

Supplementary Materials for “Solute diffusion and partitioning in multi-arm poly(ethylene glycol) hydrogels”

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Links to Datasets

All data files:

<https://doi.org/10.6084/m9.figshare.c.6186694.v2>

Non-LPEM data (measurements and SPN predictions):

<https://doi.org/10.6084/m9.figshare.21046987.v1>

LPEM prediction data and R script:

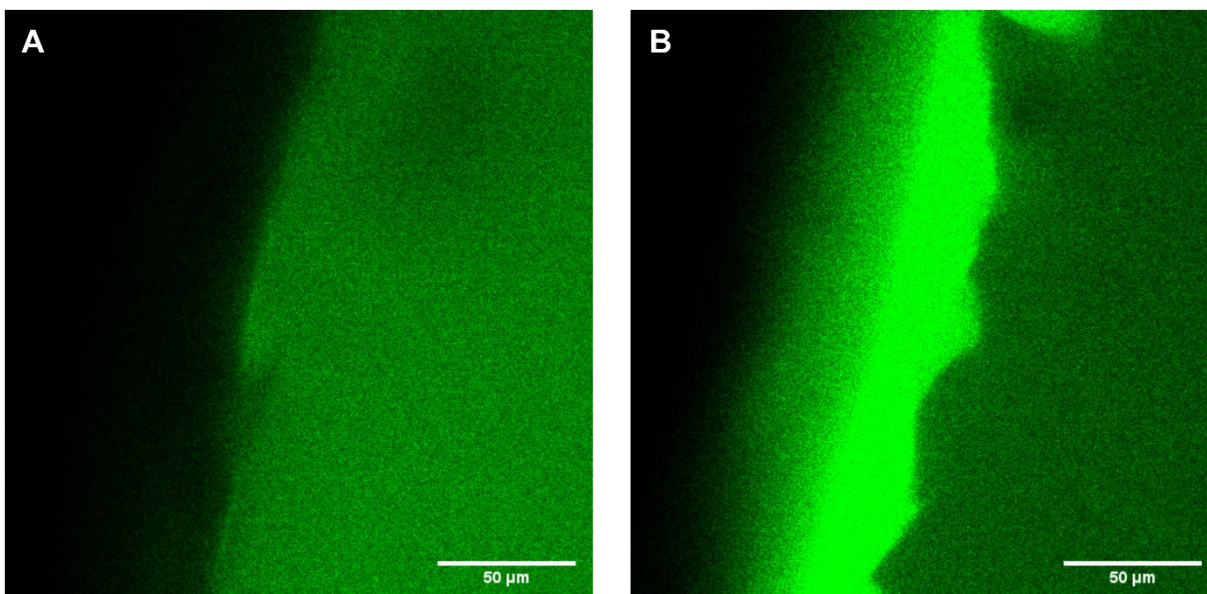
<https://doi.org/10.6084/m9.figshare.21046819.v1>

GraphPad Prism Files:

