

## MULTI-OBJECTIVE OPTIMIZATION OF PYRUVIC ACID BIOPROCESS WITH A MATLAB-SUPERPRO DESIGNER INTERFACE

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*Lucrarea tratează optimizarea multi-criterială economică și ecologică pentru bioprocesul de obținere al acidului piruvic din glucoză folosind o tulpină mutantă de Escherichia coli. Abordarea utilizată constă în cuplarea Matlab și SuperPro Designer într-o buclă de optimizare, folosind o interfață grafică originală. Optimizarea este posibilă datorită schimbului automat și repetat de variabile dintre algoritmul de optimizare din Matlab și simularea procesului de obținere al acidului piruvic cu SuperPro Designer.*

*This paper deals with economical and ecological multi-criterial optimization of the bioprocess of pyruvic acid production from glucose using a mutant Escherichia coli strain. The used approach consists in coupling Matlab and SuperPro Designer into an optimization loop using an original Graphical User Interface. The optimization is possible due to an automatic and repeated exchange of variables between Matlab optimization algorithm and pyruvic acid obtaining process simulation with SuperPro Designer.*

**Keywords:** biochemical processes, pyruvic acid, simulation, optimization

### 1. Introduction

Modeling, simulation, and optimization play today a crucial role in achieving a full bioprocesses potential exploitation.

SuperPro Designer is a valuable tool which facilitates process simulation of fine chemical and biochemical products.

Many chemical and biochemical engineering simulators are not equipped with optimization tools. For these simulators, an optimization application implies a continuous exchange of variables between the process simulator and an external optimization algorithm.

The general objectives of this paper are to develop a multi-objective cost-environmental optimization strategy and apply this procedure to the bioprocess of pyruvic acid production from glucose using a mutant *Escherichia coli* strain.

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## 2. Multi-objective optimization strategy

The proposed methodology involves three steps [1]: process simulation, formulation of the multi-objective optimization problem, and multi-objective optimization and the choice of the best compromise.

### a) Process Simulation

SuperPro Designer was chosen for this work due to his unique ability of communicating with other software through Designer Type Library.

### b) Formulation of the multi-objective optimization problem

In order to solve the multi-criterial optimization problems of cost-environment type, a vectorial objective function with two components was defined:

$$f(x_1, x_2, \dots) = (y_1, y_2) \quad (1)$$

where:

$y_1$  - the economic component formed by one or more economical indexes (e.g.  $y_1$  = TCI - total capital investment);

$y_2$  - the ecological component represented by an index which describes the bioprocess impact on the environment (e.g.:  $y_2$  =  $EI_{bioprocess}$  - environmental index of bioprocess);

$x_1, x_2, \dots$  - the independent process variables.

The objective function represent the key factor of the proposed algorithm, being the link between Matlab and SuperPro Designer and making possible the data transfer between these two softwares.

In order to create the objective function, a friendly Graphical User Interface (GUI) was elaborated as a new, extended version of a previous one [2]. This GUI automatically generates the objective function code. It contains two modules: Module one - generating the economic component  $y_1$  of the objective function, and Module two - generating the environmental component  $y_2$  of the objective function.

#### - Module one:

The available variables from SuperPro Designer are classified in seven categories, corresponding to seven buttons on the interface (Fig.1). The list of category with the variables is posted behind each button, in order to be picked out by the user. Example: variable  $x_1$  corresponding to the glucose flow in S-116 stream is part of the StreamVariables category. The item "Specified ingredient (purecomponent/mixture) mass flow in stream" is selected from this list (Fig. 2).

