Multiobjective Optimization of Multiproduct Batch Plants Scheduling Under Environmental and Economic Concerns

Elisabet Capón-García, Aarón D. Bojarski, Antonio Espuña, and Luis Puigjaner
Dept. of Chemical Engineering, CEPIMA, Universitat Politècnica de Catalunya, ETSEIB, Av. Diagonal 647, Barcelona 08028, Spain

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In batch process scheduling, production trade-offs arise from the simultaneous consideration of different objectives. Economic goals are expressed in terms of plant profitability and productivity, whereas the environmental objectives are evaluated by means of metrics originated from the use of life cycle assessment methodology. This work illustrates a novel approach for decision making by using multiobjective optimization. In addition, different metrics are proposed to select a possible compromise based on the distance to a nonexistent utopian solution, whose objective function values are all optimal. Thus, this work provides a deeper insight into the influence of the metrics selection for both environmental and economic issues while considering the trade-offs of adopting a particular schedule. The use of this approach is illustrated through its application to a case study related to a multiproduct acrylic fiber production plant, special attention is put to the influence of product changeovers. *AIChE J,* 57: 2766–2782, 2011
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Introduction

Process industry faces increasing environmental, social and economic requirements which entail complex decision making. Specifically, batch process scheduling, which is important for the maximization of the production facility utilization while meeting market demands,[1] should cope with a wide variety of criteria to obtain good schedules according to the decision maker's preferences. In this respect, the consideration of multiple criteria decision making provides the path to deal with complex problems involving multiple and conflicting objectives. As a result, a set of compromise solutions, known as Pareto solutions,[2] is usually obtained; from them, the decision maker should choose the most suitable.

Regarding the increasing environmental concerns in chemical industry, more accurate approaches to assess process sustainability are required. Several authors highlight the importance of considering life-cycle assessment (LCA) of production processes at process synthesis, product design and its integration with processing.[3,4] Therefore, waste minimization, material recovery and utilities rationalization have been mainly dealt as integral parts at the design stage of batch plants.[4–7]

In the literature, different methodologies are proposed that account for environmental considerations in process design, planning and scheduling applied to the case of batch industries. Stefanis et al.[7] propose a methodology that embeds principles from LCA to incorporate environmental considerations in the optimal design and scheduling of batch and

Correspondence concerning this article should be addressed to L. Puigjaner at luis.puigjaner@upc.edu.

semi-continuous processes. Process economics and pollution metrics are adopted as the design objectives in a multi-objetive formulation. Such methodology is illustrated through some examples from the dairy industry. A combinatorial process synthesis is proposed by Chakraborty et al.[8,9] using multiobjective goal programming under economic and environmental criteria. The decision variables are operational variables, which depend on the design superstructure being optimized, and the presented case study consists of the design of plant-wide waste treatment facilities related to the batch industry. The economic function beholds operating cost and the environmental function uses the waste reduction algorithm (WAR[10,11]). Dietz et al.[12] define a multicriteria design framework for multiproduct batch plants, which aims at minimizing both investment costs and environmental impact. The problem is solved through a multiobjective genetic algorithm (moGA), and a discrete event simulation environment is used to solve the scheduling and planning problem level in the design process.

Once plant design is fixed, process operation decisions, i.e., scheduling related, are the only subject to modifications and undoubtedly have a strong influence on the economics and environmental impact. Song et al.[13] consider the scheduling problem, modeled by a MILP formulation, of a refinery process taking into account the environmental impact. The ε-constraint method is used to obtain a set of Pareto solutions for the multiobjective optimization which considers global environmental impacts by means of the critical surface-time 95 (CST95) assessment methodology. Berlin et al.[14] consider a case study of the dairy industry, where the production sequencing affects the environmental impact from a life-cycle perspective. They developed a heuristic method to minimize production waste based on production rules. Their methodology is further applied by Berlin and Sonesson[15] to a case study with two dairy products. The authors conclude that the environmental impact of processing cultured milk products can be greatly reduced by adopting sequences with fewer changes of product. Park et al.[16] present a goal constrained programming (GCP) algorithm for the multiobjective optimization with priority for the scheduling of cutting papers, and various optimal schedule sets are provided.

As reported by the former authors, different scheduling of product provides trade-offs between economic and environmental aspects. However, integrating these issues at the operational level may generally be a nontrivial task, since day-to-day decisions require almost immediate solutions, which can only be provided for models of limited complexity given the capabilities of the current software–hardware systems. This work aims at gaining insight into those trade-offs of batch process scheduling when alternative methods for product changeover are available. In general, the process of converting a line or equipment from running one product batch to another, i.e., product changeover, is time consuming and it may involve a variety of operations such as cleaning or unit configuration. One significant issue to be considered when product changeover occurs is concerned with cleaning operations, that may be regularly performed between two consecutive batches for the sake of product quality or plant safety. In addition, their environmental impact and economic cost may vary largely depending on the cleaning technique. Thus the consideration of multiple changeover possibilities increases the number of production schedules to be considered and the appearance of eventual trade-offs.

Several mathematical formulations have been recently proposed to solve the scheduling problem of multistage batch plants under sequence dependent changeovers. Erdirik-Dogan and Grossmann[17] present a time slot based formulation which incorporates mass balances and propose a bilevel decomposition algorithm for dealing with medium sized problems. Maravelias and Grossmann[18] propose a continuous time MILP model, based on the state task network (STN) representation and apply it to the case of multiproduct batch plants. The resource task network (RTN) representation is adopted by Castro et al.[19] for two new continuous-time formulations to optimize multistage batch plants, and compare them with alternative approaches to the problem, such as constraint programming and global sequencing variables. Alternative formulations, which can deal specifically with sequential processes, are based on the general and immediate precedence concepts. The former is firstly introduced by Mendez et al.,[20] whereas Gupta and Karimi[21] present an immediate precedence model for multiproduct batch plants including sequence dependent changeover time.

Compared to the general precedence formulation, the immediate precedence model eases the mathematical formulation required for the consideration of sequence dependent schedules and the product batching problem. Consequently this work represents the scheduling problem, using the immediate precedence model.[21] The model has been extended to consider possible use of different product changeover cleaning methods and to measure the results by using different sets of metrics.

When considering the scheduling problem, the objective function nature depends on the decision maker criteria, which are based both on his/her experience and the nature of the problem. Hence, a unique objective function is not suitable for all scheduling problems. Therefore, several possible objective functions and their scope are discussed along this work. As for economic objective functions, both plant productivity and profit are considered, whereas metrics derived from the LCA methodology are adopted to assess the environmental impact from ‘‘cradle to gate’’ of the production process. Makespan is also considered as a process wide resource usage efficiency metric.

The analysis of the decision maker’s alternatives under conflicting objectives is performed by means of multiobjective optimization. Specifically, the normalized normal constraint method, presented by Messac et al.,[22] is applied to obtain a set of Pareto solutions, which are compromise solutions of the multiobjective problem. Furthermore, different metrics are proposed to select a compromise among the Pareto solutions.

Finally, the methodology is illustrated through a case study based on a multiproduct batch facility producing acrylic fibers.

Problem Statement

This work represents a comprehensive step over the approaches presented in the former section by systematically assisting in the product scheduling under economic and environmental impacts considerations. The resulting model is solved by using moMILP/MINLP algorithm, which allows observing possible trade-offs between selected indicators. The problem can be stated as follows.

Given:

Process operations planning data

- a given time horizon;
- a set of materials: final products, intermediates and raw materials;
- a set of expected final products minimum and maximum demands;
- a fixed batch topology consisting of a set of equipment technologies for processing stages;
- a set of fixed product recipes for processing, concerning mass balance coefficients, resources utilization and processing times;
- a set of different product changeover methods;

Economic data

- direct cost parameters such as production and raw material costs;
- changeover cost parameters associated to every possible product sequence combination;
- selling price for every final product;

Environmental data

- raw material production environmental interventions
- product manufacturing environmental interventions
- equipment change over environmental interventions

The goal is to determine:

- the number of batches required to meet the demand (batching);
- the assignment and sequencing of the batches (scheduling);
- the appropriate changeover methods required between batches;
- the amount of final products to be sold;
- the environmental impact associated to each process schedule;

such that different sets of metrics, discussed in the following sections, are optimized. Within this model, and to avoid emission double counting, raw material emissions are not aggregated to product manufacturing, similarly cleaning environmental interventions are considered separately.

Mathematical Scheduling Model

To model the scheduling problem, a mathematical formulation based on the immediate precedence concept[21] has been adopted. The model has been extended to consider different interbatch cleaning methods, additional objective functions (e.g., makespan, productivity and environmental impact) and product batching. The model is decomposed in two parts. First, the product batching problem is considered based on demand and acceptable product batch sizes. This allows for the subsequent scheduling problem to opt for the number of batches to be produced instead of fixing them beforehand. In this sense, given a demand that could be fulfilled and a fixed batch size, the maximum number of batches has to be set accordingly.

Next, the allocation, sequencing and timing of the batches resulting from the first problem and associated tasks (i.e., cleaning) are modeled and optimized along a production time horizon according to different objective functions. Scheduling decisions, such as product sequencing, affect environmental considerations. In this work, the environmental impact associated with the products and the different cleaning methods for changeovers among products are assessed. As a result, the mathematical programming model considers product flows, raw materials and utilities consumptions, and changeover operations to simultaneously deal with environmental and productivity features. It is worth mentioning that the proposed multiobjective approach is still valid regardless the selected mathematical model.

