

Simulation and Multi-Objective Optimization of Bioprocesses with Matlab and SuperPro Designer using a Client-Server Interface

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The paper deals with multi-objective economical-environmental optimization of bioprocesses. For optimization purposes, hundreds or more process simulations are necessary. The presented procedure consists in coupling Matlab with the process simulator SuperPro Designer, using Component Object Module (COM) technology. A client-server interface based on COM technology using Matlab and Visual Basic scripts was developed in order to call SuperPro Designer simulator repetitively, inside loops, for various sets of input variables. The potential of this method was exemplified in the frame of multi-objective optimization of the bioprocesses of penicillin V production from glucose, using *Penicillium chrysogenum*. To take into account the conflicting situations that may be encountered, respectively between economical and environmental demands, a multi-objective genetic algorithm based on Pareto front was used. The obtained results are useful both for technological, and economical reasons.

1. Introduction

Typically, system optimization in bioprocess engineering applications has focused on some economical objectives, such as the profit or the capital investment. Biochemical processes are characterized by a large number of parameters and their variations. For real applications, the existence of multiple criteria, often conflicting, which must be optimized simultaneously (i.e., multi-objective optimization), is quite common. Although this is a more realistic and desirable approach, there is not a unique solution. A set of optimal solutions, based on different criteria (i.e. the set of Pareto optimal points) can be obtained. In the case of bioprocesses, the identification of this set of optimal solutions is a very challenging task.

This work proposes a strategy for multi-objective optimization of bioprocesses. The procedure involves three major steps:

- (i) Process modeling;
- (ii) Formulation of the multi-objective optimization problem;
- (iii) Multi-objective optimization and choice of the best compromise solution.

2. Presentation of the proposed procedure

The proposed procedure consists in coupling the SuperPro Designer with Matlab. In this way, the SuperPro Designer simulator benefits from the available toolboxes

(optimization, statistics, etc.), computation and visualization advanced features given by Matlab. The SuperPro Designer functionality is greatly extended.

The general process optimization involves these three steps:

(i) Process modeling:

This is carried out by SuperPro Designer simulator, which is one of the most useful and used simulator for technological processes of fine chemical and biochemical products. The main advantages of this simulator consist in a large data base of specific chemical compounds and unit operations, and the evaluation of economical and ecological process performance indexes. Unfortunately, like most of all chemical and biochemical engineering simulators, SuperPro Designer is not equipped with optimization tools. For optimization purpose, hundreds or more evaluations of the objective function, and consequently the same number of complete simulations, are necessary. Therefore, for optimization applications, an off-line, classical use of the simulator isn't possible. Due to this fact, the application of chemical and biochemical engineering simulators were not involved up today in the full search of the optimum solutions.

(ii) Formulation of the multi-objective optimization problem:

In order to solve the multi-criteria optimization problems of economic-environment type, one needs to define a vector objective function with two components $f(x_1, x_2, \dots) = (y_1, y_2)$ where y_1 is the economic component formed by one or more economical indexes and y_2 is the ecological component formed by an environment index which describes the bioprocess impact towards the environment (e.g. the environmental index of bioprocess $EI_{Bioprocess}$); x_1, x_2, \dots are the independent variables.

The link between Matlab and SuperPro Designer for the data transfer between these was realized by a Matlab graphical user interface (GUI). This was created and applied to generate automatically the objective function source code. The details regarding the GUI will be given in the implementation section.

(iii) Multi-objective optimization and choice of the best compromise:

Because the two criteria considered presents antagonist goals, a Multi-objective Genetic Algorithm with a Pareto front was chosen for optimization.

The Matlab Genetic Algorithm generates a population whose individuals are vectors $\mathbf{v}_i = (x_1, x_2, \dots, x_n)$ where x_1, x_2, \dots, x_n are the values of the involved process variables, n being the total number of process variables taken into account, and i is the population size (i.e. for $n = 2$, x_1 is the glucose flowrate (kg/h), and x_2 is the fermentation time (h))

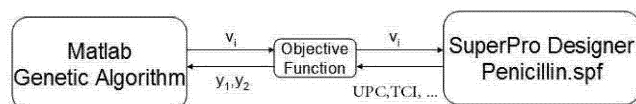


Figure 1: Variables flow in the optimization application

Each vector from the population is taken by module Objective Function and sent to the simulator. The simulator computes the mass and energy balances and the economic indexes and returns to Objective Function the required data to compute the two components y_1 , and y_2 .

In this way, to each vector \mathbf{v}_i , a fitness vector $\mathbf{y} = (y_1, y_2)$ is associated. This will be used in the frame of Genetic Algorithm.

