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# POPULATION BALANCE APPROACH FOR PREDICTING POLYMER PARTICLES MORPHOLOGY

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Polymer particles morphology can be defined as a pattern of phase-separated domains comprising a multi-phase polymer particle [1]. Properties of a polymer particle strongly depend on its morphology, and thus the control of particle morphology is a key factor for success in producing high-quality polymers materials, such as coatings, adhesives and additives [2].

Currently, an accurate prediction of particles morphology is still a challenge due to its complexity. Several modelling approaches, describing the dynamics of the morphology of a single particle, have been suggested in the last few years [3, 4, 5]. However, the single-particle approaches only provide a partial view of realistic systems, containing millions of particles. Furthermore, such models are computationally demanding even with the use of High Performance Computers.

In contrast to currently available computationally expensive and restricted single-particle approaches, we recently proposed [6] a Population Balance Equations (PBE)-based model to predict the size distribution of polymer agglomerates, composing the morphology of interest. The PBE model provides a view of the whole population of polymers particles, taking into account the relevant kinetic and thermodynamic effects behind the morphology formation [7].

The numerical treatment of such a model is not trivial due to the following difficulties. First, reactants

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and particles concentrations may be coupled, leading to a challenging integration of the resulting system of equations. Then, numerical solutions require substantial computational resources since, in practical engineering processes, the computed solution may extend over several orders of magnitude and can exhibit very sharp moving fronts.

We propose three novel numerical approaches which help to obtain accurate and efficient numerical solutions of the introduced model. While the Optimal Scaling (OS) [8] procedure, designed for the dimensionless reformulation of equations expressed in physical units, assures computationally tractable orders of magnitude for the PBE terms, the novel Generalised Method of Characteristics (GMOC) allows for the integration of PBE models with coupled dynamics. Finally, the Laplace Induced Splitting Method (LISM) combines a splitting integration scheme with Laplace induced analytical solutions to enhance accuracy and speed of the numerical treatment.

We discuss the main features of OS, GMOC and LISM methodologies and present numerical results demonstrating the potential of the proposed techniques.

## References

[1] Sawye L.C., Grubb D.T. (1987). *Introduction to polymer morphology*. Dordrecht, Netherlands: Springer.

[2] Schuler B., Baumstark R., Kirsch S., Pfau A., Sandor M., Zosel A. (2000). *Structure and properties of multiphase particles and their impact on the performance of architectural coatings*. Progress in Organic Coatings, 40(1-4), 139-150. https://doi.org/10.1016/S0300-9440(00)00136-3

[3] Asua J.M., Akhmatskaya E. (2011). *Dynamical modelling of morphology development in multiphase latex particles*. Springer Berlin Heidelberg.

[4] Akhmatskaya E., Asua J.M. (2012). *Dynamic modeling of the morphology of latex particles with in situ formation of graft copolymer*. Journal of Polymer Science Part A: Polymer Chemistry, 50(7), 1383-1393. https://doi.org/10.1002/pola.25904

[5] Akhmatskaya E., Asua J.M. (2013). *Dynamic modeling of the morphology of multiphase waterborne polymer particles*. Colloid and Polymer Science, 291, 87-98. https://doi.org/10.1007/s00396-012-2740-9.

[6] Rusconi, S. (2018). *Probabilistic Modelling of Classical and Quantum Systems*. PhD thesis, UPV/EHU - University of the Basque Country. http://hdl.handle.net/20.500.11824/812

[7] Hamzehlou S., Leiza J.R., Asua J.M. (2016). *A new approach for mathematical modeling of the dynamic development of particle morphology*. Chemical Engineering Journal, 304(15), 655-666. https://doi.org/10.1016/j.cej.2016.06.127

[8] Rusconi S., Dutykh D., Zarnescu A., Sokolovski D., Akhmatskaya E. (2019). *An optimal scaling to computationally tractable dimensionless models: Study of latex particles morphology formation*. Computer Physics Communications, 106944. https://doi.org/10.1016/j.cpc.2019.106944

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