First stage: product batching

The problem consists of the assignment of production to batches, so that the maximum demand of each product can be fulfilled. The number of batches considered must be enough to allow the complete assignment of production. Each batch i can be assigned to at most one product p (Eq. 1), and the total demand of each product has to be assigned, considering a fixed product batch size (Eqs. 2 and 3). Given that the problem being addressed considers a fixed batch topology, product batch sizes BS_p are fixed. Please note that a fixed amount of produced product is not required, but only minimum ($D_p^{\min}$) and maximum demands ($D_p^{\max}$) are enforced on each p product.

$$\sum_p Y_{ip} \leq 1 \qquad \forall i \tag{1}$$

$$\sum_i BS_p Y_{ip} \leq D_p^{\max} \qquad \forall p \tag{2}$$

$$\sum_i BS_p Y_{ip} \geq D_p^{\min} \qquad \forall p \tag{3}$$

An additional aim of this stage consists of the definition of process features for each batch, that is, the assignment to each batch of the processing time through the different processing stages, selling price, and the environmental impact. Therefore, Eqs. 4 and 5 establish the time required to fulfill stage k of batch i, and the related o operations: loading (load), preparation (pre), processing (pro), and unloading (unl) which all depend on the product p assigned to that batch. In the case of operation cleaning time, it has been assumed that it only depends on the products sequence, and different cleaning methods cannot be used within the same batch. Equations 6–8 are posed for batch selling price and product environmental impact.

$$T_{ik} = \sum_p time_{pk} Y_{ip} \qquad \forall (i,k) \tag{4}$$

$$T_{ik}^o = \sum_p time_{pk}^o Y_{ip} \qquad \forall (i,k) \tag{5}$$

$$BP_i = \sum_p BP_p Y_{ip} \qquad \forall i \tag{6}$$

$$BS_i = \sum_p BS_p Y_{ip} \qquad \forall i \tag{7}$$

$$EnvIm_i = \sum_p EnvIm_p Y_{ip} \qquad \forall i \tag{8}$$

Moreover, Eqs. 9 and 10 define the changeover time between any pair of batches for a given cleaning method c, depending on the products assigned to the batches. Similar equations are considered for changeover cost and environmental impact associated to every k stage and each pair i,i' of batches.

$$ChT_{ii'kc} \geq chanT_{pp'kc} - BigM \cdot \left(2 - Y_{ip} - Y_{i'p'}\right) \qquad \forall i, i', p, p', k, c | i \neq i' \tag{9}$$

$$ChT_{ii'kc} \leq chanT_{pp'kc} + BigM \cdot \left(2 - Y_{ip} - Y_{i'p'}\right) \qquad \forall i, i', p, p', k, c | i \neq i' \tag{10}$$

Finally, Eq. 11 enforces that each batch can only be assigned if all previous ones have already been, to avoid degenerated solutions.

$$\sum_p Y_{ip} \leq \sum_p Y_{i+1p} \qquad \forall i | i < \max(i) \tag{11}$$

Regarding the objective function to optimize the first part, we have decided to use the total profit; this way, the maximum number of batches is preassigned, and we provide with a starting point that does not restrict artificially the following optimization stage.

Second stage: batch scheduling

Once the batching problem is solved, the production and sequencing of the previously assigned batches, which are gathered in a set (*dynI*), are decided at this stage. A special feature of the proposed formulation is the production of a starting and finishing batch, required to address the cleaning for the first and last batches, which produce no product, but represent the initial and final still state of the plant. For nomenclature reasons, an unreal product, whose processing time, cost and environmental impact are zero, is assigned to the aforementioned two batches.

As for timing constraints, Eq. 12 establishes the end time of stage k of batch i, as a function of the starting time (Ts_{ik}) and operation o time ($\overline{T^{o}_{ik}}$), in case that such batch is eventually produced, that is, the binary variable (W_i) is 1.

$$Tf_{ik} = Ts_{ik} + \overline{T_{ik}} W_i \qquad \forall (i,k) | i \in dynI \tag{12}$$

In addition, the timing constraints among the different stages are necessary. Equation 13 defines the fact that for two consecutive stages, the unloading start time of the first one must be equal to the loading start time of the following one. This requirement is merely a consequence of the assumption of no intermediate storage of products between stages; however, this Eq. 13, can be easily modified if a different intermediate storage policy is adopted.

$$Ts_{ik+1} + \overline{T^{\text{prep}}_{ik+1}} = Tf_{ik} - \overline{T^{\text{unlo}}_{ik}} \qquad \forall (i,k) | i \in dynI,\ k \in kcon \tag{13}$$

When two stages are simultaneous, that is, their loading, operation and unloading occur at the same time, Eq. 14 enforces the load starting time of both stages to be equal. This constraint allows for modeling of fed-batch stages, e.g., a filter that requires a feed and outlet pump to work simultaneously for its operation.

$$Ts_{ik+1} + \overline{T^{\text{prep}}_{ik+1}} = Ts_{ik} + \overline{T^{\text{prep}}_{ik}} \qquad \forall (i,k) | i \in dynI,\ k \in kpar \tag{14}$$

Equation 15 imposes that the loading start time of a given $k + 1$ stage is equal to the time at which the operation of the previous stage k starts. This condition is useful for semicontinuous operations.

$$Ts_{ik+1} + \overline{T^{\text{prep}}_{ik+1}} = Tf_{ik} - \overline{T^{\text{unlo}}_{ik}} - \overline{T^{\text{proc}}_{ik}} \qquad \forall (i,k) | i \in dynI,\ k \in kpum \tag{15}$$

An additional timing constraint is defined by batch changeover time. Not only does production sequence affect the changeover time, but the changeover method c as well. Hence, Eq. 16 defines the changeover time for two consecutive batches in a given stage k, depending on the cleaning method used. Therefore, the binary variable $X_{ii'c}$ is 1 in case batch i is immediately processed before batch i' using cleaning method c.

$$Ts_{i'k} \geq Tf_{ik} + \overline{ChT_{ii'kc}} X_{ii'c} - BigM2(1 - X_{ii'c}) \qquad \forall (i, i', k) | (i, i') \in dynI,\ i \neq i' \tag{16}$$

The production horizon H defines the maximum time at which the last stage of any batch is allowed to finish, see see Eq. 17. Equation 18 is valid due to the fact that all product batch sizes are fixed, that is, they do not vary between batches; (they were previously predefined at the first stage).

$$W_i H \geq Tf_{ik} \qquad \forall (i,k) | i \in dynI \tag{17}$$

As for production constraints, Eq. 18 imposes that a minimum demand for each product p must be fullfilled.

$$\sum_{i \in dynI} W_i \overline{BS_i} \geq D^{\min}_p \qquad \forall p \tag{18}$$

It is necessary to define the sequence in which the batches are produced. Therefore, any batch i, with the exception of the first and the last, must have an immediate predecessor and an immediate successor. This condition is enforced by Eqs. 19 and 20, respectively.

$$\sum_{i',c|i'\in dynI,i\neq i'} X_{ii'c} = W_i \qquad \forall i|i \in dynI,\ i < \max(dynI),\ i > 1 \tag{19}$$

$$\sum_{i',c|i'\in dynI,i\neq i'} X_{i'ic} = W_i \qquad \forall i|i \in dynI,\ i < \max(dynI),\ i > 1 \tag{20}$$

The sequencing conditions for the first and last batches, which are fixed and assigned to the still state, are imposed by Eqs. 21 to 24.

$$\sum_{i',c|i'\in dynI,i\neq i'} X_{ii'c} = 1 \qquad \forall i,p|i = 1,\ p = 0,\ \overline{Y_{ip}} = 1 \tag{21}$$

$$\sum_{i',c|i'\in dynI,i\neq i'} X_{i'ic} = 0 \qquad \forall i,p|i = 1,\ p = 0,\ \overline{Y_{ip}} = 1 \tag{22}$$

$$\sum_{i',c|i'\in dynI,i\neq i'} X_{ii'c} = 0 \qquad \forall i,p|i = \max(dynI),\ p = 0,\ \overline{Y_{ip}} = 1 \tag{23}$$

$$\sum_{i',c|i'\in dynI,i\neq i'} X_{i'ic} = 1 \qquad \forall i,p|i = \max(dynI),\ p = 0,\ \overline{Y_{ip}} = 1 \tag{24}$$

Environmental Assessment

Environmental aspects are being incorporated into the design of chemical processes due to pressures from regulation policies and a global trend toward sustainability in businesses.[23] Different studies have been carried out to identify the most significant environmental effects of a process and to suggest modifications with the aim to achieve environmental improvements. As a result, a wide range of process design frameworks have been proposed: the methodology for obtaining minimum environmental impact process (MEI, or MEI methodology),[7] the WAR[11] proposed by the United States Environmental Protection Agency (US-EPA) which uses the pollution balance concept, or the introduction of ‘‘eco-vectors’’[24] for the calculation of life cycle inventories for process industries and the environmental fate and risk assessment tool (EFRAT),[25] are only some representative examples. Most of these examples embed the concepts of LCA, developed to set an environmental management system (EMS) through the ISO 1404X series.[26] Within LCA, the overall life cycle of a process or product is analyzed, taking into account upstream and downstream flow from the process from cradle to grave. Consequently, the LCA technique is also selected in this work as the best suited environmental tool for process development and optimization.

The implementation of a LCA for a given process or product requires the gathering of data regarding process environmental interventions (e.g., raw material consumption, uncontrolled emissions and waste generation). This set of data is organized in a life cycle inventory (LCI) which is the basis for the environmental impact calculation, as specified in the ISO 1404X series.

Waste generation, fugitive emissions and raw material or utility consumption are the key components for the compilation of LCIs. Specifically, in the case of batch industries, the LCI is directly related to product recipes and product changeover procedures.

