

Modeling of a two-stage polymerization considering glass fibre sizing using molecular dynamics

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Electronic Supplementary Information

1 Benzene distribution

In order to be able to investigate the spatial distribution of the various constituents, a reasonable approach must be chosen. Especially molecules like (P-)MDI or the unsaturated polyester consist of numerous atoms, which can be distributed widely over the system. Reducing them to their centre of mass would not result in a useful distribution. Instead, specific functional groups are chosen. For example, all molecules (except the coupling agent) contain benzene rings. In addition, they can be distinguished by their uniquely bonded atoms. This allows easy tracking of all benzene rings across the system and during polymerization reactions.

Figure S1 shows the styrene benzene during radical polymerization. During the reaction, the small styrene molecules level out the initial uneven distribution due to diffusion. The benzene distribution of the larger molecules such as (P-)MDI and the unsaturated polyester is shown in Figure S2 and Figure S3, respectively. Despite the fact that they also exhibit some additional artificial charges during the polyurethane reaction, significant diffusion is not observed. In contrast, they show diffusion during the radical polymerization, as they smooth the initial uneven distribution.

2 Silicon distribution of coupling agent

For the distribution of the coupling agent, hence γ -MPS, the silicon atom of the molecules is used to represent the position of the free hydrolysed as well as the coupling agent pre-attached to the fibre surface. Figure S4 shows this distribution during the polymerization reactions. As before, no significant diffusion can be observed during the polyurethane reaction. Nevertheless, the pre-attached layer with the very high peak at the fibre surface as well as the absence of γ -MPS in the pure resin layer can be observed. During the free radical polymerization, as with the other constituents, diffusion takes place, smoothing out the initial distribution.

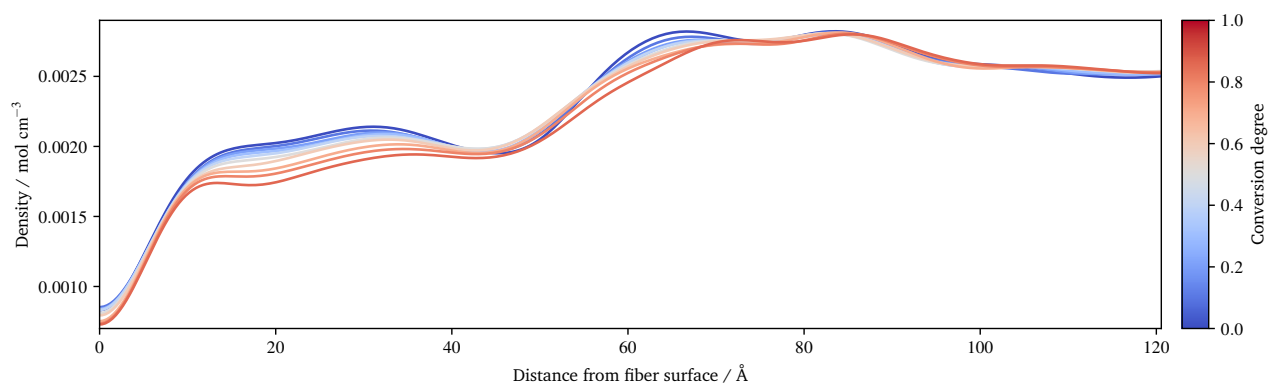


Fig. S1 Spatial distribution of the benzene of styrene during radical polymerization.

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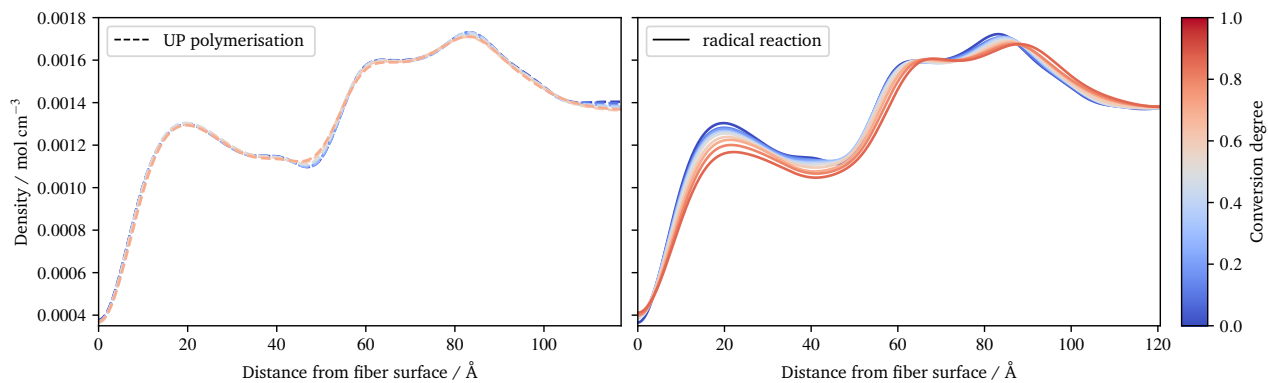


