Application of environmental and economic metrics to guide the development of biocatalytic processes - DTU Orbit (22/06/2019)

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The increasing industrial interest in biocatalytic processes is predominantly driven by the need for selective chemistry, with high reaction yield (Y-reaction) and few side reactions, as well as the need for optically pure chiral molecules (in particularly in the pharmaceutical industry). Interestingly, it is often argued that the mild conditions frequently used in biocatalytic reactions (ambient temperature and pressure, neutral pH and aqueous-based media) automatically lead to environmentally-friendly and cost-effective production processes. However, such a conclusion is not justified without the use of adequate tools to evaluate the performance of a process, in particular during process development. Nevertheless, at the early development stage, evaluation of biocatalytic processes is not a trivial task, not only due to the lack of data, but also because at this stage many of the biocatalytic processes are not yet fully optimized. Hence, in this paper we propose the use of a range of tools which can be used to guide process development, research tasks and support decision-making. Three sets of metrics are identified, each for use at different stages of process development (route selection, early development and late development), each with different objectives.

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