics, and Helfrich membrane mechanics into the ChronoChemistry action, we derived explicit, testable inequalities for prebiotic persistence and compartment stability. These *high-fidelity* thresholds convert origin-of-life narratives into quantitative design: geometry, gradients, and materials can be tuned to cross the boundary where chemistry becomes metabolism. The next

series, *HMR–BIO*, will inherit these thresholds to model living coherence—metabolic cycles, tissue fascia as structural coherence, and neural phase integration—completing the physics→chemistry→biology bridge.

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