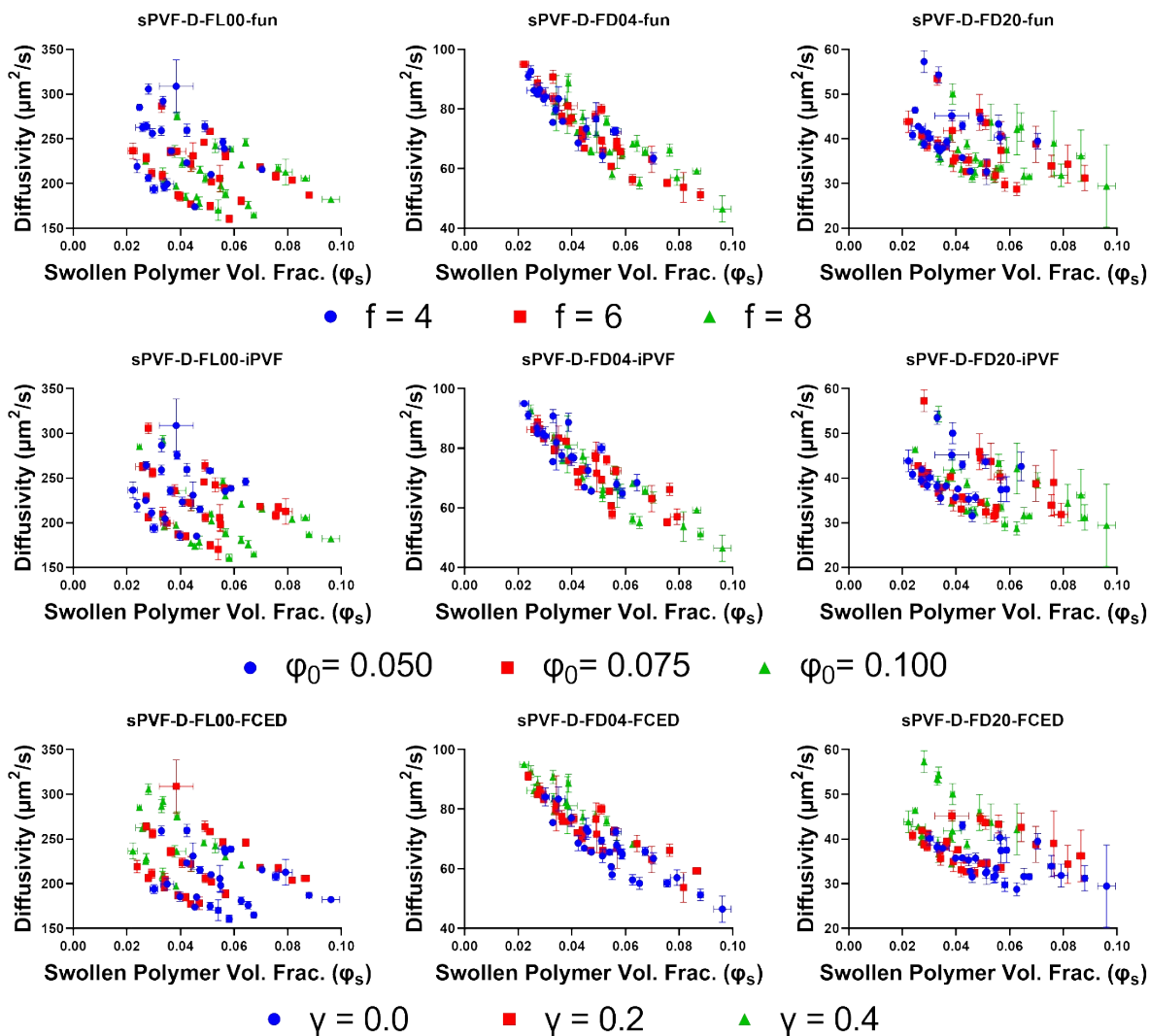
<https://doi.org/10.6084/m9.figshare.21047074.v2>

Written Protocols:

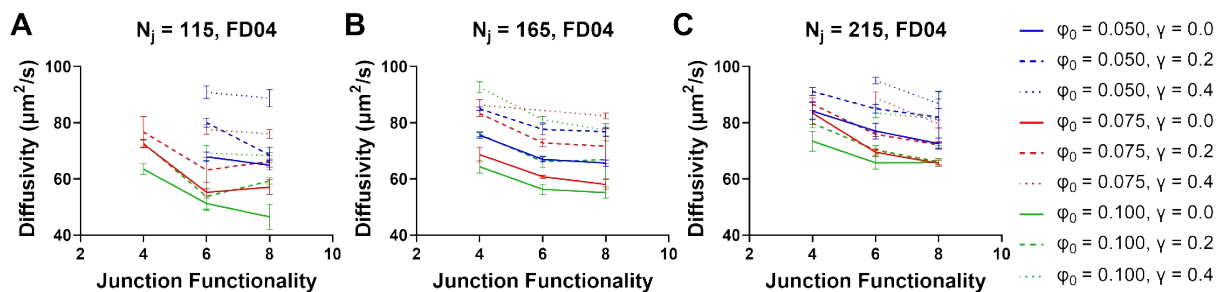
<https://doi.org/10.6084/m9.figshare.21606312.v1>



