Electronic Supplementary Material (ESI) for Soft Matter.

New Approach for SANS Measurement of Micelle Chain Mixing During Size and Morphology Transitions

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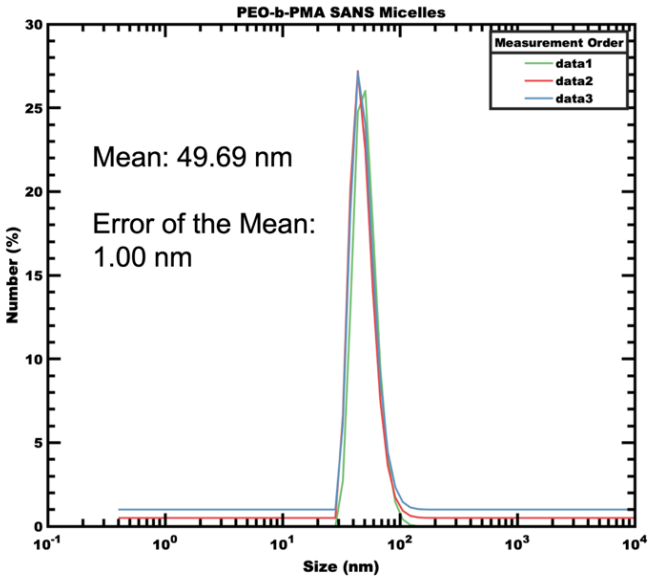

Figure S1. *DLS data of PEO-b-PMA micelles in MeOD/H2O solution.*

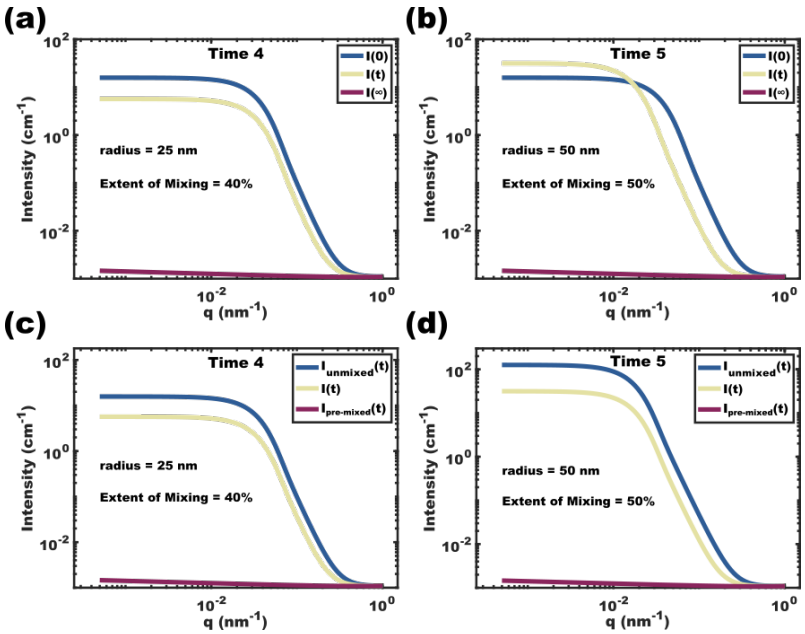

Figure S2. I vs q scattering curves for scenario 1S for time steps 4 and 5. The R(t) method is appropriate for Time step 4 (a) but reveals a flaw with intersecting curves for time step 5 (b) due to comparison to a reference pattern with a changed size. The SRR(t) method rather uses appropriate reference patterns for both Time step 4 (c) and 5(d).

