From industrial wastewater to high performance bioplastics: knowledge integration for efficient decision-making

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Abstract: The potential processes for the production of bioplastics from industrial wastewater are characterised by the combination of technologies of uneven maturity. This contribution deals with integration of knowledge of different sources, namely: mathematical models, literature data processed in a meta analysis and experimental data from the most novel technologies. From this knowledge integration, the evaluation of the environmental performance of the whole value chain is performed by life cycle assessment. Carrying out this evaluation in an early-stage of development is intended to help decision-making in the optimisation and selection of technologies and target efforts in the improvement of sustainability hot-spots.

Keywords: Industrial wastewater; mathematical modelling; life-cycle assessment

Introduction and background

The recovery of resources from industrial wastewater and further transformation into high performance biodegradable plastics is an ambitious objective which fulfils the objectives of circular economy and sustainable development goals (SDGs) 6 and 14: i) a potentially harmful water pollutant if discharged is converted instead into an added-value product; ii) ensuring biodegradability in marine conditions, the pollution by plastic in the seas is greatly minimised. In the framework of H2020 project USABLE-PACKAGING (www.usable-packaging.eu), we are carrying out a comprehensive analysis of a selection of representative value chains, from the industrial effluent to the final bioplastic product and potential by-products to ensure the economic and environmental sustainability of this valorisation route. In particular, we are integrating knowledge from different sources, namely from deliberately designed experiments, mathematical models and literature reviews, for the holistic assessment of the environmental performance of several scenarios, defined based on different wastewater characteristics (i.e. substrate) and a diverse range of bioplastic applications (i.e. final product).

The challenges inherent to the production of high performance bioplastic from a residual source are multiple. First, wastewater must be transformed so that: i) its COD content is converted into volatile fatty acids (VFA), and subsequently, mixed-culture microorganisms use them to accumulate bioplastics or ii) for some glycogen-rich fish-canning effluents are first hydrolyzed to glucose and then transformed into PHA by halophilic microorganisms such as *Halomonas boliviensis*, which can outcompete other microorganisms thanks to the high salinity of the medium. Then, the accumulation process must be done under controlled conditions to maximize the percentage of PHA with respect to the bacteria cell biomass and its yield . Finally, bioplastic must be recovered from the bacterial cells, purified and combined to match the characteristics requested by final users.

Knowledge integration framework

The development of a new value-chain unavoidably faces the coexistence of technologies with different levels of maturity, as some conventional technologies are being complemented by lab- and pilot-scale developments or adapted to the new process. Likewise, the sources of knowledge available to design or optimise a whole novel process are scattered and have different levels of detail, validity, robustness, etc. (Prat et al. 2012).

In this work and with the aim of assisting in the sustainable development of the value-chain transforming industrial wastewater into bioplastics, we are developing a knowledge integration framework (Kalakul et al. 2014), which is represented in Figure 1 and composed by:

- Experimental data from novel bacterial cultures with a potentially higher productivity into PHA
- Literature meta analysis of PHA extraction methods, including solvent selection and yield, mechanical treatments, enzymatic digestion, etc. allowing to match the PHA accumulating biomass with the final PHA application.
- Mathematical models describing PHA production bottlenecks: the production of volatile fatty acids from wastewater and the posterior accumulation of PHA.
- Life-cycle assessment of the whole value chain fed with the data provided by each of the different sources, leading to a preliminary evaluation of the process sustainability. This evaluation provides the tools, in an early-stage of development, for selecting the right technology when different options are available and targeting the development efforts in the sustainability hot-spots of the value-chain.

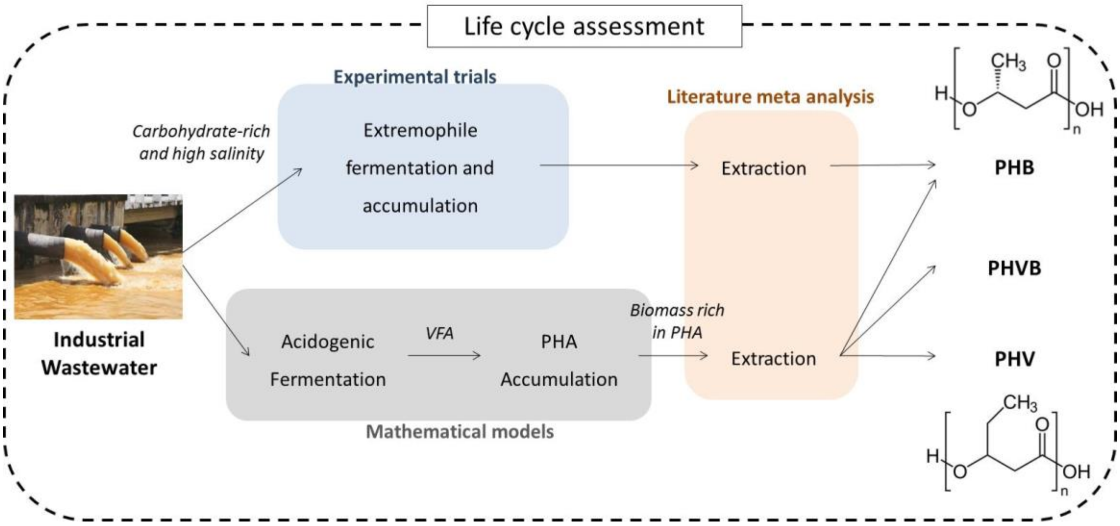

Figure 1. Flowsheet of transformation of industrial wastewater into PHA and structure of the knowledge integration framework featuring in different colours the origin and extent of the data that ultimately are used in life-cycle assessment of the whole value chain.

