Achieving Target Emulsion Drop Size Distributions using Population Balance Equation Models of High Pressure Homogenization

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Supporting Information

Table S1: Bulk properties of the emulsion system.

Density of water (ρ_c)	997.05 kg/m ³
Density of sunflower oil (ρ_d)	917.36 kg/m ³
Viscosity of water (η_w)	0.88 mPa.s
Viscosity of sunflower oil (η_d)	47.8 mPa.s
Interfacial tension of sunflower oil in water at 25°C	27 mN/m

Table S2: Objective function values at six different homogenization pressures

Pressure (bar)	Objective function (Ψ) using parameters $K_1 - K_5$ optimized at 400 bar	Objective function (Ψ) using parameters $K_2 - K_5$ optimized at 400 bar and fitted equations for K_1 and ϵ
100	0.426	0.098
200	0.123	0.058
300	0.074	0.051
400	0.029	0.031
600	0.064	0.032
800	0.186	0.063
Total	0.902	0.333

Table S3: Model predicted and experimental results for a target DSD generated from a log-normal distribution with $\mu = 0.5 \mu\text{m}$ and $\sigma^2 = 0.5$ using a weighting factor of $W = 0.01$.

Total surf-actant (wt%)	Pressure (bar)					Ψ_2	Ψ_3	$\Psi_2 + W\Psi_3$
	1 st pass	2 nd pass	3 rd pass	4 th pass	5 th pass			
						Model prediction		
1.527	736	—	—	—	—	0.715	4.060	0.756
1.591	776	617	—	—	—	0.177	4.590	0.223
1.322	800	626	599	—	—	0.027	2.703	0.054
1.186	766	555	555	566	—	0.0060	1.883	0.025
1.160	234	353	439	487	552	0.0073	1.742	0.025
						Experimental result		
1.186	766	555	555	566	—	0.126	1.883	0.145

Table S4: Effect of the objective function weighing factor W on model predicted results for four passes and a target DSD generated from a log-normal distribution with $\mu = 1.0 \text{ } \mu\text{m}$ and $\sigma^2 = 0.5$.

W	Total surf- -actant (wt%)	Pressure (bar)				Ψ_2	Ψ_3	$\Psi_2 + W\Psi_3$
		1 st pass	2 nd pass	3 rd pass	4 th pass			
0.001	1.345	425	529	546	552	0.0025	2.700	0.0052
0.005	1.234	600	549	558	565	0.0045	2.040	0.0147
0.01	1.186	766	555	555	566	0.0060	1.880	0.0248
0.05	1.043	800	554	530	572	0.0291	1.082	0.0832
0.1	0.955	532	535	493	571	0.0566	0.755	0.132