Optimal design of batch plants under economic and ecological considerations: Application to a biochemical batch plant

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Abstract

This work deals with the multicriteria cost-environment design of multiproduct batch plants, where the design variables are the equipment item sizes as well as the operating conditions. The case study is a multiproduct batch plant for the production of four recombinant proteins. Given the important combinatorial aspect of the problem, the approach used consists in coupling a stochastic algorithm, indeed a Genetic Algorithm (GA) with a Discrete Event Simulator (DES). To take into account the conflicting situations that may be encountered at the earliest stage of batch plant design, i.e. compromise situations between cost and environmental considerations, a Multicriteria Genetic Algorithm (MUGA) was developed with a Pareto optimal ranking method. The results show how the methodology can be used to find a range of trade-off solutions for optimizing batch plant design.

Keywords: Multicriteria optimization; Genetic algorithm; Batch plant design; Environmental impact

1. Introduction

The design of multiproduct and multipurpose batch plants is a key problem in chemical engineering. The problem formulation generally involves mathematical programming methods such as MINLP (Mixed-Integer Non-Linear Programming). The main limitation of such methodologies is the difficulty, even impossibility, to describe with a high degree of sophistication, the real constraints that may be encountered (various storage policies for instance ...). Moreover, the number of equations to take as constraints often renders the problem impossible to solve. An alternative proposed in [1] consists in coupling a Discrete Event Simulator (DES) in order to evaluate the feasibility of the production at medium term scheduling, with a master optimization procedure based on a Genetic Algorithm (GA). The optimization variables take only discrete values and the problem exhibits a marked combinatorial feature (the equipment sizes are considered as discrete values). This approach was then generalized in [2] to consider multicriteria design and retrofitting. The choice of a hybrid method GA/DES was then all the more justified as several criteria were simultaneously taken into account: a trade-off between investment cost, equipment number and a flexibility index based on the number of campaigns necessary to reach a steady state regime was thus investigated.

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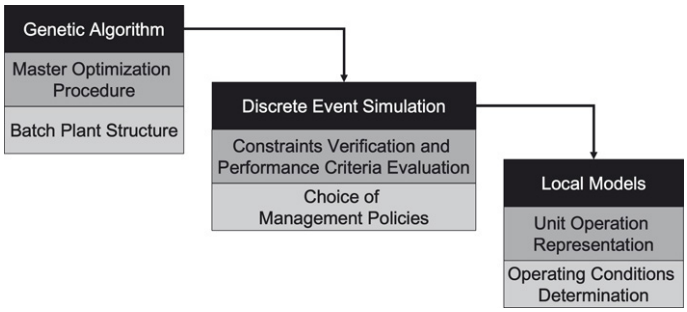

Fig. 1. General methodology for optimal batch plant design.

The Multicriteria Genetic Algorithm (MUGA) developed was based on the combination of a Monocriterion Genetic Algorithm (MOGA) and a Pareto Sort (PS) procedure.

This work is thus motivated by the need to take into account the capital cost as well as the environmental impact from the earliest design stage. A simplest version of the previously developed DES model has been implemented to model multiproduct batch plant features.

The originality of the global model is that it takes into account computed values for operating times deduced from embedded local models for unit operations. Let us recall that the constant time and size factor model [3] is the most widespread to design multiproduct batch processes. These models are used to optimize the plant design by proper selection of batch sizes of each product, the operating times of semi-continuous units and the structure of the plant. Only the works presented in [4–7] include process performance models to compute time and size factors and select process variables as optimization variables.

In this perspective, the approach proposed in this work is to offer a general methodology for ecological and economic assessment for batch plant design problems.

This paper is organized as follows: Section 2 presents the basic principles of the general framework. Section 3 discusses some key points of the implementation. Section 4 displays and discusses some significant results obtained for a case study, i.e., the design of a batch plant dedicated to the production of proteins. In the final section, the conclusion is presented and the guidelines established.

2. Methodology

The framework for batch plant design proposed in this study (see Fig. 1) integrates simple unit operation models into the batch plant wide model, which is then embedded in an outer optimization loop. The approach adopted in this work [8] consists in coupling a stochastic algorithm, indeed a Multicriteria Genetic Algorithm (MUGA) with a Discrete Event Simulator (DES). The DES was developed using the C++ object-oriented language, keeping the approach proposed in [1]. In their works, a four layer framework was proposed, resulting in the development of a standard library for the simulator classes that are general to any case, thus minimizing the task of treating different study cases or the variants of a given one (i.e. design or scheduling objectives). In this approach, at the lowest level, the common engine can be found. Most of the events at the next level are common to all batch plant simulations, but some case studies could need the definition of a particular event. Only few equipment items are common to all batch plants (i.e. storage vessels) whereas most of them are particular to each problem and must be defined. The upper layer is the supervisor, which must be generally adapted to each study case.

The objective of the master GA involved is to propose several good and even optimal solutions, whereas the DES checks the feasibility of the proposed configuration and evaluates different criteria with both economic and ecological targets.

Indeed, engineering design problems are usually characterized by the presence of many conflicting objectives that the design has to fulfill. Therefore, it is natural to look at the engineering design problem as a multiobjective optimization problem (MOOP). References to multiobjective optimization could be found in [9–11]. As most optimization problems are multiobjective by nature, there are many methods available to tackle these kinds of problems. Lately there has been a large development of different types of multiobjective genetic algorithms, which is also reflected in the literature. The big advantage of genetic algorithms over other methods is that a GA manipulates

a population of individuals. It is therefore tempting to develop a strategy in which the population captures the whole Pareto front in one single optimization run. This approach was adopted in this study.

The MUGA developed in this study involves different procedures:

(1) A method for encoding solutions in strings of digits (or chromosomes); here, a chromosome represents a workshop configuration and the corresponding operating conditions. The encoding procedure will be presented in detail in what follows.

(2) An initial population has to be randomly generated.

(3) An evaluation function which takes a string as input and returns different fitness values which measure the quality of the solution that the chromosome represents relative to each criterion. Since this work is related to minimization cases (investment cost, limitation of pollution), the individual fitness F_i is calculated by:

$$F_i = C_{\max} - C_i$$

where C_i is one of the objective function value for individual i, $C_{\max}$ is the maximum objective function value computed on the current population for the corresponding criterion.