Objective Function Selection

The main objective of batch production planning and scheduling is to optimize capacity utilization of batch manufacturing facilities and fulfill customer orders within a specific time horizon.[27] In any case, as a main building block of enterprise-wide optimization, the scheduling level pursues the overall company objectives which arise from economic, environmental and social aspects.

Economic criteria are of utmost importance in process industry. Hence, multiple economic objectives can be adopted in process scheduling, depending on the decision maker preferences, which stem from industrial demands. Thus, either an absolute economic measure, such as total profit, or a time relative measure, such as productivity could be adopted to assess the optimal decisions. The former criteria could be more suitable for those industrial environments where prices and demand have low uncertainty, and working hours are fixed; whereas process productivity is more interesting in those environments where late orders may arrive and variable costs are more important than fixed costs, and consequently the main objective is to produce the most profitable products using the least time. In academic studies related to scheduling, the economic objective function is usually regarded with time metrics, such as makespan, lateness or earliness.[1,28] However, makespan is only equivalent to productivity under certain conditions. Specifically, productivity and makespan are equivalent, if (i) the produced quantity is fixed, or (ii) under time constraints and variable production quantities if all products are equivalent from a profitability point of view, that is, they have the same profit and production time along the different stages. Only in such cases, productivity maximization can be reduced to makespan minimization.

Otherwise, companies must face nowadays tighter environmental regulations. Hence, environmental objectives have to be considered as part of the optimization process.[29] The objectives could be again expressed in absolute measures, for example, the minimization of the total environmental impact, which could lead to do not produce at all unless a minimal demand should be satisfied; or a relative measure, such as the minimization of the total environmental impact per mass of product produced. In this case, the lack of production would lead to higher penalties.

For the presented formulation, the total profit objective function, which considers product benefits ($\overline{BP_i}$) and changeover costs ($\overline{ChCost_{ii'kc}}$), is defined by Eq. 25. Parameter $\overline{BP_i}$ includes the product selling price minus its raw materials and utilities (e.g., electricity, heat, and water) costs associated directly with its production, while $\overline{ChCost_{ii'kc}}$ considers the cost associated with the inter-batch cleaning operations. The estimation of profit using Eq. 25 has been similarly performed by other authors[17] and is customary of scheduling decision level. The productivity (Eq. 26) results from dividing the total profit by the production schedule makespan (Eq. 27).

$$z^{\text{profit}} = \sum_i \overline{BP_i} W_i - \sum_{i,i',c|i\neq i'} X_{ii'c} \sum_k \overline{ChCost_{ii'kc}} \tag{25}$$

$$z^{\text{prod}} = \frac{z^{\text{profit}}}{Mk} \quad (26)$$

$$Mk = Tf_{ik} \qquad \forall i,k|k = max(k),\, i = max(i) \quad (27)$$

On the other hand, total environmental impact, which includes both the batch production process ($\overline{EnvIm_i}$) and batch changeover environmental impact ($\overline{EnvIm_{ii'kc}}$), is expressed by means of Eq. 28, whereas relative environmental impact can be obtained dividing the total environmental impact by the produced quantity (Eq. 29).

$$z^{ei} = \sum_{i,i',c|i\neq i',i'\in dynI} X_{ii'c} \sum_{k} \overline{EnvIm_{ii'kc}} + \sum_{i|i\in dynI} W_i \overline{EnvIm_i} \quad (28)$$

$$z^{rei} = \frac{z^{ei}}{\sum_{i|i\in dynI} W_i \overline{BS_i}} \quad (29)$$

In the case of using any combination of objective functions defined in Eqs. 25, 27 or 28, the resulting formulation entails an MILP; whereas the consideration of either Eqs. 26 or 29 in combination with the former results in an MINLP. Please note that the nonlinearity is only associated with the objective functions and not the scheduling model (Eqs. 1–24).

Multiobjective Approach and Metrics Selection

Different objective functions may be used in the scheduling problem according to the decision maker's criteria. Multiple objective programming methods aim at finding suitable solutions of mathematical problems with multiple conflicting objective functions, and different alternative strategies can be applied to solve a multiobjective problem.[2,30]

One typical approach consists of aggregating the different objectives in a single objective function with varying numerical weights. Unfortunately, these coefficients usually lack of physical meaning, and entail an arbitrary assignment of values. Thus, there is not a unique optimal solution for multiobjective problems, but rather a set of feasible solutions which may be suitable. The preferred approach consists of providing a set of Pareto optimal solutions: a Pareto solution is one for which any improvement in one objective can only take place if at least another objective worsens. Pareto optimal solutions are also termed dominating solutions, while the remaining possible optimization solutions are dominated. This latter approach implies that the decision maker is interested in all possible trade-off solutions resulting from no previous prioritization of the objective functions. Particularly in the case of objective functions related to the environment, economic metrics are always prioritized in companies and constraints on the environmental interventions (emissions, concentrations, etc.) are given by stringent environmental policies. However, a view of process operation that sees environment as an objective and not just as a constraint on operations can lead to the discovery of operating policies that improve both environmental and economic performance.[29]

The techniques for generating a set of Pareto optimal solutions should have some desirable properties. Namely, they should be able to find all available Pareto points, generate them evenly along the possible solutions in the feasible region (understood as the collection of points that satisfy all problem constraints), and they should not generate and explore dominated solutions.[22] However, all the available techniques present deficiencies in some of the former aspects. For example, the weighted sum must be carefully applied since it does not generate all available Pareto points, and the Pareto frontier does not represent an evenly set of solutions of the feasible region.[31] Finally, normal boundary intersection (NBI)[32] and normal constraint method (NC)[22] generate points that are not in the Pareto frontier, but NBI is more prone to generate dominated solutions. In general, all previous procedures require a filtering step to distinguish and classify dominated from nondominated solutions. This work implements the NC method described in Messac et al.[22] modified to obtain a reliable set of possible Pareto solutions, and applies a Pareto filter algorithm developed by Cao.[33]

The Pareto frontier (PF) associated with the problem at hand is discrete and results from a set of integer variables being defined (e.g., sequence, cleaning method), consequently evenly separated solutions cannot be expected. A key point in the NC method is the number of solutions that should be generated to obtain evenly separated Pareto solutions over the PF. Thus, the application of the NC method requires special attention. The selection of the number of solutions to be explored is performed by dividing the utopian line (hyperplane, in case of more than two objectives being considered), and exploring each constrained segment. This utopian hyperplane is obtained by the solution of the single objective optimizations as described in Messac et al.[22] To explore a high number of points will lead to an excessive computational effort, whereas an inadequate number of solutions would result in a fictitious PF that contains dominated solutions due to unexplored Pareto optimal solutions.

In addition, in a strategy based on constraints, if the solution space is discrete, an increase in the number of divisions of the utopian hyperplane in question does not guarantee the generation of new Pareto solutions. Although the total number of problems discussed is increased, their solution can lead to already explored discrete solutions. Hence, we propose an iterative approach to be applied to generate a reliable estimation of the PF. The number of divisions of the utopian hyperplane is incremented on each iteration and the points explored are added as new solutions. Different termination criteria are possible, (i) PF similarity and (ii) PF similarity percentage. The first termination criterion consists of checking the PF at the end of each iteration, if no changes are found in two consecutive iterations the PF is accepted as solution to the multiobjective problem. The latter termination criterion imposes the end of the iteration procedure, when the number of new Pareto solutions divided by the total number of explored solutions is lower than a specific tolerance (*tol*) percentage. Specifically in our case, a minimum of fifty points (nd_0) are initially generated and in the next iteration at least fifty new different points are further studied (nd_1). These parameters values (nd_j and *tol*) can be changed according to the problem characteristics. The convergence of the proposed algorithm depends strongly on the global convergence of the optimization method used to solve each of the constrained problems, which in some

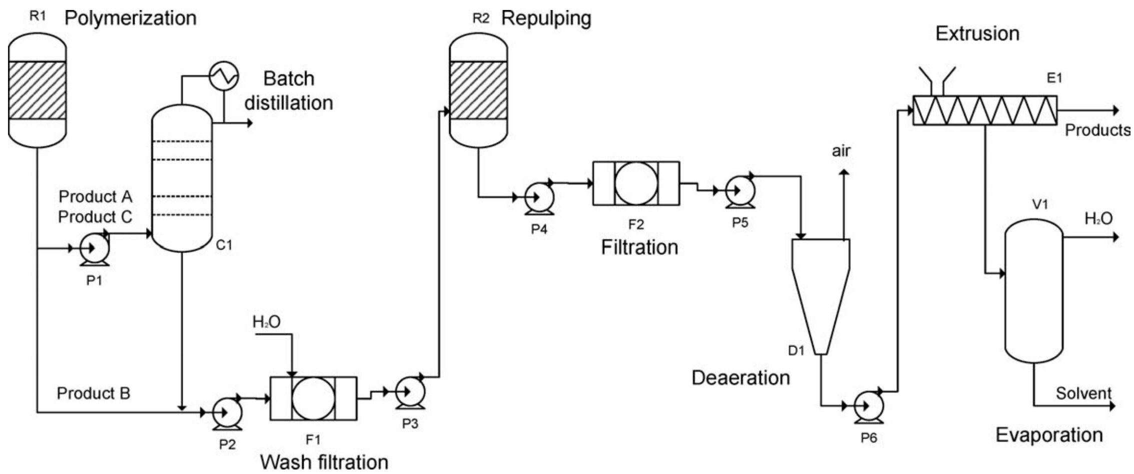

Figure 1. Flowsheet of the production process of acrylic fibers manufacturing.

cases (MINLP) might require the estimation of an initial starting point. The algorithm is shown next, Algorithm 1.

