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A New Approach to the Rough Set Multicriteria Optimisation Method

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A New Approach to the Rough Set Multicriteria Optimisation Method

A New Approach to the Rough Set Multicriteria Optimisation Method

by

Shadi Vafaeyan

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Abstract

In the recent years, enormous amount of attention has been given to multicriteria optimisation problems. These are problems with conflicting objectives, to which it is impossible to obtain an optimum solution that contains the best value for every criterion simultaneously, therefore the decision maker must decide on a reasonable compromise. There have been numerous developments of optimisation methods to aid the decision-maker in addressing such problems. These methods can be divided to two categories based on the use or not of the Pareto domain (PD). The Pareto domain is the set of all non-dominated solutions to the muticriteria problem, where no solution is better or worse than any other in the set when all the criteria are considered equal in importance.

This thesis is a collection of two papers that focuses on a new approach to the Rough Set multicriteria optimisation technique. Rough Set method (RSM) requires the determination of the PD as the first step to the optimisaton process. In the suggested new approach to RSM, a more systematic way in the selection of points from the PD, that is given to the expert for ranking and then the generation of rules by which the entire PD is ranked, is presented. The RSM that operates based on this new approach was applied to three case studies in paper 1 and to "Beer quality optimisation" in the second paper. The results were compared to the ones obtained by the traditional RSM, Net Flow method and the simple Least Squares method. In conclusion, the new RSM showed to be the most reliable and robust method of all.

Résumé

Au cours des dernières années, une attention particulière a été portée aux problèmes d'optimisation multicritère. Presqu'invariablement, ces problèmes comportent des objectifs qui s'opposent et il est donc impossible de tous les satisfaire à la fois. Un compromis raisonnable doit donc être trouvé. Plusieurs méthodes ont été développées pour venir en aide au preneur de décisions afin qu'il adopte le meilleur compromis possible. Ces méthodes peuvent être regroupées sous deux catégories dépendant si le domaine de Pareto est utilisé ou non. Le domaine de Pareto englobe toutes les solutions non-dominées de sorte qu'aucune solution est meilleure ou pire qu'une autre solution dans ce domaine si tous les critères d'optimisation sont pris en compte.

Cette thèse comprend essentiellement deux articles qui traitent d'une nouvelle approche de la méthode d'optimisation basée sur les ensembles flous (Rough Set). Cette méthode requiert que le domaine de Pareto soit préalablement déterminé. Une méthode plus systématique pour choisir le petit ensemble de points du domaine de Pareto, qui seront présentés à l'expert, est proposée. L'expert a la tâche d'ordonner ces points selon sa préférence. Ce petit ensemble de points classés par l'expert sert à établir des règles qui à leur tour servent à ordonner tout l'ensemble de Pareto. Cette méthode d'optimisation a été implantée pour trois études de cas dans le premier article et pour l'optimisation de la qualité de la bière dans le second article. Les résultats sont comparés à ceux de deux autres méthodes d'optimisation : le bilan des flux (Net Flow) et les moindres carrés. Les résultats montrent que la méthode proposée est plus fiable et robuste que les autres méthodes utilisées.

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I would like to thank my supervisor, Professor Jules Thibault, for his support.

I am dedicating this work to my uncle Farough. I am forever grateful for his continued support and encouragement throughout the ups and downs of this process and for all the stages of my life. I could not have done it without him.

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Chapter 1

Introduction

1.1 Multicriteria Optimisation

In recent years a great deal of attention has been given to multicriteria optimisation processes. Almost everyone faces some sort of multicriteria problem on a daily basis. For example in buying a sweater, the quality and cost are two opposing criteria. A cashmere sweater is much more expensive than an acrylic sweater. Basically, a step towards one criterion (better quality) is a step away from the other (lower cost). The levels of complexity of multicriteria problems are much higher in different fields of industry, science, medicine and many more. At a more complex level, these problems involve multiple conflicting criteria that must be optimized simultaneously. These criteria need to be maximized, minimized or get as close as possible to a desired target. There is no unique solution that optimizes all criteria at the same time; therefore the decision-maker must come up with a reasonable compromise that best addresses all the criteria. The decision-making process of such problems is not as easy as the one in a simple sweater buying problem, at a more complex level; it becomes overwhelming to decide which solution is the best possible optimum. A multicriteria Optimisation problem can be defined as follows (Halsall-Whitney, 2004).

