Digital Twins of Block Copolymer Synthesis by Controlled Polymerization Methods

F. Kandelhard, J. Schymura, E. Pashayev & P. Georgopanos
Helmholtz-Zentrum Hereon, Institute of Membrane Research
Contact: prokopios.georgopanos@hereon.de

Introduction

- Block Copolymers are versatile material class with applications in polymer membranes.
- Larger quantities of materials are necessary, therefore the scale-up of these processes is mandatory (Fig. 1).
- Digital twins can be valuable in this task.
- Established methods for the synthesis of block copolymers are anionic polymerization [1,2] and controlled radical polymerizations (i.e., reversible addition-fragmentation chain-transfer (RAFT) polymerization). [3]
- Development of digital twins for the scale-up of both methods as they have different advantages and disadvantages. [1, 2, 3, 4]

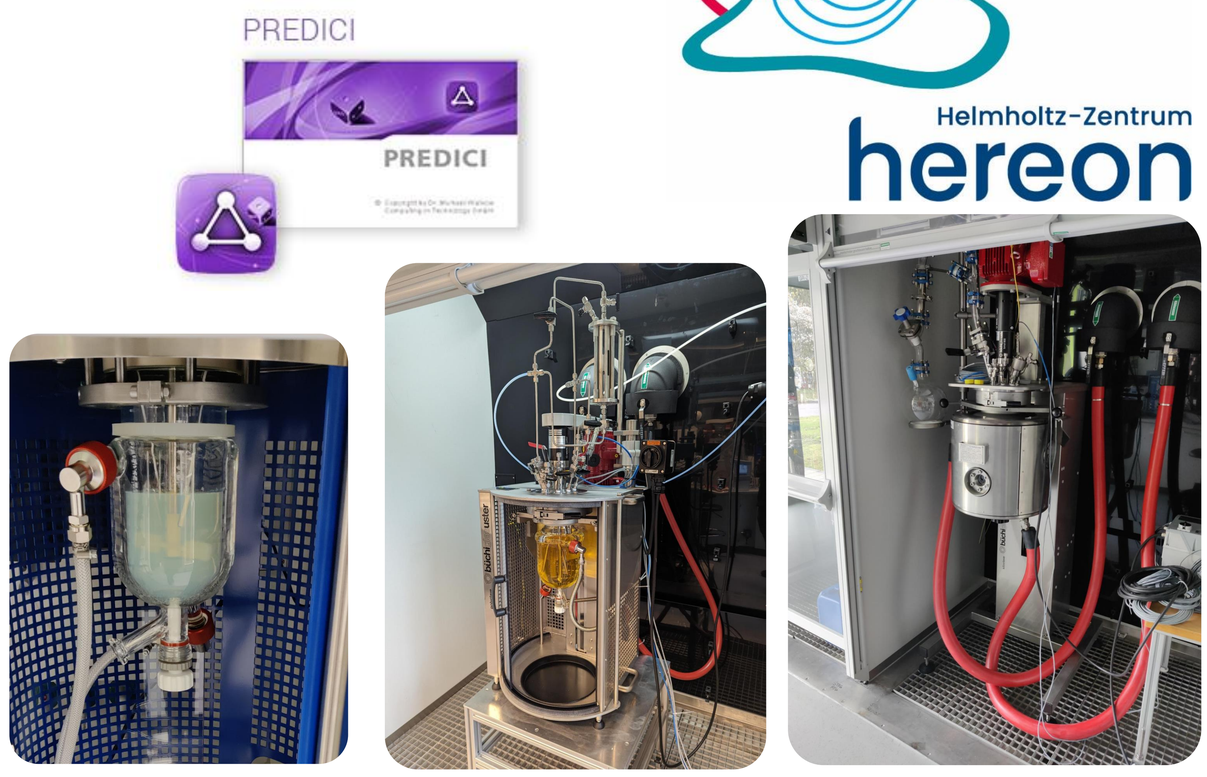

Figure 1: Reactors for the scale-up of lab polymer synthesis with volumes of 0.5 L, 2 L and 15 L.

