Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

Computational Fluid Dynamics of DNA Origami Folding in Microfluidics

SUPPLEMENTARY INFORMATION

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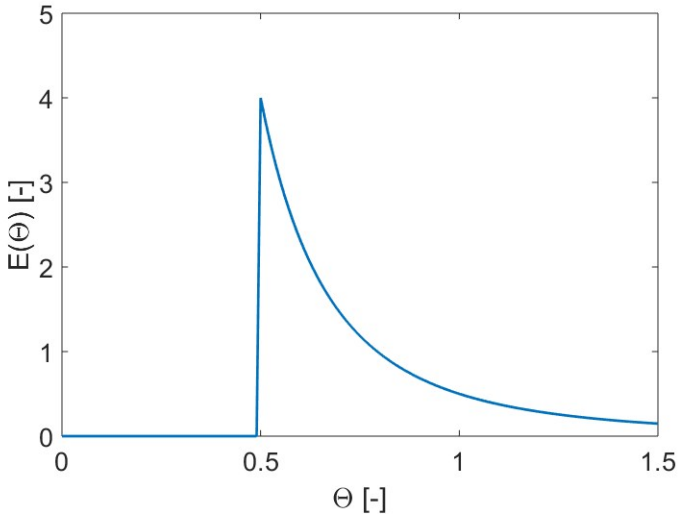

Fig. S1. The dimensionless residence time distribution function of a laminar flow reactor.

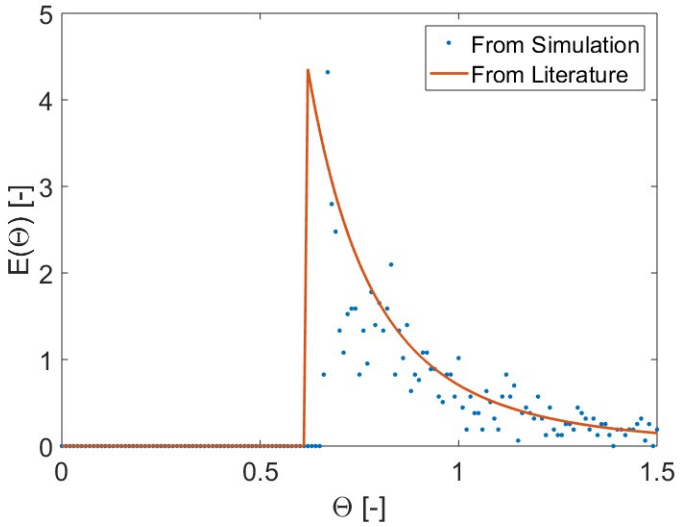

Fig. S2. The dimensionless residence time distribution function of a Dean flow reactor (in red), and the dimensionless residence time distribution function by CFD calculations when De = 1 (in blue).

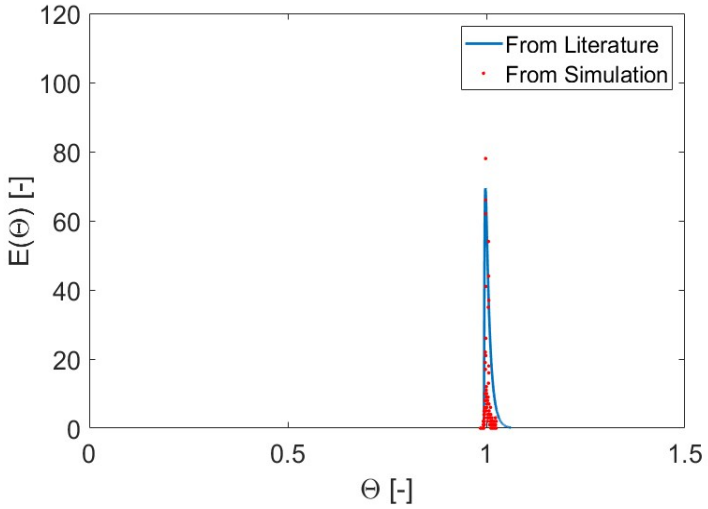

Fig. S3. The dimensionless residence time distribution function of slug flow reactor of slug length of 0.5 mm.