(4) An adaptive plan involving evolution and mutation, based on string crossover and mutation operators.

The cycle {Evaluation, Selection, Crossover and Mutation} is repeated until a stop criterion is reached. After this cycle, the Pareto sort is applied. Concerning selection and multicriteria aspects involved, it must be emphasized that for a given survival rate, the selection process is achieved via a classical Goldberg biased roulette wheel [12], relative to each criterion. For this purpose, the initial population is randomly partitioned into sub-populations (the number of sub-populations corresponds to the number of criteria considered simultaneously). A same number of individuals is chosen for each sub-population.

The genetic algorithm includes the following steps (see Fig. 2):

Step 1: an initial population is generated randomly, this procedure guarantees a diversified initial population covering the complete space search.

The following steps are performed in order to pass from the actual population (k) to the next one ($k + 1$). First an intermediate population is generated in Steps 2–4.

Step 2: an elitism procedure selects the best individual for each criterion, which is saved in an intermediate place.

Step 3: an equal number of individuals is chosen for each criterion using Goldberg's biased roulette.

Step 4: the intermediate population is completed with individuals generated by the cross-over procedure. Let us note that the individuals to whom this procedure is applied are chosen randomly from the population k. The simplest cross-over procedure is used with only one cutting point.

Step 5: the mutation procedure is applied to a fixed number of randomly chosen individuals. Only one point of the chromosome is modified, changing its value from 0 to 1 or the inverse.

Step 6: the new population becomes the current one and the Steps 2–5 are repeated until reaching the final generation.

Step 7: a Pareto sort procedure is carried out over all the individuals evaluated over generations.

At the end of the algorithm, the set of Pareto non dominated solutions is obtained.

The optimization problem may involve either continuous (i.e. the operating conditions) or discrete (parallel equipment number, equipment size) variables.

A binary system was chosen for encoding, as it simplifies the genetic operators, i.e., crossover and mutation. The encoding method presented was developed for the cases where the equipment items are identical at a given stage. The continuous variables were discretized and encoded in a binary way by a variable change (Fig. 3), using the same bit number (i.e., eight bits). Fig. 4 shows a code section used for operating stage encoding. For each stage, the equipment item number is encoded in a binary way (part A in Fig. 4). The number of bits reserved to this variable sets the maximum equipment item at the stage. For equipment size (L for large, M for medium, S for small), a number of bits equal to the available sizes for the equipment items was reserved (part B in Fig. 4): the chosen size takes a positive value whereas zero is allocated to the other places. When equipment items are composed of several parts, the same approach is repeated for each component (part B and B' in Fig. 4).

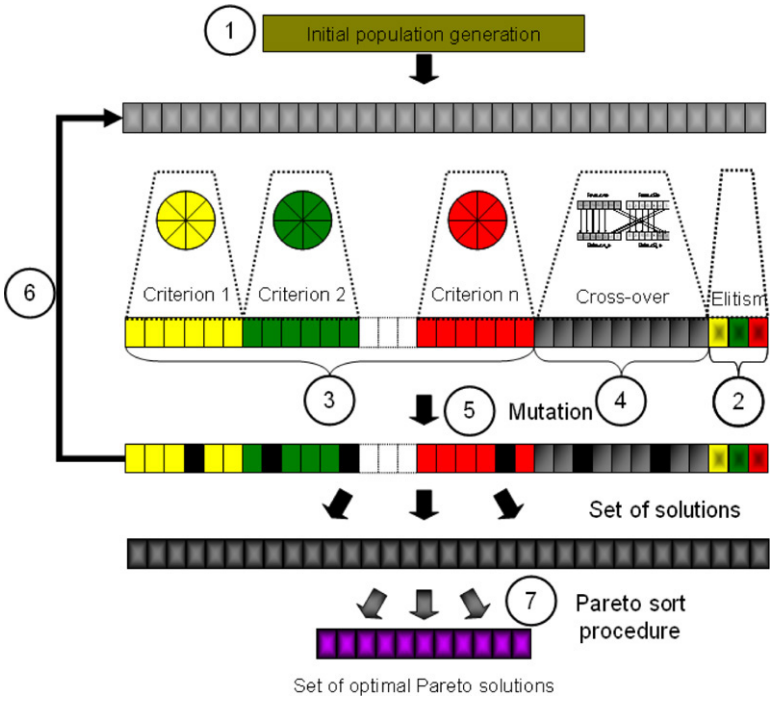

Fig. 2. MultiObjective Genetic Algorithm (MUGA).

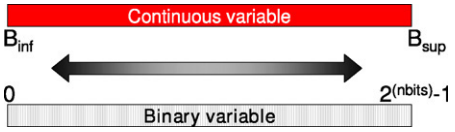

Fig. 3. Continuous variables encoding.

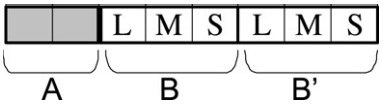

Fig. 4. Operating stage encoding method.

3. Implementation

3.1. Presentation of the illustrative example

The previous methodology was applied to a batch plant for the production of proteins taken from the literature [5].

This is a multiproduct batch plant, with four products to be manufactured by fermentation and eight treatment stages. This example is used as a test bench since short-cut models describing the unit operations involved in the process are available. The batch plant involves eight stages for producing four recombinant proteins, on one hand two therapeutic proteins, Human insulin (I) and Vaccine for Hepatitis B (V) and, on the other hand, a food grade protein, Chymosin (C) and a detergent enzyme, cryophilic protease (P). The methodology is generic for any plant producing recombinant proteins from yeast.

Fig. 5 shows the flowsheet of the multiproduct batch plant considered in this study. All the proteins are produced as cells grow in the fermenter (Fer).

Vaccine and protease are considered as being intracellular, hence, for these two products, the first microfilter (Mf1) is used to concentrate the cell suspension, which is then sent to the homogenizer (Hom) for cell disruption to liberate the intracellular proteins. The second microfilter (Mf2) is used to remove the cell debris from the solution proteins.

