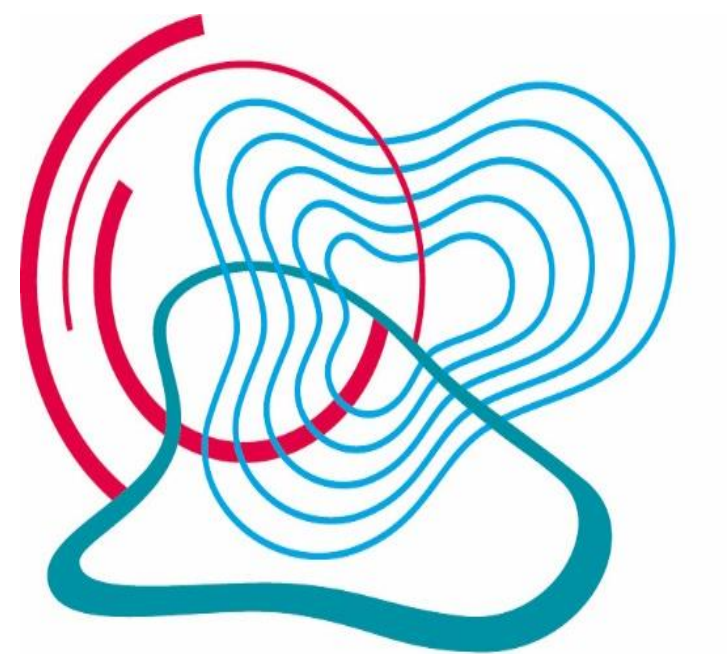


# Reaction Kinetic Modeling of the Synthesis of Polymers of Intrinsic Microporosity



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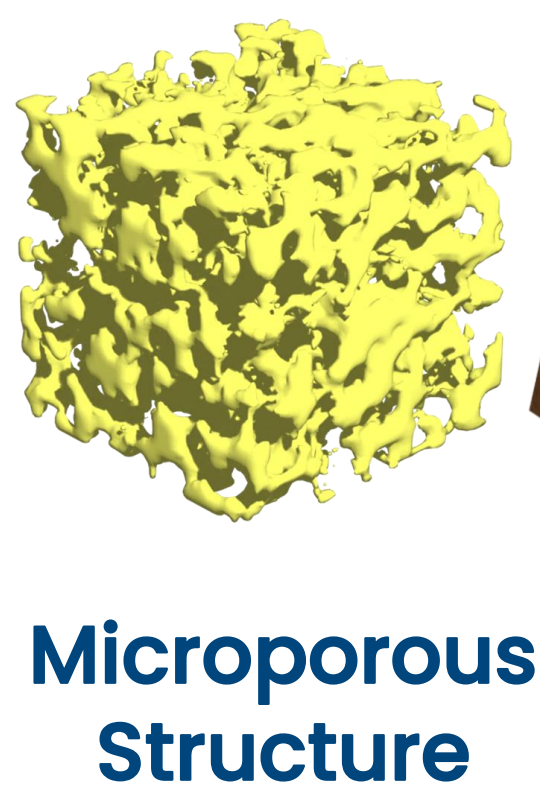
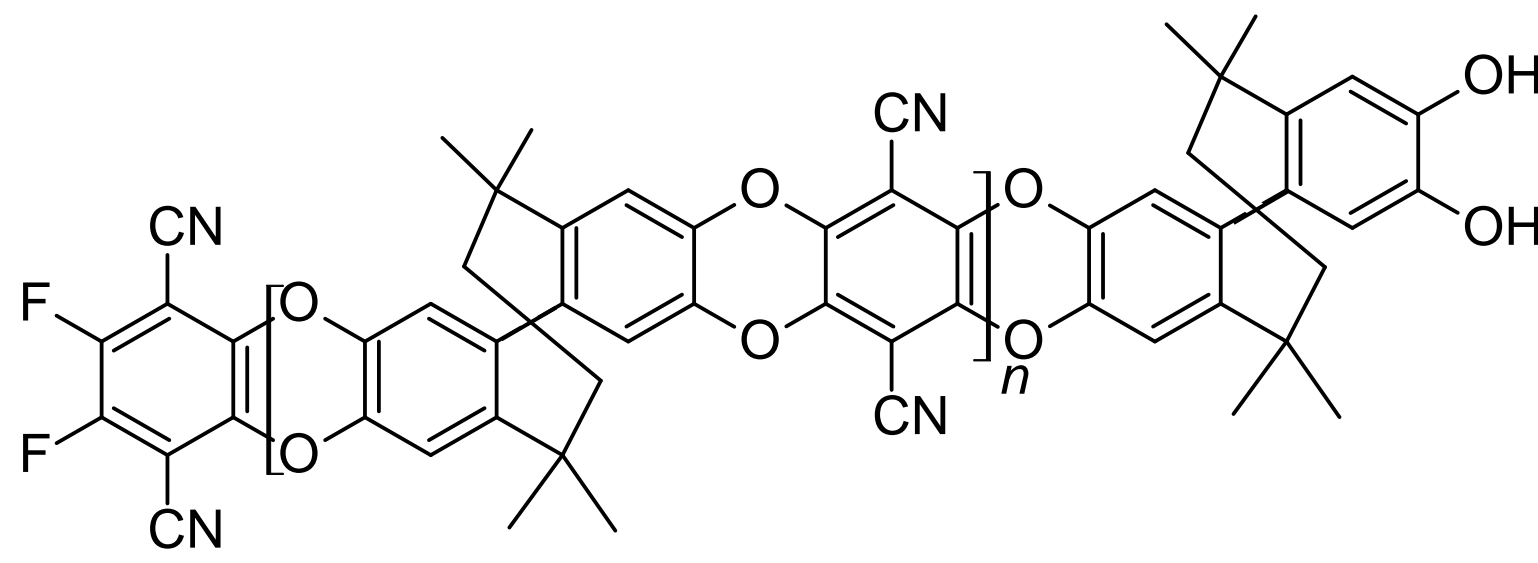
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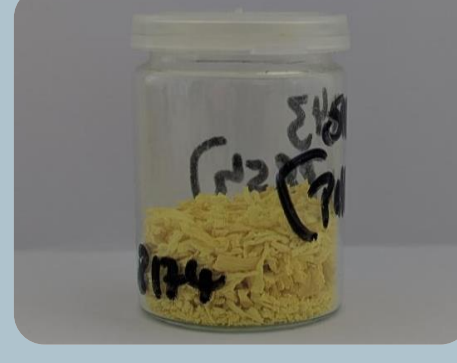
## Applications & Material [1]



