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ECONOMIC TRADEOFFS INVOLVED IN THE DESIGN OF FERMENTATION PROCESSES WITH ENVIRONMENTAL CONSTRAINTS

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A process model is used for analysing the economic tradeoffs involved in the synthesis, design and operation of a typical batch fermentation plant involving batch and semi-continuous operations with the recycle of the otherwise waste stream that results after the recovery of the product of interest from the fermentation broth. This recycle contributes to a more complete substrate consumption, water reuse and reduction of the environmental impact of the process. Process variables are optimized simultaneously with the plant structure by formulating the whole optimization problem as a non linear programme (NLP). The environmental concern about producing large amounts of fermentation broth waste was accounted for by penalizing its production combined with allowing their recycle to the different types of fermenters based on process considerations. Optimal design and operation are pursued, analysing the economic tradeoffs involved in selecting the number and operation mode of biomass grow and metabolite fermenters, sugar substrate blending to each fermenter, recycle of fermentation broth waste, initial and final concentrations of biomass, substrate and metabolite, and the role of idle times in the process. The paper reports some optimal plant structures and figures for process variables not implemented in industrial practices but supported by process analysis arguments, thus suggesting that they may be worth exploring.

Keywords: mathematical modelling; fermentation; downstream processing; batch processes; optimization; environment.

INTRODUCTION

Batch processes involve batch and semi-continuous operations that need to be scheduled. The constant time and size factors model (Biegler *et al.*, 1997) is used to optimize the plant design by proper selection of the batch sizes, the operating time of semicontinuous units and the structure of the plant (number of units in parallel at each stage and intermediate storage).

If process variables e.g., extents of reactions or reflux ratios are to be optimized too, in a first simpler approach, algebraic process performance models (Salomone and Iribarren, 1992) can be used to describe the time and size factors as functions of the process variables. In this approach the differential equations are analytically integrated, resulting in algebraic equations. The same constant size and time factors model is used, with the process performance models as additional constraints.

If more detailed dynamic models are needed to properly describe the batch units, the approach is to discretize the differential equations, as do Bhatia and Biegler (1996) with a reactor–distillation process, or to resort to dynamic simulation modules as do Salomone *et al.* (1996) with fermenters. In both cases the plant structure was fixed.

Barrera and Evans (1989) were the first in proposing an approach for the simultaneous optimization of process variables and the plant structure. They proposed a multilevel approach where the plant structure is at an upper level, the sizing of units at an intermediate level and the optimization of the process variables at a lower level. The approach presented feasibility problems because the optimization at the level of the process variables violated either size constraints imposed at the intermediate level or production targets imposed at the upper level.

Pinto *et al.* (2001) approached the problem for a fermentation process, with a mixed integer non-linear programming (MINLP) model that puts together the MINLP formulation used by other authors to optimize the structure with fixed time and size factor models, adding process

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performance models to describe the time and size factors as functions of the process variables.

Asenjo *et al.* (2000) working with the same fermentation process model, proposed to do a first optimization in a one unit per stage–free intermediate storage scenario. Then, they used the values of the process variables at this optimal solution to generate a fixed size and time factors model for optimizing the plant structure, and finally optimized the process variables with this plant structure fixed. Allgor *et al.* (1999) described this multilevel approach as a sequence of *ad hoc* iterations between the structural and process variables optimization sub-problems.

It should be noted that the simultaneous optimization of the structure and process variables for the particular batch reactor–batch distillation process received considerable literature attention, which rendered efficient optimization approaches based on an analysis of the distillation regions.

On the other hand, the fermenters–downstream process did not receive enough attention. There is a considerable number of contributions in the area of synthesis of the sequence of unit operations of the downstream process e.g., in Steffens *et al.* (2000) or in the particular chromatographic protein purification sub-process e.g., in Vasquez *et al.* (2001). But not in deciding the number of fermenter units at each stage and optimizing the size of the fermenters and downstream process subject to scheduling constraints, even if it has a considerable economic impact (Petrides *et al.*, 1995).

