MATHEMATICAL MODELING FOR 1,6-HEXANEDIOL DIACRYLATE PHOTOPOLYMERIZATION IN PRESENCE OF OXYGEN

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A fundamental model was developed for photopolymerization of 1,6-hexanediol diacrylate (HDDA) with the bifunctional initiator bis-acylphosphine oxide (BAPO) to account for inhibition effects of oxygen. Real-time FTIR vinyl-group conversion data were used to support parameter estimation and model testing. A sensitivity-based estimability analysis confirmed that all of the oxygen-related parameters were estimable using data obtained from 8 dynamic experiments. The resulting model and parameter estimates provide good predictions for experiments involving thin films up to 12 μm, with a variety of BAPO levels (1 wt% to 4 wt%) and relatively low light intensities (200 to 1000 W/m2).[1]

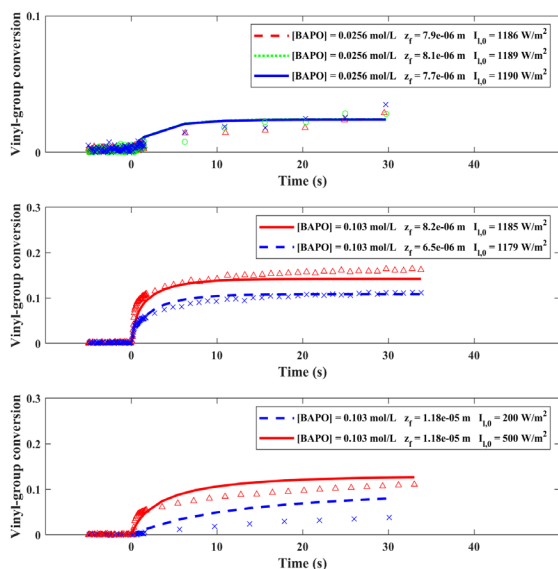Because spatial variation in oxygen concentration and other species were neglected in the current model, it does not do an adequate job of predicting conversion vs. time behaviour in thick films using high light intensities. A more comprehensive model is being developed using partial differential equations that account for oxygen and monomer diffusion to account for gradients in species concentrations. The p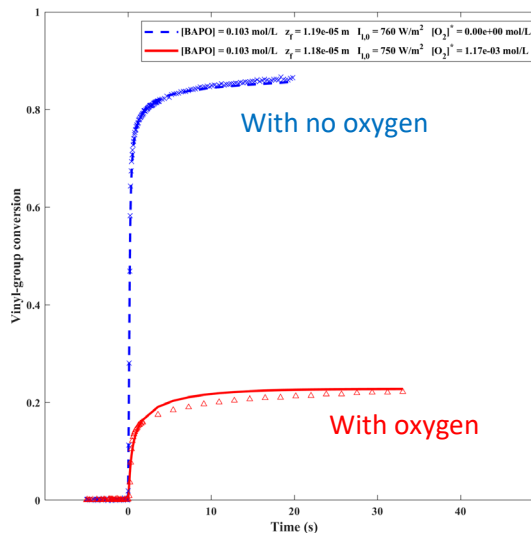arameters estimates obtained in the current study will be used as starting values for this more comprehensive model, which should provide more accurate predictions for thicker films.

Figure 1 – Experimental data and corresponding model predictions for experiments with oxygen at air level

Figure 2 – Model predictions and the corresponding FTIR measured values for experiments in the absence (✗) and in the presence of oxygen (△) using [BAPO] = 4 wt%, z_f ~ 12 μm, and $I_{l,0}$ ~ 750 W/m2

Reference

[1]   Vo, A-D D., Abdi, K., Tak, J.F.U., Vandervelden, L., Willemse, R.X.E., Vanderlinden, M.N., Iedema, P.D., McAuley, K.B. (2022). Mathematical Modeling for 1,6-Hexanediol Diacrylate Photopolymerization in Presence of Oxygen. *Can. J. Chem. Eng.*, accepted 2022.