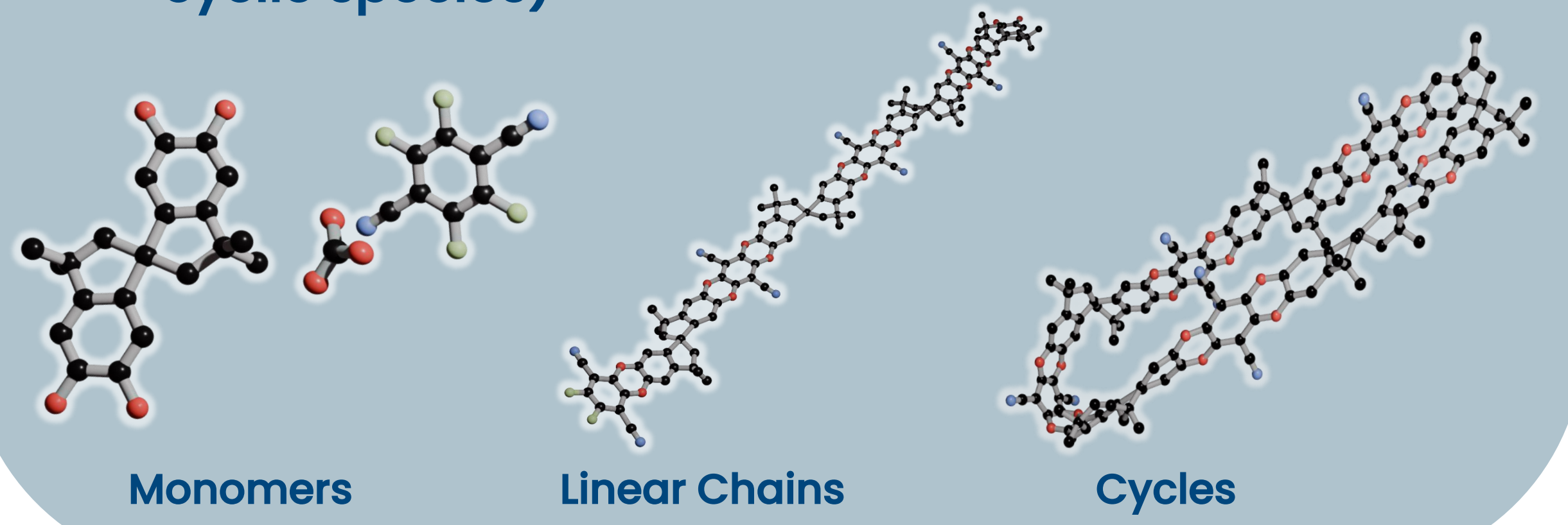
Still a ladder to climb!

