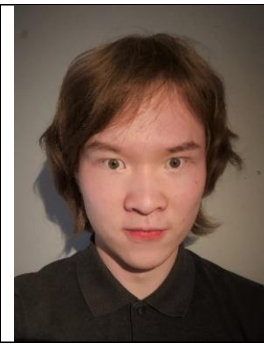
ESR 3

Project title and research strand:	Bio-based ingredients for coating formulations. Strand 3: functional polymers.
Name:	Zhou Fang
Supervisors, affiliation:	Katrien Bernaerts; Maastricht University (NL) Geert Deroover; ChemStream (BE)



Abstract

Galactaric acid is a molecule derived from sugar beet pulp, a waste stream from sugar production. Due to the presence of secondary OH groups that might trigger branching or cross-linking, it is risky to directly use this molecule for polyester synthesis. The goal of this thesis is to extend the value chain of galactaric acid by exploring the possibility of transferring the acetal-protected from (GalX) and catalytic converted form (2,5-Furandicarboxylic acid, FDCA) of galactaric acid as building blocks into degradable thermosetting polyester resins. It was found that the cross-linking can be carried out by two means including initiator-free UV and thermal treatment. Cured thermosetting polyesters were proved to be degradable after the end of their service lives serving as coating and adhesive resins thanks to the labile linkages including acetals and esters. Moreover, to accelerate the development of bio-based polyesters, machine learning models were developed for predicting the glass transition temperature (T_g) of new polyesters derived from FDCA with high accuracy. Overall this research proved that it is feasible to put the derivatives of galactaric acid into applications and the synthetic approach as well as the models developed in this thesis may contribute to the circular material transformation.

Visual Summary – Poster

Maastricht University

Faculty of Science and Engineering

Synthesis of sugar beet pulp-derived polyester resins

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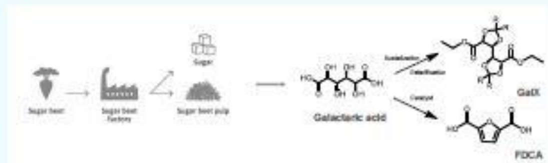
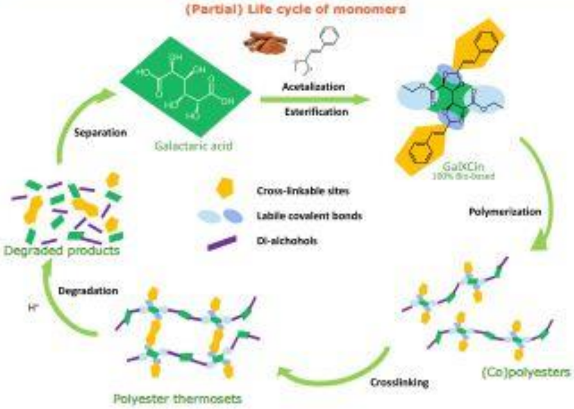
Background

Galactaric acid is a molecule derived from sugar beet pulp, a waste stream from sugar production. Due to the presence of OH groups that might trigger branching, it is risky to directly use this molecule for polyester synthesis

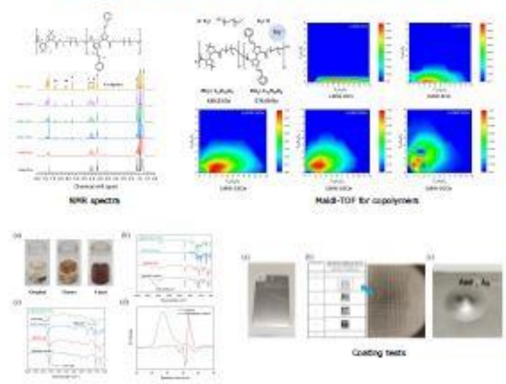
The goal of this thesis is to explore the possibility of transferring the acetal-protected from (GalX) and catalytic converted form (FDCA) of galactaric acid into polyester resins in the framework of sustainable concepts such as degradable thermosets and machine learning-assisted synthesis that may contribute to the circular material transformation



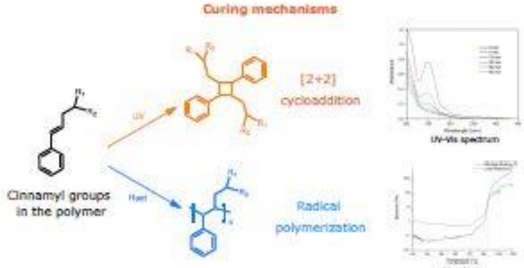
(Partial) Life cycle of monomers



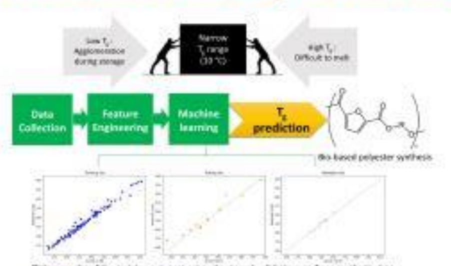
Extensive characterizations and structure-property study



Curing mechanisms



Machine learning model for predicting the T_g of furan-based polyesters



Conclusions

This work shows the feasibility of using cinnamaldehyde-modified GalX to synthesis unsaturated polyesters. Two curing pathways, namely UV-induced [2+2] cycloaddition and thermal-triggered radical polymerization were found to be attainable. A wide range of characterizations regarding polymer properties, cross-linking kinetics, film properties, coating and adhesive tests were systematically carried out. These tests also revealed the structure-property relations of these polyesters. Moreover, degradation of cross-linked polyesters were achieved in acidic media thanks to labile linkages, realizing an partially closed-loop of monomer's life cycle.

As a supplement of experimental work, machine-learning models were developed for accurately predicting the glass transition temperature of FDCA-derived co-polyesters with the minimum root mean square error < 5 ˚C for the validation data set based on synthesis. It is believed that this powerful tool can accelerate the development of bio-based co-polyester resins for industrial applications

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