By doing so, we move from the assessment and optimisation of individual process to the global vision, so inter-relationships arise and the whole picture is more clearly presented (Rodriguez-Garcia et al. 2014).

Experimental trials

The production of PHA from mussel processing water (MPW) will be evaluated using as producing organism the halophilic bacteria *Halomonas boliviensis*. This bacterium has been previously used in the production of PHA from VFA (García-Torreiro et al. 2016a) and from cereal mash, integrated in an ethanol biorefinery (García-Torreiro et al. 2016b). Based on the characterisation of the MPW, the conversion will be conditioned for adapting its characteristic to the growth requirements of *H. boliviensis*. Finally, the effect of the most important parameters on PHA production such as salinity, C/N ratio, or the addition of special nutrients will be evaluated.

Literature meta analysis

The methods for bioplastic extraction and purification were reviewed searching for keywords "PHA extraction", "PHA purification", "PHA" AND "downstream" in Scopus database (for scientific articles) and Espacenet (for patents). Each method was characterised by the following categories: type of PHA, PHA application, yield, resources, by-products, pre- and posttreatment, technology readiness level (TRL). For solvent or enzymatic extraction, the use of a different solvent (or enzyme) was classified as a different method.

Modelling framework

The mathematical model consists of several modules following the sequential flowsheet model paradigm, where modules connected by interfaces transforming the outputs of a module on the inputs of the following one. The acidogenic fermentation is modelled following the framework described by Regueira et al. (2019). It is based on a metabolic model where a virtual versatile microorganism is able to perform all the metabolic functions and has access to all the metabolites ("enzyme soup" approach). The actual pathways expressed during the fermentation are the ones that maximise the energy harvest (in terms of ATP) of the whole community. The different model features are summarised in figure 2. This kind of models has been successfully applied to describe and predict the products of mixed-culture anaerobic fermentations (Regueira et al. 2018).

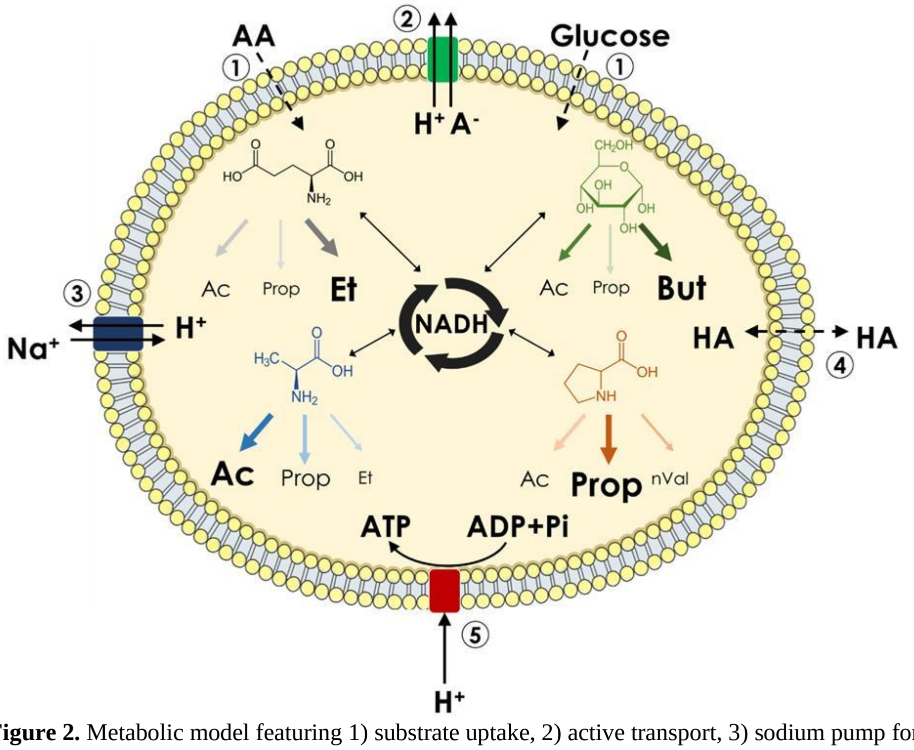

Figure 2. Metabolic model featuring 1) substrate uptake, 2) active transport, 3) sodium pump for pH regulation, 4) passive transport and 5) ATP production (Regueira et al. 2019).

Life-cycle assessment

The ambitious Plastic Strategy (EC 2018) involves the development of different measures to decrease the impact of plastic on the environment, being one of them the search for alternative feedstocks for plastic production provided that they result in genuine environmental benefits compared to the non-renewable alternatives under a life cycle perspective. So, the LCA methodology has already been used to assess the environmental performance of PHA production against competing materials (Yates and Barlow 2013), raising the fact that different methodological choices, such as the selection of the impact categories considered or the definition of the system boundaries, have to be done and there is still room for improvement and consensus.

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