3. Implementation

The Matlab GUI application used to generate the objective function is based on Component Object Module (COM) technology. This is a new feature that has become available since the release of version 6.0 of SuperPro Designer. Using COM technology, it is possible to add code so that the applications behave as an Object Linking and Embedding (OLE) Automation Server. The SuperPro Designer COM Server can thus be used by client applications to perform various tasks including: data exchange between the SuperPro Designer simulation variables (input/output) and other applications, exporting of SuperPro Designer reports, charts, and pictures to specified files or to the clipboards, etc. The object exposed by the SuperPro Designer server is the Designer Type Library. The use of the methods of this library to interoperate with other Windows applications requires the use of a common scripting language, and Visual Basic (VB) was chosen to this.

The program used for the generation of objective function contains two modules:

Module1: generate the environmental component of the objective function and it starts when EnvironmentalAssesment.m is called.

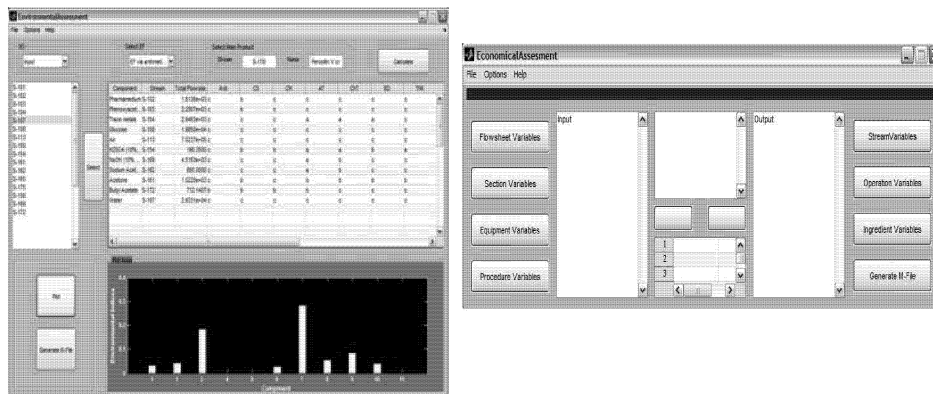


Figure 2: Matlab GUI used for generation of environmental and economical components of the objective function

Module2: generates the economical component and it starts when EconomicAssesment.m is run in Matlab.

4. Case Study

The previous methodology was applied to a batch plant for penicillin V production from glucose, using *Penicillium chrysogenum*.

(i) Process modeling:

The process model was taken from Heinzle (2006).

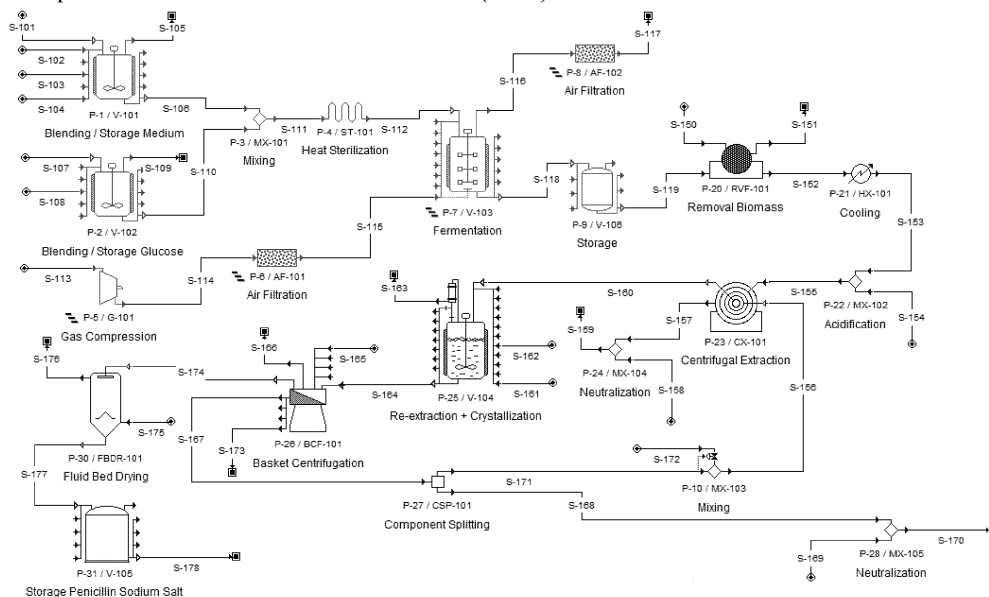


Figure 3: The penicillin V process flow diagram

An annual production of 2,300 t of penicillin is assumed and realized using 10 parallel bioreactors.

(ii) Formulation of the multi-objective optimization problem:

The optimization application consists in generation of Pareto front for $f(x_1, x_2, x_3, x_4) = (y_1, y_2)$ where $y_1 = UPC + w \cdot TCI$ (where UPC is the unit production cost in \$/kg of product, TCI is the total capital investment in \$, and w is a scale and weighting coefficient), and $y_2 = EI_{Bioprocess}$, respectively the environmental index of bioprocess. The process variables are: x_1 - glucose flowrate in stream S-109; x_2 - fermentation time in fermentor P-6; x_3 - yield butyl acetate recycling in P-15; x_4 - crystallization time in P-25.