In this paper we use the NLP formulation proposed by Corsano *et al.* (2004) for representing the structure of fermentation networks, with the aim of simultaneously optimizing process variables and plant structure of fermentation processes. The process model includes the fermentation stages followed by a downstream process for recovery of the product of interest, with environmental constraints on the waste fermentation broth (Corsano, 2005).

The multiple optimal solutions nature of the problem is explored, finding that the NLP formulation is robust, i.e., the optimal structures arrived at were not dependent on the initial values of the continuous optimization variables. And an analysis is done of the economic tradeoffs involved in selecting the number and operation mode—in parallel or in series—of biomass grow and metabolite fermenters, the sugar substrate blending to each fermenter, the recycle of fermentation broth waste, the initial and final concentrations of biomass and substrate and the role of idle times in the process. This analysis arises from considering the simultaneous optimization of the synthesis, design and operation of the fermentation and downstream processes.

The paper is organized as follows: The study case process is described, afterwards, the models for each unit and their interconnections are presented. Following, is the main contribution of the paper, presenting an analysis of the tradeoffs involved in the optimizations. Finally, the conclusions of this work are presented.

STUDY CASE PROCESS DESCRIPTION

We consider a typical fermentation plant consisting of four stages: biomass production fermentation, metabolite production fermentation, centrifugation of the biomass and a downstream operation for separating the product of interest from the fermentation broth. The process example used here is the production of ethanol, for which a simplified scheme of the process is shown in Figure 1.

The objective of the first batch stage is the production of biomass. The first biomass fermenter, if there were more than one fermenters in series at this stage, is inoculated with a broth containing biomass prepared in laboratory while the next ones are fed by the outlet stream of the preceding unit. At this stage typically large amounts of air are supplied.

The metabolite production stage is also a batch item, fed with the biomass from the first stage and an appropriate fermentation broth. This stage typically works without air supply. We used the yeast and ethanol fermentations superstructure model presented in Corsano *et al.* (2004) to represent these stages. This superstructure model considers the possibility of duplication in series or in parallel for both the biomass and metabolite fermentation stages. The fermenters are modelled by discretizing their mass balances ordinary differential equations. The extents of reaction at each fermenter are process optimization variables.

The final fermentation broth is discharged through a disk stack centrifuge that operates in a semi-continuous mode. The objective of this stage is to separate the biomass from the liquid fermentation broth that contains the metabolite. We used a fixed size factor model for this semi continuous item because its sizing equation does not depend on any of the selected process optimization variables.

The last stage of the process is a batch distillation. The batch distiller is a combination of two batch items: the distiller feed vessel and the distillate tank, and three semi-continuous items: the evaporator, the condenser and the column itself. The analytical process performance model presented by Zamar *et al.* (1998) for batch distillation was adopted, where the size of these items depends on the value of two process optimization variables: the internal reflux ratio and the number of separation stages.

The four stages are connected through the mass balances on the batches that leave one stage to enter into the next. In the case of the fermenters, each one needs an additional stream of substrate. We considered process integration to procure this raw material: two are external carbohydrate sources which are purge streams from a sugar plant i.e., residues of a sugar production process, which can become raw materials of this process: concentrated molasses are the mother liquors of the last sugar crystallization stage and diluted filter juices are the filter permeate of a precipitated phase in an early purification stage of the sugar cane juice.

A third source of carbohydrate is the residual fermentation broth after recovering of the alcohol, that still contains a sugar concentration which we consider a process optimization variable. In this case the residue of the process, known as 'vinasses', can become a raw material of the same process.

The flow sheet of the plant to be optimized feeds each fermenter by blending streams coming from four feed tanks containing: molasses, filter juices, spent fermentation broth and fresh process water. The amounts taken from each source to each fermenter are process optimization variables.

It should be pointed out that from an industrial perspective, this selection of available raw materials implies a