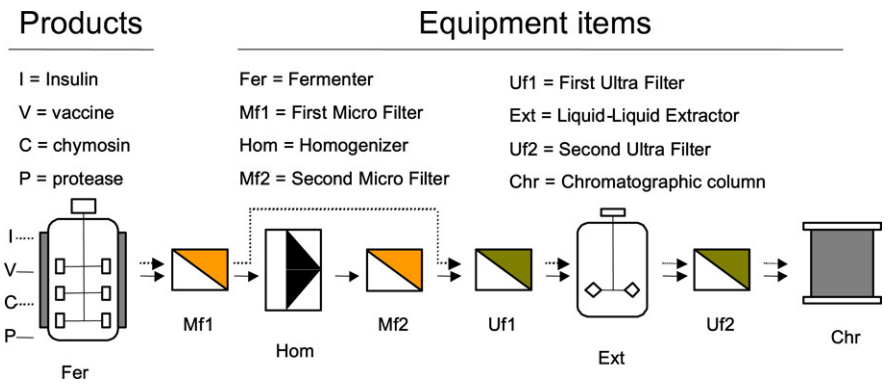

Fig. 5. Multiproduct batch plant for proteins.

The ultrafiltration (Uf1), prior to extraction, is designed to concentrate the solution in order to minimize the extractor volume. In the liquid–liquid extractor (Ext), salt concentration (NaCl) is used to first drive the product to a poly-ethylene-glycol (PEG) phase and again into an aqueous saline solution in the back extraction.

Ultrafiltration (Uf2) is used again to concentrate the solution. The last stage is finally chromatography (Chr), during which selective binding is used to better separate the product of interest from the other proteins.

Insulin and chymosin are extracellular products. Proteins are separated from the cells in the first microfilter (Mf1), where cells and some of the supernatant liquid stay behind. To reduce the amount of valuable products lost in the retentate, extra water is added to the cell suspension.

The homogenizer (Hom) and microfilter (Mf2) for cell debris removal are not used when the product is extracellular. Nevertheless, the ultrafilter (Uf1) is necessary to concentrate the dilute solution prior to extraction. The final step of extraction (Ext), ultrafiltration (Uf2) and chromatography (Chr) are common to both the extracellular and intracellular products.

3.2. Environmental impact evaluation

Considering environmental impact (EI), let us recall that several methodologies are available in the literature. The most important concept refers perhaps to the Life Cycle Assessment (LCA) [13] considering all the wastes generated in order to produce the different products in the upstream stages (i.e., raw material production, energy generation, etc.), in the study stage (i.e. solvents, non-valuable by-products, etc.) and in the downstream steps (i.e. recycling, incineration, etc.). The aim of LCA is to consider the wide chain in order to prevent pollution generation and to compare the different alternatives to produce a product. Another concept used the Pollution Balance (PB) principle to carry out a pollution balance [14] equivalent to the balance made for mass or energy. This means that a process can not only pollute but also consume a polluting product and will be a benign process.

Finally, the Pollution Vector (PV) methodology [15] consists in evaluating the environmental impact by means of an impact vector over different environments (i.e. water, air, etc.) defined as the mass emitted on an environment divided by the standard limit value in this environment.

Given the production recipes for the different products and the general flow-sheet, the first step consists in applying the LCA methodology to determine all the products contributing to the environmental impact (Fig. 6). For information availability reasons, the study was reduced to the process being studied, which is of course a limited application of LCA. Products (i.e. vaccine) and raw materials (glucose, NH_3) were considered not having an environmental impact. After that, a PB is applied, using the PV to quantify the environmental impact. In this case, an adapted definition of the pollution vector was introduced, because the standard limit values for the polluting product were not found in the literature. This vector has two components; the former is the total biomass quantity released and the latter concerns the PEG volume used. Even if the solvent can be recycled, it cannot be carried out at 100%, so the environmental impact is considered to be proportional to this quantity. The pollution indexes were thus defined as the emitted quantities divided by the mass of the manufactured products. Let us remark that environmental impact minimization can be viewed as a multicriteria problem in itself.

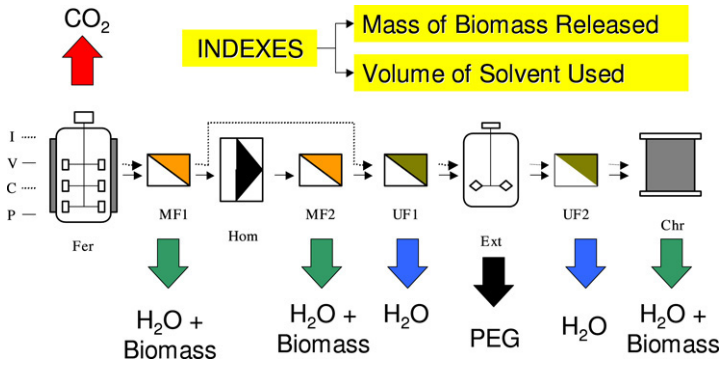

Fig. 6. Environmental impact evaluation.

The global index of each environmental impact criterion is defined as a weighted sum respect to the production of each product index (Eq. (1)).

$$I_k = \frac{I_k^{\text{ins}} \cdot P_{\text{ins}} + I_k^{v} \cdot P_{\text{vac}} + I_k^{\text{chy}} \cdot P_{\text{chy}} + I_k^{\text{pro}} \cdot P_{\text{pro}}}{P_{\text{ins}} + P_{\text{vac}} + P_{\text{chy}} + P_{\text{pro}}} \tag{1}$$

where I_k is the pollution global index, I_k^i is the k pollution index of i product defined as the kilograms of the pollutant k by kilograms of manufactured product i and P_i is the total production of the i product.

The cost criterion considered in this study is classically based on investment minimization because there was not enough information to evaluate the operational cost of the batch plant (raw material cost, utilities cost ...) and to embed it in a net present worth computation.

The optimization criterion involving investment cost for equipment and storage vessels ICost is calculated by (Eq. (1)):

$$\text{ICost} = \sum_{i=1}^{N_{\text{OP}}} \sum_{j=1}^{N_{\text{EQ}}} \left(A_i + B_i V_{ij}^{C_i} \right) + \sum_{k=1}^{N_{\text{SK}}} \left(A_k + B_k V_{sk}^{C_{ki}} \right) \tag{2}$$

where N_{OP} is the number of operations, $N_{\text{EQ}i}$ is the number of equipment items (for operation i), N_{SV} is the number of storage vessels, A_i, B_i and C_i are the cost coefficients for operation i, A_s, B_s and C_s are the cost coefficients for storage vessels, V_{ij} is the volume of equipment ij and V_{sk} is the volume of storage vessel k.

