Experimental and theoretical investigation of glycol-based hydrogels through waterflooding processes in oil reservoirs using molecular dynamics and dissipative particle dynamics simulation.

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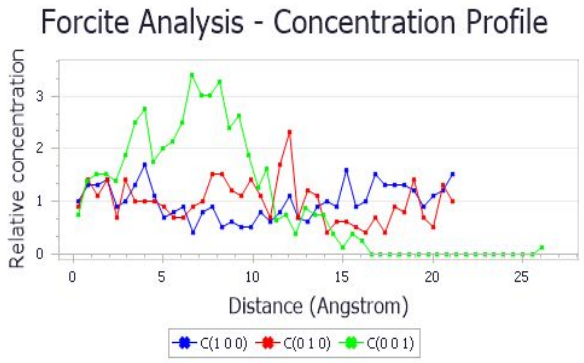
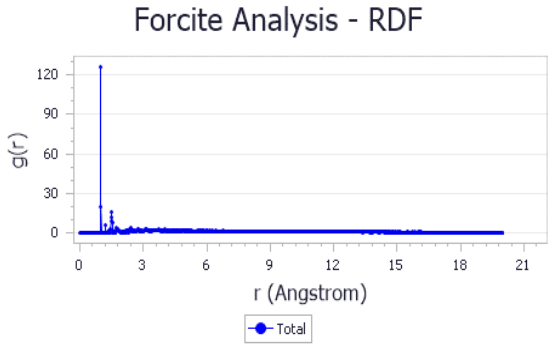
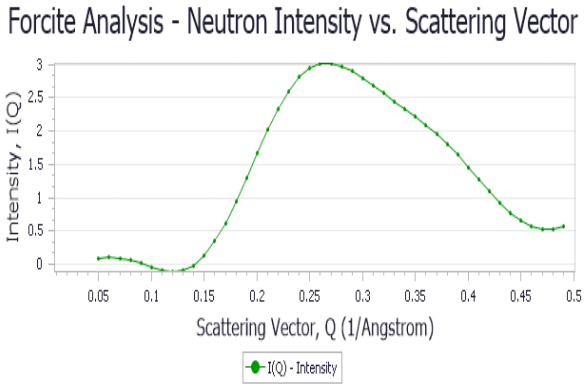
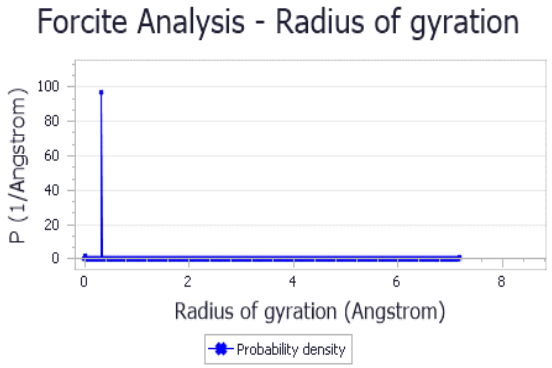
(a) Forcite Analysis in case of PEG-hydrogel

