

Poster 6

Population Balance Model for Emulsion Polymerisation Under Pseudo-Bulk Conditions: Combined Particle Size Distribution and Molecular Weight Distribution

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The aim of this research is to develop a model of the emulsion polymerisation process accounting for particle size distribution (PSD) and molecular weight distribution (MWD). Mathematical models provide theoretical insight into this complex process as well as proving invaluable for process design, optimisation and control. The final latex product properties are strongly correlated with the entire PSD and with the MWD. These complex objectives are driven by multiple sub-processes (nucleation, growth and coagulation).

This work will address a detailed population balance model of both the PSD and MWD. The PSD information is incorporated through a population distribution of the polymer particles with respect to their size in combination with a population distribution of the total live polymer radicals/particle¹. The MWD information is incorporated through population balances on the live radicals and dead polymer chains distributed with respect to their chain length. Computational efficiency is maximised by employing the method of moments for the radical and polymer populations². This moments approach is consistent with the state-of-the-art in terms of measurements (of the global average molecular weights). An assumption of pseudo-bulk reaction conditions is assessed with respect to its effect on PSD and MWD, thus elucidating the effect of compartmentalisation on the process. Model validation is being undertaken using capillary hydrodynamic fractionation (CHDF) to measure PSD and gel permeation chromatography (GPC) for global molecular weight.

References:

- [1] Immanuel, C. D., Doyle III, F. J., Cordeiro, C. F., & Sundaram, S. S.(2003). *AIChE Journal*, 49, 1392-1404.
- [2] Park, M. J., Dokucu, M. T., Doyle III, F. J.(2005). *Macromol. Theory Simul.*, 14, 474-490.