The models representing the operation units involved in the global process are presented in detail in [16] and will not be recalled here.

The optimization problem considered can be formulated as follows:

$$\begin{aligned} &\min f_1(y) \\ &\min f_2(x) \\ &\text{s.t. } g(x, y) \leq H \end{aligned}$$

where, f_1 represents the investment cost and f_2 the environmental impact. The x vector, $x = [x_1, x_2, \ldots, x_n]$ represents the operating conditions and $y = [y_1, y_2, \ldots, y_n]$ refers to batch plant configuration.

The optimization problem involves 44 variables, which may be either continuous (i.e. the operating conditions) or discrete (parallel equipment number, equipment size).

In Tables 1 and 2, all the optimization variables and their corresponding type (discrete or continuous) are listed.

A set of data must be fixed by the user concerning the optimization problem definition before the implementation of the design methodology. These data are presented in Tables 3–5:

In Table 3, the annual demand for each product is presented.

Table 4 presents the available range in terms of size for each equipment type. Three sizes are available for each equipment item: large (L), medium (M) and small (S). Table 5 presents the classical expressions used for computing the investment cost of the equipment items, following a classical scaling law. Of course, a thorough economic study

Table 1
Continuous optimization variables: operating conditions

Continuous variables	
Name	Description (operating conditions)
$C_{i,\mathrm{fer}}$	Insulin final concentration at the fermentation stage
$C_{v,\mathrm{fer}}$	Vaccine final concentration at the fermentation stage
$C_{c,\mathrm{fer}}$	Chymosin final concentration at the fermentation stage
$C_{p,\mathrm{fer}}$	Protease final concentration at the fermentation stage
$C_{i,\mathrm{mf1}}$	Insulin final concentration at the first microfiltration stage
$C_{v,\mathrm{mf1}}$	Vaccine final concentration at the first microfiltration stage
$C_{c,\mathrm{mf1}}$	Chymosin final concentration at the first microfiltration stage
$C_{p,\mathrm{mf1}}$	Protease final concentration at the first microfiltration stage
$W_{i,\mathrm{mf1}}$	Water added at the first microfiltration stage (insulin)
$W_{c,\mathrm{mf1}}$	Water added at the first microfiltration stage (chymosin)
$W_{v,\mathrm{mf2}}$	Water added at the second microfiltration stage (vaccine)
$W_{p,\mathrm{mf2}}$	Water added at the second microfiltration stage (protease)
$R_{i,\mathrm{ext}}$	Phase ratio at the liquid–liquid extraction for insulin
$R_{v,\mathrm{ext}}$	Phase ratio at the liquid–liquid extraction for vaccine
$R_{c,\mathrm{ext}}$	Phase ratio at the liquid–liquid extraction for chymosin
$R_{p,\mathrm{ext}}$	Phase ratio at the liquid–liquid extraction for protease

Table 2
Discrete optimization variables: equipment item number and size

Discrete variables	
Name	Description (equipment items number and size)
N_{sto}	Storage vessel number
N_{fer}	Equipment items number at the fermentation stage
N_{mf1}	Equipment items number at the first microfiltration stage
N_{hom}	Equipment items number at the homogenization stage
N_{mf2}	Equipment items number at the second microfiltration stage
N_{uf1}	Equipment items number at the first ultrafiltration stage
N_{ext}	Equipment items number at the liquid–liquid extraction stage
N_{uf2}	Equipment items number at the second ultrafiltration stage
N_{chr}	Equipment items number at the chromatographic separation stage
$NP_{v,\mathrm{hom}}$	Vaccine pass number through the homogenization stage
$NP_{p,\mathrm{hom}}$	Protease pass number through the homogenization stage
V_{sto}	Storage vessel volume
V_{fer}	Fermenter volume
$V_{\mathrm{mf1,ret}}$	First microfilter retentate vessel volume
$S_{\mathrm{mf1,fil}}$	First microfilter filtration surface
$V_{\mathrm{mf1,per}}$	First microfilter permeate vessel volume
S_{hom}	Homogenizer size
$\mathrm{Cap}_{\mathrm{hom}}$	Homogenizer capacity
$V_{\mathrm{mf2,ret}}$	Second microfilter retentate vessel volume
$S_{\mathrm{mf2,fil}}$	Second microfilter filtration surface
$V_{\mathrm{mf2,per}}$	Second microfilter permeate vessel volume
V_{uf1}	First ultrafilter retentate vessel volume
$S_{\mathrm{uf1,fil}}$	First ultrafilter filtration surface
V_{ext}	Liquid–liquid extractor volume
V_{uf2}	Second ultrafilter retentate vessel volume
$S_{\mathrm{uf2,fil}}$	Second ultrafilter filtration surface
S_{chr}	Storage vessel volume
$S_{\mathrm{chr,col}}$	Chromatographic column volume

would also include the operating cost estimation and analysis of profitability. Since this kind of analysis only requires reliable economic data for a real process and does not induce additional difficulties in the chosen resolution strategy, a

Table 3
Product demands

Product	Production (kg/year)
Insulin	1500
Vaccine	1000
Chymosin	3000
Protease	6000

Table 4
Available equipment item sizes

Equipment item size	Large	Medium	Small
Fermenter (m^3)	6	3	1
First micro filter-retentate vessel (m^3)	6	3	1
First micro filter-filtration surface (m^2)	5	2.5	1
First micro filter-permeate vessel (m^3)	6	3	1
Homogenizer-holding vessel (m^3)	6	3	1
Homogenizer-capacity (m^3/h)	0.5	0.25	0.1
Second micro filter-retentate vessel (m^3)	6	3	1
Second micro filter-filtration surface (m^2)	5	2.5	1
Second micro filter-permeate vessel (m^3)	6	3	1
First ultra filter-filtration surface (m^2)	50	25	10
First ultra filter-permeate vessel (m^3)	6	3	1
Liquid–liquid extractor	6	3	1
Second ultra filter-permeate vessel (m^3)	6	3	1
Second ultra filter-filtration surface (m^2)	5	2.5	1
Chromatographic separation-holding vessel	6	3	1
Chromatographic separation-column	1	0.5	0.25
Storage vessel	6	3	1

Table 5
Cost coefficients

Unit	Size	Cost
Fermenter	V_j (m^3)	$63\,400 \cdot V^{0.6}$
Micro- and ultrafilter	$V_{\text{retentate}}$ (m^3)	$5750 \cdot V^{0.6}$
	V_{permeate} (m^3)	$5750 \cdot V^{0.6}$
	A_{filter} (m^2)	$2900 \cdot A^{0.85}$
Homogenizer	V_{holding} (m^3)	$5750 \cdot V^{0.6}$
	Cap (m^3/h)	$12\,100 \cdot \text{cap}^{0.75}$
Extractor	V_{extr} (m^3)	$23\,100 \cdot V^{0.65}$
	V_{holding} (m^3)	$5750 \cdot V^{0.6}$
Chromatography column	V_{chrom} (m^3)	$360\,000 \cdot V^{0.995}$
Storage vessel	V_{sto}	$5750 \cdot V^{0.6}$

capital cost-based study was finally adopted for the preliminary economic evaluation of the project for manufacturing biological products.

