Title: Effect of wetting on micelle fragmentation in confined channels

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Abstract: We use coarse-grained molecular-dynamics (MD) simulations to study the fragmentation of sodium dodecyl sulfate micelles under Poiseuille-like flow in a die-extruder geometry. The effect of flow confinement and wetting on spherical micelles is explored. We demonstrate that the interplay between flow and the wettability of the channel determines the size of daughter micelles inside the channel.

Micelle wetting and fragmentation in confined channels

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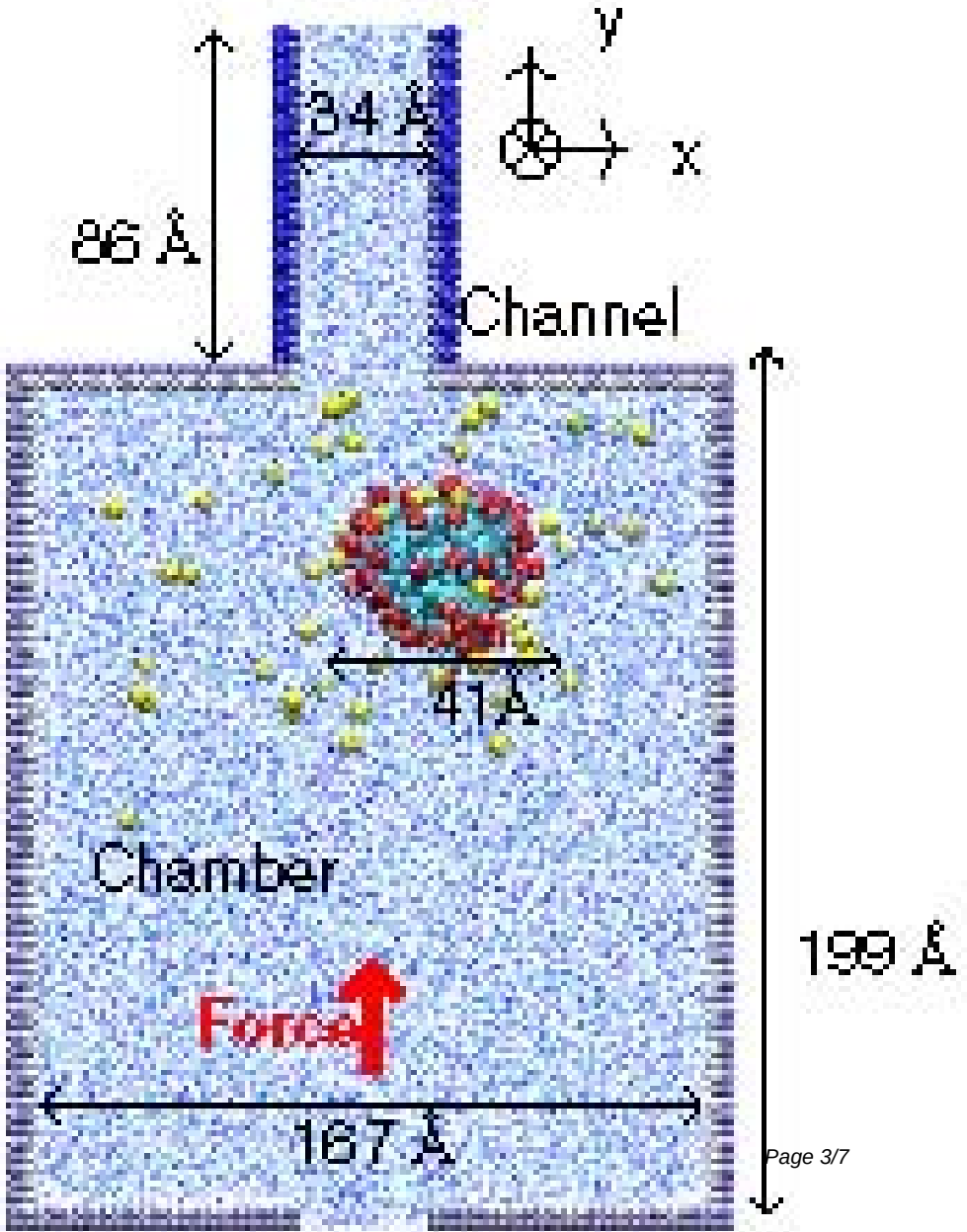
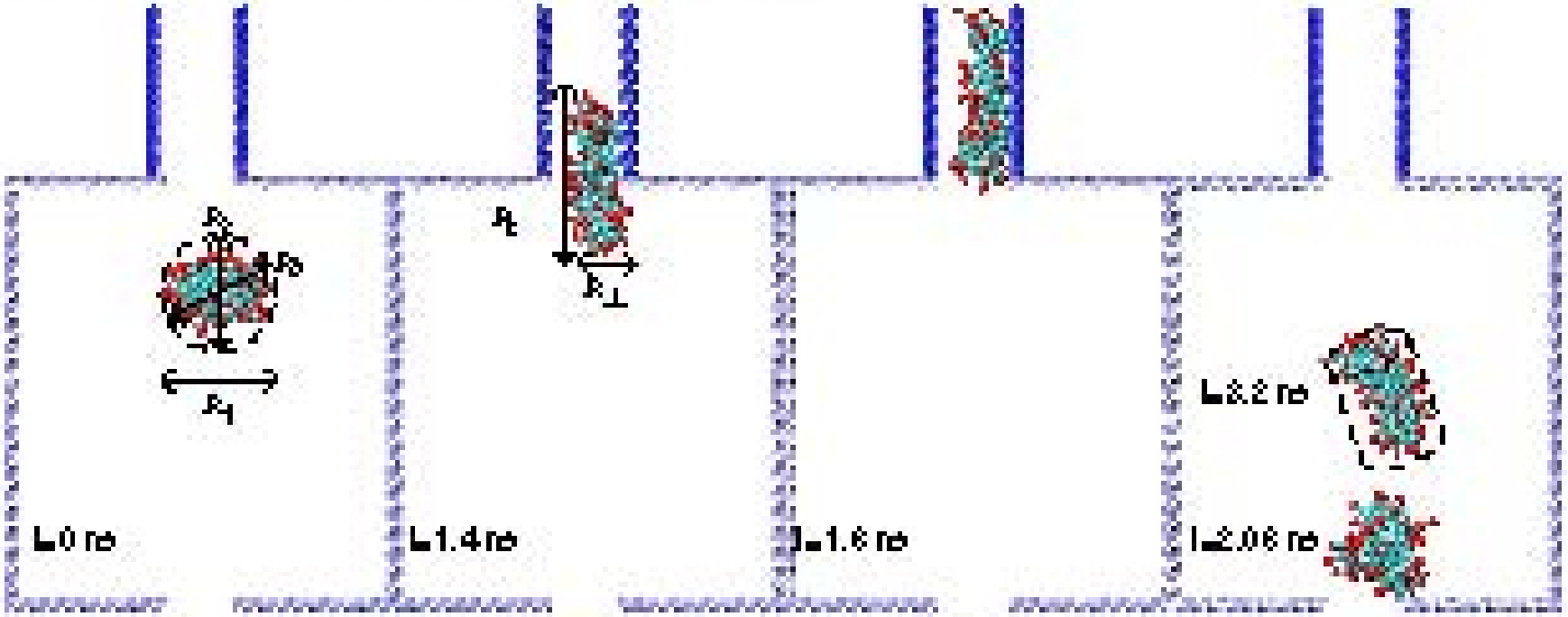
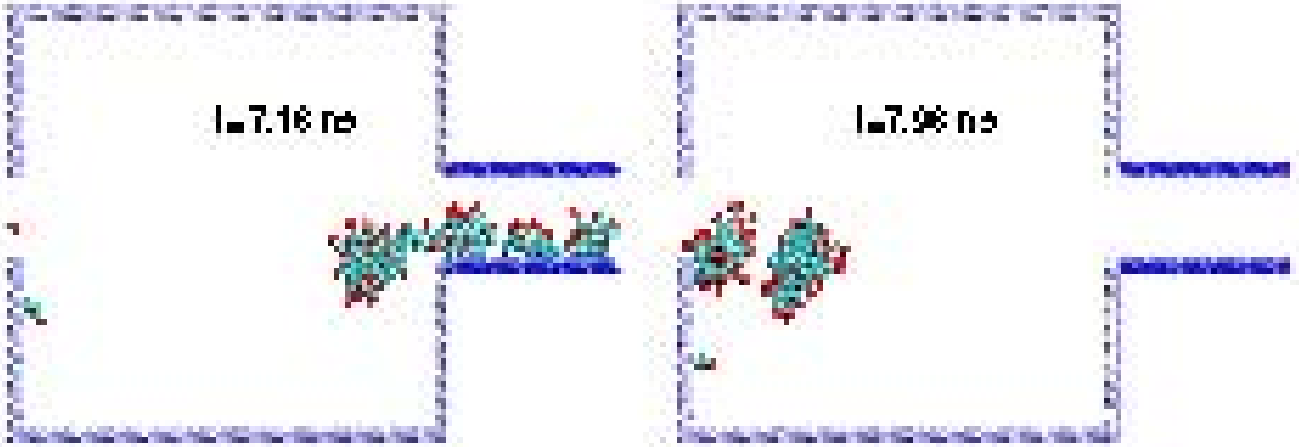
Micelle under flow