## Challenges & Goals

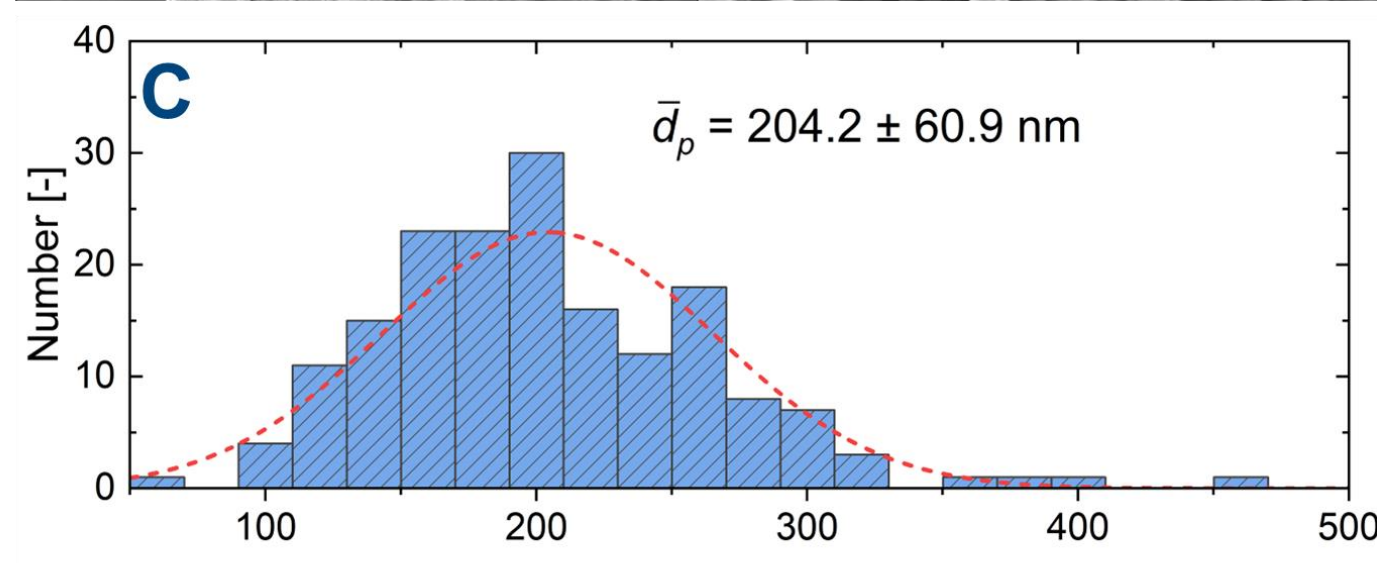
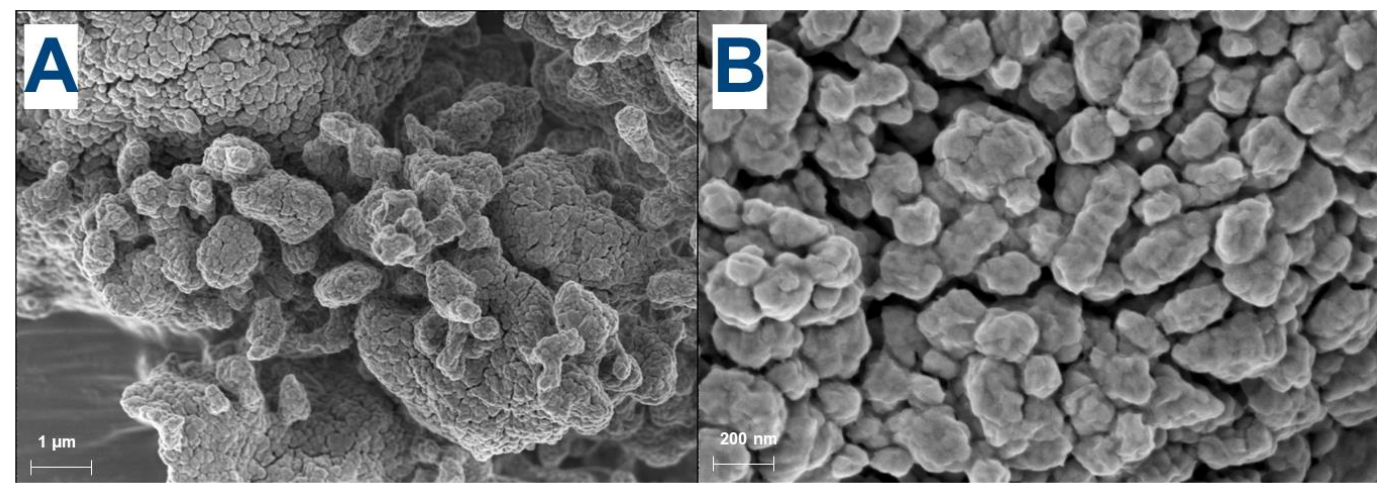
Scale-Up