Table 6 presents the lower and upper variable bounds.

Table 7 displays the parameters of the genetic algorithm used for multicriteria batch plant design. In this work, the generation number was fixed as twice the population size. The global survival rate is relatively low as compared to standard values for optimization of test mathematical functions [2]. Moreover, a high mutation rate was set. Although a systematic study was not carried out to find these values, they were chosen from several preliminary tests and agree with previous works [2] where similar problems were treated. Elitism was used in order to avoid losing the best solution for each criterion. Considering the stochastic aspect of GAs, several optimization runs were carried out

Table 6
Variable bounds

Variable	Lower bound	Upper bound
$C_{i,\mathrm{fer}}$, $C_{v,\mathrm{fer}}$, $C_{c,\mathrm{fer}}$, $C_{p,\mathrm{fer}}$ (kg/m^3)	35	55
$C_{i,\mathrm{mf1}}$, $C_{v,\mathrm{mf1}}$, $C_{c,\mathrm{mf1}}$, $C_{p,\mathrm{mf1}}$ (kg/m^3)	150	250
$W_{i,\mathrm{mf1}}$, $W_{c,\mathrm{mf1}}$ (m^3/m^3)	0.5	3.0
$NP_{v,\mathrm{hom}}$, $NP_{p,\mathrm{hom}}$	1	3
$W_{v,\mathrm{mf2}}$, $W_{p,\mathrm{mf2}}$ (m^3/m^3)	1	3
$R_{i,\mathrm{ext}}$, $R_{v,\mathrm{ext}}$, $R_{c,\mathrm{ext}}$, $R_{p,\mathrm{ext}}$ (m^3/m^3)	0.05	1.5
N_{sto}	0	7
N_{fer}, N_{mf1}, N_{uf1}, N_{ext}, N_{uf2}, N_{chr}	1	8
N_{hom}, N_{mf2}	1	4

Table 7
Genetic algorithm parameters

	Bicriteria solvent-biomass	Bicriteria cost–solvent	Bicriteria cost–biomass	Tricriteria cost-EI
Population size	300	450	450	600
Generation number	600	900	900	1200
Survival rate	0.5	0.5	0.5	0.5
Mutation rate	0.4	0.4	0.4	0.4
Elitism by criterion	1	1	1	1

for each multicriteria optimization. Given that solutions obtained in one optimization run could be dominated by the solution of another one, a Pareto sort procedure is applied to the set of solutions obtained at each optimization run, and the non-dominated solutions are those proposed by the methodology.

4. Results and discussion

Two strategies were tested either monoproduct or multiproduct campaigns with a batch of each product to be produced. In the latter case, the starting order of the different batches was fixed altering intracellular and extracellular products.

The MUGA presented in this work was first used to demonstrate that the two EI criteria considered, that are respectively the total biomass quantity and the PEG volume, present antagonist goals (Fig. 7). Very similar results were obtained at each optimization run, so only the results after the final Pareto sort procedure are presented in Fig. 7. Moreover, it must be noted that slight differences are obtained between both production policies because the environmental impact depends only on the mass balance that is a function of the continuous variables.

This antagonist behavior can be explained at the liquid–liquid extraction stage. The more solvent is used, the more efficient the stage becomes and, consequently, the fewer products are lost, reducing the environmental impact index computed as Kg of biomass released by Kg of final product.

The same approach was also applied to the cost–environment criteria. First, the amount of solvent used and the investment cost were considered.

For illustration purposes, Fig. 8 shows the results obtained at each optimization run for the monoproduct production policy, performed with an identical parameter set to guarantee the stochastic nature of the GA. In this case, the results are not superposed as it was the case for the bicriteria optimization biomass-solvent, which show the need of carrying out several optimization runs for the same problem.

In Fig. 8, it can be seen that each optimization run is oriented to a section of the search region. The first optimization comes up with the better solution for the cost criterion, the second for the environmental criterion and the third is a compromise between both. The final Pareto sort procedure is carried out over these solutions. The final results for both production policies are presented in Fig. 9. Let us note that the Pareto zone is constituted of sparse points, since the adaptation function related to the investment cost takes discrete values.

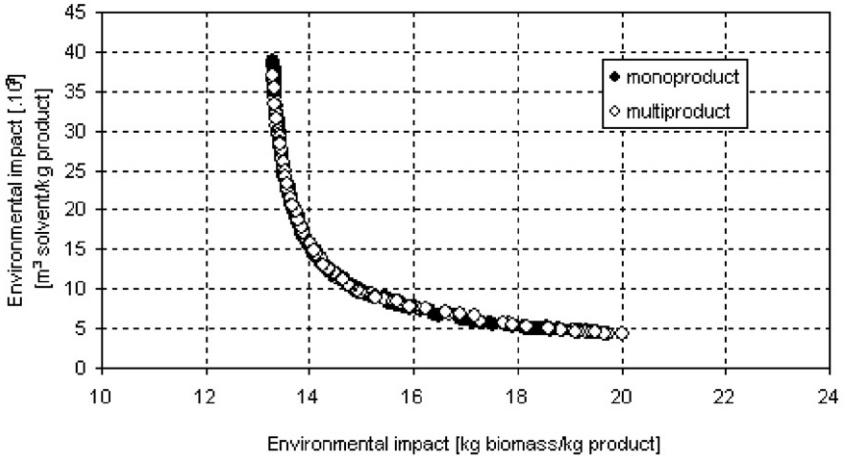

Fig. 7. Pareto's optimal solutions for biomass released — solvent amount criteria (bicriteria case).