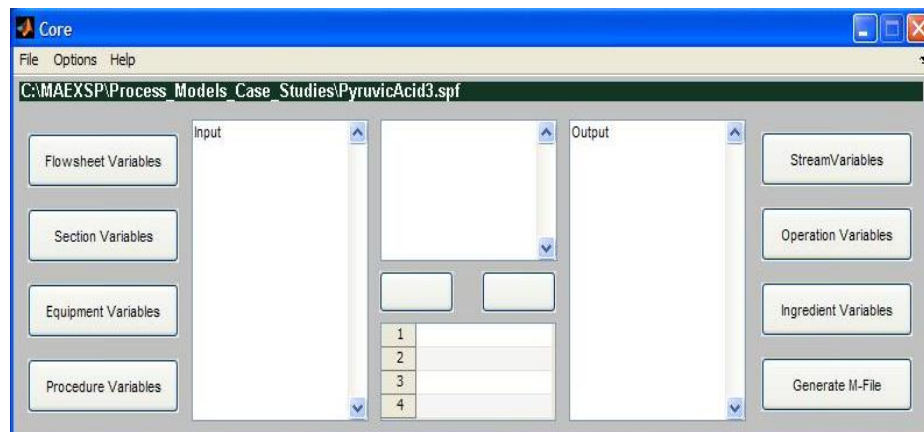


Fig. 1. Matlab Graphical User Interface used for generation of economic component of the objective function

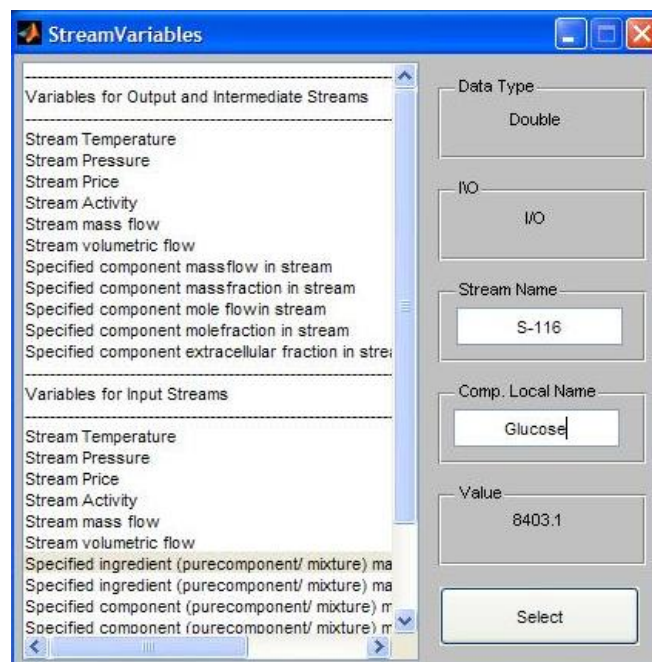


Fig. 2. Stream Variables list

The following additional data are also required:

StreamName: S-116;

Comp.Local Name: Glucose.

The objective function is generated by clicking the "Generate M-File" button (Fig.1).

**- Module two:**

The environmental component of the objective function is represented by an index ( $EI_{Bioprocess}$ ) that indicates the environmental relevance of the whole bioprocess.  $EI_{Bioprocess}$  is calculated by the method proposed by Heinzle and Biwer [3]. The method requires material flows (provided by SuperPro Designer and used to compute Mass Indices, which is a metric for the material intensity of the process) and ABC classification (provided by the user and used to compute Environmental Factors  $EF_i$  – a metric for the environmental impact of each component  $i$ ). From Mass Indices and Environmental Factors, the  $EI_{Bioprocess}$  is computed (Fig.3). A detailed presentation and several applications of this procedure were given by Nica and Woinaroschy [4].

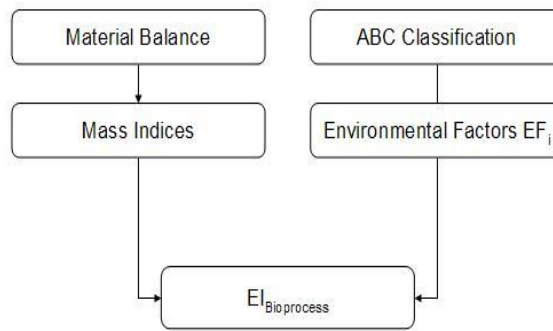


Fig. 3. Calculation of  $EI_{Bioprocess}$

After completing the interface table, the function generated by clicking the "Generate M-File" button (Fig.4) is able to calculate  $EI_{Bioprocess}$  by extracting mass flows from the SuperPro Designer and using ABC classification provided by the user.