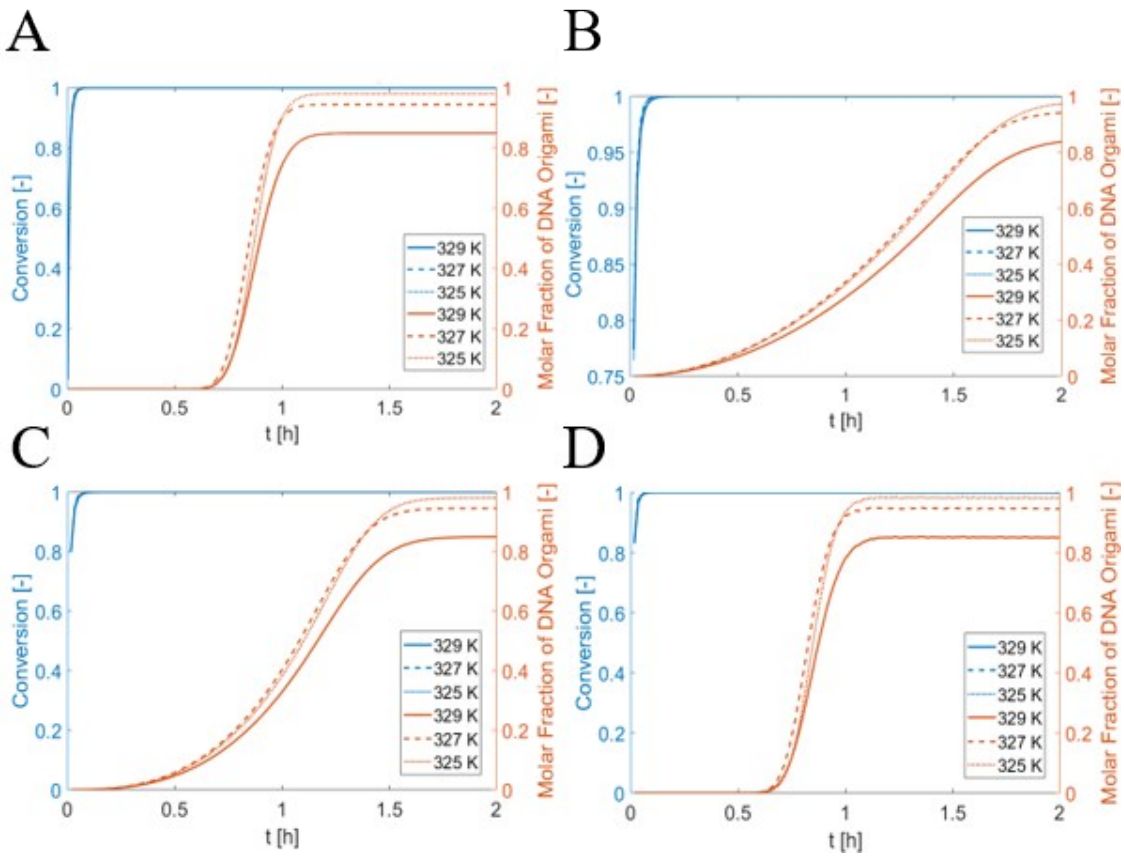

Fig. S4. The reaction temperature influence on conversion and product composition in (A) Batch reaction (B) Laminar flow reactor (C) Dean flow reactor (D) Slug flow reactor.