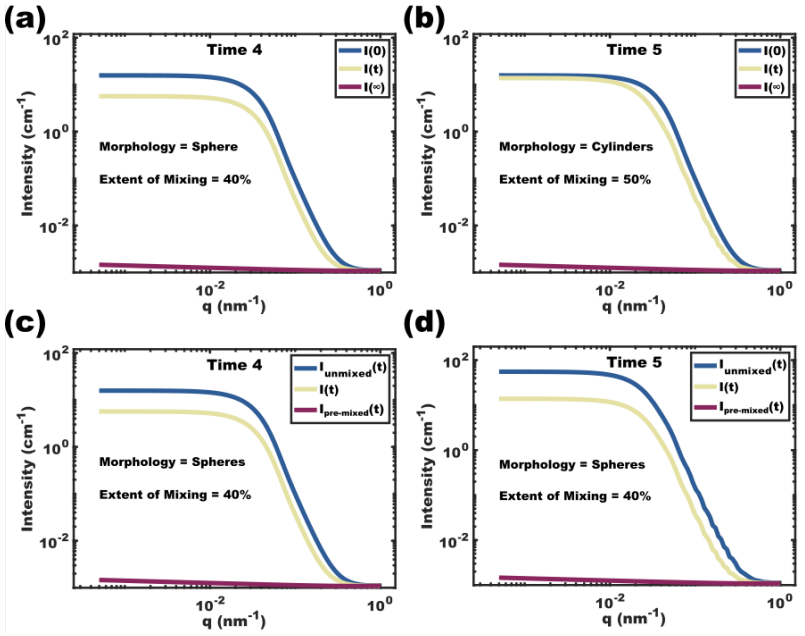

Figure S3. *I vs q scattering curves for scenario 2S. The R(t) method is appropriate for Time step 4 (a) but reveals a flaw with intersecting curves for time step 5 (b) due to comparison to a reference pattern with a changed morphology. The SRR(t) method rather uses appropriate reference patterns for both Time step 4 (c) and 5(d).*

Table S1. Simulation parameters for I(t) values in scenario 1S.

Time	SASfit Model	Radius* (nm) (X0)	Particle Number Density (N)	Dispersity (S)	Scattering Contrast (eta)
0	Sphere	25	1e-30	20	1e10
1	Sphere	25	1e-30	20	9e9
2	Sphere	25	1e-30	20	8e9
3	Sphere	25	1e-30	20	7e9
4	Sphere	25	1e-30	20	6e9
5	Sphere	50	1.25e-31	40	5e9
6	Sphere	50	1.25e-31	40	4e9
7	Sphere	50	1.25e-31	40	3e9
8	Sphere	50	1.25e-31	40	2e9
9	Sphere	50	1.25e-31	40	1e9
10	Sphere	50	1.25e-31	40	0

*Parameter with a gaussian distribution width corresponding to shown Dispersity (S) values.

Table S2. Simulation parameters for $I_{unmixed}(t)$ values in scenario 1S.

Time	SASfit Model	Radius* (nm) (X0)	Particle Number Density (N)	Dispersity (S)	Scattering Contrast (eta)
0	Sphere	25	1e-30	20	1e10
1	Sphere	25	1e-30	20	1e10
2	Sphere	25	1e-30	20	1e10
3	Sphere	25	1e-30	20	1e10
4	Sphere	25	1e-30	20	1e10
5	Sphere	50	1.25e-31	40	1e10
6	Sphere	50	1.25e-31	40	1e10
7	Sphere	50	1.25e-31	40	1e10
8	Sphere	50	1.25e-31	40	1e10
9	Sphere	50	1.25e-31	40	1e10
10	Sphere	50	1.25e-31	40	1e10

*Parameter with a gaussian distribution width corresponding to shown Dispersity (S) values.

Table S3. Simulation parameters for I(t) values for scenario 2S.

Time	SASfit Model	Radius* (nm) (X0)	Particle Number Density (N)	Dispersity (S)	Scattering Contrast (eta)	Length
0	Sphere	25	1e-30	20	1e10	N/A
1	Sphere	25	1e-30	20	9e9	N/A
2	Sphere	25	1e-30	20	8e9	N/A
3	Sphere	25	1e-30	20	7e9	N/A
4	Sphere	25	1e-30	20	6e9	N/A
5	Cylinder	25	1.33e-31	20	1e9	200
6	Cylinder	25	1.33e-31	20	8e9	200
7	Cylinder	25	1.33e-31	20	6e9	200
8	Cylinder	25	1.33e-31	20	4e9	200
9	Cylinder	25	1.33e-31	20	2e9	200
10	Cylinder	25	1.33e-31	20	0	200

*Parameter with a gaussian distribution width corresponding to shown Dispersity (S) values.

Table S4. Simulation parameters for $I_{unmixed}(t)$ values for scenario 2S.