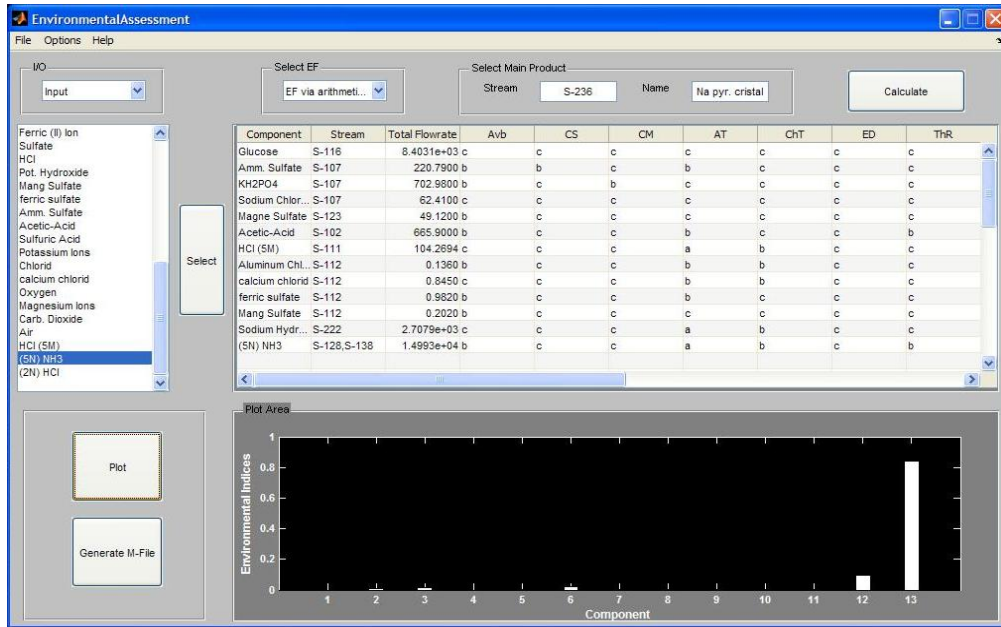


Fig. 4. Matlab Graphical User Interface used for generation of environmental component of the objective function

### c) Multi-objective optimization and the choice of the best compromise

Since the two considered criteria present antagonist goals, a Multi-objective Genetic Algorithm based on Pareto front was chosen for optimization. The solution which represents the best compromise between the economic and ecologic objective can be selected on the base of Pareto front.

The Matlab genetic algorithm (“gamultiobj” function from Genetic Algorithm and Direct Search Toolbox [5]) generates a population in which individuals  $i$  are vectors:

$$v_i = (x_1, x_2, \dots, x_n) \quad (2)$$

where  $x_1, x_2, \dots$  are the process variables,  $n$  being the total number of variables.

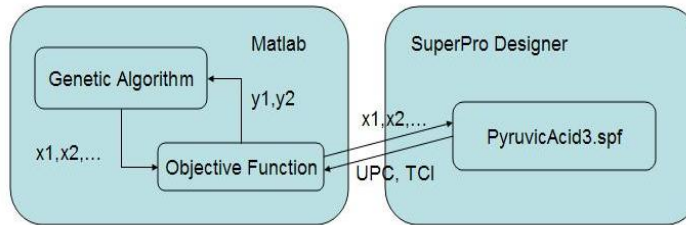


Fig. 5. Variables flow in the optimization application

Each vector from the population is taken by the objective function module and sent to the simulator (Fig.5). The simulator computes the mass and energy balances and the economic indexes, returning the required data to the objective function module, in order to evaluate the two components ( $y_1$ ,  $y_2$ ).

In this way, a fitness vector  $y = (y_1, y_2)$  is associated to each vector  $v_i$ , and this is used according to the Genetic Algorithm.

