

Supplementary Materials

Thermodynamic Modeling of Solvent-Assisted Lipid Bilayer Formation Process

Hongmei Xu ¹, Hyunhyuk Tae ², Nam-Joon Cho ^{2,*}, Changjin Huang ^{1,*} and K. Jimmy Hsia ^{1,3,*}

¹ School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore 639798, Singapore; HONGMEI001@e.ntu.edu.sg

² School of Materials Science and Engineering, Nanyang Technological University, Singapore 639798, Singapore; HYUNHYUK001@e.ntu.edu.sg

³ School of Chemical and Biomedical Engineering, Nanyang Technological University, Singapore 637459, Singapore

* Correspondence: njcho@ntu.edu.sg (N.-J.C.); cjhuang@ntu.edu.sg (C.H.); kjhsia@ntu.edu.sg (K.J.H.)

Calculation of the scaling factor ξ

In our model, we consider the supporting lipid bilayer (SLB) formation via lipid self-assembly as a thermodynamic process. However, the solvent exchange process reduces the total number of lipids available to self-assemble. Assuming that the organic solvent and the injected aqueous buffer are instantly and completely mixed in the chamber, the bulk lipid concentration evolves as [1]:

$$c_b = c_0 \exp\left(-\frac{Q}{V}t\right) \quad (\text{S1})$$

where c_0 , Q , and V are the initial lipid concentration in the organic solvent before the aqueous buffer injection, the solvent exchange flow rate, and the volume of the chamber, respectively. The scaling factor ξ is deduced by taking the average of the lipid bulk concentration within the time range of lipid formation. It is known that, only when the water fraction ψ exceeds a critical value ψ_c , the lipids start to form conventional micelles and self-assemble into SLBs on the substrate, which corresponds to the time t_c . When the lipid concentration becomes so low that the reaction quotient equals to the chemical equilibrium constant, the lipid adsorption will stop. We assume the water volume fraction is ψ_k when SLB formation stops, and the corresponding timepoint is t_k . The corresponding water fractions at $t = t_c$ and $t = t_k$ are given by:

$$\begin{aligned} \psi_c &= 1 - \exp\left(-\frac{Q}{V}t_c\right) \\ \psi_k &= 1 - \exp\left(-\frac{Q}{V}t_k\right) \end{aligned} \quad (\text{S2})$$

Hence, the time average of lipid bulk concentration can be calculated as:

$$\bar{c}_b = \frac{\int_{t_c}^{t_k} c_0 \cdot \exp\left(-\frac{Q}{V}x\right) \cdot dx}{t_k - t_c} = \frac{(1 - \psi_c) - (1 - \psi_k)}{\ln(1 - \psi_c) - \ln(1 - \psi_k)} \cdot c_0 \quad (\text{S3})$$

The scaling factor ξ is defined as:

$$\xi = \frac{\bar{c}_b}{c_0} = \frac{(1 - \psi_c) - (1 - \psi_k)}{\ln(1 - \psi_c) - \ln(1 - \psi_k)} \quad (\text{S4})$$

The measured ψ_c is in the range of 0.4 - 0.8 [2]. Taking $\psi_c = 0.7$ and $\psi_k = 0.001$, we obtain $\xi \approx 0.05$.

References

1. Bird, R.B.S.W.E.L.E.N. *Transport phenomena*; 2007.

Citation: Xu, H.; Tae, H.; Cho, N.-J.; Huang, C.; Hsia, K.J. Thermodynamic Modeling of Solvent-Assisted Lipid Bilayer Formation Process. *Micromachines* **2022**, *13*, 134. <https://doi.org/10.3390/mi13010134>

Academic Editor: Toshihisa Osaki

Received: 22 December 2021

Accepted: 11 January 2022

Published: 15 January 2022

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2022 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

2. Hohner, A.O.; David, M.P.C.; Rädler, J.O. Controlled solvent-exchange deposition of phospholipid membranes onto solid surfaces. *Biointerphases* **2010**, *5*, 1-8, doi:10.1116/1.3319326.