Algorithm 1: Pareto frontier generation.

Data: Number of utopian line divisions (nd_0), tolerance (tol).
Result: A reliable Pareto frontier estimate PF^*
begin
explore S_0 solutions using nd_0 and count np_0^{explored};
generate first Pareto frontier estimate PF_0 from S_0;
count Pareto points np_0^{PF}
$j \leftarrow 1$;
np_j^{PF}, $np_j^{\text{explored}} \leftarrow np_0^{\text{explored}} + 1$;
while $np_j^{PF} \neq np_{j-1}^{PF}$ or $\frac{np_j^{PF} - np_{j-1}^{\text{PF}}}{np_j^{\text{explored}}} \geq tol$ **do**
select j-th number of utopian line divisions nd_j;
explore j-th solutions S_j using nd_j;
$S_j \leftarrow [S_j, S_{j-1}]$;
perform a Pareto filter of explored solutions PF_j from S_j;
count Pareto points np_j^{PF};
count total explored solutions np_j^{explored} in S_j;
$j \leftarrow j + 1$;
$PF^* \leftarrow PF_j$

Once the PF is generated, the decision maker should choose the solution to be adopted.[2] Metrics that may assist the decision-maker to choose a final solution can be derived from the values of the different objectives expressed in terms of the normalized distance from their individual (single objective) optimal solution. The point which considers the best possible single objective outcomes is known as utopian point, while the one which considers worst solutions is the nadir point. The best compromise solution could be thought as the one that minimizes the overall distance to the utopian point (Eq. 30), as proposed by Hwang and Yoon[34] in the Technique for Order by Similarity to Ideal Solution (TOPSIS). An alternative strategy consists of measuring the distances from the PF solutions to the nadir point. Therefore another compromise solution could be chosen as the one whose geometric distance to the nadir is maximum (Eq. 31).

$$\mu^{\text{best}} \rightarrow \min \left\{ \sum_g \left(\frac{\mu_g^* - \mu_g}{\mu_g^* - \mu_g^0} \right)^2 \right\} \tag{30}$$

$$\mu^{\text{best}} \rightarrow \max \left\{ \sum_g \left(\frac{\mu_g - \mu_g^0}{\mu_g^* - \mu_g^0} \right)^2 \right\} \tag{31}$$

Case Study

The proposed methodology is illustrated in a case study which was originally posed by Grau et al.[35] It consists of a multiproduct batch process plant that produces three acrylic fiber formulations by a suspension polymerization process (Figure 1) requiring 14 processing stages. Due to minimization of inventory costs, the possible storage of polymer (considered as intermediate product) after stages deaeration (stages 11,12) has been disregarded and polymer extrusion (stage 13) is performed right after polymer deareation is done. Production recipes contain a detailed description of the product batch sizes,[35] as well as operational times (Table 1) and energy demands[35] of each of the production stages. Production costs and sales price are shown in Figure 2.

Between any two batches, a changeover operation must be carried out. Three different changeover cleaning methods, which differ in time, cost and environmental impact, are defined as summarized in Table 2.

To ease the computation of the environmental impacts, instead of adding up all the LCI results associated with the consumption/use of raw materials, utilities and cleaning agents, the Life Cycle Impact Assessment (LCIA) results from each of the activities (e.g., water use, steam generation or raw material production) have directly been used. These LCIA results hold the combined environmental impact of each activity from a cradle to gate point of view. The LCIA methodology applied is IMPACT 2002.[36] Simapro[37] has been selected to calculate these LCIAs from the corresponding LCIs[38] and the LCIA information is used in the model. It is found that the environmental impact of raw materials is quite large compared to the remaining quantities. This fact

Table 1. Operation Times and Equipment Associated to Each Stage for All Possible Produced Products [h]

		Product A					Product B					Product C				
Stage	Equipment	P	L	O	U	TOT	P	L	O	U	TOT	P	L	O	U	TOT
1	R1	0.2	0	2	0.3	2.5	0.2	0	3	0.75	3.95	0.2	0	1	0.3	1.5
2	P1	0.2	0	0.3	0	0.5	0	0	0	0	0	0.2	0	0.3	0	0.5
3	C1	0.5	0.3	2.5	0.75	4.05	0	0	0	0	0	0.5	0.3	2	0.75	3.55
4	P2	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95
5	F1	0.5	0	0.75	0	1.25	0.5	0	0.75	0	1.25	0.5	0	0.75	0	1.25
6	P3	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95
7	R2	0.3	0.75	1	0.75	2.8	0.3	0.75	0.75	0.75	2.55	0.3	0.75	0.5	0.75	2.3
8	P4	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95
9	F2	0.5	0	0.75	0	1.25	0.5	0	0.75	0	1.25	0.5	0	0.75	0	1.25
10	P5	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95
11	D1	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95
12	P6	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95
13	E1	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95	0.2	0	0.75	0	0.95
14	V1	0.3	0.75	3.5	0	4.55	0.3	0.75	3	0	4.05	0.3	0.75	1.5	0	2.55

P, for preparation; L, loading; O, processing; U, unloading.

was expected given that this impact is significantly larger than either the environmental impact associated with the use of utilities or changeover operations. Hence, this analysis distinguishes between them accordingly. As for environmental impact of the production itself, the LCI entailing residues, noncontrolled emissions, raw materials, steam, water, and electricity consumption is calculated using good engineering practices, and it is based on the available literature data.

Raw materials consumption estimation

Raw materials (solvent, monomers and initiators) addition for fiber production is considered at stage 1 (polymerization). An overall reaction yield of 95% is assumed. In addition, a 40% of the total initial amount introduced in the reactor is solvent, and the remaining 60% is monomer mixture, which is composed by 85% acrylonitrile, 10% methyl metacrylate and 5% vynil chloride. The solvent is considered to be pure acetone, while vynil chloride, styrene, acrylonitrile and methyl metacrylate are the possible comonomers. Each one of the former raw materials LCI data has been retrieved from their corresponding Ecoinvent LCI.[38]

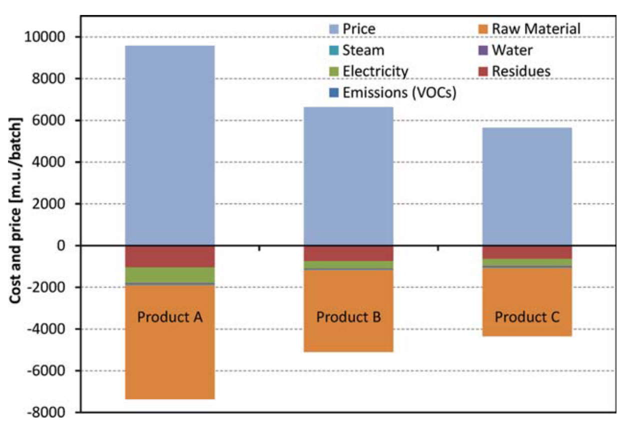

Figure 2. Batch cost and price, and environmental impact for the three acrylic fibers.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Residues generation

The remaining quantity of each batch (5% in mass) is released in the last stage (evaporation), and treated as production waste. A certain percentage of consumed water (30%) is also considered as residue to be treated. The LCI associated to its treatment as waste has been related to treatment of "heat carrier liquid, 40% $C_3H_8O_2$, to waste water treatment, class 2/CH S" in Ecoinvent.

Noncontrolled emissions

According to US-EPA (pg. 33),[39] acrylonitrile emissions in this production process occur at the pelletizer (repulping) and polymer dryer (deaeration) (stages 7 and 11 of the recipe) and estimates an air emission of 18.75 kg/Mg product released in acrylic wet spun homopolymer manufacturing. In this case, these emissions are considered as air emissions of pure acetone, disregarding any monomer emission.

Electricity consumption

Electricity consumption includes pumping required for product movement between stages that are not gravity driven and also for pumping cooling water and steam compression. In the case of pumping cooling water, a pumping $\Delta P = 1 \times 10^5$ Pa and a flow of 20 m^3/h, which requires and approximate power of 1.5 kW, is considered. On the other hand, for compressing heating steam, a yield which represents 0.6 GJ useful heat of steam/GJ electricity is used. In all cases, the LCI information for electricity consumption is considered as "Electricity, medium voltage, at grid/ES U."

Heating and cooling needs

In the case of heating, it is considered to be supplied using steam, the LCI has been gathered using the "Steam,

Table 2. Cleaning Methods Description

Cleaning method	Time	Cost	Env. Impact	Method based on the use of
1	Very low	Medium	Medium	Steam
2	Very high	Very low	Low	Water
3	Medium	High	Medium	Organic solvent

for chemical processes, at plant/RER U'' Ecoinvent unit. It is a medium-low pressure saturated steam, at 9×10^5 Pa (2029,45 kJ/kg steam). Steam is used to heat streams according to the recipe provided in Grau et al.[35] For the estimation of cooling needs, water is used to cool down the streams. All cooling requirements are computed as water cooling and assuming no electrical refrigeration required. Cooling water consumption is computed by taking into account its specific heat (liquid water is 4.18 kJ/kg), and an average ΔT for water of about 20°C.

Water consumption

Process water is considered to require softening, consequently the Ecoinvent LCI ''Water, completely softened, at plant/RER U'' is used. Process water is required in some recipe stages besides cooling. The filtering stages require a water flow of 40 m^3/h, and for the cleaning of these units a water flow of 10 m^3/h is needed.