Anionic Polymerization

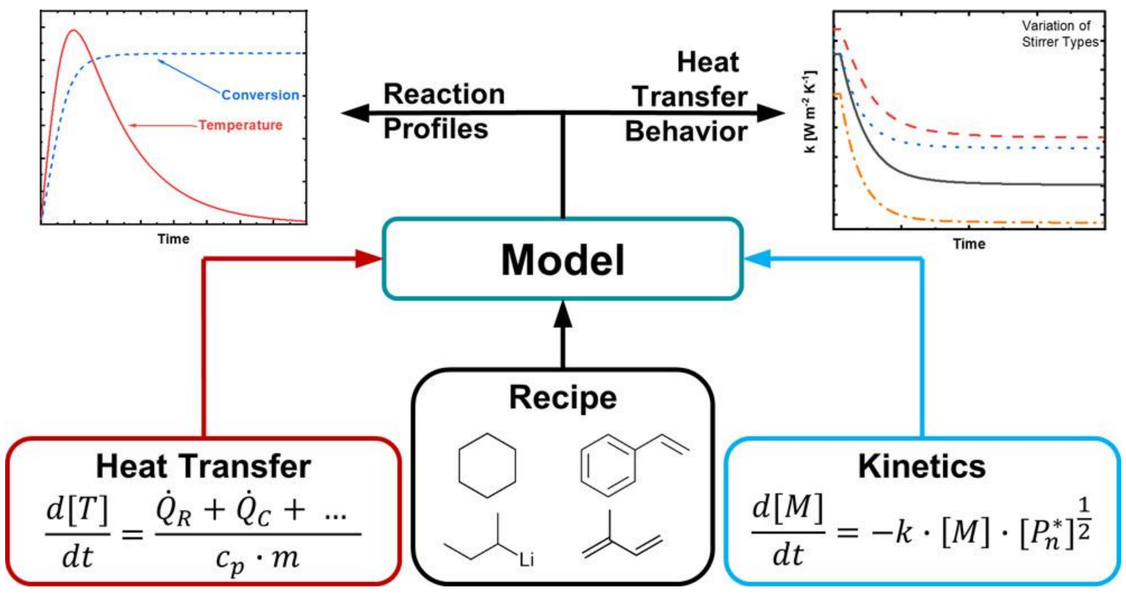

Figure 2: Schematic overview over the combined reaction kinetic and heat transfer model. [1]

- **The model (Fig. 2) is capable to describe the reaction kinetic of the PS-*b*-PI synthesis via anionic polymerization including the full molar mass distributions (Fig. 3b).**
- **The heat transfer behavior including the resulting temperature profiles are simulated (Fig. 3a).**
- **Influence of process parameters as the stirrer speed, the stirrer speed, jacket-temperature, or the recipe can be studied.**

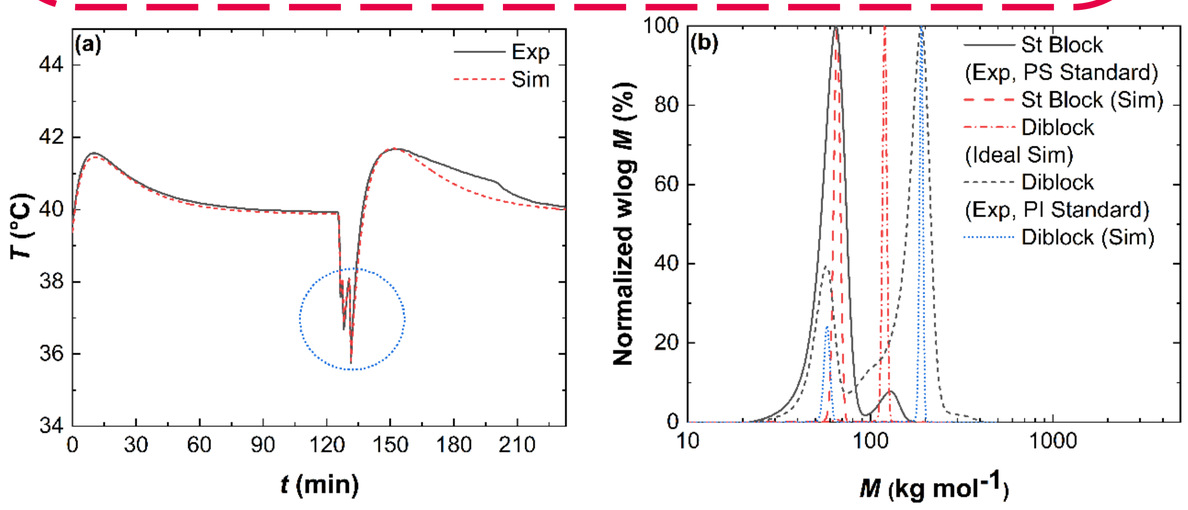

Figure 3: Simulation of the PS-*b*-PI synthesis in cyclohexane. (a) The temperature profile and (b) the molar mass distributions. [2]

RAFT Polymerization

Reaction Kinetics

$$RAFT + P_n^* \underset{k_{frag}}{\overset{k_{add}}{\rightleftharpoons}} RAFT - P$$

