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South African Journal of Chemical Engineering

journal homepage: http://www.journals.elsevier.com/south-african-journal-of-chemical-engineering

# Generic flow sheet model for early inventory estimates of industrial microbial processes. I. Flowsheet development, microbial growth and product formation

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A R T I C L E I N F O

*Article history:*
Received 11 December 2015
Received in revised form
6 September 2016
Accepted 11 October 2016

*Keywords:*
CeBER Bioprocess Modeller
Bioprocess design
Modelling
Bioreactors
Sterilisation
Agitation

A B S T R A C T

Early stage process analysis to maximize economic feasibility and minimize environmental burden is critically important for process flow sheet selection and optimization. This is equally true for bioprocesses. For many systems, including bioprocess systems, the desired material and energy balance data are not available at an early stage of design. The CeBER Bioprocess Modeller (Centre for Bioprocess Engineering Research at the University of Cape Town, Department of Chemical Engineering) has been developed to provide estimates of these material and energy balance data, as well as calculate equipment volumes and utility needs.

The model allows for aerobic or anaerobic, intra- or extracellular product formation or biomass growth in a continuous or batch process for various bioproducts produced from a selection of microorganisms using a range of raw materials. Using simple inputs, and default values drawn, the model is suitable for engineers and scientists alike.

The model also incorporates the option to select for sterilization and to specify the downstream processing train. In the bioreactor, the model takes into account aeration, agitation, reaction, biomass maintenance, yield, post microbial growth cooling and growth rate calculations, amongst others. This paper presents the model framework for the microbial growth and product formation stages.



## 1. Introduction

Industrial bioprocesses (environmental biotechnology, biocatalysis, bioremediation or similar) are becoming increasingly important for the production of chemical and energy products over conventional chemical synthesis, owing to the emphasis on the use of renewable raw materials, the specificity and complexity of biologically catalysed reactions, or both (Dorsch and Miller, 2003; Finlay, 2003; Hermann and Patel, 2007; Lynd et al., 1999; Lynd, 2008; McLaughlin et al., 2002). These biological processes are frequently claimed to provide benefit over conventional chemical processes from an environmental or sustainable process perspective (Botha and von Blottnitz, 2006; Gavrilescu and Chisti, 2005; Heller et al., 2003, 2004; Organisation for Economic Co-operation and Development, 2001; Sheehan et al., 2003; von Blottnitz and

DOI of original article: http://dx.doi.org/10.1016/j.sajce.2016.10.002.

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http://dx.doi.org/10.1016/j.sajce.2016.10.003

Curran, 2007; Harding et al., 2007, 2008), owing largely to their mild operating conditions, aqueous systems and the nature of the bio-system used.

To support claims of benefit, in terms of reduced environmental burden or increased process sustainability, rigorous process analysis is required using tools such as Life Cycle Assessment or carbon- and water footprinting. These approaches require availability of material and energy inventories, as do techno-economic assessments. Where these are available at an early stage of process design, they can be used to inform process selection. Further, such analysis can be used to target process improvements. In order to perform the environmental or economic studies required, a good knowledge of the process as well as the material and energy balance data are needed. This information is often found through physical data collection or from a detailed software modelling exercise (including, for example, AspenPlus or SuperPro Designer). Such an exercise typically requires a software package that is more complex than needed, may not be freely available, is unsuitable for biological processes or requires a specialist user to manipulate. Alternative, simplified tools are also available but concentrate on costing only, are limited to a single product, include pharmaceutical processes only and/or use modified results from the software mentioned earlier as inputs to a next step (Boukouvala et al., 2012, 2013; Claypool and Raman, 2013; Sen et al., 2013).

In order to obtain fast, accurate data estimates, the 'CeBER Bioprocess Modeller' has been developed to allow for the use of a limited set of inputs (using zero inputs will give a generic bioprocess flowsheet) to calculate the material and energy approximations. This data can then be used to perform environmental or economic assessments or aid in further process design. The approach to the generic flowsheet model is based on first principles, supplemented by data from advanced modelling studies and industrial practice.

## 2. Model specifications

### 2.1. *Desirable function for the model*

There are three main desirable features of the generic flowsheet model:

1. It should act as a first estimate bioprocess simulation tool;
2. It is required to calculate all relevant information required for a comprehensive environmental or economic assessment; and
3. It should require minimal input data.