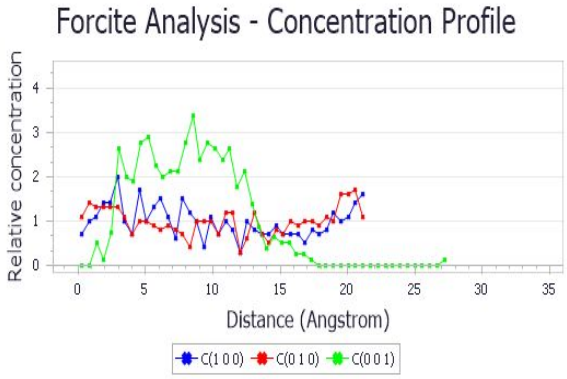


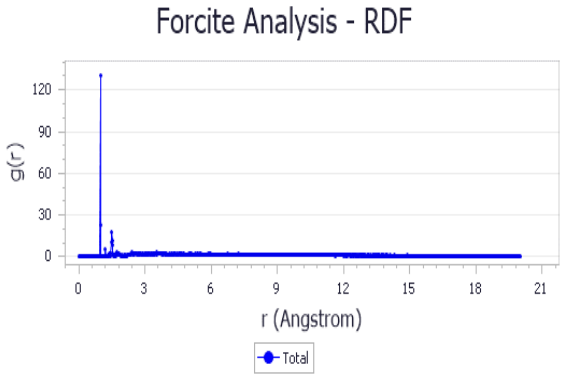






(b) Forcite Analysis in case of PPG-hydrogel





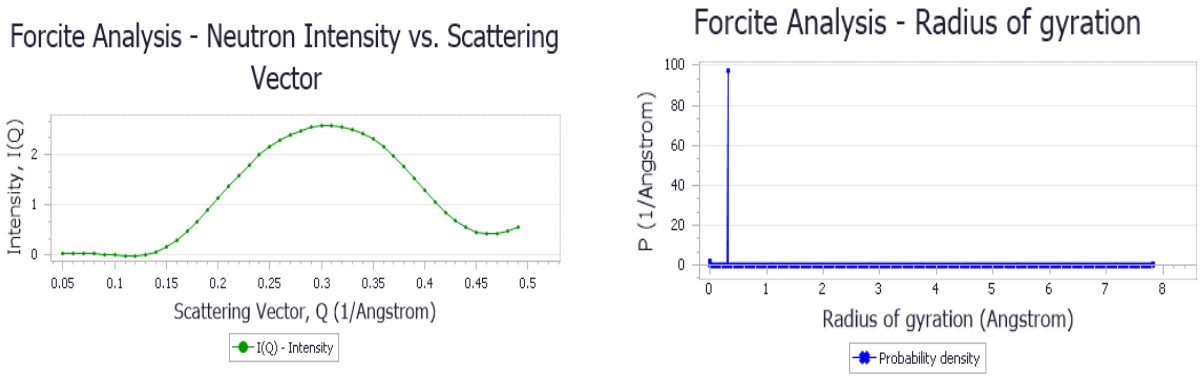
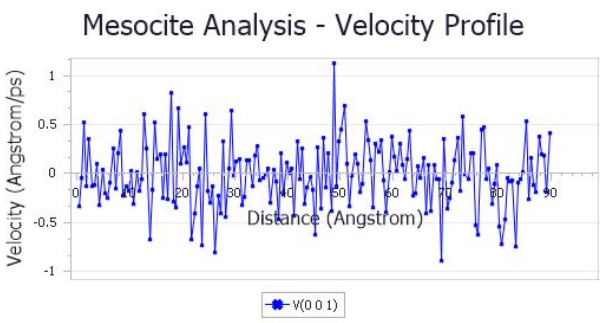
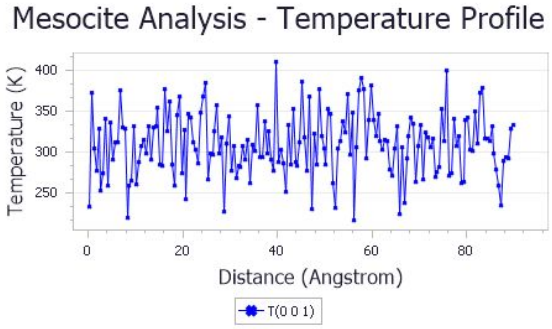


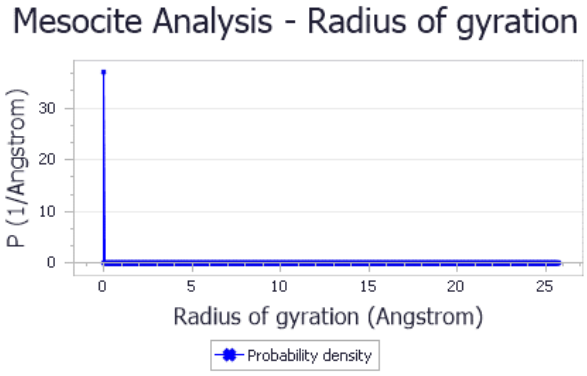
Figure S1: Concentration profile, radial distribution function (RDF), scattering, and radius of gyration obtained from Forcite Module analysis in case of PEG-and PPG-hydrogels respectively