Understanding Reaction Kinetics & Formation of Polymer during the Reaction (incl. propagation of linear chains, formation of the ether-bonds and cyclic species)



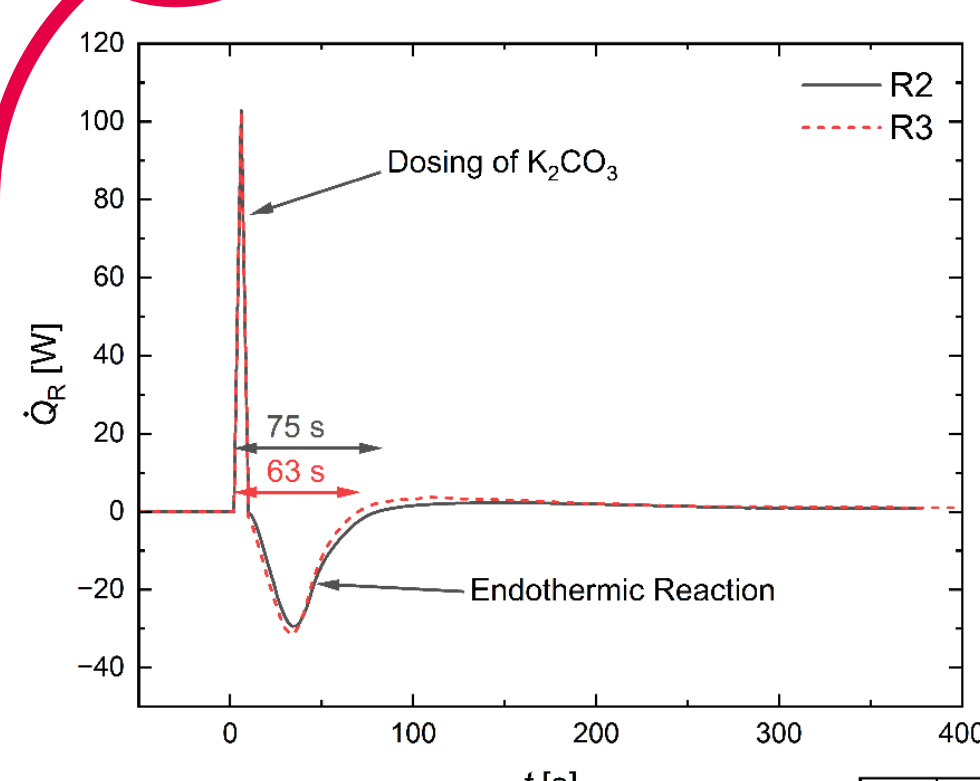
## How to do it? – Bridging Experiments & Models [2]



