1. ABOUT THE DATASET

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Title: Pore size data outputs

Creator(s): Kalila Rohana Cook

Organisation(s): University of Leeds

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Description: This dataset consists of raw data file outputs from each simulation run for the pore size test results. The *‘PoreSizes'* folder contains subfolders with this repeated data set type but with parameters varying for each volume fraction/reaction probability/simulation run number.

Each data set is found in directory path: *‘PoreSizes > ‘{x}percentVF’ > ‘R{y} > ‘Run{z}’*, where *{x}percentVF* = x% monomer volume fraction, *R{y}* = monomer-monomer reaction probability of y% and *Run{z}* = simulation repeat number, with z ranging from 1-10.

Each data set contains files for

* Position coordinates for updated monomer positions (‘UpdatedParticlePositions.csv’)
  + monomer position coordinates in 3D at the end of the simulation at the fully crosslinked state. These coordinates were used to produce the pore distribution snapshots of Fig. 6a and c.
* Supercomputer job script output (‘{JOB\_NAME}.sh.o{JOBID}’)
  + Supercomputer job script output. {JOB\_NAME} corresponds to varying volume fraction/reaction probability filename. '{JOBID}' corresponds to varying assigned supercomputer job script ID. Each file contains pore size distribution histograms used to produce the pore size distribution histograms of Fig. 6b and d.
* Pore distribution snapshots (‘{VOLUMEFRACTION\_REACTIONPROBABILITY}Pores.png’)
  + Pore distribution simulation snapshots pictured in Fig. 6a and c.

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Related publication: Cook, K. R., Head, D., & Dougan, L. (2023). Modelling Network Formation in Folded Protein Hydrogels by Cluster Aggregation Kinetics. Soft Matter (Accepted). https://doi.org/10.1039/D3SM00111C.