

Minutes of the meeting of the IUPAC Subcommittee on “Modelling of Polymerization Kinetics and Processes” in Cairns on July 3rd 2018

Attendees:

Robin Hutchinson, Sabine Beuermann, Atsushi Kajiwara, Marco Drache, Shigero Yamago, Anatoly Nikitin, Graeme Moad, Simon Harrisson, Atsushi Goto, Bert Klumperman, Per Zetterlund, Greg Russell, Igor Lacik, Chris Fellows, Philipp Vana, Dagmar D’hooge, Kris Matyjaszewski, Marianne Gaborieau, Patrice Castignolles, Kash Bhullar

Topics

Note: the slides shown during the meeting are attached to the minutes

Robin reported about membership, recent activities and projects, citations of publications. It was noted that younger researchers working on kinetics should be approached with respect to becoming a member of the group. Suggestions should be sent to either Robin or Sabine. It was pointed out that Simon Harrisson is not on all lists – which has to be changed soon. In addition, it should be investigated whether all members are still interested in being a member. Greg notified the group that Gerhard Zifferer passed away.

Robin reported on some aspects of the IUPAC Polymer Division meeting held on June 30th/July 1st. Special emphasis was put on a larger interdivisional initiative to distribute critically evaluated data more openly and make them accessible free of charge. Robin is a member of an interdivisional project set up to develop guidance for the production and use of high-visibility evaluated data recognized widely as “Evaluated by IUPAC”, chaired by David Shaw (Div V). In addition, he has worked with Stewart Chalk from the IUPAC Committee on Publications and Cheminformatics Data Standards, who set up a test webpage for the critically evaluated propagation rate coefficients of methyl acrylate (link: <https://sds.coas.unf.edu/poly/>). The webpage gives the publication that came out of an IUPAC project together with an Arrhenius diagram of the entire data set. In addition, the original publications are given and the associated data points are displayed. During the discussion it was suggested to show the individual data sets always together with the over Arrhenius fit of the data. In addition, only the Arrhenius parameters of the global fit should be displayed. Further, it was discussed whether copyright issues occur, if the first page of the publication is shown. In addition, the question came up how the data should be cited – either the publication or the IUPAC webpage. This point should be clarified on the webpage. Further, it was noted that the addition of a k_p calculator to provide values at a desired temperature would be nice for the user, ensuring that correct data will be used. Robin will provide the link of the test webpage to the group and comments are welcomed until the end of August. Finally, it has to be clarified who is responsible for putting the data on the web, and the best way to link the material to the IUPAC site.

The status of the ongoing projects was given by the task group leaders:

project 2009-050-1-400: the project is finalized with Graeme's review article in Prog. Polym. Sci. Peroxide initiators will not be considered.

project 2013-045-1-400: the project is finalized with the publication of the critically evaluated data for vinyl acetate in 2017. A summary paper will be written for Pure. Appl. Chem.

project 2013-047-1-400: Sabine reported that the relevant reactions and associated kinetic rate coefficients were put together in her group. At the end of the summer the data collection will be distributed to the taskgroup members for discussion and identification of additionally required elemental reactions / kinetic data.

project 2013-051-1-400: Greg reported that there is no progress on the project due to his engagement as IUPAC Polymer Division president. Most likely, after his presidency the project will be revitalized.

project 2015-034-1-400: Atsushi reported that data on hyperfine constants and activation energies were collected. A report will be written until fall.

project 2017-028-1-400: The project led by Tanja and Robin just started and had its first meeting on July 2nd. It was decided that firstly, the techniques used to evaluate backbiting rate coefficients will be evaluated. A survey is intended to be provided by the end of 2018. Data provided in the current literature appear to agree at low temperatures up to 60°C. However, at higher temperatures a need for more experimental data was identified. Until the end of the year some of the taskgroup members will carry out additional experiments. Hopefully, the situation will be more clear then.

Future activities:

It was pointed out that face to face meetings are very important for making progress. Lately, the subcommittee met less frequently, due to the fact that kinetics and modelling conferences or sessions at large conference become rare. In an effort to promote meetings at the last Pacifichem conference (2015) and at the MACRO 2018 conference special sessions were initiated. Similarly, it is intended to have a kinetics / modelling session at Pacifichem 2020. Another meeting may be set up for the Polymer Reaction Engineering conference taking place in June 11 to 14th 2019 in Hamburg.

Greg suggested to initiate a project on propagation rate coefficients for acrylates with long ester groups. Currently, there are very little data available in the literature. Scientifically, it is less interesting to investigate these monomers. However, it may be an option that a couple of independent groups experienced in PLP determine additional data, which will then be published in a joined publication, that could be considered as a benchmark value paper. This point requires some further thinking and discussion before a project may be started.

Simon suggested to start a project on reactivity ratios, for example for styrene and methyl methacrylate. After a discussion it appeared to be an interesting project that should be pursued. In addition, it should be considered whether copolymerization propagation rate coefficients can be included. Firstly, the data available have to be identified.

After the discussion of potential future projects the meeting was ended.