Supporting Information

Liquid-liquid Dispersion and Selectivity of Chemical Reactions in the Inline Teethed High Shear Mixers

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Appendix I: Validation of the CFD methods

I.1 Mesh independence validation

The power consumption can also be calculated by energy dissipation:

$$P = \iiint_V \rho \varepsilon dV \tag{S1}$$

The comparison of power values P_1 calculated based on torque with the power P_2 calculated based on energy dissipation are listed in Table S1. The values of P_1 and P_2, as well as the difference with accepted error between P_1 and P_2, maintain constant when the number of cells is above 3.2 million for the inline mixer and 5.0 million for the batch mixer, which confirms the good quality of the meshes adopted in our work. In addition, it is generally accepted that the calculated method based on the energy dissipation rates significantly underestimates the power value [1, 2]. Hence, the method based on torque is adopted in our work to predict the power with higher accuracy.

Table S1. Mesh independence validation of HSMs

Item	HSMs	V/m^3	Cells	P_1/W		P_2/W	
				N = 12500 rpm	N = 21000 rpm	N = 12500 rpm	N = 21000 rpm
mesh(a)	inline	1.69×10^{-5}	1.35 million	42.34	204.41	31.32	154.36
mesh(b)	inline	1.69×10^{-5}	3.20 million	44.48	223.01	36.02	183.67
mesh(c)	inline	1.69×10^{-5}	4.66 million	45.20	224.20	36.16	183.73
mesh(d)	inline	1.69×10^{-5}	5.80 million	44.50	226.40	36.04	184.67
mesh(e)	batch	2.99×10^{-4}	2.92 million	74.60	349.50	57.71	261.89
mesh(f)	batch	2.99×10^{-4}	5.00 million	72.20	340.69	59.44	269.51
mesh(g)	batch	2.99×10^{-4}	7.07 million	71.95	339.30	59.51	271.51.

Previous work has validated that Tr/200 applied in this paper was adequate for the flow and power simulations of HSMs [3]. Furthermore, time step size independence has

been checked in Table S2.

Table S2. Time-step size independence validation of high shear mixers

Item	time step size	Torque/(N·m)	
		N = 12500 rpm	N = 21000 rpm
inline HSM	Tr/100	0.035	0.092
	Tr/200	0.034	0.101
	Tr/300	0.034	0.100
	Tr/400	0.032	0.099
batch HSM	Tr/100	0.057	0.157
	Tr/200	0.055	0.155
	Tr/300	0.056	0.156
	Tr/400	0.055	0.155

I.2 Experimental validation

The batch HSM was wrapped by 10 cm rubber and plastic insulation to minimize heat losses. Each experiment was conducted until achieving a temperature rise of 10 ℃ at least, and the temperature data monitored by thermocouple was recorded every 20 seconds. All the experiments were repeated at least three times. The experimental power consumption P_{exp} can be calculated by eq (S2):

$$P_{exp} = \rho_M V C_p \Delta T/\Delta t \quad \text{(S2)}$$

where V is the total volume of fluid in the tank, C_p represents the specific heat, ΔT denotes the temperature rise and Δt is the time variation. Friction losses were measured without rotor at different rotor speeds and excluded from the total power consumption. The comparison of the simulated and average experimental power consumption are listed in Table S3, and the satisfactory agreement in the values indicates the validation of the CFD model applied in this paper.

Table S3. Comparison of simulated and average experimental power consumption in the batch HSM

N/rpm	P_{exp}/W	P_{cal}/W
3000	1.26	1.02
7700	17.77	16.97
12500	81.56	72.78

Appendix II: Selection of feeding flow rate Q_B for the batch HSM

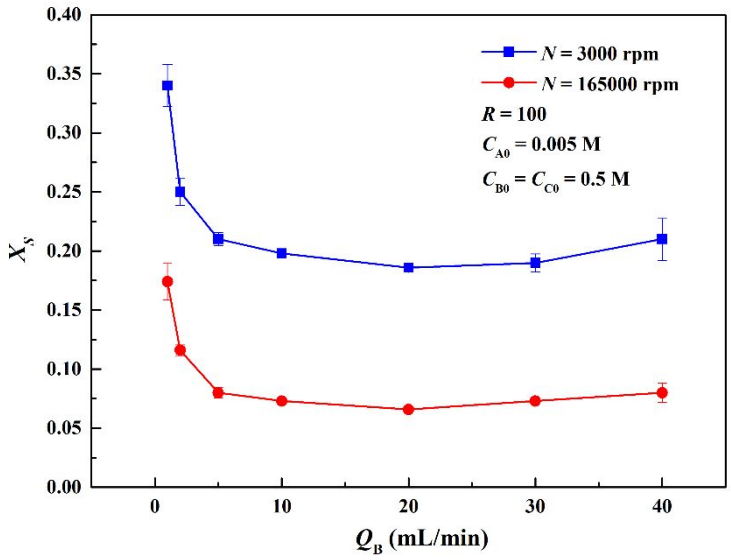

Figure S1. Effect of feeding flow rate Q_B on X_S at different rotor speeds in the batch HSM.

Reference

(1) Singh, H.; Fletcher, D. F.; Nijdam, J. J. An assessment of different turbulence models for predicting flow in a baffled tank stirred with a Rushton turbine. *Chem. Eng. Sci.* **2011,** *66*, 5976.

(2) John, T. P.; Fonte, C. P.; Kowalski, A.; Rodgers, T. L. A comparison of power and flow characteristics between batch and in-line rotor-stator mixers. *Chem. Eng. Sci.* **2019,** *202*, 481.

(3) Qin, H.; Xu, Q.; Li, W.; Dang, X.; Han, Y.; Lei, K.; Zhou, L.; Zhang, J. Effect of Stator Geometry on the Emulsification and Extraction in the Inline Single-Row Blade-Screen High Shear Mixer. *Ind. Eng. Chem. Res.* **2017,** *56*, 9376.