Changeover characterization

Despite the fact that product changeover involves different operations, in this article we focused on cleaning operations. According to Allen et al.,[40] the nature of the cleaning process should be considered taking into account several aspects: (i) nature of the vessels to be cleaned (capacities, materials of construction and shape), (ii) the cleaning schedule, (iii) the residual quantity of chemical left to be cleaned in the vessel, (iv) the cleaning agent (aqueous/organic, chemical solubility/miscibility), and (v) the requirements of waste treatment for the used cleaning agent. Mainly in the batch industries where individual unit operations are utilized for multiple products, many pieces of equipment are subject to long clean-out periods using large solvent volumes and/or aqueous detergents. It is current practice to try to use clean-in-place (CIP) procedures instead of break down and rebuild approaches where unit operation allows it.[41] Although in some cases the unit operation requires its break down and rebuild (e.g., plate filtration) most vessel cleaning is performed using CIP.

Regarding clean up scheduling (ii), it depends on the process or product and cleaning between batches could be due to product requirements (color changes in paint manufacturing), or process requirements (solidification of product in a filter requires its clean up). Estimation of point (iii) requires knowing vessel characteristics and some rough estimate of the viscosity and surface tension of the liquid to be cleaned; however, as a rule of thumb, the amount in weight percent left in vessels ranges from 3 to 0.03%.[40] With regard to (iv) in the case of aqueous cleaning agents, these are sent to waste water treatment (WWT) plants, while organic solvents are recycled or incinerated. In general, the actual amount of clean up agent will depend on the amount of this agent that can be recycled/reused in other cleaning operations.

In the case study, three different product changeovers are possible. Each of them has associated different costs, inventory/impact and duration (Table 2). Since cleaning options are very different, a comparison based on used volume or energy would be too simplistic, and we have decided to use the environmental impact and cost of those stages to select among

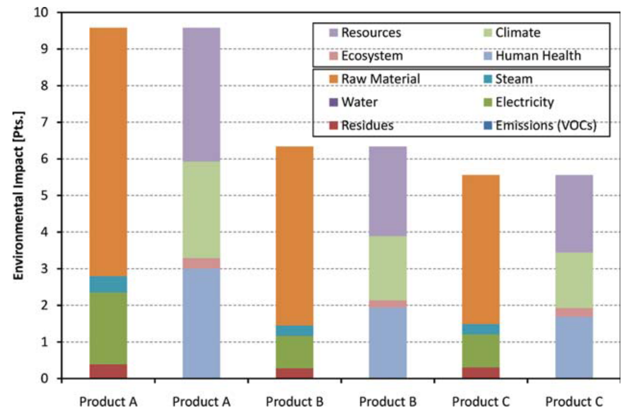

Figure 3. Environmental impact distributed along different items, left column operation related, while right column in different end point categories.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

them by including such aspects in the objective function calculations. A few assumptions have been made regarding the LCI for each of the three available changeover policies.

- Regarding costs, they have been assigned according to the cleaning requirements and general engineering principles used for the estimation of former production costs.
- Electricity consumption [GJ] has been considered to be a function of changeover time (*ChanT*), it is calculated considering the *ChanT* [h] multiplied by the power of a pump with a flow of 20 m^3/h and a Δ P of 2×10^5 Pa, which is nearly 1.5kW. Electricity consumption also includes electricity requirements for steam compression.
- As for water consumption, a pump of 20 m^3/h is considered in the water cleaning method; so the changeover time multiplied by the pump capacity is approximately the water consumption in that operation.
- Similarly to the estimation of water consumption, solvent is estimated considering a pump capacity and the required changeover time. Solvent recycle has been disregarded.

Figures 2 and 3 present the batch cost and environmental impact for the production a batch of each product. Raw materials represent the most important operating cost for all products, followed by residues treatment and electricity. However, there are no great differences in production costs among products because their recipe is similar in terms of raw materials and processing stages. In the case of Figure 3, environmental impacts for each product are shown in two different columns distributed in different items. One of them in terms of raw materials, utilities consumption, residues treatment and emissions and the other column using the different end point environmental impact categories that IMPACT 2002 implements (resource usage, global climate change, damage to ecosystem and human health impacts). In the first case, the highest contribution to environmental impact is due to raw materials production, followed by electricity and thirdly water consumption and residues which have approximately the same impact. The distribution along end point categories shows similar impacts to resource use, climate change and human health, while smaller effects to ecosystem quality.

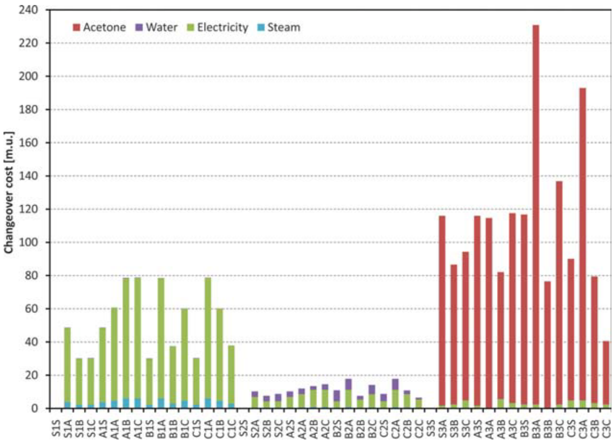

Figure 4. Changeover costs between pairs of products (S-still state, A, B, C) for the three methods (1, 2, 3).

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

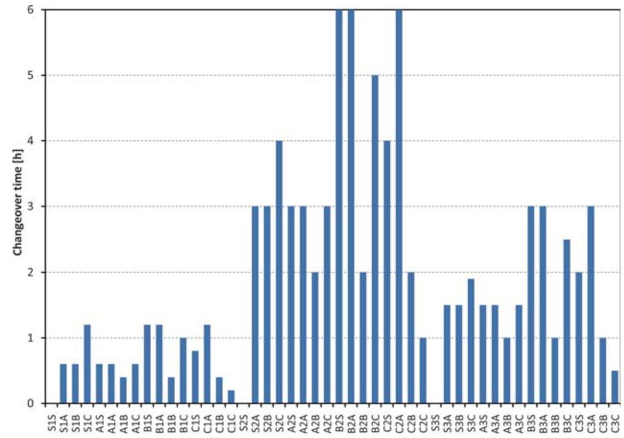

Figure 6. Changeover time between pairs of products (S-still state, A, B, C) for the three methods (1, 2, 3).

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Figures 4–6 show the changeover costs, environmental impacts and time for each pair of products using the three available cleaning methods. The differences briefly outlined in Table 2 can be appreciated, and the contribution of each operating resource to the total cost is unveiled. Therefore, the high operating cost of method 3 is basically due to fresh acetone consumption. In the case of changeover 1, cost is basically due to electricity consumption, whereas steam represents a smaller fraction of total cost, and electricity and water are the main costs of cleaning method 2.

Results

The previous case study is solved considering a demand of 2 batches of each product, and that a minimum of the 50% of the demand (i.e., 1 batch) of each product must be satisfied. Three different combinations of objective functions are studied which result in different multiobjective problems, namely (i) a three-objective optimization considering makespan, profit and environmental impact, and two biobjective optimization problems which consider: (ii) productivity and environmental impact, and (iii) productivity and relative environmental impact. The selection of the former problems was done based on the consideration of ''extensive'' and ''intensified'' system characteristics. The extensive characteristics are mainly driven on the amount of product produced, while the latter are centered on efficiency, by relating the metric directly linked to production to others such as time or amount produced. In this sense, the first case considers only extensive metrics, the second considers a mixture of them, while the third case analyzes only intensified metrics. The

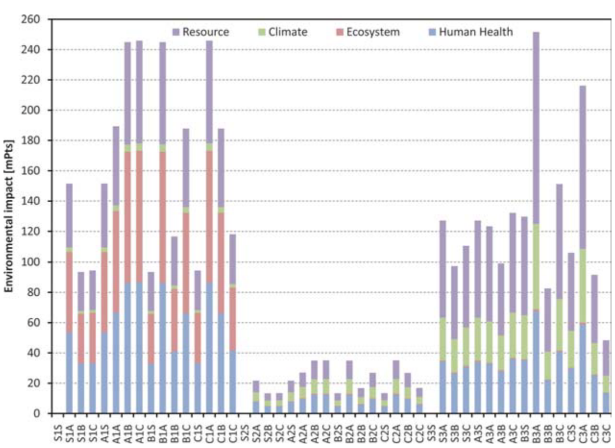

Figure 5. Changeover environmental impacts between pairs of products (S-still state, A, B, C) for the three methods (1, 2, 3).

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

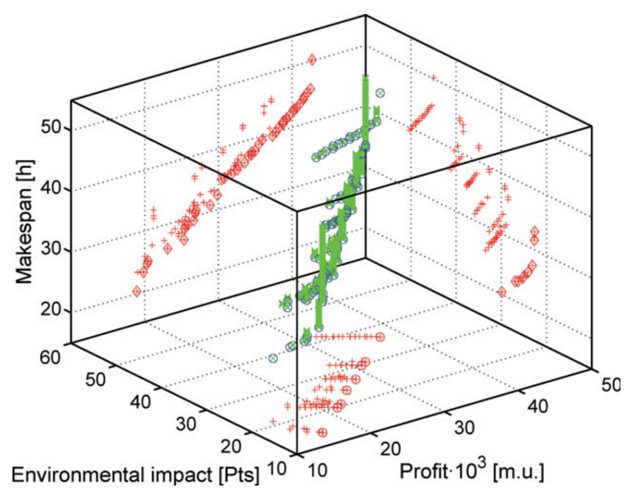

Figure 7. Case, Solutions for three objective optimization considering profit, environmental impact and makespan.