$$\textit{Max/Min/Target} \quad F(x) = \left[f_1(x_1..x_2), f_2(x_1..x_n), \ldots. f_n(x_1..x_n)\right] \tag{1.1}$$

$$\textit{Subject to} \quad G_{i=1...k}(x) \geq 0,$$

$$H_{i=1...m}(x) = 0, \quad i = 1,2,3,...n \text{ or } k \text{ or } m$$

$$\textit{Where} \quad x_{i=1...n}^{(Lower\ Bound)} \leq x_{i=1...n} \leq x_{i=1...n}^{(Upper\ Bound)}$$

This problem has created the need for powerful aid methods that could be easily applied to different categories of multicriteria optimisation problems and lead the decision-maker to the best possible solution. Many multicriteria optimisation techniques have been developed to assist the human expert in finding a suitable compromise amongst all the objective criteria. These methods can be categorized as two main groups: a) aggregating and b) non-aggregating. The aggregating group consists of methods that depend on the a priori knowledge of the human expert that must be known at the beginning of the optimisation process; at this early stage expert's preference may bias the results. The aggregating functions do not require the determination of the Pareto domain (Andres-Toro et al., 2002). Methods that solve the multicriteria problem by combining all the criteria, through a linear combination, to form a single scalar criterion function (e.g. weighted sum of individual objectives) or a geometric average of the objective functions (multiplication of the objective functions), are examples of aggregating group. In certain cases the focus of such methods is only on a single objective and the other objectives are transformed into constraints (Massapequa et al., 1999). Although these techniques are known for their simplicity of implementation and computational efficiency (Andres-Toro et al., 2002), there are many drawbacks to their use especially when the objectives under consideration are conflicting. Combining multiple objectives into a single objective does not provide the decision-maker with information about the trade-offs among the various objectives or about alternative operating conditions. Furthermore when multiple criteria are transformed into a single criterion composed of the weighed sum of all the criteria, the optimisation relies heavily on the selection of weights. This is not a trivial task and every time different weights are used, a different optimum is obtained. When a single objective is chosen to be optimized and the remaining objectives are transformed into constraints, the final solution may be biased. This can result in misleading conclusions. It may not be easy to decide which criterion to optimize (Halsall-Whitney, 2004).

The non-aggregating methods, on the other hand, require the prior or simultaneous determination of the Pareto domain. These methods are considered to be more general and more accurate; they can simultaneously optimize multiple and conflicting objectives. These techniques have the ability to generate multiple solutions in a given iteration that cover the entire search space (Halsall-Whitney, 2004). The goal is to find the non-dominated zone of solutions amongst which the human expert can select the best possible one (Massebeuf et al., 1999). Two known examples of this category are Net Flow method (NFM) and Rough Set method (RSM). These methods essentially determine the Pareto domain and then rank all the Pareto-optimal solutions to find the best optimum, using the conscious and intuitive preferences of the decision maker. The Pareto Domain (PD) is the set of all non-dominated solutions where no one solution is better than any other in the domain when compared on all objective criteria. Based on the domination criterion, a point dominates another if it is strictly better for at least one criterion and better or equal for the others (Deb, 2001). The PD provides the decision-maker with information about the trade-offs and alternative solutions arising from the use of multiple conflicting objectives. The Pareto domain will converge to one solution, without conflict between the objectives (Deb 2001).

There are three main common steps to multicriteria optimisation that are done by the PD-based optimisation methods. The first step is to develop a comprehensive model of the process that clearly represents the relationships between the input and the output variables. Second, the solution zone is reduced to a set that only contains all the non-dominated solutions (i.e. the PD). Finally, the third step is to rank this reduced non-dominated set of solutions using the knowledge and preferences of the decision-maker to obtain the best optimal solution. Ranking the PD is the main challenge in this process; hence it is crucial to use a robust procedure to obtain the knowledge of the decision-maker in the best efficient way to meet this challenge.