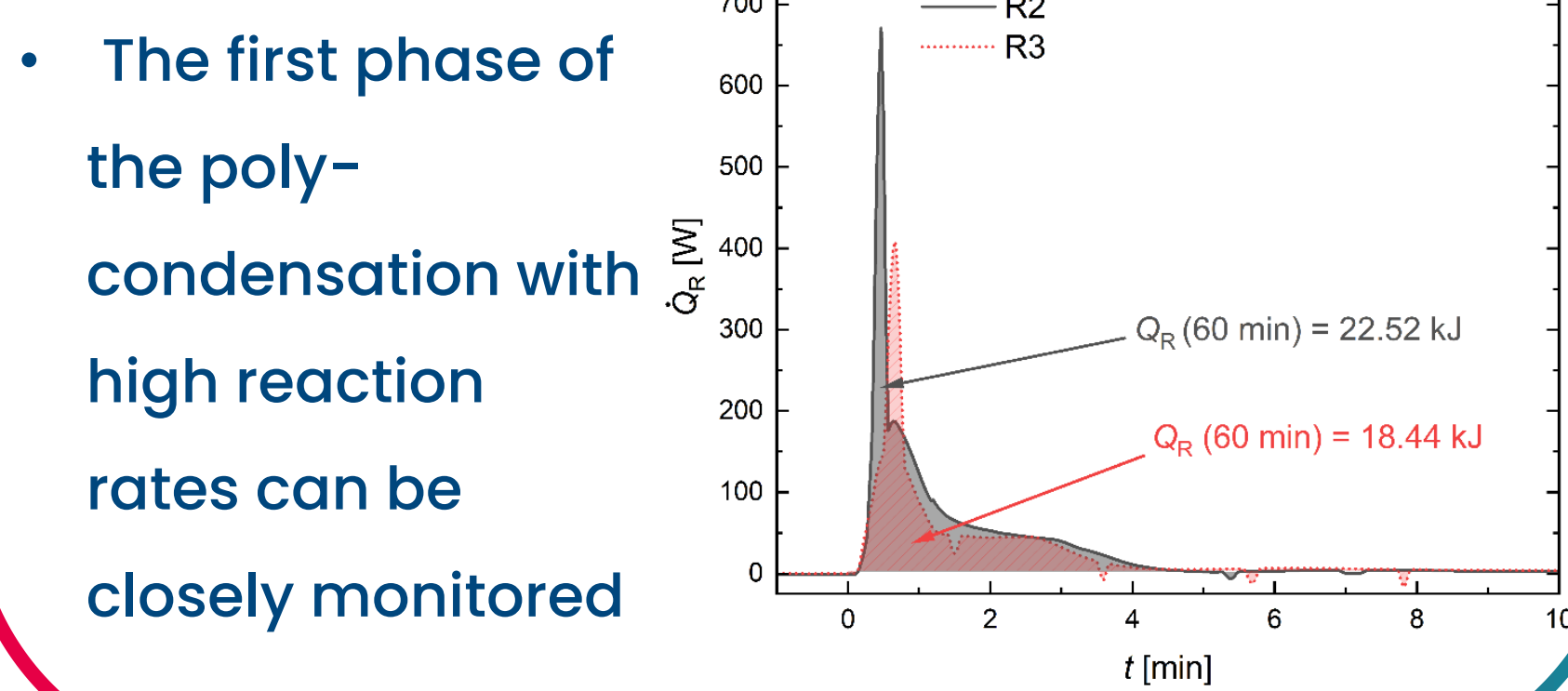
- Particle size of K<sub>2</sub>CO<sub>3</sub> as investigated by SEM (A, B)
- The size distribution (C) influences the reaction rate