Green crosses are all explored solutions; nondominated solutions are encircled in blue (Pareto frontier); red plus symbols are projections of all explored solutions in their corresponding two dimensional planes and red diamonds solutions are nondominated solutions in such planes. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 3. **Case (1), Iterations in the Number of Pareto Points Generation, for the Multiobjective Optimization Considering Profit, Environmental Impact and Makespan**

	Initialization	Iteration 1	Iteration 2	Iteration 3	Iteration 4	Iteration 5	Iteration 6
Number of utopian line divisions (nd_j)	11	21	31	41	46	51	56
Number of explored points	58	256	701	1479	2468	3679	5143
Total Pareto solutions (np_j^{PF})	26	42	59	71	76	85	89
Changing Pareto frontier solutions	26	16	20	12	6	10	4
Pareto solutions $z^{\text{profit}} - z^{ei}$	10	11	13	15	15	16	16
Pareto solutions $z^{\text{profit}} - Mk$	10	18	31	34	36	40	42
Pareto solutions $z^{ei} - Mk$	4	4	5	7	7	9	9
Computation time $\times 10^3$ [s]	3.60	11.97	30.25	69.40	107.89	152.43	210.45

mathematical formulation and the NC method have been implemented in GAMS, and solved using CPLEX 11.2 in the MILP case (problem i), and BARON 8.1 in the MINLP (problems ii and iii). Due to the convergence of the MILP and MINLP solvers from their default starting points, no need for initial starting point estimation was required. However, the computation effort in solving each constrained optimization might be reduced if the solver is fed with a good initial solution. Pareto filtering of the solutions has been done in Matlab,[33,42] and the algorithmic strategy (Algorithm 1) was implemented in Matlab and the whole solving process automated using Matgams.[43]

Case 1

Considers the multiobjective optimization of profit, environmental impact and makespan. Figure 7 contains the Pareto solutions in the three dimensional space. Given the fact that fixed batch sizes are considered, the Pareto frontier is a collection of points that represent different production sequences. The evolution of the proposed algorithm in terms of the resulting Pareto solutions are presented in Table 3. A total of 5143 MILP have been solved to optimality, which result in 89 nondominated solutions. The average solving time for each optimization problem was about 44 seconds. The iterative procedure has been stopped when the percentage of new Pareto solutions divided by the total number of explored points is below 0.1%, ($tol = 1 \times 10^{-5}$).

PFs of the two dimension projections do not contain all the Pareto points of the three dimensional problem, but show existing trade-offs between any two objectives. Therefore, the projections of the solutions on two dimensional planes and their respective Pareto points are further discussed.

Figure 8 presents the PF for the two-objective optimization of total profit and total environmental impact, which was considered separately (as Case 1a) from the three objective Case (1). A total number of 3000 points along the utopian line have been solved to optimality (green crosses), from which 24 nondominated Pareto solutions (blue circles) are obtained after applying the Pareto filter.

The solution with highest profit satisfies the total demand (i.e., 2 batches of each product), whereas the most environmentally friendly option only processes the minimum amount of each product (1 batch for each product). In any case, the same changeover cleaning method 2 is selected in all solutions, because it is the most economic and environmental advantageous (see Figures 4 and 5), despite the time required, which is not considered in this case. Pareto points are found to be grouped between the two extreme optimal solutions in six clusters, whose difference consists of the number of batches of each product. Regarding the most environmentally friendly solution cluster, product C offers more increment in profit and less environmental impact. The following less environmentally advantageous sequence with higher gain in profit includes an additional batch of product B instead of C; and then, a batch of A instead B or C. Next, an additional batch is considered in the production sequence, and finally, the complete fulfillment of demand entails the highest economic profit. In every cluster, solutions differ in the production sequences. To start producing with fiber C is slightly more environmentally friendly and less economically profitable than with fiber A.

Table 4 shows that the compromise solution according to the minimum distance to the utopian point consists of sequence 2A2A2C2B2 (such string represents the ordered sequence of batches, where the capital letters A, B, and C, stand for the product, and the numbers 1, 2, and 3 for the cleaning method being used), which is located approximately in the middle of the whole range of both objective functions. If the maximum distance to the nadir point was selected as decision criterion, there would be two possibilities: either the solution of maximum profit or the solution of minimum

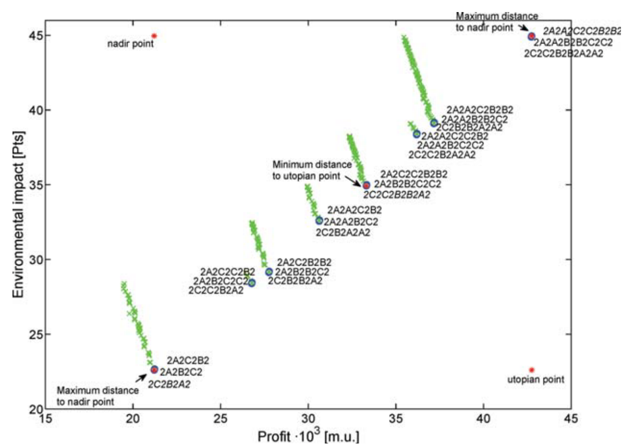

Figure 8. Case (1a). Solutions for two-objective optimization considering profit and environmental impact.

Green crosses are all explored solutions; nondominated solutions are encircled in blue (Pareto frontier); red stars are nadir, utopian points; and sequences in italics represent compromise solutions shown in Table 4. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 4. Case (1a). Utopian, Nadir and Solutions of Compromise According to the Different Metrics Considering Profit and Environmental Impact

$z^{profit} \cdot 10^3$ [m.u.]	z^{ei} [Pts]	Sequence	Distance Utopian	Distance Nadir
21.213$^-$	22.595*	2C2B2A2	1.000	**1.000**
33.310	34.921	2A2A2C2B2	**0.704**	0.719
42.7455*	44.956$^-$	2A2A2C2C2B2B2	1.000	**1.000**

* defines utopia and $^-$ nadir. Distances are reported normalized.

environmental impact, since both of them have the same maximum normalized distance to the nadir solution.

On the other hand, the biobjetive projections for environmental impact versus makespan (Case 1b), and profit versus makespan (Case 1c), are given in Figures 9 and 10. The solution with lowest makespan contains one batch of each product, and includes changeover 1, whose time is the shortest, as it could be expected (see Figure 6). Sequences starting with fiber A have higher environmental impact but lower makespan than those with C. In addition, those sequences starting with product A dominate other sequences in the profit and makespan biobjective problem, even though starting with product A has the highest cost regarding the other two products.

For the overall three objective optimization, the utopia, nadir and solutions of compromise selected according to the proposed criteria are shown in Table 5. Sequence 2A2A2C2B1 is the one whose distance to the utopian is minimum; whereas solution 2A2B1C1 has the highest distance to the nadir point.

It is important to note that in this case, single objective optimal solutions are bounded by the minimum and maximum demand requirements. Regarding minimum requirements, in the case of environmental impact and makespan, their ultimate minimum will be zero which is associated to not producing any product, while in the case of profit, its optimization fulfills all required demand. If these bounds are changed the behavior would be the same, consequently special attention has to be put in the modelling of demand requirements given that for these metrics, its selection will be of paramount importance.

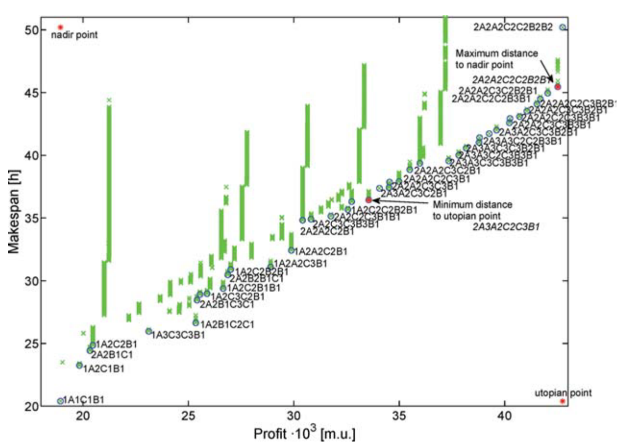

Figure 9. Case (1b), Solutions for two-objective optimization considering profit and makespan.

Green crosses are all explored solutions; blue circles the nonnominated solutions (Pareto frontier); red stars are nadir, utopian points; and sequences in italics represent compromise solutions. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

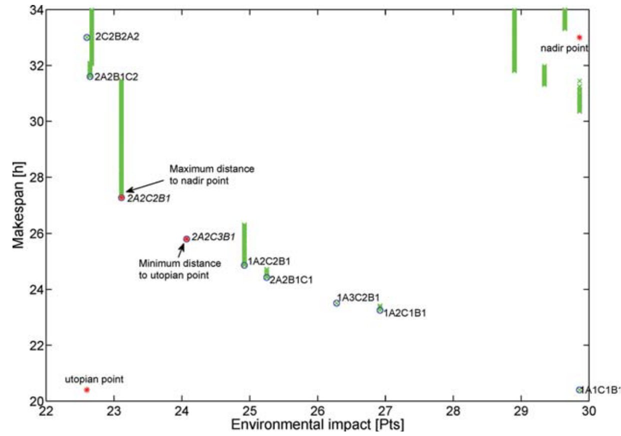

Figure 10. Case (1c), Solutions for two-objective optimization considering total environmental impact and makespan.