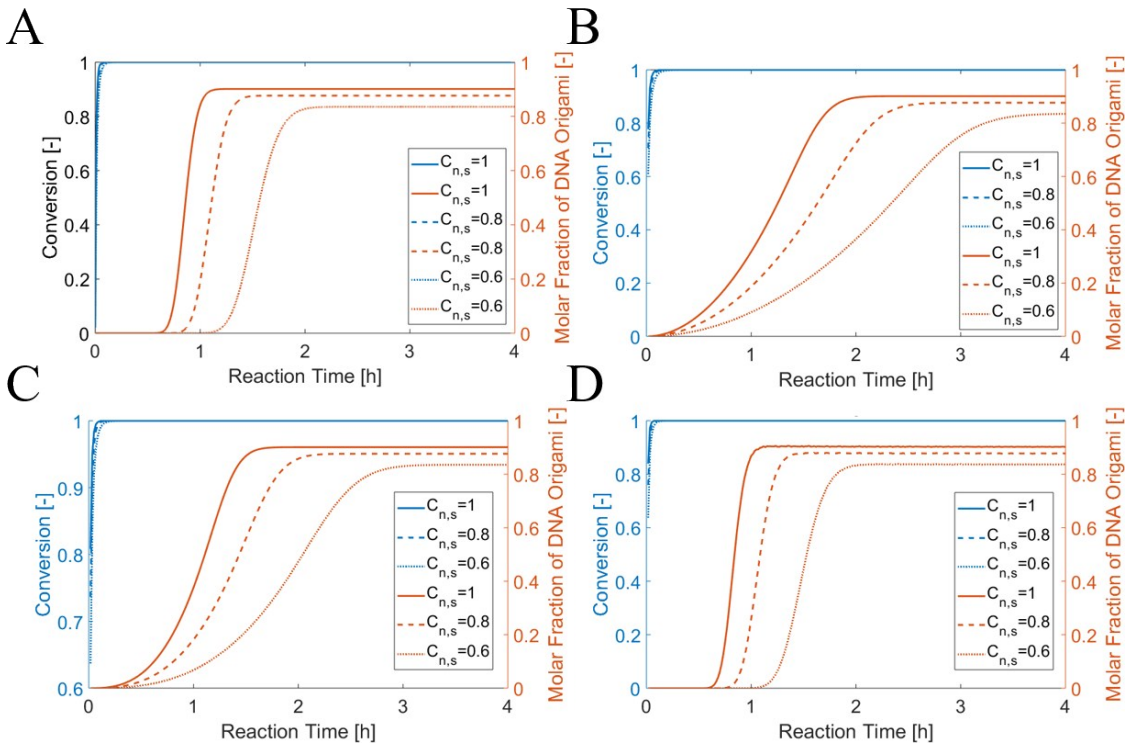

Fig. S5. The staple concentration influence on conversion and product composition in (A) Batch reactor (B) Laminar flow reactor (C) Dean flow reactor (D) Slug flow reactor.

Kinetics data interpretation method

Agarose gel electrophoresis data of Fig. 3(C) in Sobczak et al.'s paper[1] was interpreted and regenerated in Fig. 2 in this manuscript. In their work, electrophoresis data of time-resolved folding of DNA origami at constant 328 K was plotted as a function of reaction time from 0 to 60 min. Scaffold strand and DNA origami positions were labeled as "U" and "F" respectively. The amount of substance was represented by the blue-red colormap. Using MATLAB image viewer tool box, we were able to extract the pixels and their RGB values at each point. We fixed y-axis position at the same level of the "F" label and varied the x-axis position in order to collect the R-value at each pixel. Later, we normalized the data we collected in respect to 255 (maximum R-value) and then subtracted the blue background from them to get the molar fraction of DNA origami. 7 pixels centered at each electrophoresis bar was used to generate the mean molar fraction and the standard deviation as well. The result was plotted with simulation results at the same condition in Fig. 2.

Reference

(1) Sobczak, J.-P. J.; Martin, T. G.; Gerling, T.; Dietz, H. *Science* **2012**, *338* (6113), 1458–1461.