Support Information

Reproduction of super-multicomponent self-assembled structures and their functionality using coarse-grained molecular simulation - the example of cleansing foams

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S1. Simulation model

In this study, we adopted a coarse-grained method to eliminate the complex effects including a chemical reaction. Mesoscopic representation of the molecular components of cleansing foams are chosen in this simulation. Since there are an enormous amount of ingredients used in cosmetic products, we modeled commonly used molecules, as shown in Fig. S1. We modeled 13 molecules including 8 surfactants, 3 polyols, citric acid, and water (as solvent).

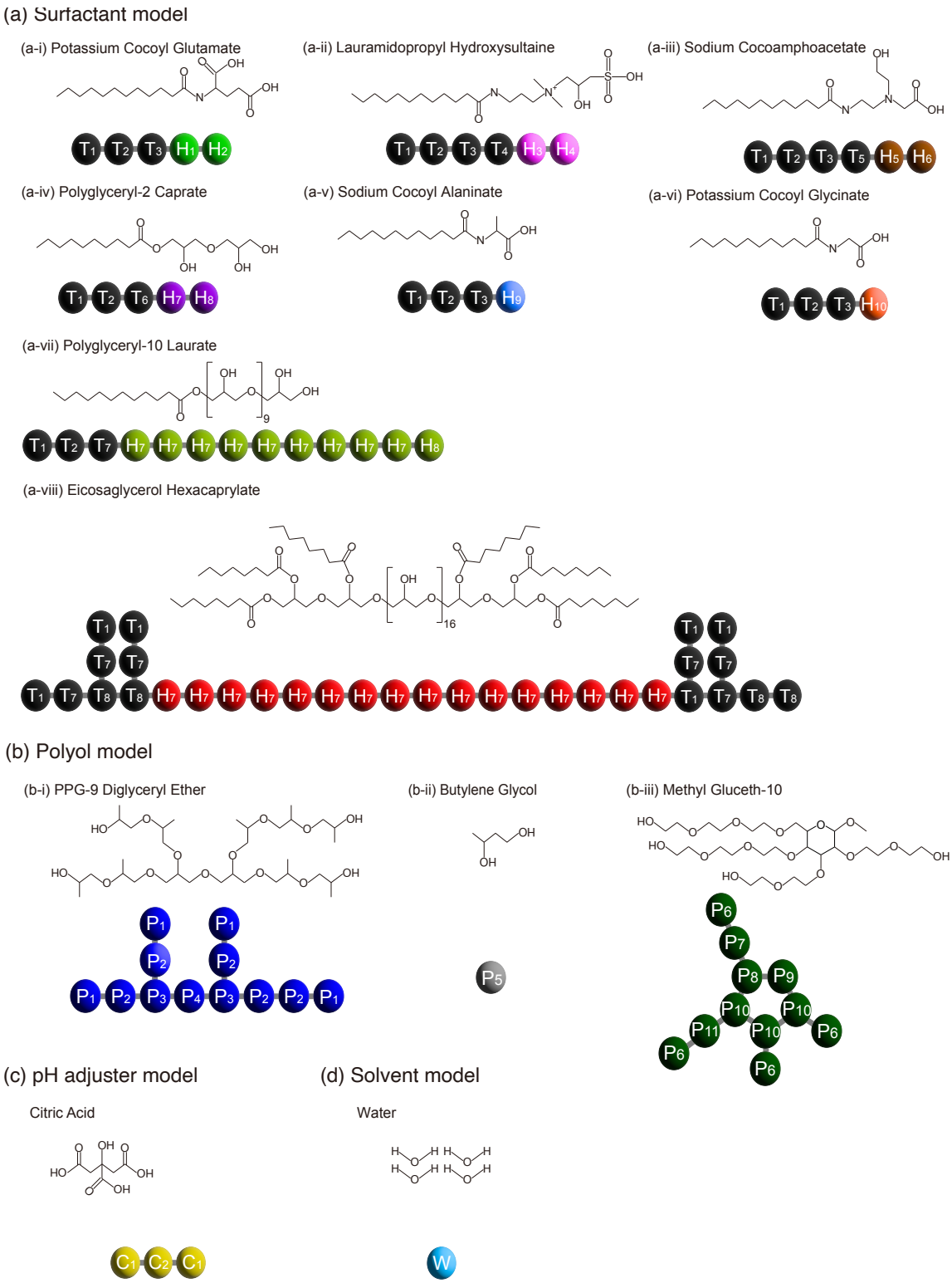


Fig. S1 Coarse-grained simulation models of the molecules we used in this study. Those molecules include (a) Surfactants, (b) polyols, (c) pH adjuster, and (d) solvent.