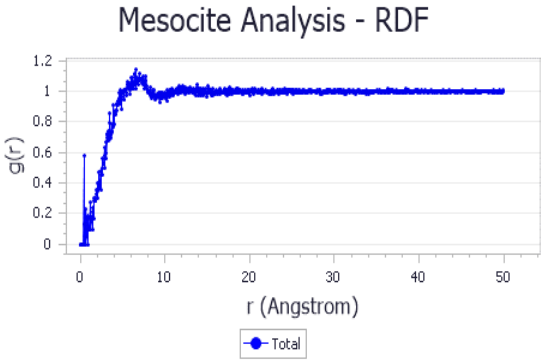
Figure S1 indicates that an increase in the radius of gyration (R_g) confirms that the molecules are more overextended and aligned perpendicularly towards the water/ oil boundary.

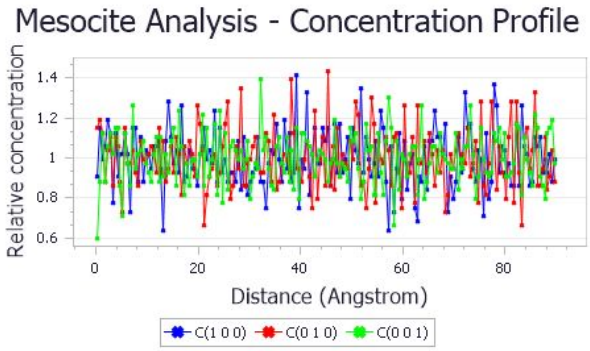
(a) DPD analysis results in the case of PEG-hydrogel



