Data on of interfacial hydrolysis kinetics of an aromatic acid chloride

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Data on the interfacial hydrolysis of trimesoyl chloride (TMC) is presented. The reaction is a side reaction in the process of interfacial polycondensation leading to polyamide films used in reverse osmosis, and affects the kinetics of film formation and properties of the film. We have developed (Behera and Suresh, 2019) a methodology for the kinetic study of this hydrolysis, and the data used it to determine and model the kinetics of hydrolysis of TMC are presented here. In order to provide the context, we first establish the circumstances under which it can be competitive with the main reaction. The data show that pH has a significant effect on the kinetics of hydrolysis, and the hydrolysis can be self-limiting under most circumstances. The presence of a surfactant, often present in such systems, can influence the kinetics in significant ways. The kinetic model has been tested against experimental data obtained with different initial TMC concentrations, and at different concentrations of a commonly used surfactant, Tween 85. The data here support the results and conclusions presented in the main paper i.e. (Behera and Suresh, 2019) and details, including parametric effects, are presented in this data-in-brief.

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1. Data

This section describes the actual data files presented in this article. Fig. 1 of this article presents the FTIR scans of polyamide polymer samples. The monomer concentrations used for the preparation of polymer samples are mentioned in the figure description. The fast-acting pH probe was connected to a dynamic pH meter along with Agilent data acquisition system.

1.1. The evidence of hydrolysis

In our earlier paper [2], we have tried to study the polyamidation kinetics under such conditions, based on qualitative considerations, that the importance of hydrolysis is minimized (low amine concentrations, no surfactant, etc). Here, through FTIR of the polymer samples (Fig. 1), we provide the evidence for hydrolysis by showing the presence of –COOH groups in the polymer, and proceed to determine the conditions under which it is competitive with the main reaction. The FTIR analysis of the polymer, for a typical combination of monomer concentrations was presented in Fig. 2 of the main paper [1], and other combinations are shown in Fig. 1 below. In all cases, a CO stretching of carboxylic acid at a wavenumber of 1720 cm$^{-1}$ [3,4] and COOH stretch [5] at a wavenumber of 3082 are seen.

Specifications Table

| Subject area       | Chemical Engineering    |
|--------------------|-------------------------|
| More specific subject area | Reaction Engineering |
| Type of data       | Tables, image (FTIR spectroscopy), graphs, figures |
| How data was acquired | Vertex 80 FTIR system, (Bruker, Germany), kinetic data using the experimental method and apparatus described. |
| Data format        | Calculated and analyzed data are plotted in Figures 2 and 3. Raw data for these figures are available in tabular form in the supplementary file. |
| Experimental factors | Hydrolysis kinetics data were collected from the experimental set-up described in the paper [1], in which the hydrolysis experiment was carried out. The hydrolysis data were in terms of drop in pH with time. The fast-acting pH probe was connected to a dynamic pH meter along with Agilent data acquisition system. |
| Data source location | Indian Institute of Technology Bombay |
| Data accessibility | The experimental hydrolysis kinetics data of aromatic acid chloride monomer along with model validation of the same are included in this paper |
| Related research article | Behera, Subhalaxmi and Akkihebbal K. Suresh. 2017. “Kinetics of Interfacial Polycondensation Reactions- Development of a New Method and Its Validation.” Polymer 127:28–44. Behera, Subhalaxmi and Akkihebbal K. Suresh. 2019. “Kinetics of Interfacial Hydrolysis of an Aromatic Acid Chloride.” Chemical Engineering Research and Design 146:154–61. |
Fig. 2 below shows a comparison of the fall in pH with time, in the first 20 s of reaction, between polyamidation and hydrolysis. These data here (Fig. 2(a) and (b-f)) supplement the data presented in Figures 17 and 16 of the main paper [1] and support the conclusions arrived at.

1.2. Hydrolysis kinetics

Fig. 3 presents the results of hydrolysis reaction with different surfactant concentrations in the organic phase, over a wide range of surfactant concentrations, and supplements the data provided in Fig. 3 of the main paper [1]. The range of concentrations of surfactant covers values both above and below the CMC of the surfactant used, Tween-85. Also shown is the fit of the model presented in the main paper to this data.
2. Experimental design, materials, and methods

2.1. Experimental design

Two sets of experiments have been designed. The first is to confirm the occurrence of hydrolysis phenomena by FTIR spectroscopy of polymer sample, and gauge its importance relative to the main polyamidation reaction under a variety of experimental conditions. The second is the set of kinetic studies, culminating in a kinetic model.

2.2. Materials

De-ionized water, purged with Nitrogen at a pressure of 0.3 Bar to expel other dissolved gases such as carbon dioxide (which could have an influence on pH), was used as the aqueous phase. The organic phase solvent, n-Hexane (purity>99%), was obtained from Merck, Germany. The organic phase monomer TMC, (purity>98%) was obtained from Sigma Aldrich Chemical Co., USA. The aqueous phase monomer mPDA (purity>99%) was obtained from Merck, Switzerland. A surfactant is often employed in interfacial syntheses and could influence the reactions in significant ways; hence the kinetic studies...
in our work included experiments in the presence of a surfactant. In such experiments, Tween-85 (Fluka, Switzerland) was the surfactant used. Tween-85 is a non-ionic surfactant with a CMC (critical micelle concentration) of 1.395 vol%.

2.3. Experimental method

The experimental method involves conducting the hydrolysis reaction by adding an emulsion of the organic phase containing the acid chloride monomer TMC in water, to the required volume of the aqueous phase, and monitoring the fall in pH with time with a fast acting pH probe connected to a data acquisition system (Agilent). The reaction is conducted under high shear to eliminate all transport resistances. The required auxiliary quantities such as interfacial area per unit volume, are determined as described in our earlier work [2].

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Conflicts of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2019.104337.

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