### 1 Particle Size

### 2 Calorimetry

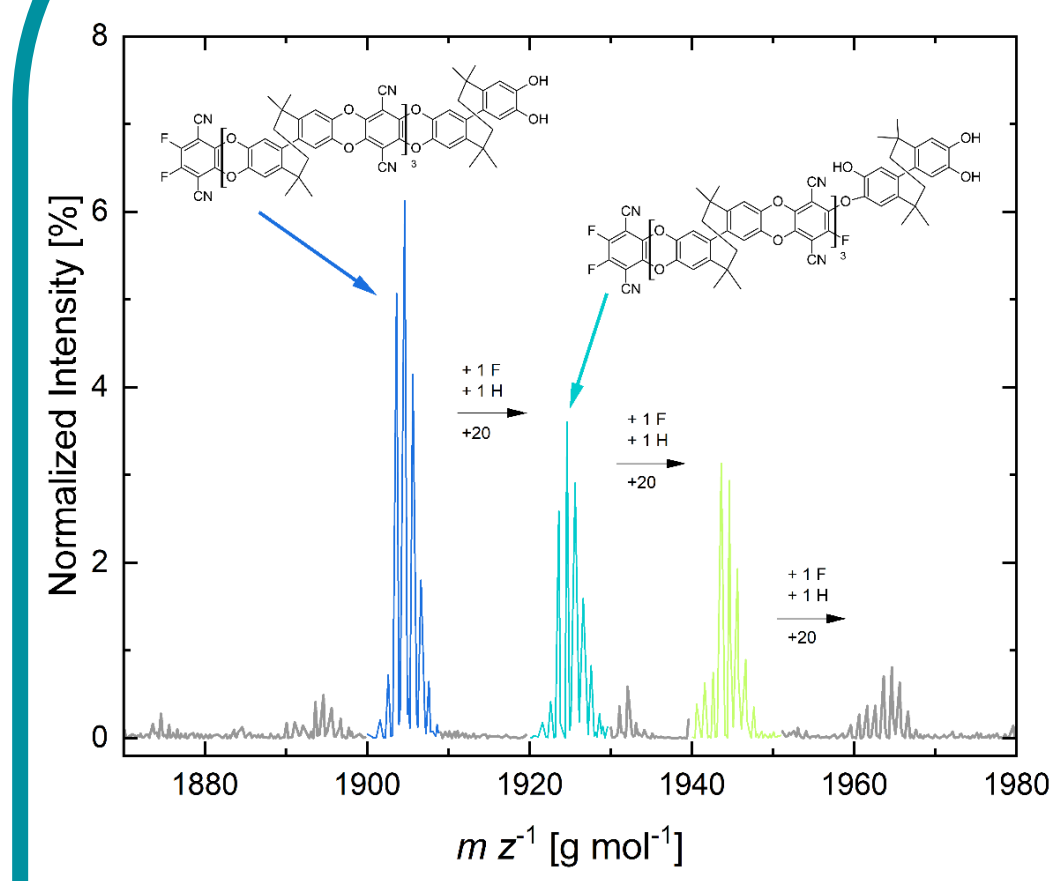


- Reaction calorimetry enables the investigation of the deprotonation step



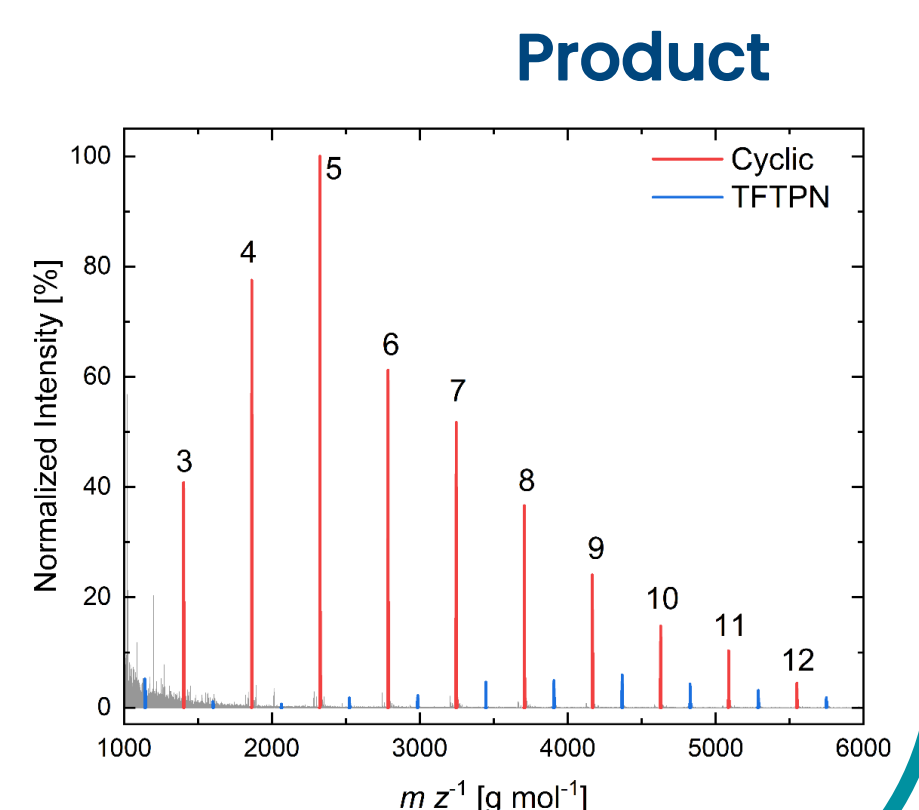
- The first phase of the polycondensation with high reaction rates can be closely monitored

After 3 min



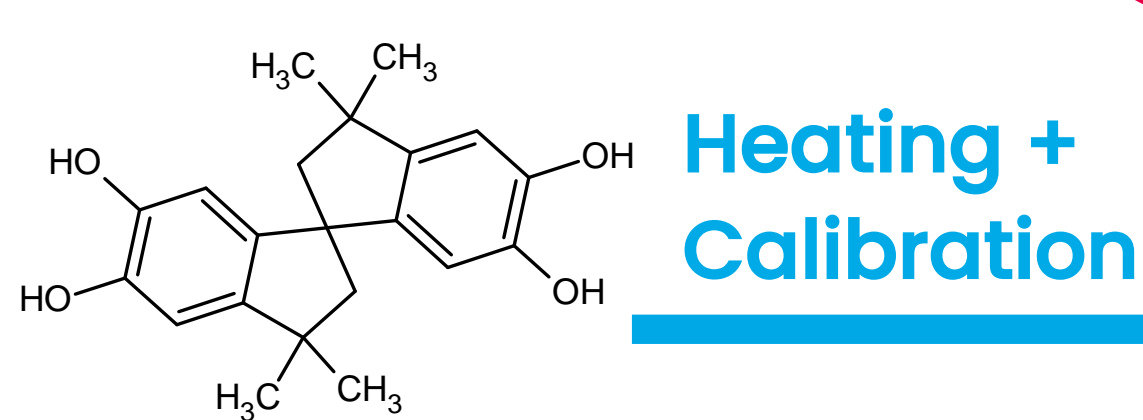
Underreacted species at the beginning of the reaction  
→ Sequential formation of the ether bonds during polycondensation