### 3. Multi-objective optimization of pyruvic acid bioprocess

The pyruvic acid bioprocess (Fig.6) is that presented by Heinzle and Biwer [3]. Pyruvic acid is produced in a bioreactor from glucose, using an acetate auxotroph strain of *Escherichia coli*. The fermentation is run as repeated fed-batch with four cycles. At the end of each cycle, a part of the fermentation broth is removed. The first cycle includes biomass growth and product formation. The biomass remains in the bioreactor, which is refilled with fresh medium. In cycles 2-4, no further acetate is added, and pyruvic acid is produced with the resting cells. For the bioreactor model, the cycles 2-4 are lumped together.

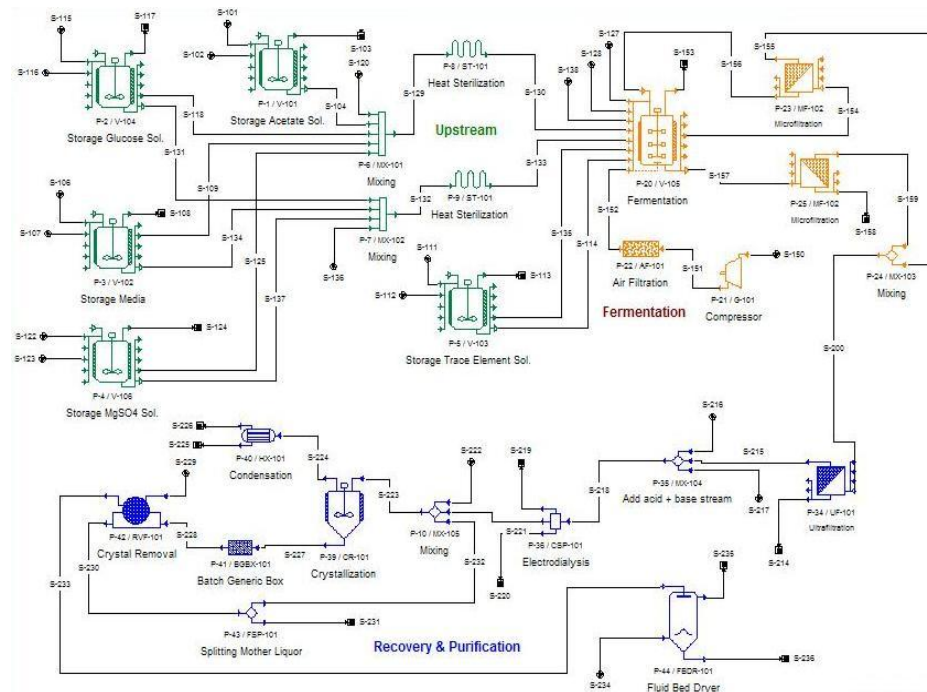


Fig. 6. Pyruvic acid bioprocess

The objective function chosen for this optimization application is:

$$f(x_1, x_2, x_3, x_4, x_5) = (y_1, y_2) \quad (2)$$

where:

$y_1$  - UPC: unit production cost (\$/kg PyruvicAcid), or

TCI: total capital investment (\$);

$y_2$  -  $EI_{\text{Bioprocess}}$ ;

$x_1$  - glucose flowrate in stream S-116 (kg/batch);

$x_2$  - acetic acid flowrate in stream S-102 (kg/batch);

$x_3$  - fermentation time for the first cycle in fermentor P-20 (h);

$x_4$  - fermentation time for cycles 2-4 in fermentor P-20 (h);

$x_5$  - crystallization time in P-39 (h).

In order to maintain the stoichiometric reaction model of the bioreactor, it is necessary to modify the flows of other participants (potassium dihydrophosphate, ammonia) in the fermentation process. Also, the pyruvic acid flowrate varies, and the amounts of sodium hydroxide in stream S-222 used for crystallization need to be adjusted. This modification can be automatically done using the GUI.