Fig. S2 Spatial distribution of benzene of (P)-MDI during polyurethane reaction (left) and radical polymerization (right) for different conversion degrees.

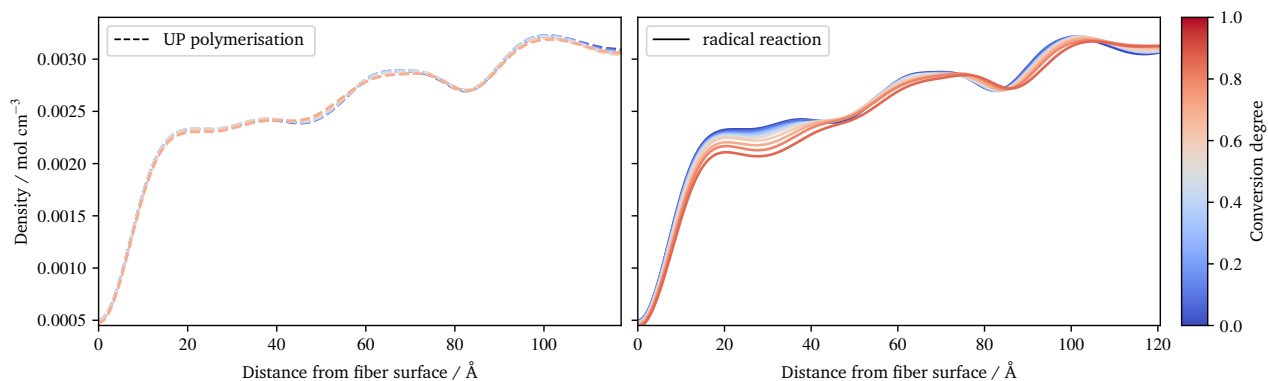


Fig. S3 Spatial distribution of benzene of the unsaturated polyester during polyurethane reaction (left) and radical polymerization (right) for different conversion degrees.

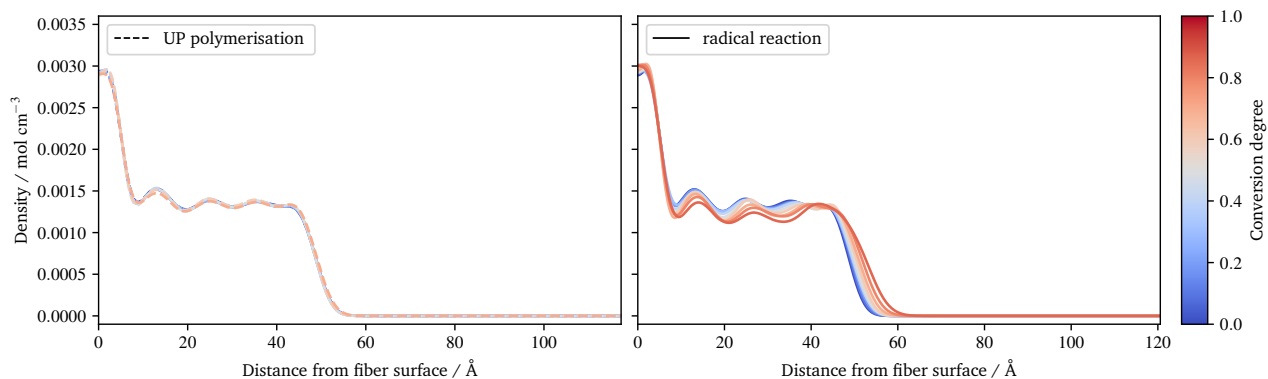


Fig. S4 Spatial distribution of silicon atoms of γ -MPS molecules during polyurethane reaction (left) and radical polymerization (right) for different conversion degrees.