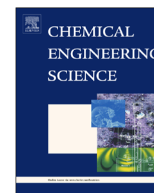
Chemical Engineering Science 114 (2014) 114–127

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces



Global sensitivity analysis and meta-modeling of an ethanol production process

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HIGHLIGHTS

- Ethanol removal from bacterial fermentation *via in situ* gas stripping model.
- Global sensitivity analysis applied for identification of critical parameters.
- Results comparable to data of *Geobacillus thermoglucosidasius* growth on cellobiose.
- Conditions under which gas stripping is a practical recovery method established.
- Metamodels of the process developed and performance compared to mechanistic model.

ARTICLE INFO

Article history:
Received 9 September 2013
Received in revised form
26 March 2014
Accepted 18 April 2014
Available online 26 April 2014

Keywords:
Bioethanol production
Thermophilic bacteria
Global sensitivity analysis
Sobol indices
Meta-modeling
Random sampling – high dimensional model representation

ABSTRACT

Traditional ethanol fermentation becomes inhibitory to microbial growth at ethanol concentrations that depend on the producer organism, leading to reduced ethanol productivity. Continuous ethanol removal from the fermenter could increase productivity and potentially reduce the cost of product recovery. In this work, continuous ethanol removal *via in situ* gas stripping in a stirred tank reactor has been investigated as a means of reducing growth inhibition and improving productivity. A dynamic mathematical model that couples ethanol fermentation with gas stripping has been developed. This has been linked to a flash separation model to represent the initial steps of product recovery. Global sensitivity analysis was used to reduce the number of uncertain parameters, the values of which were estimated with satisfactory accuracy using experimental data for ethanol production from a metabolically engineered strain of the thermophile *Geobacillus thermoglucosidasius* growing on cellobiose. Simulation results show that continuous ethanol fermentation with product removal by gas stripping is feasible, with the associated energy requirement, costs of gas compression and fermenter agitation being a function of the stripping gas flow rate. Finally, the conditions under which gas stripping is a practical product recovery method were established.

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1. Introduction

Bioethanol for use as an additive to gasoline for petrol engines is produced in significant quantities in the US and Brazil, and increasing amounts in the rest of the world. In the US, nearly 50% of all gasoline supply is blended with ethanol up to 10% in most cases (Yacobucci and Schnepf, 2007), while in Brazil the legal blend has been 25% ethanol and 75% gasoline since 2007 (Portaria N.° 143, de 27 de Junho de, 2007). The traditional method for bioethanol production is batch fermentation of *Saccharomyces cerevisiae*. The natural tolerance of *S. cerevisiae* to alcohol means that final concentrations can be more than 12% (v/v), and the ethanol produced is subjected to further processing steps including distillation and dehydration. The distillation step requires significant energy input and thus accounts for a substantial part of the processing cost.

While *S. cerevisiae* readily converts sucrose (from sugar cane) and glucose (from starch), it has a very limited substrate range when second generation, lignocellulosic substrates are considered. This includes an inability to metabolize pentoses and deal with polymeric substrates. Rather than engineer these capabilities into *S. cerevisiae*, an alternative strategy is to convert a metabolically versatile organism into an ethanologen. Given that large scale

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http://dx.doi.org/10.1016/j.ces.2014.04.027
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fermentation generates metabolic heat, and that most cellulases and similar enzymes seem to work optimally at 55 °C or above, the use of thermophilic microorganisms, many of which are naturally involved in biomass degradation, provides the opportunity to utilize a wider range of substrates and also carry out the fermentation process close to the boiling point of ethanol.

This leads to another option; the concept of simultaneous fermentation and product removal. By working close to the boiling point of ethanol, it could be removed continuously into the gas phase. Park and Geng (1992) have reviewed methods for combining fermentation with product separation. These include fermentation under vacuum (Cysewski and Wilke, 1977), fermentation coupled with pervaporation (Muller and Pons, 1991; Shabtai et al., 1991), fermentation coupled with liquid–liquid extraction (Matsumura and Märkl, 1984), fermentation coupled with perstraction (Christen et al., 1990) and fermentation coupled with adsorption (Lencki et al., 1983). Recently, a technical and economic evaluation of various ethanol recovery schemes was presented in Haelssig et al. (2008), who conclude that distillation with two columns or with a vapor recompression system are the most financially viable options, whereas flash fermentation followed by distillation is the most energy efficient alternative. Continuous product removal would reduce product inhibition, by keeping the ethanol produced during fermentation below inhibitory levels. This is particularly important when the natural tolerance to alcohol is less than that of *S. cerevisiae*.