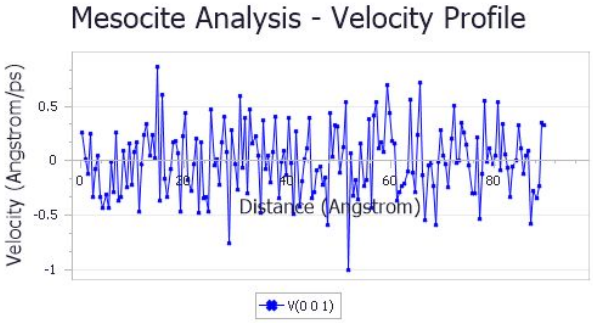


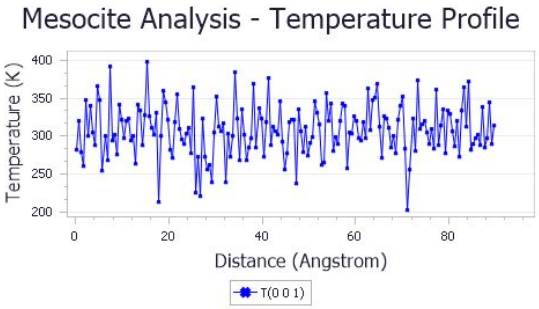






(b) DPD analysis results in the case of PPG-hydrogel





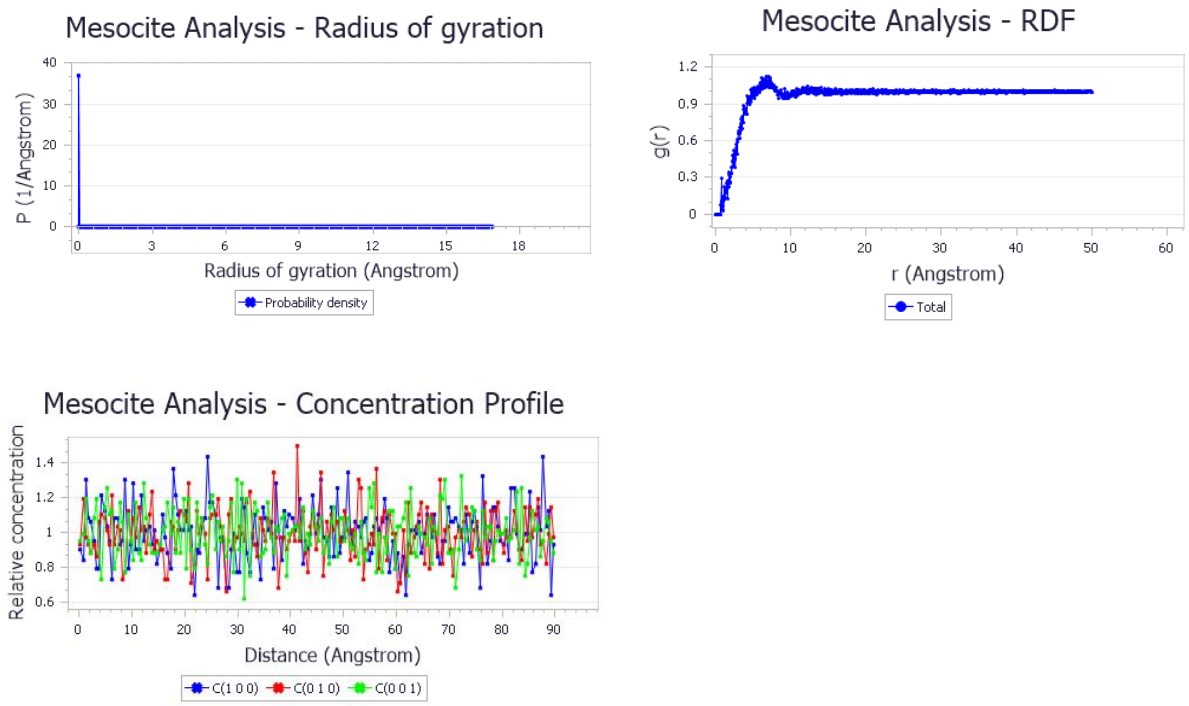


Figure S2: The DPD simulation analysis in case of PEG-and PPG-hydrogels

1. Spectral analysis

FT-IR bands of the **PPG and PEG surfmers** are displayed in Figures (S3 a and b), respectively. The broadbands at 3434 - 3390 cm^{-1} resort to (-OH) group vibration. The intense bands at 2981 cm^{-1} and 2882 cm^{-1} correspond to the CH_2 symmetrical stretching vibration. The broadband at1720 and1635 cm^{-1} was assigned to the C=O stretching vibration of conjugated anhydride. The band at 1635 cm^{-1} represents the C=C of the alkene stretching. The band at 1453 cm^{-1} resorts to CH_2 group scissoring. Bands at 1381 cm^{-1} and 1296 cm^{-1} can be attributed to C-O-C asymmetric stretching vibrations. The intense bands at 945 and 815 cm^{-1} are assigned to the stretching vibrations of the C-C skeleton. IR spectra of poly(propyleneglycol) based hydrogels **(PPG- hydrogel)** and poly(ethylene glycol) based hydrogel **(PEG-hydrogels)** are displayed in Figures S3 c and d. They exhibit broadband in the range of 3500-3000 $cm^{-1,}$ which resorted to (-OH and -NH) stretching vibrations in AMPS and AM, respectively. The disappearance of characteristic peaks of vinyl groups indicates that the complete polymerization has been achieved [1-2].