The model should not be location specific. Hence, certain aspects of the model may not use the most appropriate options for different geographic regions *e.g.* the use of natural gas or coal, dependent on local availability. The option to modify these, to introduce location specificity as required, should be included. Further, the model is required to provide a framework to allow for the addition of more complex modelling.

### 2.2. *Model description*

The complete model allows for aerobic or anaerobic microbial growth with solid or liquid, intra- or extracellular product formation in a batch or continuous set-up. Sterilization, inoculation, microbial growth and product formation operations are followed by biomass recovery by solid–liquid separation, cell disruption (if required), product recovery, purification and formulation. Downstream processing is limited to six recovery, concentration or purification steps followed by a final formulation step (Fig. 1). The addition of chemicals (and reaction of these) is allowed in downstream

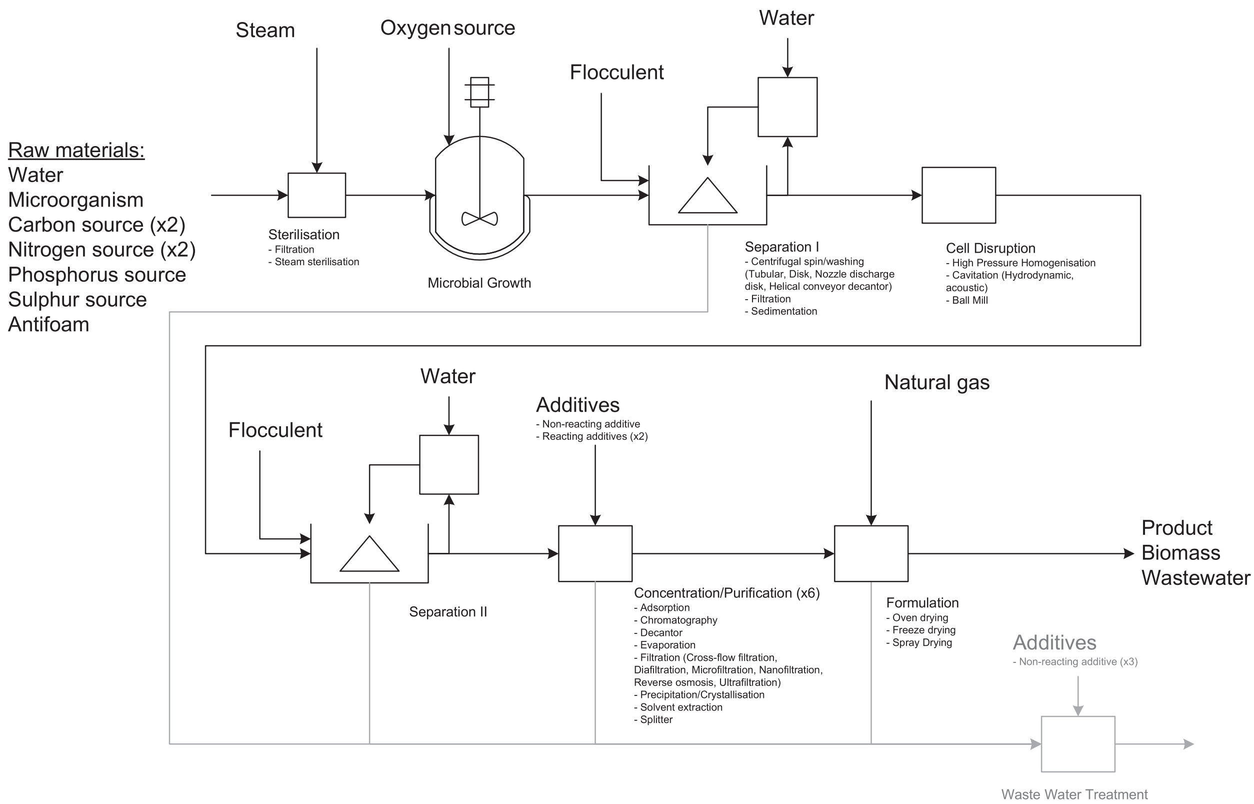


**Fig. 1 – Outline of the process flow sheet used in the generic bioprocess model.**