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Review

Bioprocesses: Modeling needs for process evaluation and sustainability assessment

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ABSTRACT

The next generation of process engineers will face a new set of challenges, with the need to devise new bioprocesses, with high selectivity for pharmaceutical manufacture, and for lower value chemicals manufacture based on renewable feedstocks. In this paper the current and predicted future roles of process system engineering and life cycle inventory and assessment in the design, development and improvement of sustainable bioprocesses are explored. The existing process systems engineering software tools will prove essential to assist this work. However, the existing tools will also require further development such that they can also be used to evaluate processes against sustainability metrics, as well as economics as an integral part of assessments. Finally, property models will also be required based on compounds not currently present in existing databases. It is clear that many new opportunities for process systems engineering will be forthcoming in the area of integrated bioprocesses.

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1. Introduction

Process systems engineering offers many tools for the chemical engineer. Today, for example, modeling, simulation and process evaluation tools are routinely applied to optimization problems in

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the bulk chemicals and fuels sector, where small process improvements yield significant economic returns. In the last 20 years bioprocesses have become more common. In particular they have found application in the production of high value products such as pharmaceuticals (and their intermediates). The process engineering emphasis in these cases is on rapid process implementation (rather than optimized development). However, in recent years bioprocesses have also been applied to bigger volume products such as fine chemicals, bulk chemicals and fuels. In these cases process improvement is the emphasis since this will yield significant returns. In addition to the direct process improvements, bioprocesses have also frequently been justified on the basis that they are processes with potentially lower environmental impact than their chemical synthetic counterparts. The main synthetic operations in bioprocesses include fermentation, microbial catalysis and enzyme catalysis. Downstream options are dependent on the nature of the product (macromolecular or low molecular weight compounds ('small molecules')). Small molecules are frequently processed in a similar way to other chemical products, although dilute aqueous solutions bring specific problems which need to be addressed, both from the viewpoint of process optimization and the environmental footprint. For instance, the downstream processing of some small molecule bioprocesses could include large amounts of organic solvents for extraction from aqueous solutions. In these cases, the organic solvents require processing, recycle, control and ultimately safe disposal. Macromolecules require more specialist operations such as filtration or chromatography. However, in all cases the molecules are frequently sensitive to extremes of pH and temperature, placing specific restrictions and constraints on processing methods. Biocatalyst recovery (frequently for recycle) also necessitates filtration and centrifugation.

From this discussion it is clear that engineers and others involved in implementing new processes need to address a range of questions. For example: when should a bioprocess, rather than a chemical process, be implemented? If a bioprocess is to be implemented, can the existing infrastructure (feedstock, utilities and plant) be used? How can process plant be adapted for different biomass in different geographical regions? What is the optimum biorefinery? What options exist for process integration? What are the environmental, health and safety issues of bioprocesses in comparison with chemical processes? What is the environmental footprint of a bioprocess compared with its chemical counterpart? How can bioprocesses be designed to maximize process efficiency, minimize environmental impact, as well as maximize sustainability?

Many of these questions can currently be addressed qualitatively, but to have real value it is necessary to assess the questions on a quantitative basis. In order to achieve this effectively therefore, computer-based tools are required. Over the last decades, process systems engineering has already developed many of the appropriate tools. Nevertheless, some further developments are required. For example, in the case of bioprocesses an extra option available to the engineer is the improvement of the catalyst itself. This requires models which take into account catalyst properties. In addition, one can see life cycle inventory and assessment (LCI/A) modeling tools and methods as a logical extension of process systems engineering. LCI/A methodologies allow for the estimation of environmental impact across the entire life cycle of a process or product. LCI/A estimations rely heavily on the characterization of the process and its unit operations using process systems engineering modeling and simulation techniques.

Hence we are now at the point where process engineering tools need to be applied to the complete set of bioprocesses, including pharmaceuticals, fine chemicals, bulk chemicals and fuels. In this paper the specific role of process systems engineering and life cycle inventory and assessment in the development, design and improvement of sustainable bioprocesses will be discussed.

2. Scope

Biotechnology is an enormous sector of industry from high value, low volume products (such as pharmaceuticals) to low value, high volume products (such as biofuels). To date the majority of implemented bioprocesses have focused on the former group. The emphasis here has been on implementing processes effectively to meet the tough regulatory demands placed on such products. Rapid process implementation, rather than optimization, has been the necessary focus of process engineering (e.g. Pollard & Woodley, 2007; Woodley, 2008). The latter group of bio-based products (and associated processes), represent a different challenge. These are the new sectors of industrial (also called 'white') biotechnology where new opportunities exist for alternative feedstocks based on renewable resources such as biomass and clean processes with reduced solvent inventories, renewable catalysts and mild conditions for reaction and separation (e.g. Dale, 2003). Here there remain some significant hurdles to achieve full-scale implementation. For example, for cost-effective synthesis one can start from fermentation of starch or sugars (ultimately from biomass given suitably cost-effective pretreatment). However, fermentation by its very nature is a rather inefficient process with a significant amount of substrate/reactant required for cell energy, cell growth and other products. This inherent weakness for use in chemical synthesis has stimulated genetic and metabolic engineering methods to improve strains. A parallel development with protein engineering has developed around enzymatic catalysis. Furthermore, the new 'bio-economy' will require the development of a suitable infrastructure and, like the oil-based counterpart will demand very high yield processes meaning that process engineering for the future implementation and development of these processes will have an increasingly important role, alongside the biological methods for biocatalyst improvement. In addition, the timely identification of environmental, health and safety issues to be managed will be crucial to facilitate the development of sustainable bioprocesses. Most importantly it is imperative that any claims of 'greenness' are considered in the wider framework of sustainability. Attempting to assess and compare the sustainability of bioprocesses must have a holistic scope based on life cycle thinking, which is strongly based on the output of systems engineering modeling and simulation techniques. Given the maturity of the field of process systems engineering it is clear that many new opportunities will be forthcoming.

3. Industrial biotechnology processes

Three major types of bioprocess can be identified dependent on the nature of the biocatalyst. These are outlined beneath and the key process features are outlined in Table 1.

3.1. Fermentation processes

For a significant number of chemicals, the use of fermentation has become a standard alternative to fossil-based feedstocks and technology. Nevertheless the possibility of growing microbial cells on a variety of sugars (derived from renewable biomass) has re-invigorated interest in this area. The consequence is that fermentation at a large-scale will become more common in the future chemical industry. Many different types of fermentation process (using different strains to produce different products) can take place in the same process plant which is a significant advantage. The plant is relatively simple and the challenges lie in adequate mixing (sometimes with materials having complex rheology), suitable oxygen input (for aerobic processes) and process control. Downstream, the separation process depends on the product, but will nearly always need to avoid high temperatures and extremes of pH. The solvent is water, meaning that the dilute product stream combined