- First cyclic species appear after 7 min (conversion > 80%)
- Low molar mass species in the product are cyclic



MALDI-TOF

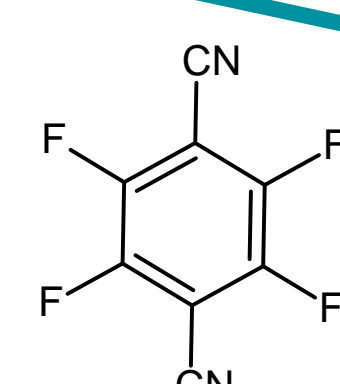
3



Heating + Calibration

K<sub>2</sub>CO<sub>3</sub>

Deprotonation

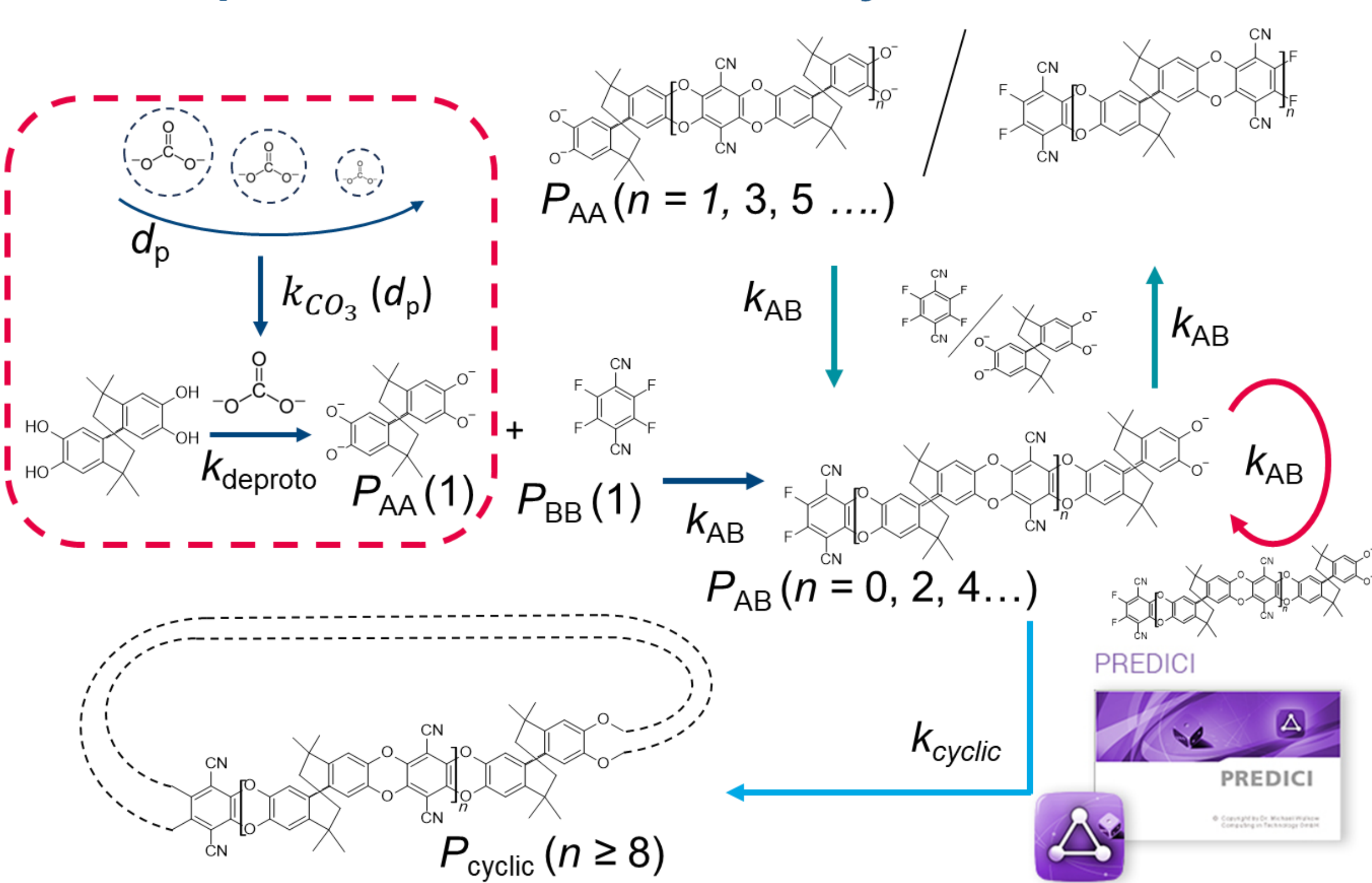


Polycondensation

## Reaction Kinetic Model

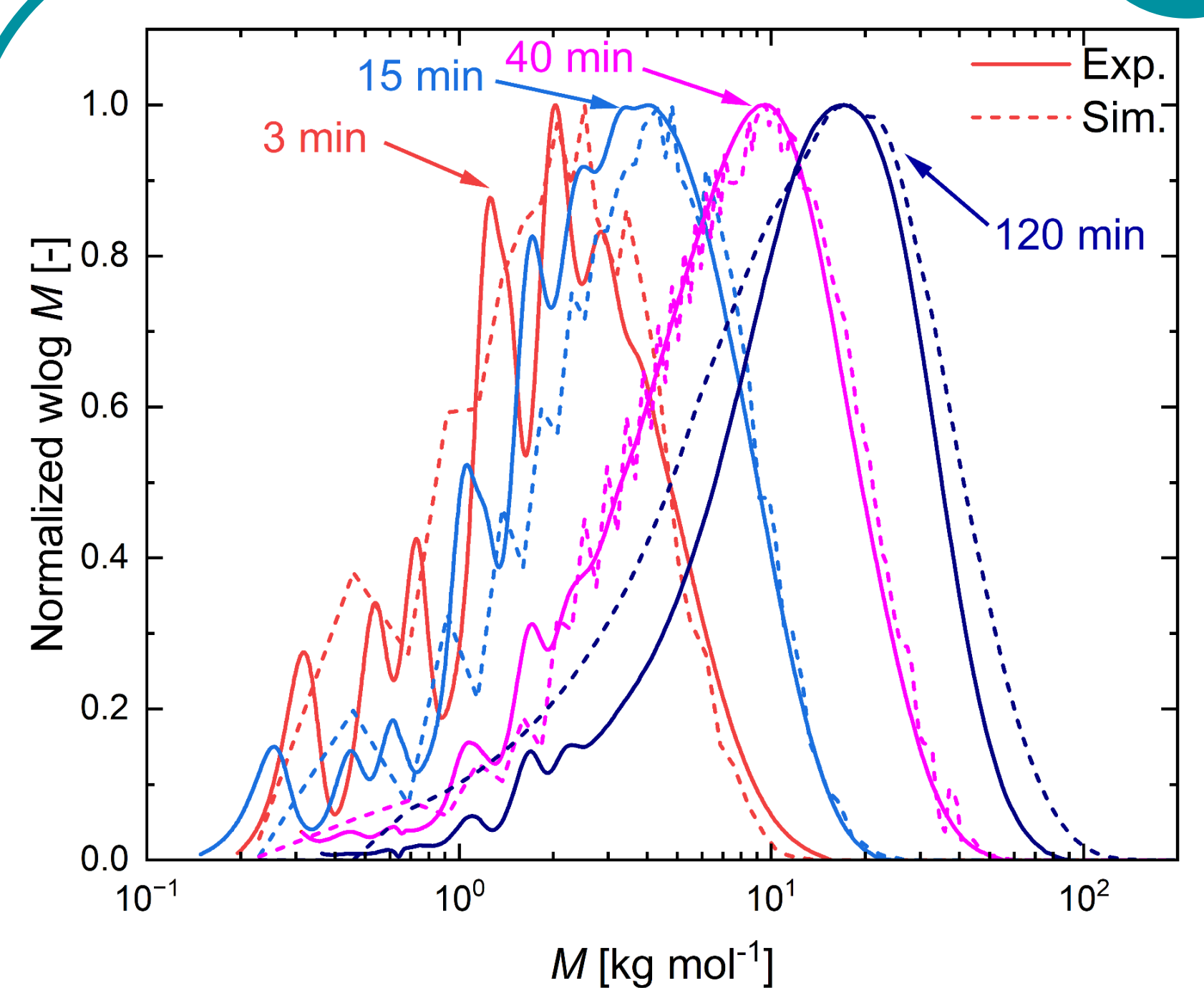
### 1. Deprotonation

### 2. Polycondensation



The reaction kinetic model describes both the deprotonation and the polycondensation steps

## Molar Mass Distribution



- Parameter estimation of two reactions coefficients:
  - $k_{AB} = 1.05 \cdot 10^{-2} \text{ L mol}^{-1} \text{ s}^{-1}$
  - $k_{cyclic} = 8.00 \cdot 10^{-2} \text{ s}^{-1}$
- The model can predict the evolution of the molar mass distribution over the course of the reaction

## Literature:

[1] Lau et al., *Prog. Mater. Sci.*, 2024, 145, 101297.

[2] F. Kandelhard et al., *Adv. Funct. Mater.*, 2025, 35, 2413358.