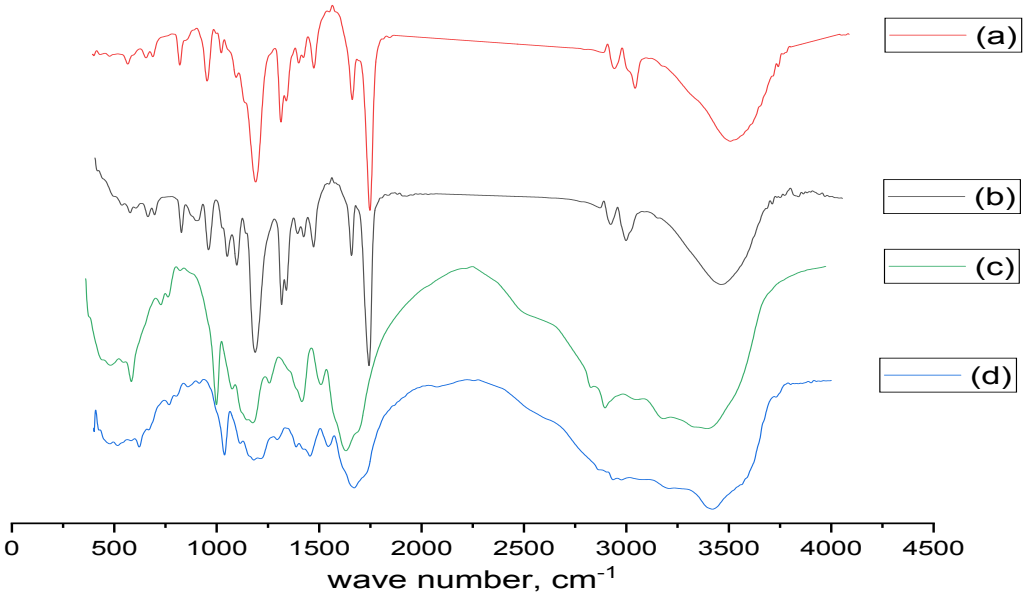


Figure S3: FT-IR spectra of (a) PPG-surfmer; (b) PEG-surfmer; (c) PPG-hydrogel; and (d) PEG-hydrogel

^{1}H-NMR spectra of PEG- and PPG surfmers and hydrogels, as displayed in Figure S4, indicate that PEG- and PPG-surfmers show nearly similar chemical shifts. Moreover, PEG- and PPG- hydrogels exhibit the characteristic chemical shifts of surfmers in addition to typical chemical shifts of monomers, as summarized in Table S1. The absence of a vinyl bond shift confirms complete polymerization occurrence [2].

Table S1: Summary of chemical shifts (^{1}H-NMR)

Cpd	Chemical shift (δ, ppm)	Peak identification
PEG- and PPG-surfmers	1.93 (S, 6H, 2(-**CH_3**)	Terminal alkyl groups
	2.2- 4.2 (s, 4H, O-**CH_2**- **CH_2**-O) 2.2- 4.4 (t, 6H, O-**CH_2**- **CH_2**-**CH_2**-O)	characteristic chemical shifts of ethylene oxide typical chemical shifts of propylene oxide
	5.72 - 5.80 (s, 4H, 2 (C=**CH_2**)	characteristic chemical shifts of vinyl bond
PEG- and PPG-hydrogels	1.02 (s, 1H, **-OH**)	Hydroxyl group in AMPS monomer
	6.60 (s, 2H, (**NH_2**-C=O)	Amide group in AM monomer
	0.95- 1.80 (pendant methyl and backbone methylene groups)	