Herein we present an integrated mathematical model to describe ethanol production from thermophilic bacteria growing on cellobiose. The model accounts for *in situ* gas stripping followed by flash separation of the components in the reactor off-gas. We use global sensitivity analysis (GSA) and parameter estimation based on experimental data for the fermentation process to increase model confidence. GSA can provide valuable information regarding the dependence of the model outputs to its uncertain parameters. It is superior to other SA methods, such as those based on correlation or regression coefficients, because, unlike linear regression, it works for non-linear and non-additive models. GSA methods evaluate the effect of a factor while all other factors are varied as well and thus they account for interactions between variables and do not depend on the choice of a nominal point like local sensitivity analysis methods. Reviews of different GSA methods can be found in Sobol' and Kucherenko (2005) and Saltelli et al. (2008). The variance-based method of global sensitivity indices developed by Sobol' (2001) became very popular among practitioners due to its efficiency and ease of interpretation. For large-scale models the direct application of variance-based GSA measures can be extremely time-consuming and impractical. One of the very important and promising developments of model analysis is the replacement of complex models with equivalent operational metamodels (also known as surrogate models). Once they are built, metamodels can be run in seconds. They can also be subsequently used for GSA. This approach to GSA is considerably cheaper than the traditional variance-based methods in terms of computational time.

In this paper we apply two different meta-modelling methods, namely Radial Basis Functions (Buhmann, 2003) and Quasi Random Sampling–High Dimensional Model Representation (Li et al., 2002; Feil et al., 2009; Zuniga and Kucherenko, 2013) and compare their efficiency. We finally explore the fermentation operating space, in terms of agitation and stripping rates, to identify conditions under which gas stripping is a feasible product recovery method.

2. Model development

We have developed a dynamic model of ethanol fermentation with *in situ* gas stripping. A batch fermenter is modeled as a perfectly mixed stirred tank reactor with constant volume. The model predicts the concentrations of biomass, substrate and of products, in both liquid and gas phases, with respect to time. In order to alleviate product inhibition and aid the recovery process, gas stripping for *in situ* ethanol removal is applied. Thus, a constant volumetric flow rate of gas *G*, is flowing through the fermenter to extract the products from the broth. Mass transport of the products from liquid to gas phase is assumed to take place *via* equilibrium and convection. The model also considers the transfer of water from the liquid to the gas phase *via* evaporation and convection.

2.1. Material conservation equations

A material balance for biomass within the bioreactor is given by the following equation:

$$\frac{dX}{dt} = \mu X \tag{1}$$

where X is the biomass concentration (g L^{-1}) in the bioreactor and μ is the specific growth rate measured in h^{-1}. The specific growth rate is given by

$$\mu = \mu_{max} \frac{S}{K_S + S}\left[1 - \left(\frac{P}{P_m}\right)\right] \tag{2}$$

where μ_{max} is the maximum specific growth rate of biomass (h^{-1}), S is the concentration of substrate, in this case cellobiose, (g L^{-1}), K_s is the half-saturation constant also known as affinity constant for biomass growth on cellobiose (g L^{-1}), P_m is the ethanol concentration at which growth is completely inhibited(g L^{-1}), and P represents the actual ethanol concentration in the fermentation broth (g L^{-1}). The model was proposed by Luong (1985) and is a combination of Monod-type kinetics, considering microbial growth based on the consumption of one carbon substrate and product inhibition. It assumes that growth inhibition occurs at all product concentrations; whereas it is often observed only above a threshold concentration. However, as it is usually applied where inhibition is apparent, the error is not significant. The maximum specific growth rate is given by the Monod equation only in the case where the product concentration is negligible.

The material balance for the concentration of cellobiose is estimated by the following equation:

$$\frac{dS}{dt} = -q_s X \tag{3}$$

where q_s is the specific substrate consumption rate (g substrate (g biomass)$^{-1}$ h^{-1}), which is given by the following maintenance model first proposed by Pirt (1965):

$$q_s = \frac{\mu}{Y_{X/S}} + m_s \tag{4}$$

$Y_{X/S}$ represents the biomass yield with respect to substrate consumpti(g biomass (g substrate)$^{-1}$) and m_s is the maintenance factor (g substrate (g biomass)$^{-1}$ h^{-1}). The first term of Eq. (4) accounts for biomass growth, while the second term accounts for the energy required for cell maintenance. Maintenance metabolism allows product formation to continue in the absence of growth.

Similarly, mass balances for the fermentation products of primary metabolism can be carried out. Considering that products exist both in liquid and gas phases, mass balances are formulated for both phases. The index i in the following equations stands for metabolic products ethanol, acetic acid and succinic acid. Let us consider first the mass balances in gas phase, as can be seen in Eq. (5), below:

$$V_g \frac{dP_{gi}}{dt} = -GP_{g_i} + V_l r_{eqb_i} + V_l r_{conv_i} \tag{5}$$

where G represents the stripping gas flow rate (L h^{-1}), P_g corresponds to the concentration of the product in the gas phase

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