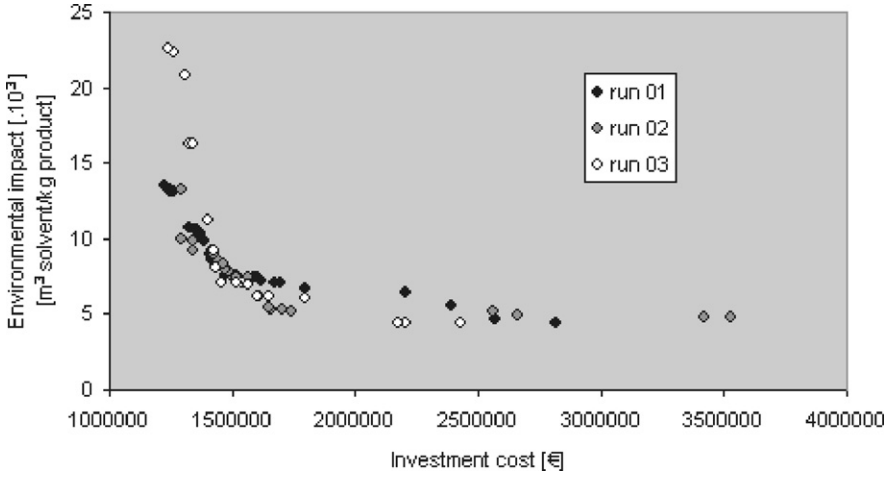

Fig. 8. Pareto's optimal solutions for the bicriteria case (solvent used–investment cost) under monoproduct policy.

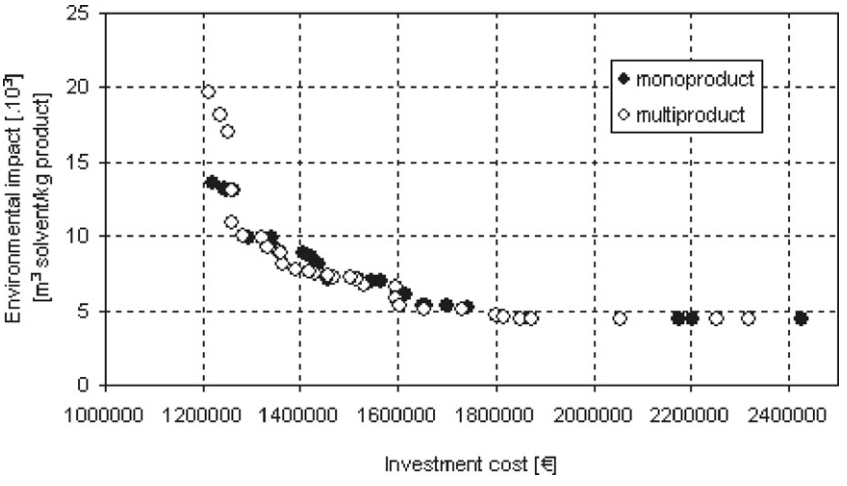

Fig. 9. Pareto's optimal solutions for the bicriteria case (solvent used–investment cost) under mono- and multiproduct policies.

Table 8
Bicriteria cost–solvent optimization results.

	Monoproduct			Multiproduct		
	Cost	Solvent (10^3)	Solutions	Cost	Solvent (10^3)	Solutions
Run 1	1 221 890	4.445	32	1 303 730	5.070	21
Run 2	1 290 490	4.779	23	1 211 100	5.006	28
Run 3	1 238 050	4.415	23	1 257 200	4.406	23
Best	1 140 990	4.386	–	1 139 100	4.386	–

Table 9
Values range for the not considered criterion

	Biomass for cost–solvent		Solvent for cost–biomass	
	Minimum	Maximum	Minimum	Maximum
Monoproduct	14.393	20.3691	36.0292×10^{-3}	40.581×10^{-3}
Multiproduct	14.261	22.889	34.9659×10^{-3}	41.877×10^{-3}

Table 10
Bicriteria cost–biomass optimization results

	Monoproduct			Multiproduct		
	Cost	Biomass	Solutions	Cost	Biomass	Solutions
Run 1	1 143 080	13.303	10	1 252 280	13.307	15
Run 2	1 235 340	13.300	10	1 289 530	13.303	13
Run 3	1 129 290	13.305	15	1 116 950	13.302	22
Best	1 140 990	13.299	–	1 139 100	13.305	–

Slight differences were found between both production policies. The antagonist behavior between these two criteria, investment cost — amount of solvent used, can be explained by a compromise between the solvent yield and the process global yield. When process yield is penalized, a bigger, and consequently more expensive, batch plant is required.

In order to evaluate the search performance of the GA, Table 8 presents the best solution obtained at each optimization run for each criterion considered as well as the best solution obtained with a monocriterion approach. Even though the methodology was not able to find the best solution, the values are relatively near (around 5% more expensive for the investment cost criterion). It must be noted that in the monocriterion optimization (not presented here), the best value was obtained only once and, in the other cases, the solutions were around 2%–3% more expensive, which justifies the results when several criteria are taken into account simultaneously. The number of solutions obtained in each optimization run was around 25. It is important to note that in each case, the solutions are uniformly distributed in the search space; this means that there is no preferential search region in the multicriteria search as shown in Fig. 8.

It is also interesting to see where the results are placed with respect to the criterion not considered here, in this case the amount of biomass released. Table 9 presents the range of values for this criterion for both production policies.

They have the same order of magnitude for both policies. Moreover, the minimal value of the range is close to the best value obtained in monocriterion optimization (see Table 10), which allows one to predict less antagonism between investment cost and biomass released criteria.

The last bicriteria optimization considers the investment cost and biomass released. As for the previous case, three optimization runs were carried out for each production policy. The results obtained after the final Pareto sort procedure are presented in Fig. 10 and are similar for both production policies as was shown for the cost–solvent criteria.