Time	SASfit Model	Radius* (nm) (X0)	Particle Number Density (N)	Dispersity (S)	Scattering Contrast (eta)	Length
0	Sphere	25	1e-30	20	1e10	N/A
1	Sphere	25	1e-30	20	1e10	N/A
2	Sphere	25	1e-30	20	1e10	N/A
3	Sphere	25	1e-30	20	1e10	N/A
4	Sphere	25	1e-30	20	1e10	N/A
5	Cylinder	25	1.33e-31	20	2e10	200
6	Cylinder	25	1.33e-31	20	2e10	200
7	Cylinder	25	1.33e-31	20	2e10	200
8	Cylinder	25	1.33e-31	20	2e10	200
9	Cylinder	25	1.33e-31	20	2e10	200
10	Cylinder	25	1.33e-31	20	2e10	200

*Parameter with a gaussian distribution width corresponding to shown Dispersity (S) values.

Table S5. Simulation parameters for $I_{mixed}(t)$ values for scenario 2S.

Time	SASfit Model	Radius* (nm) (X0)	Particle Number Density (N)	Dispersity (S)	Scattering Contrast (eta)	Length
0	Sphere	25	1e-30	20	0	N/A
1	Sphere	25	1e-30	20	0	N/A
2	Sphere	25	1e-30	20	0	N/A
3	Sphere	25	1e-30	20	0	N/A
4	Sphere	25	1e-30	20	0	N/A
5	Cylinder	25	1.33e-31	20	0	200
6	Cylinder	25	1.33e-31	20	0	200
7	Cylinder	25	1.33e-31	20	0	200
8	Cylinder	25	1.33e-31	20	0	200
9	Cylinder	25	1.33e-31	20	0	200
10	Cylinder	25	1.33e-31	20	0	200

*Parameter with a gaussian distribution width corresponding to shown Dispersity (S) values

Table S6. Simulation parameters for cylinder scenario 3S based on the SASfit model "CYL+Chains(RW)_Rc." The initial "Particle Number Density (N)" was scaled for each time step with proportion to the fraction shown in Figure 5b. Unlisted variables were set to 0.

Particle Number Density (N)	Dispersity (S)	Core Radius (X0)*	Core Block Volume (v_core)	Corona Block Volume (v_brush)	Scattering Contrast of core (eta_core)	Scattering Contrast of corona (eta_brush)	Scattering Contrast of solvent (eta_solv)	R_g	d	Cylinder Height (H) (nm)
2e-28	4.0	10.0	24.31	7.345	2e10	1.6e10	1e10	10	1	50

*Parameter with a gaussian distribution width corresponding to shown Dispersity (S) values.

Table S7. Simulation parameters for small spheres in scenario 3S based on the SASfit model "BlockCopolymerMicelle." The initial "Particle Number Density (N)" was scaled for each time step with proportion to the fraction shown in Figure 5b. The initial "Scattering Contrast of Core (eta_core)" was scaled at each time step with proportion to the extent mixing shown in Figure 5b. Unlisted variables were set to 0.

Particle Number Density (N)	Dispersity (S)	Aggregation Number (X0)*	Core Block Volume (v_core)	Corona Block Volume (v_brush)	Scattering Contrast of core (eta_core)	Scattering Contrast of corona (eta_brush)	Scattering Contrast of solvent (eta_solv)	R_g	d
7.5e-28	66.93	172.31	24.31	7.345	2e10	1.6e10	1e10	10	1

*Parameter with a gaussian distribution width corresponding to shown Dispersity (S) values.

Table S8. Simulation parameters for large spheres in scenario 3S based on the SASfit model "BlockCopolymerMicelle." The initial "Particle Number Density (N)" was scaled for each time step with proportion to the fraction shown in Figure 5b. The initial "Scattering Contrast of Core (eta_core)" was scaled at each time step with proportion to the extent mixing shown in Figure 5b. Unlisted variables were set to 0.

Particle Number Density (N)	Dispersity (S)	Aggregation Number (X0)*	Core Block Volume (v_core)	Corona Block Volume (v_brush)	Scattering Contrast of core (eta_core)	Scattering Contrast of corona (eta_brush)	Scattering Contrast of solvent (eta_solv)	R_g	d
9.4e-29	551.4	1378.5	24.31	7.345	2e10	1.6e10	1e10	10	1

*Parameter with a gaussian distribution width corresponding to shown Dispersity (S) values.

Table S9. Background parameters for all scenario 3S calculations included the contribution of SASfit model "Dozier Star" with the below parameters.

N	Dispersity (S)	Forward Scattering I(0)*	R_g	Alpha	Nu	F
1e-26	150.0	200.0	2	2e25	0.6	400

*Parameter with a gaussian distribution width corresponding to shown Dispersity (S) values.