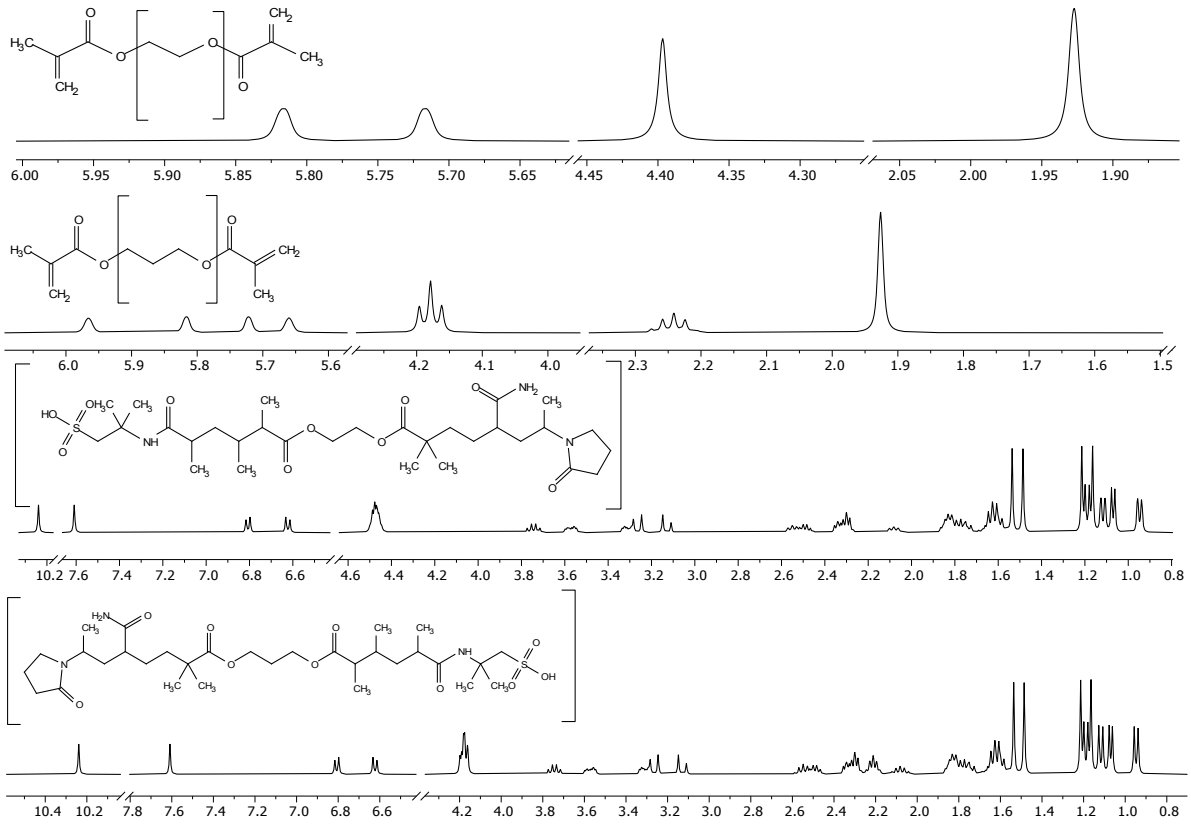


Figure S4: [1]H-NMR of PEG- and PPG- surfmers and hydrogels

The TGA-thermograms of the PEG- and PPG-hydrogels as displayed in Figure S5 exhibit four degradation stages; the first phase occurs at 25-250°C and is assigned to the vaporization of bounded water [3-4]. The second stage at 250-325°C related to the disintegration of the amide groups on the hydrogel chains [5-6]. The third stage at 325-385°C corresponds to the complete degradation of other side chain moieties, including sulfonic groups in AMPS and pyrrolidone rings, in addition to the breakdown of carbon-nitrogen bonds [6-7]. The fourth stage occurs at 385-600°C and related to the complete degradation and carbonization of the polymer skeleton [6]. TGA- thermograms of PEG- and PPG- hydrogels are closely associated with each other, as exhibited in Figure S5. However, at a temperature higher than 385°C, the weight loss in PPG-hydrogel is higher than the weight loss in PEG-hydrogel. This thermal behavior may resort to PPG has a longer carbon chain than PEG, so by thermal degradation, its weight loss is higher than PEG.

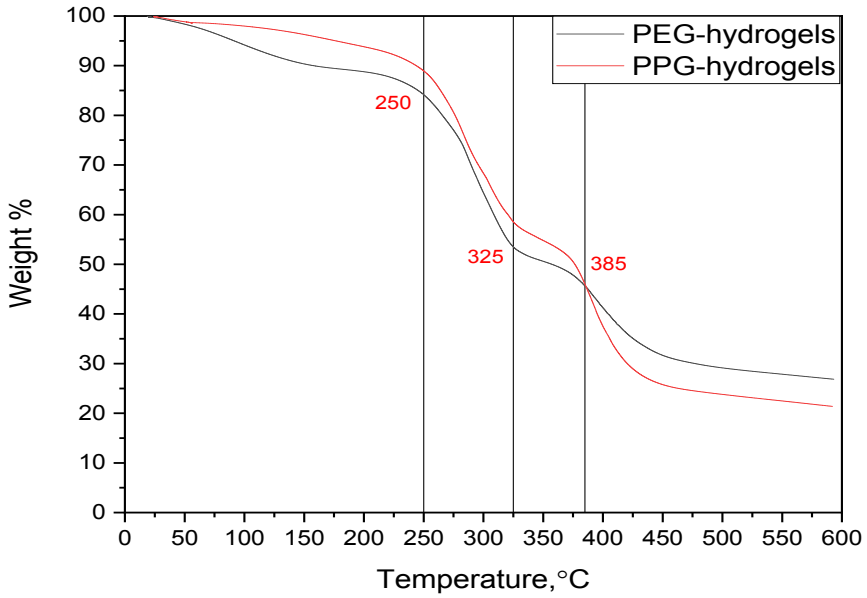


Figure S5: TGA- thermograms of PEG- and PPG hydrogels

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