#### 4. Results and discussion

Table 1 displays the parameters of the genetic algorithm used for multi-criterial optimization. The values of the population size and generation number seem to be too small. The reason of these small values was to avoid an excessive computer execution time. Despite these selections, good solutions were obtained, although they did not correspond with the global optimum.

Table 1

Parameters of the Genetic Algorithm				
		Variable	Lower Bound	Upper Bound
Population Size Generation Number	15	$x_1$	7500 kg/h	9500 kg/h
	40	$x_2$	550 h	750 h
		$x_3$	11.5 h	14.5 h
		$x_4$	19 h	26 h
		$x_5$	5 h	7.3 h

The minimizations of UPC and TCI, respectively, during the evolution of Genetic Algorithm are presented in Figs. 7 – 8. The results of optimization process are given in Table 2.

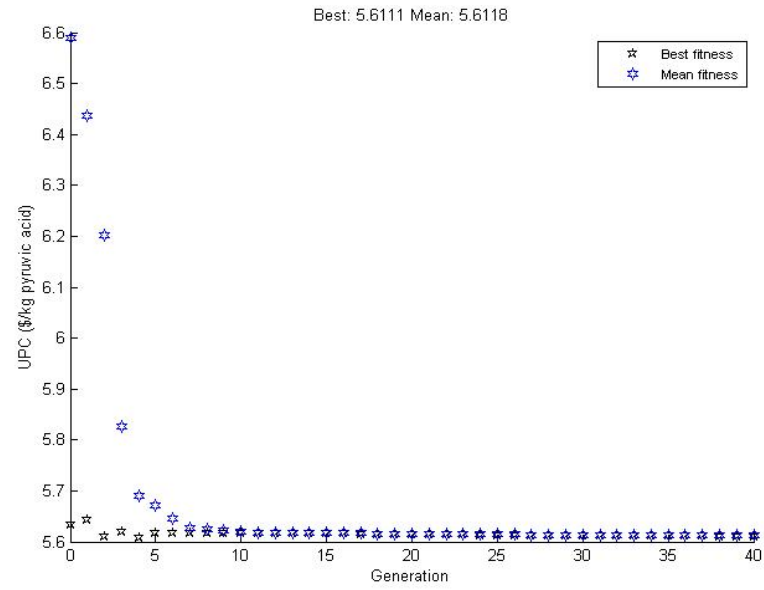


Fig. 7. Minimization of UPC

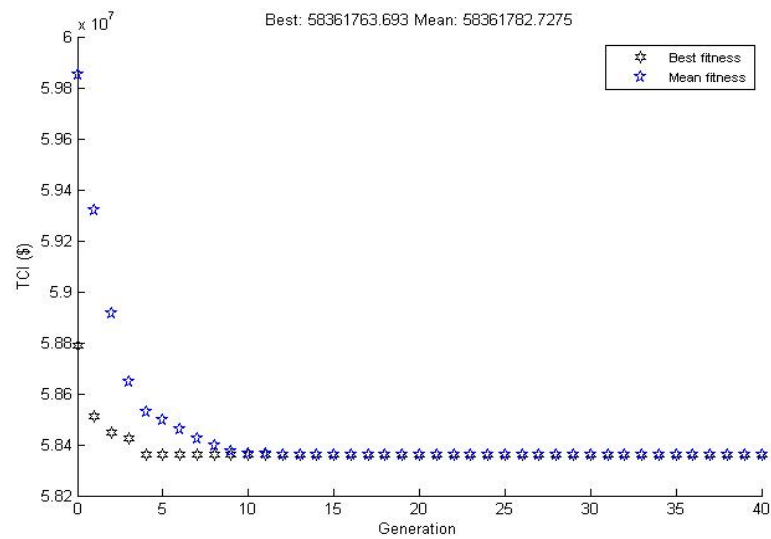