Table 10 presents the best solution obtained at each optimization run for each considered criterion as well as the best solution obtained with a monocriterion approach. As for the criterion related to the amount of biomass released, the best value is obtained at each optimization run, as was the case for the amount of solvent in the previous bicriteria

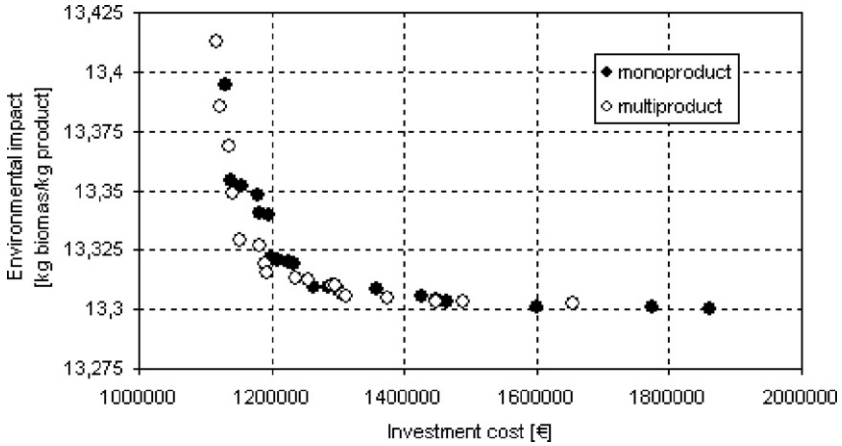

Fig. 10. Pareto's optimal solutions for biomass released – investment cost (bicriteria case).

Table 11
Multicriteria cost-environmental impact results

	Monoproduct			Multiproduct		
	Cost	Solvent (10^3)	Biomass	Cost	Solvent (10^3)	Biomass
Run 1	1 232 630	4.43776	13.303	1 130 860	4.39352	13.3003
Run 2	1 207 900	4.42136	13.3038	1 265 100	4.44696	13.3034
Run 3	1 279 110	4.39088	13.3043	1 124 630	4.45884	13.3014

optimization. The number of solutions is slightly inferior to the previous results. This can be explained by the lower antagonism between the biomass and the cost criteria. As for the investment cost, for both production policies, a better solution than the one of the MOGA was found (not presented here). Even these solutions are only 2% better than the previous. This shows the drawback of the stochastic optimization methods because they can not guarantee the solution optimality. Besides, it must be noted that the GA parameters were not the same. In the case of the MUGA, a larger population was used, but at the same time it must be noted that the fact that several criteria were taken into account is not penalizing in the GA. The environmental impact criteria guide the search of batch plants with several equipment items diversifying the search paths.

Table 9 presents also the range of values for the criterion not considered, the amount of solvent used. These values are distant from the best values, which recalls the antagonism of this criterion with respect to the others considered as objective functions.

The results obtained show the typical compromise between cost and each environmental index. Since the conflicting behavior between each pair of criteria (investment cost, solvent used and biomass released) was demonstrated, the final multicriteria cost–environment batch plant design was carried out, keeping the two environmental criteria independent: this simply means that the same survival rate was considered for each criterion.

As for the previous optimizations, three optimization runs were carried out for each production policy. Given the similarity of the results with both production policies (see Table 11), only the results obtained with a multiproduct production policy are presented (Fig. 11).

To facilitate result interpretation, a projection over the plane of interest (relative to two given criteria) was carried out (Figs. 13, 15 and 16). It can be observed that most solutions referring to the previous bi-criteria optimization are found again. In all three cases, the points are more concentrated near the compromise zone, which is interesting for final decision. In order to evaluate the methodology, Figs. 12 and 14 show the results projected for each optimization run. In this case, we observe that several optimization runs are necessary, given the complexity of considering a third criterion; the results are not systematically superposed as for the bicriteria case study. Two options could be considered for improvement, larger population and generation number and some extra optimization runs.

Table 11 presents the best solution for each criterion for both production policies. As was above mentioned, there are only slight differences between both production policies. This also shows that the monocriterion search is not

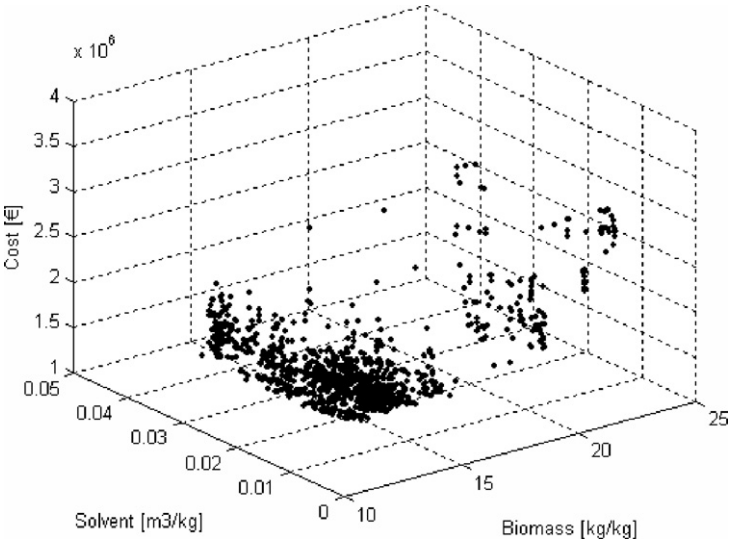

Fig. 11. Pareto's optimal solutions cost–IE (tricriteria case).

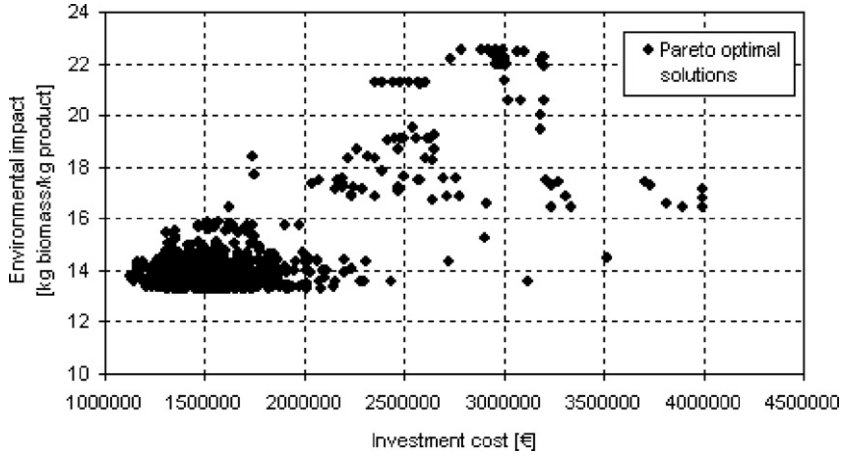

Fig. 12. Pareto's optimal solutions cost–biomass (tricriteria case).