Sensitivity Analysis

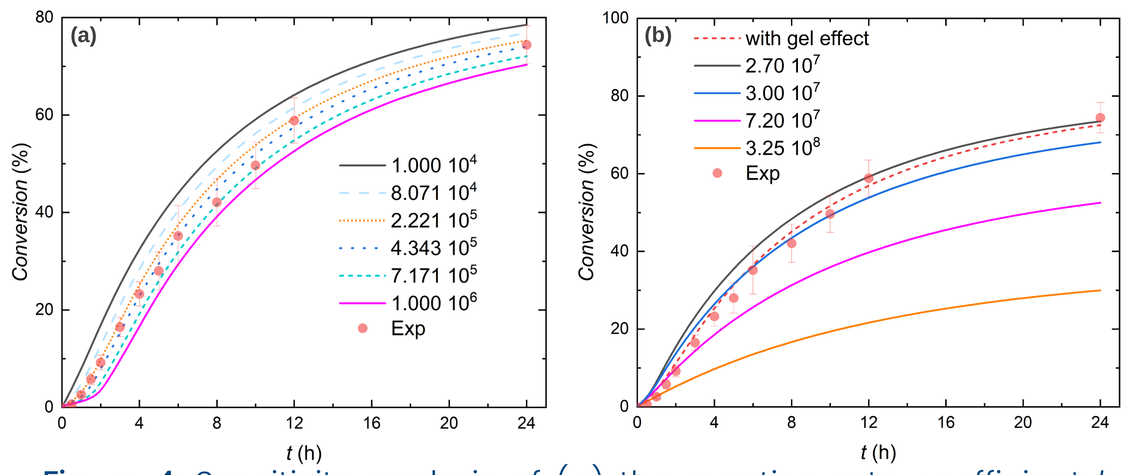

Figure 4: Sensitivity analysis of (a) the reaction rate coefficient k_{add} and (b) termination rate coefficient k_t compared to experimental data (RAFT:Initiator = 18:1). [3]

Simulation

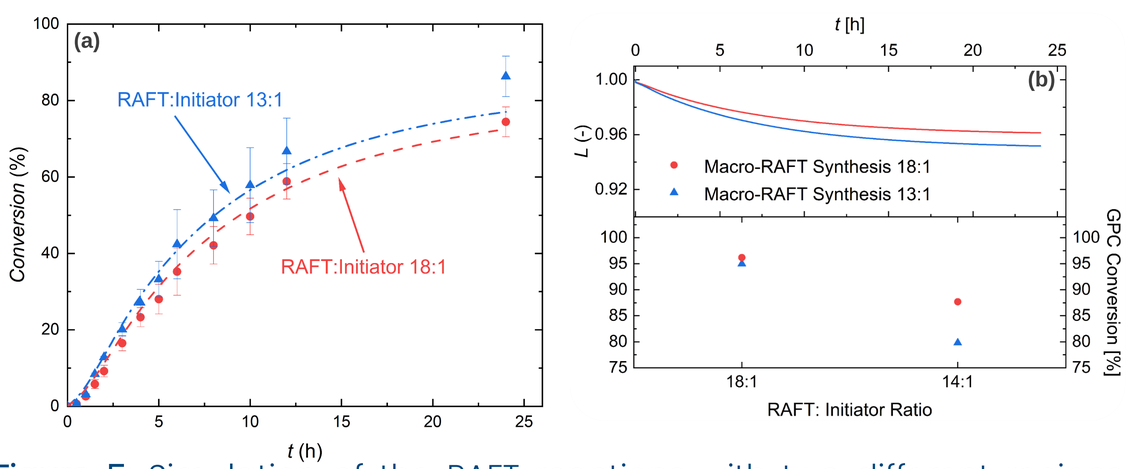

Figure 5: Simulation of the RAFT reactions with two different recipes including (a) the conversion profile and (b) the livingness of the product. [3]

Conclusion & Outlook

- **Digital twins of polymerization processes can assist the scale-up in multiple ways including the optimization of recipes and other process parameters.**
- **Both methods and their twins are still used in the department and are further developed.**

Literature:
[1] F. Kandelhard, P. Georgopanos, *Ind. Eng. Chem. Res.*, **2021,** 60, 30, 11373.
[2] F. Kandelhard, P. Georgopanos, *Chem. Ing. Tech.*, **2023**, 9, 5, 754.
[3] F. Kandelhard et al., *Ind. Eng. Chem. Res.*, **2023,** 62, 22, 8696.
[4] E. Pashayev et al., *Macrom. React. Eng.,* **2023,** 2200068.

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HELMHOLTZ GEMEINSCHAFT

Helmholtz-Zentrum **Hereon** • Max-Planck-Straße 1 • 21502 Geesthacht I Germany • T +49 4152 87-0 • contact@hereon.de • www.hereon.de
Contact: Dr. Prokopios Georgopanos • T +49 4152 87-2402 • prokopios.georgopanos@hereon.de