

Supporting information for

# Constructing solid microspheres of CL-20/MTNP cocrystal via droplet microfluidic for improved performances

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### Caution

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SI 1. Computational fluid dynamics simulation

We derived the residual curve of the calculation process in Fluent software, as shown in Figure S 1a. It can be used to judge the convergence of iterative solution. After each iteration, the residual represents the deviation between the current solution and the exact solution of the equations. It can be seen from the residual diagram that the residual curve gradually stabilized after 40000 iterations (corresponds to 2000 steps), which indicates that the simulation results have converged at this time. Secondly, we monitored the inlet and outlet flow to confirm that the calculation results meet the most basic mass conservation (Figure S1b). It can be seen that the flow at the outlet has stabilized after 2000 steps. We calculated the mass flow of 2000-6000 steps, and the mass flow of the inlet and outlet is  $2.34 \times 10^{-3}$  Kg/s. Combined with the results of grid independence verification, we can determine that the simulation results are accurate and reliable.

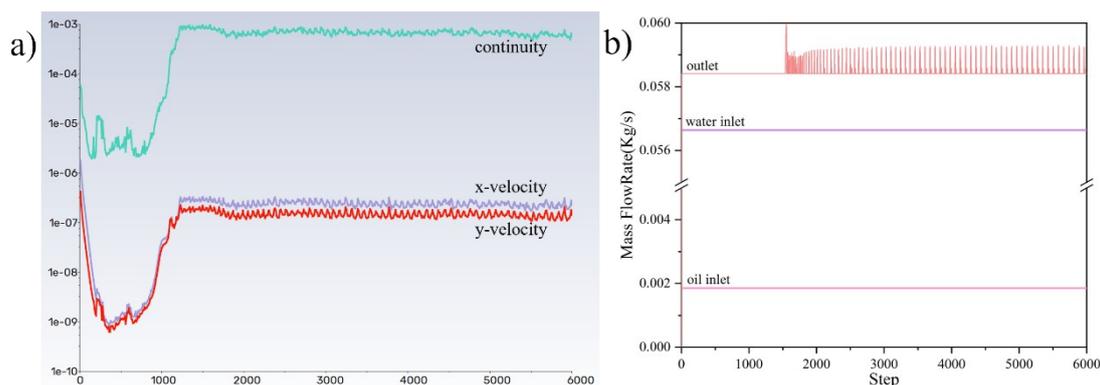


Figure S1. residual curve (a) and XRD (b) inlet and outlet flow rates

## SI 2. Powder X-ray Diffraction (PXRD)

Power X-ray Diffraction (PXRD) patterns were recorded on diffractometer using Cu-K $\alpha$  radiation ( $\lambda=1.54056 \text{ \AA}$ ) and operating at 40 kV and 40 mA. Each sample was scanned over a scan range of  $2\theta$  between  $5^\circ$  and  $80^\circ$  with a step size of  $0.015^\circ$  and a step speed of 0.2 seconds.

The XRD data were refined by Rietveld refinement. Limited by the low crystallinity of organic matter, the fitting effect was relatively general, but the calculated peak position was aligned with the experimental peak position (Figure S 2a). The XRD patterns of raw materials, physical mixtures and cocrystal microspheres were compared. The results show that the peak shape of eutectic is completely different from that of raw materials and physical mixtures, which is different from the superposition of two raw material peaks in physical mixtures.

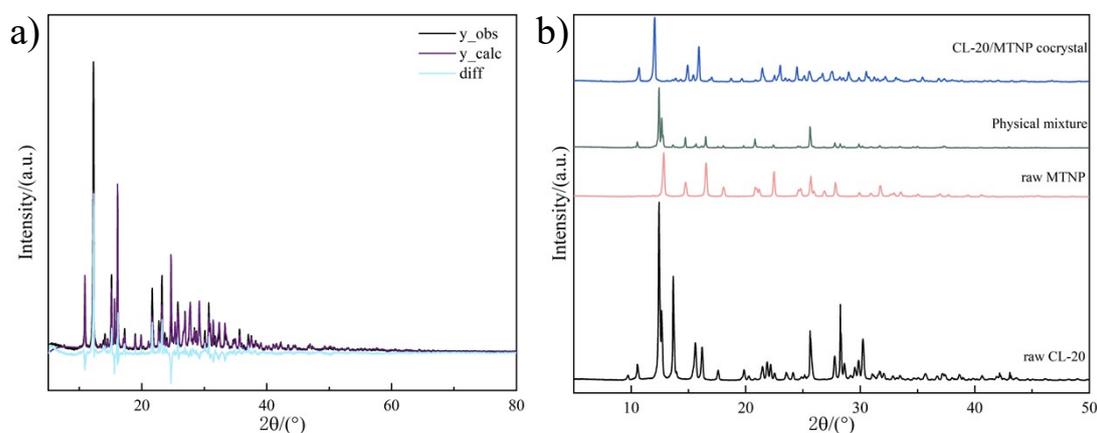


Figure S2. Rietveld refinement result (a) and XRD (b) spectra of raw materials, CL-20/MTNP cocrystal, and physical mixture.