Biocomposites from poly(3-hydroxybutyrate-co-3-hydroxyvalerate) and lignocellulosic fillers: Processes stored in data warehouse structured by an ontology

Presented by Mélanie Münch, Univ. Bordeaux (visioconference) or Patrice Buche, INRAE IATE Montpellier

Due to the rising amount of plastic waste generated each year, multiple questions are emerging about their harmful long-term effects on the environment, the eco-systems and human health. One possible strategy to mitigate these issues is to substitute conventional plastics by materials fully biodegradable in natural conditions, such as poly(3- hydroxybutyrate-co-3-hydroxyvalerate) (PHBV). In order to decrease the overall cost and environmental impact of PHBV-based materials while modulating their technical performance, PHBV can be combined with lignocellulosic fillers. In this dataset, a total of 88 formulations of PHBV-based biocomposites distributed over 5 interdisciplinary projects has been collected, involving computer scientists, data scientists and biomass processing experts for food and bio-based material production. Available data concern the technical process descriptions, including the description of each step and the different observations measured.

This dataset presents two characterizations for both the lignocellulosic fillers and the biocomposites. Lignocellulosic particles characterized and used as fillers for the production of biocomposites were either purchased as commercial grades (e.g. cellulose and wood fibers) or produced by dry fractionation of raw biomasses (e.g. wheat straw, vine shoots, olive pomace, and green park and garden waste). They were characterized in terms of biochemical composition (cellulose, lignin, hemicellulose and ashes contents) using biochemical analyses, and morphology (apparent median diameter and span value) measured by laser granulometry. On another hand, biocomposites were produced following two processing steps: first, a compounding step to mix lignocellulosic particles with the PHBV polymer matrix; and then, a shaping step to get either thermopressed films or injection moulded samples. Biocomposites were characterized in terms of thermal properties (melting and crystallization temperatures) assessed by differential scanning calorimetry (DSC) analysis, thermal stability (temperatures of thermal degradation) assessed by thermogravimetric analysis (TGA), mechanical properties (Young's modulus, strain at break and stress at break) assessed by tensile tests and water vapour permeability.

This dataset uses a vocabulary defined with experts and described by PO² (Process and Observation Ontology) [1], an ontology dedicated at its core to the representation of transformation processes through the definition of steps, relations between those and their associated observations. In our case, specific domain vocabulary has been elicited and used to define precisely the different technologies used for the biomass treatment and the biocomposites production. This vocabulary can be reused for others projects on the domain [2].

[1] Mélanie Munch, Patrice Buche, Stéphane Dervaux, Juliette Dibie, Liliana L. Ibanescu, et al.. Combining ontology and probabilistic models for the design of bio-based product transformation processes. Expert Systems with Applications, 2022, 203, pp.117406.
[2] M. Munch, P. Buche and S. Dervaux, "Biorefinery ontology," 11 01 2022. [Online]. Available: https://data.inrae.fr/ dataset.xhtml?persistentId=doi:10.15454/AIF6TX. Accessed February 28, 2022.

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