(III) Multi-objective optimization:

To solve the multi-objective optimization problems, the Matlab “gamultiobj” function from Genetic Algorithm and Direct Search Toolbox was used.

5. Results and Discussions

The results obtained show the typical compromise between economical and environmental aims. Table 1 presents the parameters of the genetic algorithm used for multi-criteria optimization.

Table 1: Parameters of the Genetic Algorithm

		Variable	Lower Bound	Upper Bound
Population Size	40	x_1	18,000 kg/h	22,500 kg/h
		x_2	120 h	140 h
Generation Number	100	x_3	70%	90%
		x_4	10 h	14 h

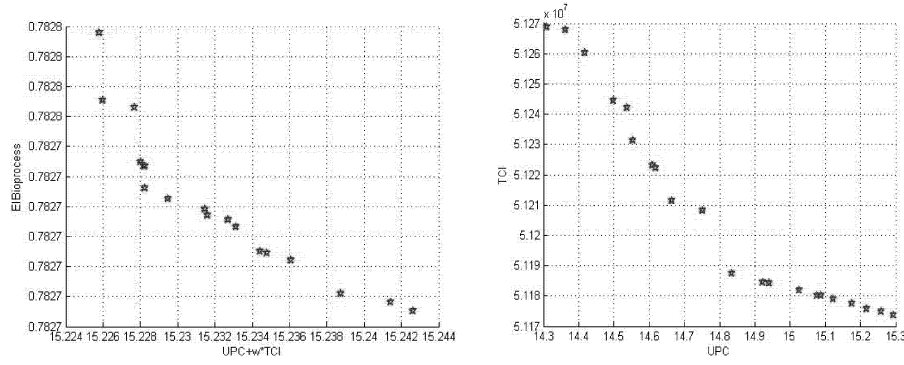


Figure 4: Pareto optimal solutions

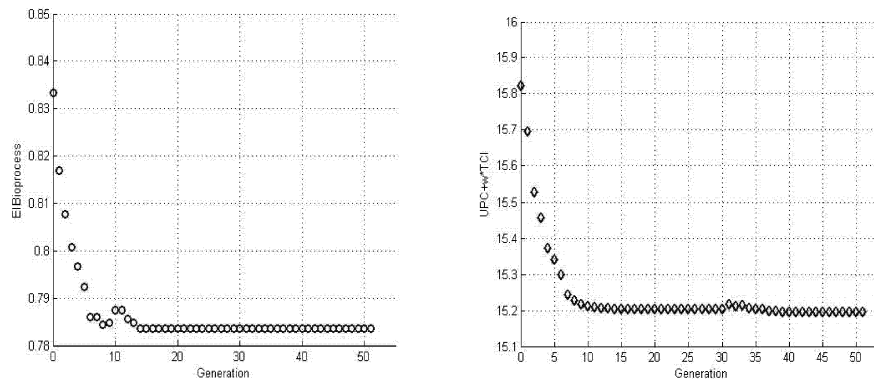
Figure 5: Uni-criterial optimizations: minimization of $EI_{Bioprocess}$ and of $UPC + w*TCI$

Table 2 presents the results of uni-criterial optimizations. It can be noticed the improvements of $EI_{bioprocess}$ from the 0.8335 to 0.7836, and of $UPC + w*TCI$ from 16.020 to 15.196. In Pareto optimal solution diagram, it can be seen that for any selected solution, economical and ecological performances of the bioprocess are improved.

Table 2: Results of uni-criterial optimization

	Initial Value	Minimization of $EI_{Bioprocess}$	Minimization of $UPC + w*TCI$
$EI_{Bioprocess}$	0.8335	0.7836	
$UPC+w*TCI$	16.020		15.196
UPC	14.22 \$/kg	14.40 \$/kg	14.20 \$/kg
TCI	51,231,929 \$	51,276,423 \$	51,248,642 \$
x_1	20,728.01 kg/batch	19,987.95 kg/batch	19,752.71 kg/batch
x_2	130 h	129.55 h	120 h
x_3	80 %	89.7 %	89.8 %
x_4	12 h	11.12 h	10.95 h

6. Conclusions

A methodology for multi-objective optimization of bioprocesses was proposed. A useful client-server application used to call the SuperPro Designer simulator repetitively, inside loops, for various sets of input variables was developed. The application was realized by VB and Matlab scripts. Unfortunately, not all the process variables are given in the Designer Type Library of SuperPro Designer server. Consequently, the selection of the independent variables is slightly restricted. Up today, the use of SuperPro Designer simulator for optimization problems on the base of a client-server application was not reported in literature. The potential of the client-server application was demonstrated in the frame of the optimization of the bioprocesses of penicillin V production using *Penicillium chrysogenum*. The corresponding results are useful both for technological, and economical reasons.

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