Exploitation of flow chemistry and machine learning for the optimization of organocatalyzed ring-opening polymerization

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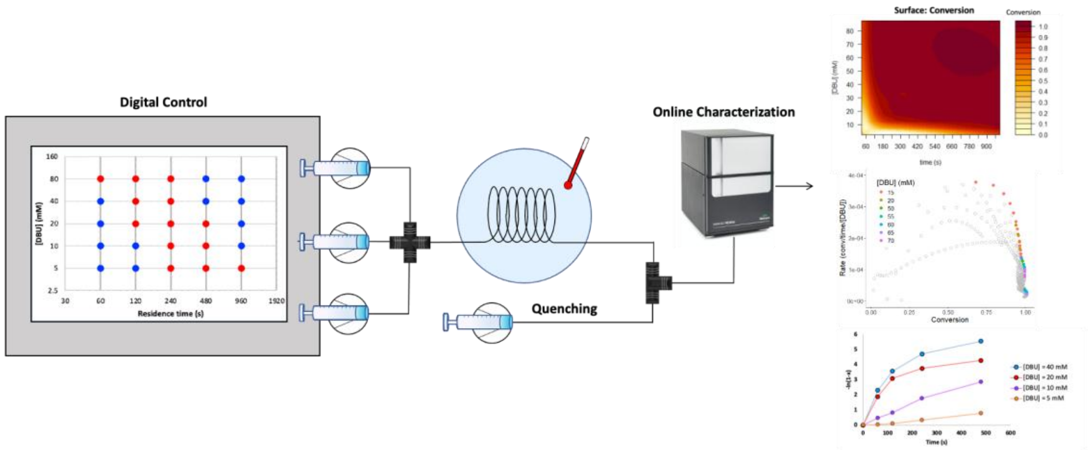
Résumé :

Although polylactide (PLA) is currently the most widely produced degradable polymer, its commercial impact remains modest compared to conventional petrochemically derived plastics.[1] This discrepancy stems from factors such as relatively high production costs, suboptimal material properties for certain applications, and slow degradation rates.[2] Recently, the optimization and discovery of new materials have undergone a major transformation driven by advances in machine learning and automated chemistry, offering new strategies to address these limitations.[3]

In this work, supported by the AMETHYST project of the PEPR DIADEM, we combined continuous flow polymerization with online SEC-HPLC characterization to study the ring-opening polymerization (ROP) of L-lactide catalyzed by DBU. High-throughput experiments were performed across a broad range of residence times, catalyst concentrations, and initiator concentrations. The resulting dataset was analyzed using a non-parametric Kernel-Based Regularized Least Squares (KRLS) model,[4] enabling accurate mapping of reaction kinetics without assuming a predefined functional form. Pareto optimization was then applied to identify conditions that maximize polymer production while minimizing catalyst cost, with predictions validated in both flow and batch. The optimized PLA exhibited high molecular weight, low dispersity, and high conversion. This approach demonstrates how integrating flow chemistry with machine learning can accelerate the discovery and optimization of scalable, well-controlled polymerization processes.[5]



Références :

[1] M. Ghasemlou, C. J. Barrow and B. Adhikari, *Food Packaging and Shelf Life*, 2024, **43**, 101279.
[2] C. Wellenreuther, A. Wolf and N. Zander, *Cleaner Engineering and Technology*, 2022, **6**, 100411.
[3] B. Lin, J. L. Hedrick, N. H. Park and R. M. Waymouth, *Journal of the American Chemical Society*, 2019, **141**, 8921-8927.
[4] I. Braga and M. C. Monard, *Neurocomputing*, 2015, **163**, 106-114.
[5] G. K. K. Clothier, D. Taton and S. Harrisson, *ACS Polymers Au,* ASAP article, doi:10.1021/acspolymersau.5c00071