Green crosses are all explored solutions; blue circles the nonnominated solutions (Pareto frontier); red stars are nadir, utopian points; and sequences in italics represent compromise solutions. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Case 2

Considers the analysis of the scheduling results when productivity and environmental impact are compared. Figure 11 presents the PF with 38 nondominated Pareto solutions (blue circles) for the biobjective optimization of productivity and environmental impact. In this case, the utopian line is divided iteratively in multiples of 50, from 50 to 150 (see Table 6). As a result, a total number of 200 points along the utopian line have been solved. In about 13% of all problems, the MINLP solver (BARON) was not able to guarantee global optimality, after a reasonable computational effort (7200 CPU seconds). The average solving time for each optimization problem was found to be 2635 seconds. The iterative procedure has been stopped when the percentage of new solutions is below 5% ($tol = 5 \times 10^{-2}$).

The most productive sequence consists of producing full demand of the three products with changeover method 1, which is the one that takes the least time. It is worth noting that the former sequence consists of AACBBC, which entails three interproduct changes and with higher overall changeover time than sequences such as AACCBB (with two interproduct changes). The reason for this issue is not evident and it can be understood from the Gantt charts in Figures 12 and 13. In sequence AACCBB, there are two pieces of equipment that are bottlenecks (C1 and V1); which results in

Table 5. Case (1) Utopian, Nadir and Solutions of Compromise According to the Different Metrics Considering Total Profit, Environmental Impact and Makespan

$z^{profit} \cdot 10^3$ [m.u.]	z^{ei} [Pts]	Mk [h]	Sequence	Distance Utopian	Distance Nadir
21.213	22.595*	33.000	2C2B2A2	0.998	1.159
42.745*	44.956$^-$	50.200$^-$	2A2A2C2C2B2B2	1.285	1.018
18.931$^-$	29.861	20.400 *	1A1C1B1	1.034	1.243
30.417	33.069	34.820	2A2A2C2B1	**0.803**	0.941
20.327	25.251	24.427	2A2B1C1	0.956	**1.253**

* defines utopia and $^-$ nadir. Distances are reported normalized.

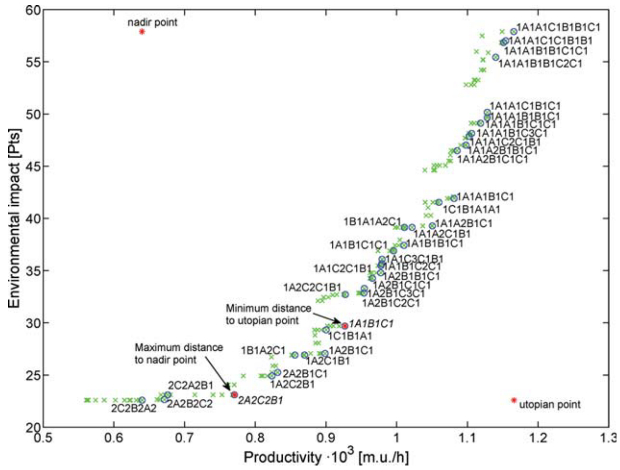

Figure 11. Case (2), Solutions for two-objective optimization considering productivity and environmental impact.

Green crosses are all explored solutions; blue circles the nonnominated solutions (Pareto frontier); red stars are nadir, utopian points; and sequences in italics represent compromise solutions shown in Table 7. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

a total makespan of 33.75 h (Figure 13). However, sequence AACBBC avoids the bottleneck in equipment C1 and has a total makespan of 33.15 h (Figure 12); consequently, its profitability increases despite the higher costs incurred by sequence changes.

Table 7 contains the solutions of compromise according to the different metrics. Note that in this case, the solution whose distance to the utopian point is minimum includes one batch of each product using cleaning method 1. In addition, Figure 11 highlights the relative position of the compromise solutions regarding the other Pareto solutions.

Case 3

Encompasses the analysis of scheduling results considering productivity and relative environmental impact metrics.

Table 6. Case (2), Iterations in the Number of PARETO Points Generation, for the Multiobjective Optimization Considering Productivity and Environmental Impact

	Initialization	Iteration 1	Iteration 2
Number of utopian line divisions	51	101	151
Number of explored points	51	101	201
Total Pareto solutions	31	38	37
Changing Pareto frontier solutions	31	7	7
Computation time $\times 10^5$ [s]	1.31	2.67	5.28

In Figure 14, Pareto solutions differ in the number of batches of each product, the sequence in which they are produced, and cleaning method used. Some of these solutions have already appeared when optimization of total profit is considered, although they are still valid, most of them are not part of the PF for this case. In the Pareto frontier solutions are not grouped as in the two-objective case of total profit and environmental impact.

The Pareto frontier for the two-objective optimization of productivity and relative environmental impact contains 34 nondominated solutions (Figure 14). In this case, the utopian line is divided iteratively in multiples of 50, from 50 up to 100 (see Table 8), when the percentage of new Pareto solutions is below 10%. The average solving time for each optimization problem was found to be 5121 seconds. When minimizing the environmental impact per unit of product, both the sequence and cleaning method is the same as when minimizing the total environmental impact, but an additional batch of fiber B is produced. The main reason stems from the fact that by dividing the produced quantity, producing the smallest quantity of the products is not advantageous from the environmental point of view. Therefore, this relative objective function measures the most environmentally efficient way of producing.

Table 9 contains the solutions of compromise according to the different metrics. In this case, both solutions are different to the extreme points. Figure 14 highlights the relative position of the solutions of compromise according to Eqs. 30 and 31, which are both different to the single objective

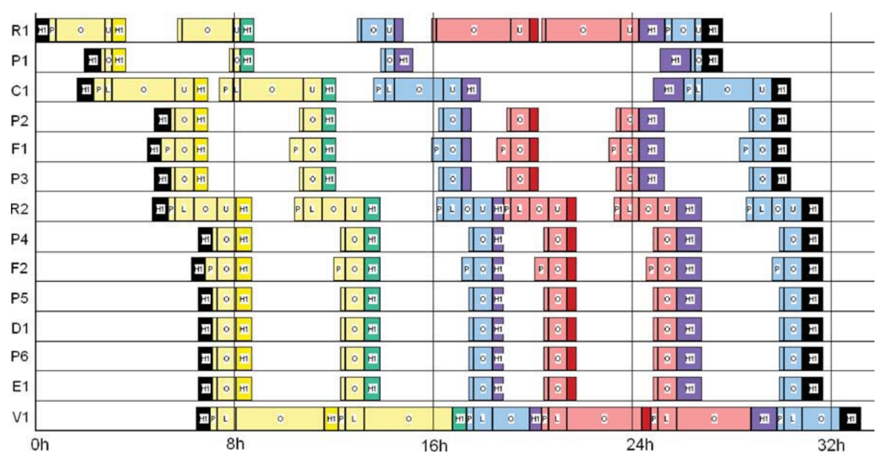

Figure 12. Gantt chart for sequence 1A1A1C1B1B1C1.

(black: starting and finishing cleaning tasks; yellow, red and blue: fibers A, B and C, respectively; darker colored areas represent changeover methods). [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

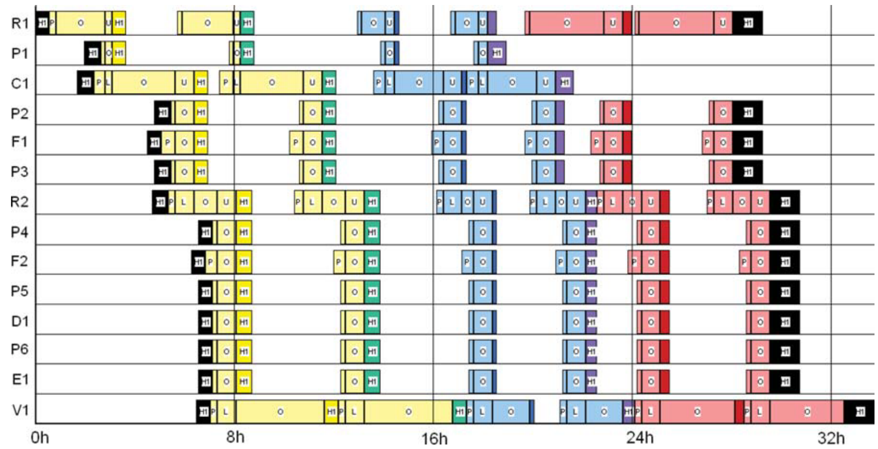

Figure 13. Gantt chart for sequence 1A1A1C1C1B1B1.

(black: starting and finishing cleaning tasks; yellow, red and blue: fibers A, B and C, respectively; darker colored areas represent changeover methods). [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

optimal solutions. Both selected sequences produce the same amount of products and in the same order, but they differ in the cleaning methods used for the changeover between pairs of batches.

To sum up, we have considered the relative environmental impact and productivity metrics for comparison. In Figure 15 it can be seen that the solutions obtained for the other metrics optimization (Case 1 and 2), are not contained in the PF found for the relative environmental impact and productivity (Case 3). It can be seen that the solution with optimal profit is dominated by other solutions whose cleaning methods are the same, but its production sequence is different. With regard to the makespan (Mk) optimization solution it is found be far way from the PF, while the environmental impact optimization is closer.

As we can see from the computational times reported in Tables 3, 6, and 8, the application of this algorithm is highly dependant on the solving time required for the optimization of each constrained problem. We found that MILPs are easier to solve, while MINLPs require longer times. Clearly the applicability of the presented model and algorithm, to practical day-to-day operation decisions is far from being optimal due to the excessive computational required time, however we have shown the algorithm conceptual validity, which is independent of the model used. Given that the bottleneck of the presented algorithm resides in the optimization step, any method or technique for decreasing this time will improve the overall algorithm solution time. These techniques might involve: an initial point estimator or the application of decomposition techniques (e.g., Benders or Lagrange) to the model. On the other hand, an algorithm improvement might lie in the selection of the new constrained problems which in our case was done blindly and systematically by subdividing the utopian hyperplane in smaller divisions. The application of any of the former techniques will render an algorithm which might be suitable for day-to-day operation.

