Goldschmidt 2022 Abstract
https://doi.org/10.46427/gold2022.11211

Quantification of Physicical Processes Driving Assembly of Protocell-like Vesicles in Micro-Scale Hydrothermal Pores

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Identifying mechanisms capable of driving protocell formation under prebiotic conditions is a long-standing unanswered question in the origin of life. Hydrothermal vents are zones of interest for these processes because they embed inherently rich biochemical environments. Previous studies demonstrated the assembly of fatty acid precursors in model open pores emulating thin cracks at the surface of hydrothermal networks ($d \leq 100$ μm) under extreme thermal gradients (100–1000 °C/mm) [1-2]. But fatty acid vesicles do not represent cell membrane components, and the physical pore sizes and magnitude of the thermal gradients applied only capture a small subset of conditions within hydrothermal systems. Here, we report studies characterizing the growth of vesicles composed of phosphatidylcholine, a primary cell membrane constituent, in model hydrothermal pores at size scales (mm-cm diameter) and temperature gradients (0.1-10 °C/mm) closer to realistic hydrothermal conditions. We use simulations and experiments to identify complex 3-D convective flow fields that optimally favor and drive the assembly of protocell-like vesicles via localized trapping and continual refeeding.

We analyzed an ensemble of ~10,000 pores extracted from vent cut images to establish size scales characterizing the bulk of the total pore volume fraction. We then selected nine cylindrical pore-mimicking geometries within these size scales for experimental study, incubating them with solutions containing small precursor vesicles (~0.2 μm) under a δT of 40 °C for 24 h. Quantification using nanoparticle tracking analysis made it possible to classify the vesicles produced after incubation into three size categories: 0.6 μm, 0.8-1.0 μm, and >1.0 μm. Next, we performed computational simulations to characterize the 3-D flow fields in each of the nine pore geometries to evaluate their ability to locally trap chemical species (quantified by the Q-criterion) and feed material into the trapping regions (quantified by the Lyapunov exponent and Poincaré maps). We apply these new insights to introduce a parametric map linking the combined processes favoring the assembly of micron-sized vesicles, laying the groundwork to pinpoint promising locations for protocell formation in hydrothermal vents.

[1] Budin*, et al.* (2009) *JACS* **131**,9628–9629
[2] Mast, *et al.* (2013) *PNAS* **110**,8030-8035