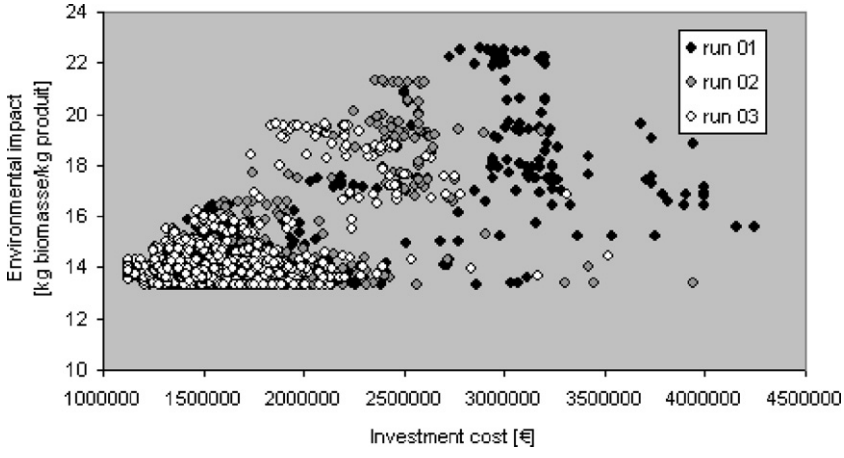

Fig. 13. Pareto's optimal solutions cost–biomass (different optimization runs).

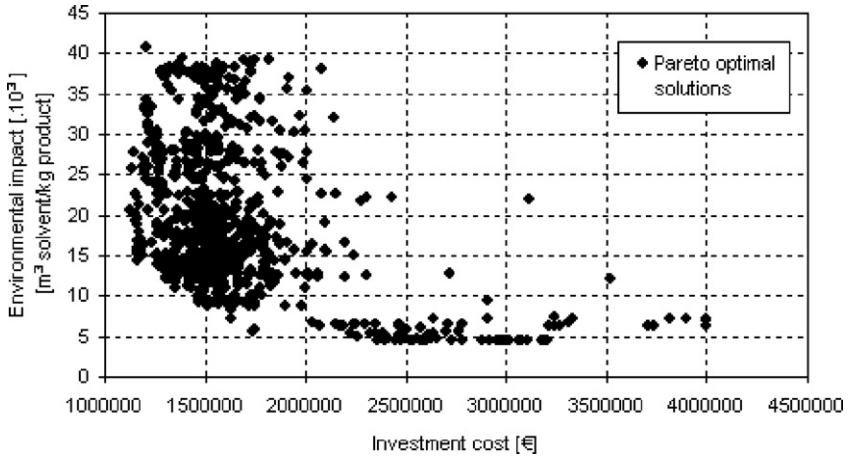

Fig. 14. Pareto's optimal solutions cost–solvent (tricriteria case).

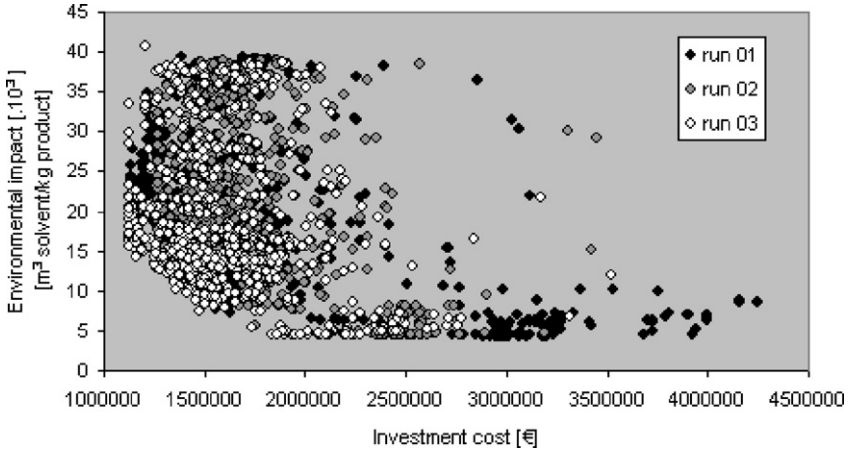

Fig. 15. Pareto's optimal solutions cost–solvent (tricriteria case).

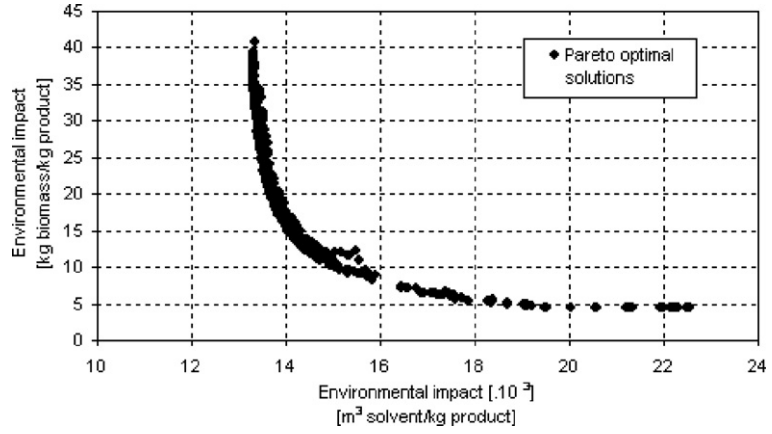

Fig. 16. Pareto's optimal solutions cost–solvent (tricriteria case).

penalized by the multicriteria one. In other words, the same GA is able to carry out both policies, even when several antagonist objective functions are considered.

5. Conclusions

A methodology was proposed for batch plant design, considering both investment cost and environmental impact minimization. An optimization scheme has been implemented using a multiobjective genetic algorithm with a Pareto optimal ranking method. This technique is ideally suited to this type of problem, where a number of conflicting considerations must be taken into account. The use of MUGA makes possible a robust optimization technique, across a non-linear search space (the objective functions are computed by the use of a discrete event simulator (DES) integrating shortcut unit operations models) linking multiple variables and objectives. The paper clearly shows that opportunities for process optimization and environmental impact minimization must be considered at the early stages of process development before the process is frozen due to regulatory reasons.

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