- LAMMPS
- MARTINI FORCE FIELD
- PBC in y,z
- NVT at T=300K°
- 10 ns under flow
- Channel surfaces are non-, low-, high-wetting.



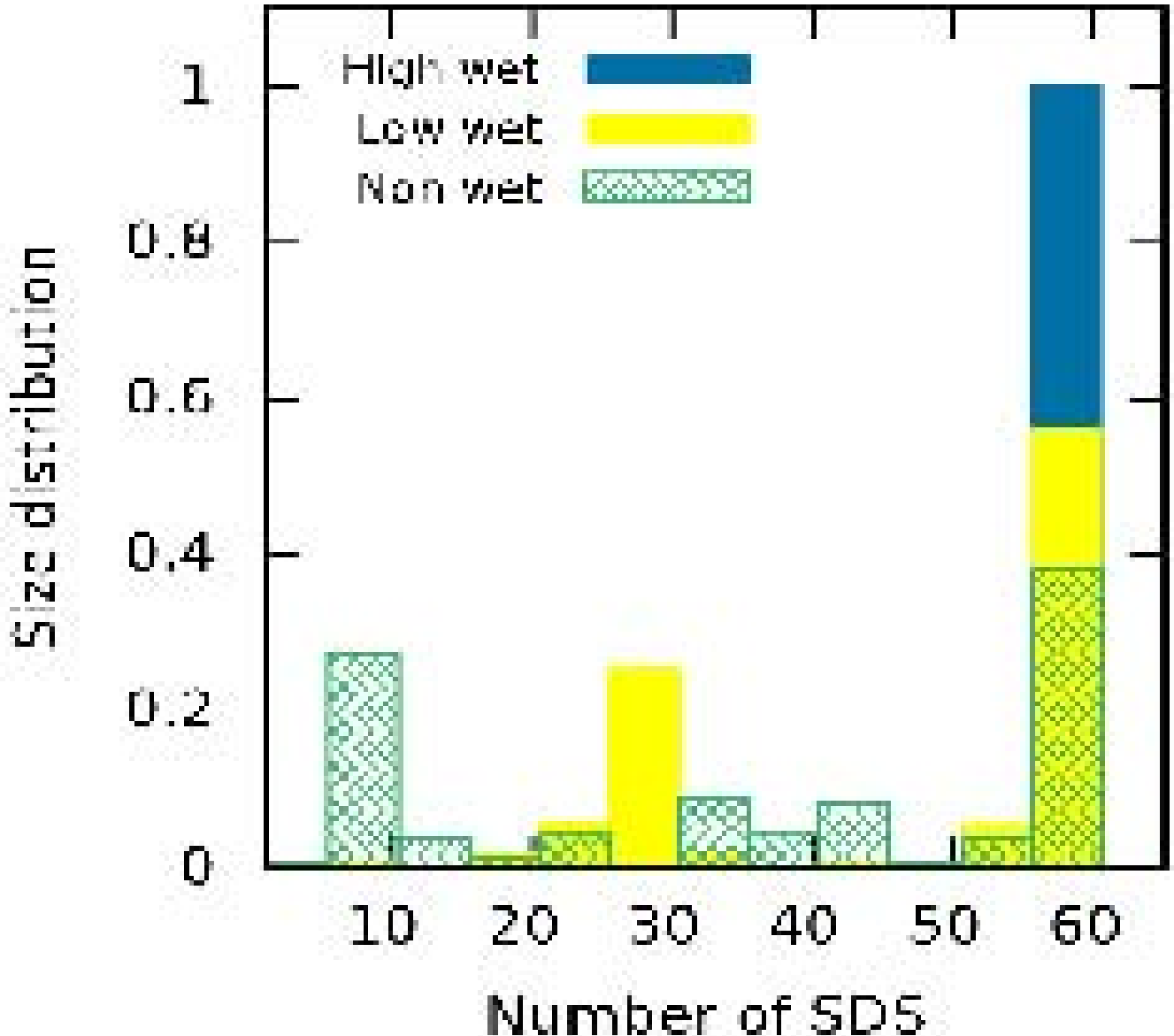


High wet, F=0.003 $\frac{Kcal}{mol\,\AA}$



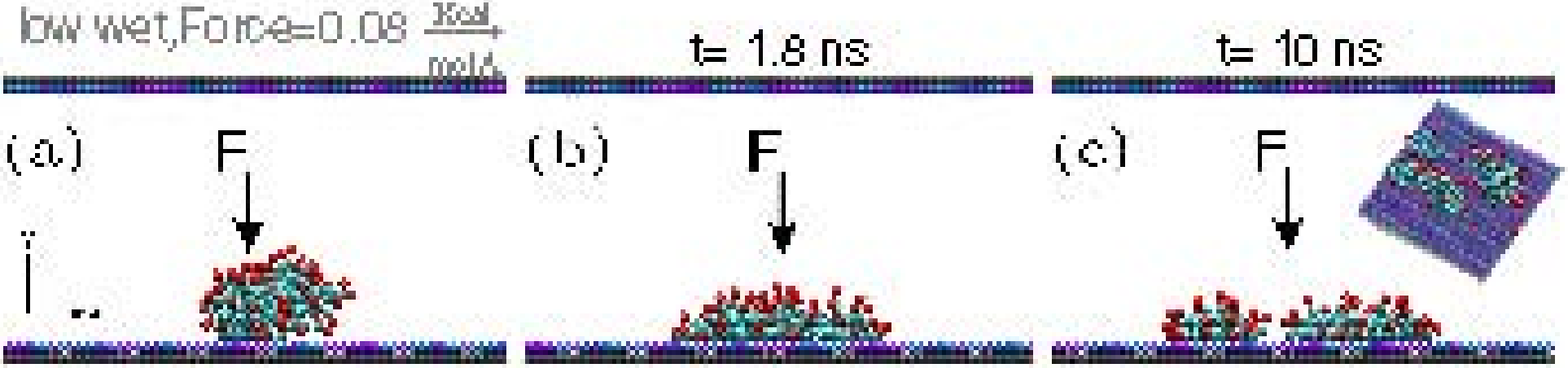
Low wet, F=0.003 $\frac{Kcal}{mol\,\AA}$

Size distribution of micelles in the first passage

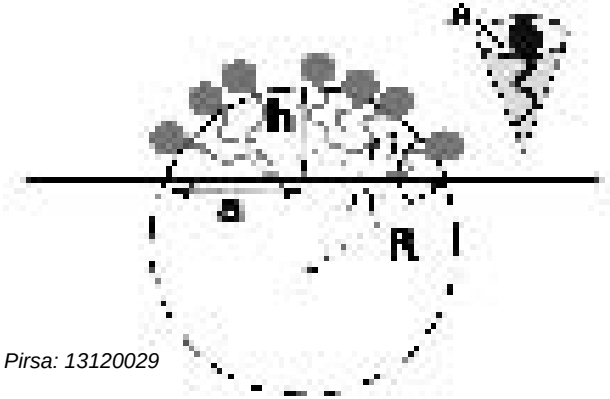


Fragmentation

Fragmentation is an interplay between self-assembly, surface adsorption and hydrodynamic forces.



g= number of SDS



$$\cos\theta = \frac{\gamma_{SDS/F} - \gamma_{SDS/W}}{\gamma_{W/SDS}} = \frac{R-h}{R}$$

$$g = \frac{2\pi Rh}{A} = \begin{cases} 7.8 \pm 18.9 & Non \\ 24.6 \pm 19.4 & Low \\ 49.3 \pm 23.1 & High \end{cases}$$

Summary

- The micellar solution under Poiseuille-like flow in the presence of different wetting surfaces was studied.
- In addition to the flow rate, the wettability of the channel surfaces dictates whether the micelle fragments.
- The balancing of hydrodynamic forces, micelle-wall interactions and self-assembly forces determines the size of the daughter micelles.