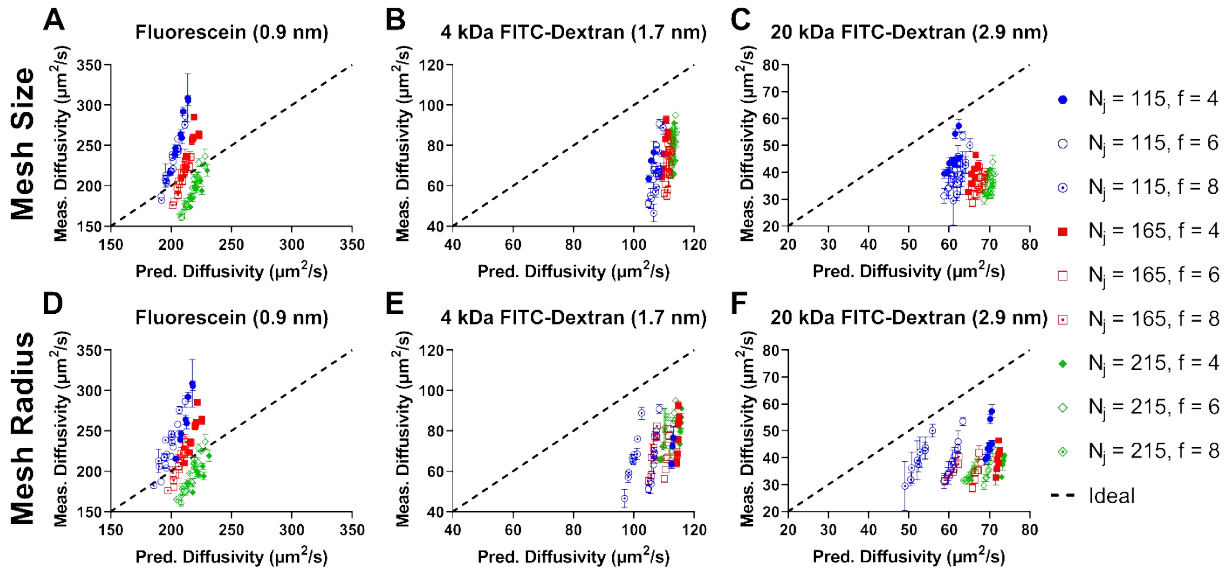
Supplementary Figure S1. Surface accumulation of (A) fluorescein and (B) 20 kDa FITC-dextran at the edge of multi-arm PEG hydrogels. ($f = 6, N_j = 165, \varphi_0 = 0.075, \gamma = 0.2$) Fluorescein, as a small, non-polymeric solute (0.9 nm hydrodynamic diameter)) shows negligible surface accumulation, whereas the larger 20 kDa FITC-dextran (2.9 nm) shows significant accumulation. Solute size-dependent surface accumulation was consistent across all hydrogel formulations.



Supplementary Figure S2. Grid of how junction functionality (f), initial polymer volume fraction (ϕ_0), and frequency of chain-end defects (γ) each affect the relationship between swollen polymer volume fraction and solute diffusivity for fluorescein (FL00), 4-kDa FITC-dextran (FD04), and 20 kDa FITC-dextran (FD20). These three structural parameters have redundant effects on the overall relationship (simultaneously decreasing swollen polymer volume fraction and increasing diffusivity or vice versa), while degree of polymerization between junctions (N_j) has a unique effect.



Supplementary Figure S3. Example of direct relationships between a structural property (junction functionality, f) and a hydrogel property (diffusivity of 4 kDa FITC-dextran). Formulations are sub-grouped by the degree of polymerization between junctions (N_j), initial polymer volume fraction (φ_0), and frequency of chain-end defects (γ). From these figures, we concluded that increasing junction functionality generally decreases the diffusivity of 4 kDa FITC-dextran, as seen in Table 1.



Supplementary Figure S4. Prediction-measurement comparison for all hydrogel formulations based on mesh size (A-C) and mesh radius (D-F). Ideal: 1:1 correlation between prediction and measurement.