S2. Solubility parameters δ, and molar volumes of DPD beads

The interaction parameters of the mesoscopic models, solubility parameters and molar volumes are calculated from J-OCTA simulation software [S1]. Table S2 shows the interaction parameters for all DPD beads we used in this study.

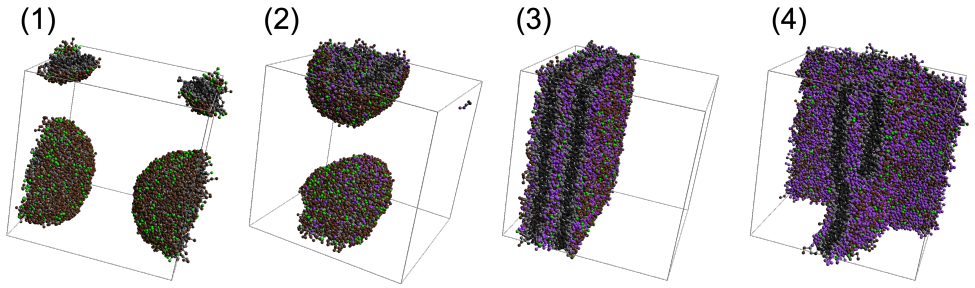
Table S2 Interaction parameters of DPD bead i. δ and V_{seg} describe solubility parameter and molar volume respectively.

Label	δ	V_{seg}
W	40.6	72.1
T_1	15.8	58.1
T_2	16.0	58.1
T_3	24.6	72.1
T_4	24.9	73.1
T_5	25.1	59.1
T_6	22.5	102.1
T_7	23.2	74.1
T_1	15.8	58.1
H_1	33.4	75.1
H_2	30.8	74.1
H_3	27.6	89.1
H_4	35.0	96.1
H_5	34.5	61.1
H_6	32.9	60.1
H_7	26.6	90.1
H_8	32.9	76.1
H_9	30.4	89.1
H_{10}	33.5	75.1
P_1	31.4	60.1
P_2	22.8	74.1
P_3	23.0	90.1
P_4	23.4	74.1
P_5	32.2	90.1
P_6	26.5	76.1
P_7	22.8	60.1
P_8	22.6	60.1
P_9	22.3	76.1
P_{10}	22.6	60.1
P_{11}	22.6	60.1
C_1	32.9	60.1
C_2	34.7	76.1

S3. Validity of Simulation model

To verify the validation of our coarse-grained simulation models using J-OCTA simulation software [S1], we conducted simulations to reproduce the morphology of cleansing agents whose morphologies are already clarified by experiments. Fig S3 shows the simulation results of four different cleansing agents whose morphologies are known from the past experiments [S2]. The morphologies of four cleansing agents (1)-(4) were determined as (1), (2) have micellar phase, and (3), (4) have lamellar phase respectively. We chose our simulation parameters such as number density ρ and system size based on this simulation. As a result, we confirmed that our coarse-graining method can reproduce the same phase morphologies as experimental ones when $\rho = 5$, and system size is $30 \times 30 \times 30\ r_C^3$.

(a)



(b)

	(1)	(2)	(3)	(4)
From the past experiments[2]	Micellar phase	Micellar phase	Lamellar phase	Lamellar phase
From our simulation results	Micellar phase	Micellar phase	Lamellar phase	Lamellar phase

Fig. S3 (a) The simulation results of four different cleansing agent morphologies. (b) The phase morphologies of cleansing agents obtained from experiments and coarse-grained simulations.

References

[S1] JSOL Corporation, J-OCTA, https://www.j-octa.com.
[S2] Shiseido Co Ltd, JP Patent 4911752B2 (2012).