COARSE-GRAINED MODELS FOR FRONTAL PHOTOPOLYMERISATION FOR NON-PLANAR MATERIAL ASSEMBLY

MG Ridwan[1], Alessandra Vitale[2], and João T. Cabral[1]

[1]Department of Chemical Engineering, Imperial College London, London SW7 2AZ, United Kingdom
[2]Department of Applied Science and Technology, Politecnico di Torino, Corso Duca degli Abruzzi, 24, 10129 Torino, Italy

We introduce a series of coarse-grained models for frontal photo-polymerisation (FPP), with varying degrees of complexity, seeking to describe material fabrication by FPP for a wide range of chemistry and process parameters. FPP is a light-driven directional solidification process which yields conversion profiles that propagate in time, in the form of travelling waves, generally under conditions of strong light attenuation and limited mass transfer. Under certain conditions, the travelling conversion profiles are time-invariant, while in general these evolve with time due to a complex interplay of mass or heat diffusion, and polymer network properties. In the simplest form, our models comprise a single equation of motion for a (scalar) conversion fraction φ and a generalised Beer-Lambert law accounting for the spatio-temporal evolution in conversion [1, 2, 3]. The non-trivial coupling of these equations can describe a range of systems, but higher order chemical conversion schemes are needed to account for experimental observations of solidification kinetics, light attenuation and spatio-temporal monomer-to-polymer conversion, acquired by profilometry, AFM and spectroscopic imaging. Our framework provides a range of simple descriptive models, with a small number of system parameters, yet providing a predictive ability for ubiquitous solidification and patterning processes, including 3D printing and non-planar assembly of materials generated via photopolymerisation.

This project received funding from the #horizoneurope20212027 programme under the Marie Skłodowska-Curie Doctoral Networks (MSCA-DN) grant agreement No 101073432.

ESPERANTO
Enhancing the Sustainability of PhotopolymERs ANd phoToinduced prOcesses

Funded by the European Union

1. Cabral, J.T.; Hudson, S.D.; Harrison, C.; Douglas, J.F. Frontal photopolymerization for microfluidic applications. *Langmuir* **2004**, *20*, 10020–10029.
2. Cabral, J.T.; Douglas, J.F. Propagating waves of network formation induced by light. *Polymer* **2005**, *46*, 4230–4241.
3. Vitale, A.; Hennessy, M.G.; Matar, O.K.; Cabral, J.T. A Unified Approach for Patterning via Frontal Photopolymerization. *Adv. Mater.* **2015**, *27*, 6118–6124.