Reactive extrusion based synthesis of thermoplastic cellulose derivatives

Summary

The overall goal of the project is elaborating sustainable and up-scalable method for synthesis of thermoplastic cellulose derivatives using fully biobased reagents and mechanochemical action of reactive extrusion. The project addresses critical issue of providing bio-based alternatives for fossil-based plastics. Cellulose is the most relevant but strongly underutilized raw material for this. The project should provide solution for conducting synthesis of thermoplastic cellulose derivatives on sustainable and energy efficient way. The work is conducted in international team in collaboration with relevant academic and industrial research partners.

Research field:	Chemical, materials and energy technology
Supervisors:	Andres Krumme Dr. Illia Krasnou
Availability:	This position is available.
Offered by:	School of Engineering Department of Materials and Environmental Technology
Application deadline:	Applications are accepted between June 01, 2024 00:00 and June 30, 2024 23:59 (Europe/Zurich)

Description

The research

Cellulose, as the most common biopolymer in the world, is an important resource for replacing fossil-based plastics as it has good mechanical properties, chemical durability and is not competing food resources. However, only minor amount of global plastic production is covered by cellulose derivatives or regenerates. This is pointing strong need to increase utilization of this sustainable, carbon neutral raw material for plastics. Unlike most of the commodity plastics, cellulose is not intrinsically thermoplastic and must be chemically modified to achieve melting behavior, expected by plastics processing industry. The cellulose modification methods known so far are resource- and energy-intensive. This stimulates development of more sustainable routes. There are two main aspects of sustainability of synthesis of thermoplastic cellulose derivatives: biobased, sustainable reactants and fast and energy efficient process. However, several perspective bio-based reactant candidates have intrinsically low reactivity with cellulose functional groups. Therefore, the synthesis process should provide strong support to the reactions. Increasing reactivity of the reactants by mechanochemical action is a perspective research area, where nearly no relevant publications exist. The most promising mechanochemical method, where both high shearing and elongational forces are present is reactive extrusion (REX) in co-rotating twin-screw extruder. REX is known in general as a method in polymer synthesis and modification, providing highest yield with the shortest time, minimum usage of energy, solvents, and reactants. The extrusion process is continuous, having therefore good perspectives for industrial up-scaling. REX can process highly viscous substances and therefore, much higher cellulose concentrations can be expected than in a batch-wise stirred reactor, significantly reducing the need of solvents. **Therefore, the main objective of the PhD project is to elaborate sustainable and up-scalable method for the synthesis of thermoplastic cellulose derivatives using fully biobased reagents and mechanochemical action of REX.**

Responsibilities and specific tasks

- Modelling and simulation of the REX process by the screw design, input material characteristics and process conditions for understanding thermo-mechanical conditions, energy balance and materials behavior/reaction evolution along the process.
- Optimizing the reaction conditions, screw profile, screw rotation speed, temperature profile, feed rates etc. for obtaining maximum reactivity in shortest time with minimum usage of energy and solvents.
- Studying effect of preparative procedures of cellulose (as swelling, partial dissolution, application of ultrasound or microwave radiation etc.) for maximizing the reaction efficiency.
- Improving the REX based laboratory pilot technology by specific components.

- Conducting LCA of the REX process addressing critical aspects of sustainability and environmental impact. Improving the process accordingly.
- Contributing to analyzing, publishing and dissemination of the results of the study as a member of the research team.

Applicants should fulfil the following requirements:

- a master's degree in polymer technology;
- a clear interest in the topic of the position;
- excellent command of English;
- practical skills in operation of extrusion instrumentation;
- strong and demonstrable writing and analytical skills;
- capacity to work both as an independent researcher and as part of the research team;
- capacity and willingness to provide assistance in organizational tasks relevant to the project and teaching and/or supervision activities.

The following experience is beneficial:

- knowledge of modelling and simulations of extrusion based processes;
- knowledge of (bio)polymer synthesis;
- knowledge of pulping and/or cellulose chemistry;
- working knowledge of compounding and/or reactive extrusion;
- knowledge of chemical engineering;
- LCA experience.

The candidate should submit a research plan for the topic, including the overall research strategy. The candidate can expand on the listed research tasks and propose theoretical approaches to be used.

We offer:

- 4-year PhD and early-stage researcher position in internationally recognized research team of biopolymer technology.
- The chance to contribute to the green turn of plastics.
- Opportunities for conference visits, research stays and networking with globally leading universities and research centers in the field of biopolymer technology.

About the laboratory

The main focus of the research of Laboratory of Biopolymer is Technology is valorization of bio-based environmental resources in everyday and high-tech applications. The aim is to find sustainable alternatives to fossil based polymeric materials by applying bio-based alternatives and recyclables.

The laboratory is looking for novel ways to sustainably valorize cellulose by applying new, recyclable solvent systems, bio-based chemical modification reagents, and energy-saving technologies as reactive extrusion.

The laboratory has a unique pilot production capability in Estonia in such important areas of polymer technology as hot mixing, extrusion, injection molding and electrospinning. Thermoplastic or thermosetting polymer composites with inorganic or bio-based additives are being developed for the efficient use of secondary raw materials in the circular economy. Solutions are also being sought for larger-scale recycling of textile waste and lignocellulosic fibers.

Activities:

- conducting studies at the bachelor's, master's and doctoral level;
- conducting basic and applied research in the field of polymeric materials, biopolymers;
- providing product development, piloting and testing services to companies.

Additional information

For further information, please contact Prof Andres Krumme (andres.krumme@taltech.ee) and visit https://biopolymer.taltech.ee/

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