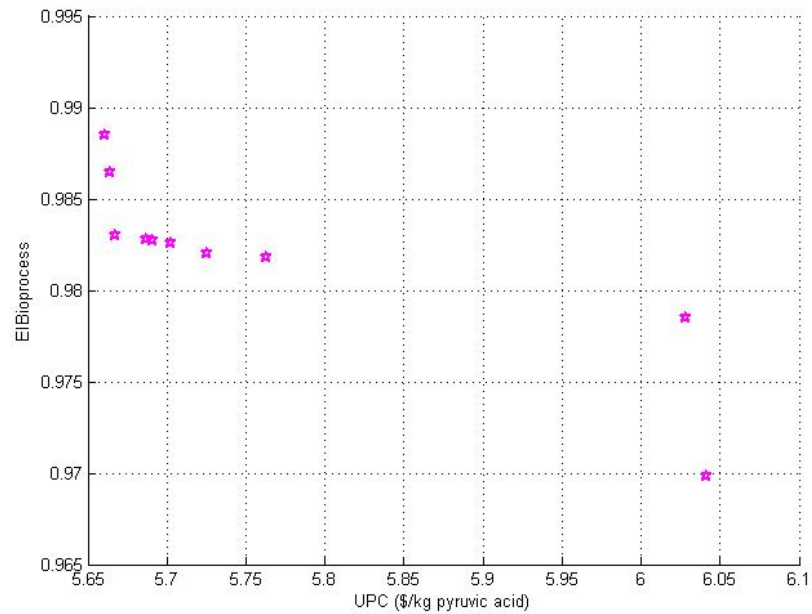
Fig. 8. Minimization of TCI



Table 2

Results of the optimization process			
	Initial Value	Minimization of UPC	Minimization of TCI
$EI_{\text{Bioprocess}}$	0.9819	0.9398	1.0942
UPC (\$/kg PA)	6.386	5.611	6.558
TCI (\$)	59,637,477	59,637,477	58,361,763
$x_1$ (kg/batch)	8,403.10	9,499.56	7,500.28
$x_2$ (kg/batch)	665.9	623.65	569.54
$x_3$ (h)	13	13.24	12.54
$x_4$ (h)	22.6	19	19
$x_5$ (h)	6.15	6.71	7.08

In Pareto optimal solution diagrams (Figs. 9 – 11), for any selected solution, in comparison with the initial case, the economical and ecological performances of the bioprocess are improved. A desired compromise between economical and environmental aims, or between two economical indexes can be selected.

Fig. 9. Pareto optimal solutions  $EI_{\text{Bioprocess}}$  -UPC

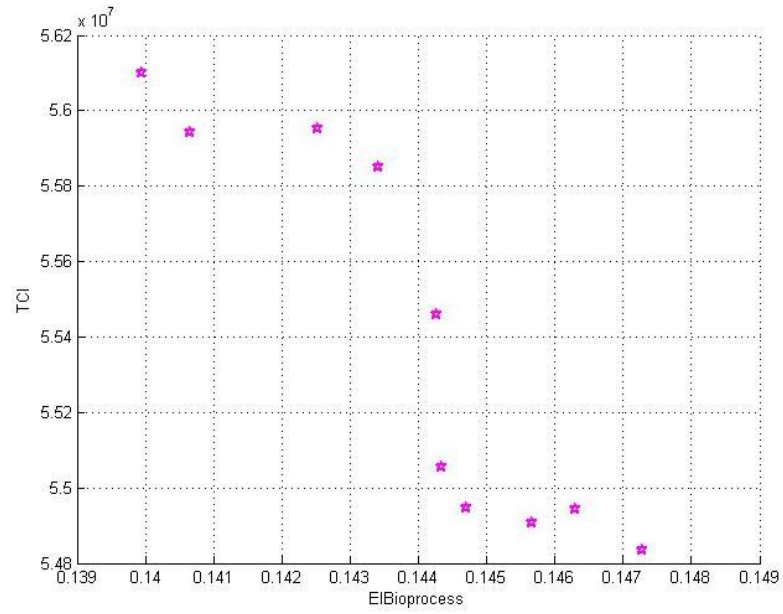
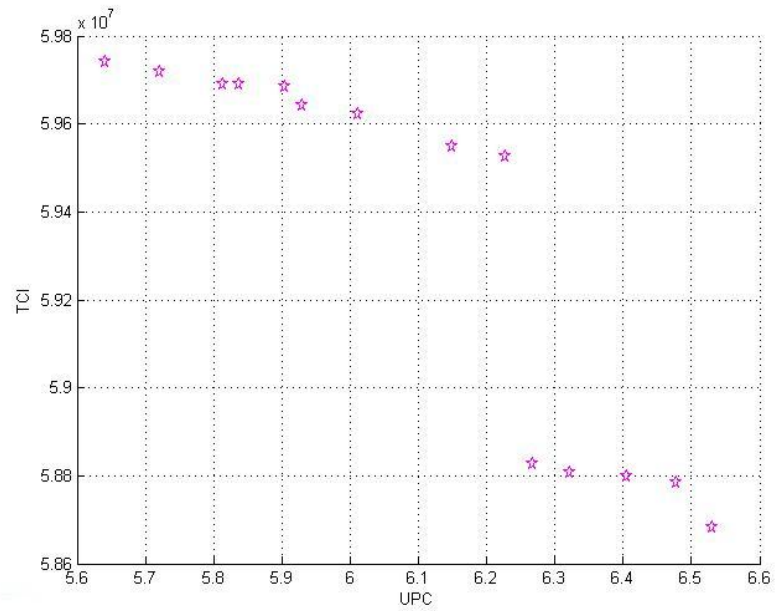
Fig. 10. Pareto optimal solutions TCI-EI<sub>Bioprocess</sub>