Table 7. Case (2), Solutions of Compromise According to the Different Metrics Considering Productivity and Environmental Impact

$z^{prod} \cdot 10^3$ [m.u./h]	z^{ei} [Pts]	Sequence	Distance Utopian	Distance Nadir
0.640^-	22.595 *	2C2B2A2	1.000	1.000
0.927	29.691	1A1B1C1	**0.497**	0.968
0.771	23.110	2A2C2B1	0.752	**1.016**
1.166*	57.898^-	1A1A1C1B1B1C1	1.000	1.000

* defines utopia and $^-$ nadir. Distances are reported normalized.

Conclusions

The consideration of environmental impact as an additional objective in the optimization of the scheduling problems rises a trade-off which can be rigorously studied using multiobjective optimization. In this context, the normal constrained (NC) method is a technique that allows for a good description of the Pareto frontier; however, a high number of solutions has to be explored and generated to avoid missing

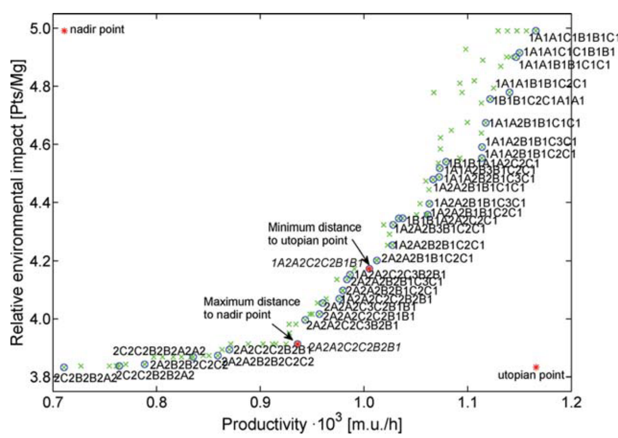

Figure 14. Case (3), Solutions for two-objective optimization considering productivity and relative environmental impact.

Green crosses are all explored solutions; blue circles the nonnominated solutions (Pareto frontier); red stars are nadir, utopian points; and sequences in italics represent compromise solutions shown in Table 9. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 8. Case (3), Iterations in the Number of Pareto Points Generation, for the Multiobjective Optimization Considering Productivity and Relative Environmental Impact

	Initialization	Iteration 1
Number of utopian line divisions	51	101
Number of explored points	51	101
Total Pareto solutions	31	34
Changing Pareto frontier solutions	31	10
Computation time $\times 10^5$ [s]	2.35	5.17

Table 9. Case (3), Utopian, Nadir and Solutions of Compromise Considering Productivity and Relative Environmental Impact

$z^{\text{prod}} \cdot 10^3$ [m.u./h]	z^{rei} [Pts/Mg]	Sequence	Distance Utopian	Distance Nadir
0.711^-	3.833*	2C2B2B2A2	1.000	1.000
0.936	3.913	2A2A2C2C2B2B1	0.510	**1.054**
1.005	4.173	1A2A2C2C2B1B1	**0.459**	0.958
1.166*	4.991^-	1A1A1C1B1B1C1	1.000	1.000

* defines utopia and $^-$ nadir. Distances are reported normalized.

Pareto optimal solutions. Hence, the proposed strategy of increasing the number of utopian hyperplane divisions to explore the Pareto frontier has demonstrated its capacity to produce reliable Pareto frontiers with limited computational effort.

Pareto frontiers provide the decision maker with highly valuable information about production schedule trade-offs. This information sheds light into production and sequencing relationships that may not be obvious. In addition, it is highly important to thoroughly consider which is the objective of the decision maker (e.g., plant manager) which could be economic, such as to maximize the profit or the productivity of the plant, or environmental, for instance to minimize the total environmental impact or the environmental

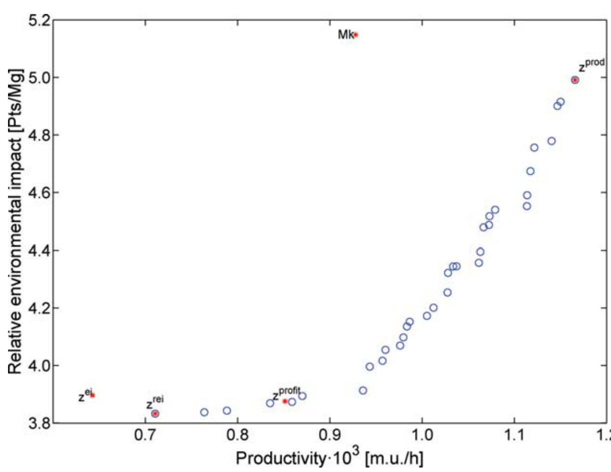

Figure 15. Pareto frontier for two-objective optimization considering productivity and relative environmental impact, and optimal single objective solutions (nondominated solutions are encircled in blue; red stars are single objective optimal solutions).

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

impact per unit of product. In this context and depending on the selected objective functions, the solutions obtained are found to be completely different despite the same economic or environmental concerns. The decision maker will reach completely different Pareto frontiers, in terms of number and sequence of product batches, as well as in selected cleaning methods by considering different objective functions.

The proposed approach for obtaining a compromise solution, which uses the concept of utopian and nadir points, allows to choose a single solution among the Pareto efficient ones. These solutions are balanced in terms of relative distance to reference points, namely the utopian and nadir of each Pareto frontier.

From a LCA point of view, ratios seem to provide more sense, at least in terms of rational use of resources, and consequently have to be considered. However the best ratios to be considered depend on the circumstances (e.g., demand characteristics), and its use greatly affects the mathematical characteristics of the problem to be solved.

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Notation

Sets and subsets

c = cleaning modes between products.
g = objective functions.
i = batches.
k = stages.
p = products (product S simulates plant "still" state).
$dynI$ = batches i that have been assigned to a product.
$kcon$ = stages k whose following stage operation is parallel to their unload.
$kpar$ = stages k which are parallel in operation to the following one.
$kpum$ = stages k whose following stage is being loaded while they are operating.

Parameters

$BigM$ = parameter with a big value, in this case its minimum value is 3 times the maximum cost, environmental impact or time between any pair of products.
$BigM2$ = parameter with a big value, in this case its minimum value is the time horizon.
$\overline{BP_p}$ = batch price of product p.
$\overline{BP_i}$ = price resulting from the production of batch i.
$\overline{BS_p}$ = batch size of product p (which is fixed).
$\overline{BS_i}$ = batch size of batch i.
$\overline{chanT_{pp'kc}}$ = changeover time between products p and p' in stage k with cleaning mode c.
$\overline{ChCost_{ii'kc}}$ = changeover cost between batches i and i' for stage k using changeover type c.
$\overline{ChT_{ii'kc}}$ = changeover time between batches i and i' for stage k using changeover type c.
D_p^{MIN} = minimum demand of product p that has to be accomplished.
D_p^{MAX} = maximum demand of product p that can be accomplished.
$\overline{EnvIm_p}$ = production impact resulting of producing a batch of product p. It includes: raw materials, electricity, residues, steam, water and emissions.
$\overline{EnIm_i}$ = production impact resulting of producing a batch i.

$EnvIm_{ii'kc}$ = environmental impact associated to changeover type c between batches i and i' for stage k.
H = time horizon.
$ptime_{pk}$ = total processing time before stage k of product p.
$\overline{T_{ik}}$ = total processing time of stage k of product i.
$\overline{T_{ik}^{\text{operation}}}$ = time parameter of stage k in batch i for the different operations, i.e., preparation, loading, cleaning, operation and unloading.
$\overline{Y_{ip}}$ = states if product p is being carried out in batch i (it is defined after the first stage, which assigns products to batches).

Continuous variables

$ChT_{ii'kc}$ = changeover time of doing i and then i' in stage k through cleaning method c.
Mk = objective function that aims at minimizing the makespan.
pT_{ik} = time of stage k in order i.
Ts_{ik} = starting time of stage k of batch i.
Tf_{ik} = finishing time of stage k of batch i.
z^{ei} = objective function that aims at minimizing the environmental impact.
z^{prod} = objective function that aims at maximizing productivity.
z^{profit} = objective function that aims at maximizing profit.
z^{rei} = objective function that aims at minimizing the relative environmental impact.
μ^{best} = vector of objectives for the best compromise solution.
μ^* = vector of objectives that contains the optimal μ_g^* objectives (utopian point).
μ^0 = vector of objectives that contains the worst μ_g^0 objectives (nadir point).
μ = vector that contains the μ_g objectives for a Pareto solution.

Binary variables

W_i = production of batch i.
$X_{ii'c}$ = assignment of cleaning method c to changeover, if batch i is produced immediately before batch i'.
Y_{ip} = assignment of product p to batch i.

Algorithm notation

j = iteration counter.
nd_0 = initial number of utopian line divisions.
nd_j = number of utopian line divisions.
np_j^{explored} = number of explored solutions at iteration j.
np_j^{PF} = number of solutions that belong to the Pareto frontier at iteration j.
PF_0 = solutions that belong to the Pareto frontier at the first iteration.
PF_j = solutions that belong to the Pareto frontier at iteration j.
PF^* = pareto frontier solutions estimated by the proposed algorithm.
S_0 = solutions explored at the first iteration.
S_j = solutions explored at iteration j.
tol = tolerance value as termination criterion.

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