Fig. 11. Pareto optimal solutions TCI-UPC

The proposed optimization strategy is fast, easy to use and doesn't require advanced programming knowledge.

The main advantages of SuperPro Designer simulator are:

- A large data base of specific chemical compounds and unit operations.
- The possibility of evaluating of the economical performance indexes.

However, SuperPro Designer was not designed for this kind of use and, unfortunately, there are several restrictions:

- Not all the process variables are given in the Designer Type Library of SuperPro Designer server [6].
- Due to the simplicity of the model associated with unit procedures, some inconsistent results can be obtained: the pyruvic acid process uses a four cycle stoichiometric fermentation model. In the first cycle, acetic acid is added, the biomass growth is increased, and pyruvic acid is produced in low amounts. In the cycles 2-4, due to the lack of acetic acid, the growing of the biomass stops, and the product formation is increased. In these conditions, it is expected that in the first cycle, increasing acetic acid flowrate would lead to a biomass production growth, and to an increase of pyruvic acid produced by resting biomass in cycles 2-4. However, from simulations results, it can be observed that an increase of acetic acid flowrate leads to a decrease of pyruvic acid production. This limitation can be overcome by the elaboration of complex models in Matlab, for the key steps of the bioprocesses in order to link them to the corresponding SuperPro Designer unit procedures, using the presented GUI.
- Continuous change of process variables may lead to unexpected error messages and run off the optimization process. This may occur in the case of complex bioprocesses.

## 5. Conclusions

A useful client-server application used to call the SuperPro Designer simulator repetitively inside optimization loops for various sets of input variables was developed. Due to the link with Matlab, SuperPro Designer functionality is greatly extended by the use of Matlab toolboxes (optimization, statistics, genetic algorithm and direct search, graphical tools, etc.). The multi-objective optimization is in agreement with the actual tendency in design and operation of economical and environmental sustainable bioprocesses. Genetic Algorithms are stochastic search techniques that evolve a population of initial solutions. More accurate solutions can be obtained by modifying Genetic Algorithm parameters (e.g. increasing of the population size and generation number) with the cost of a substantially increasing of the computer execution time. Another very important direction of improving the results quality consists in elaborating of complex models for key process units in Matlab, and implementing them in SuperPro

Designer using the presented GUI. In this way the inconvenient of the SuperPro Designer models simplicity is solved. The optimal solution, obtained by the link of Matlab with SuperPro designer using the presented new GUI can be finally refined by repeated of-line, traditional simulations, especially by changing the values of the process variables which are not present in Designer Type Library.

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