1.2 Scope of Current Research

This research focuses on the behavior of the multicriteria optimisation method the "Rough Set method" (RSM) and the development of a modified Rough Set that overcomes the existing problems involved with the traditional Rough Set method. The new Rough Set methods along with the traditional RSM are used to optimize three multicriteria optimisation case studies (Papers 1 and 2). Results are compared to those obtained by the Net Flow method (NFM) and the simple least squares (LSQ) method. The Net Flow method is a fairly robust method and acts as the expert in the evaluation of the Rough Set method. The NFM is used as an expert because it can consistently resort to the same thinking process. The results of this work is presented here as a collection of two papers. The Rough Set method is described in detail in both papers and for a more detailed description on NFM, the reader is referred to Thibault et al (2002). The two papers are summarized as follows.

1. The first paper, Selection of Pareto-Optimal Solutions for Process Optimisation Using Rough Set Method: A New Approach, investigates the robustness of three variants of RSM. These methods are implemented, along with the NFM (expert), to evaluate three multicriteria optimisation problems. The main focus is on the Rough Set method with a new approach for selection of subset of points from the PD. The Pareto domains, the set of all non-dominated solutions, were obtained using a diploid genetic algorithm (Fonteix et al., 1995) for the second case study, and a uniform grid method for the first and third case studies (Halsall-Whitney and Thibault, 2006).

2. The second paper, Multicriteria Optimisation of Beer Quality Using the Rough Set Method, proposes a new Rough Set method to optimize the beer quality. In this work, the robustness of the new RSM is examined and analyzed. A uniform grid method (Halsall-Whitney and Thibault, 2006) is used to obtain the Pareto domain. This domain is then ranked by the new RSM, NFM (expert) and the Least Squares (LSQ) method and the results are compared.

The two papers are self-contained. Therefore, there is no additional information beyond the scope of each paper required in order to make the reader understand the research.

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Chapter 2

Paper 1

Selection of Pareto-Optimal Solutions for Process Optimisation Using Rough Set Method: A New Approach

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Abstract

The optimisation of complex processes normally involves numerous conflicting objectives. There is typically no solution that provides the user with the best values for all criteria. Therefore, the decision-maker needs to decide on a reasonable compromise, and numerous multicriteria optimisation methods can assist the decision-maker in performing this task. The method of interest in this study is the Rough Set method (RSM) where the decision-maker ranks a small subset of Pareto-optimal solutions which serves to encapsulate his preferences in a simple set of preference and non-preference rules that are used to rank the Pareto domain. A new robust RSM is suggested that concentrates on the way the subset of Pareto-optimal solutions is selected and presented to the decision-maker. Three case studies are used to assess the performance of the different variants of RSM. Results show that the improved method is indeed more robust in consistently obtaining a reliable optimum solution.

Keywords: Multicriteria Optimisation, Pareto Domain, Rough Set, Net Flow, Beer Quality

1. Introduction

Multicriteria optimisation processes have attracted considerable attention in recent years. Everyone faces some sort of multicriteria optimisation problems on a daily basis. For example in designing a car, an engineer may want to increase the crash resistance for safety and decrease the weight of the car for fuel economy. These two objectives are opposing each other, where a step towards improving one objective is a step away from improving the other. These problems are not always easy to address and, at a more complex level, they involve multiple conflicting criteria that need to be optimized simultaneously. These criteria need to be maximized or minimized or to be as close as possible to a target value. The level of complexity of this decision process can become rapidly overwhelming for complex multiobjective optimisation problems routinely encountered in industry, medicine, systems science, and many other fields. In addition, in many manufacturing processes, many market, financial and environmental constraints need to be satisfied simultaneously with the multiple objectives. In situations like these, there is rarely a unique solution that yields the optimal values for all objective criteria and, therefore, the decision-maker must find a reasonable compromize to reconcile all the conflicting objectives.

This challenge has led to the development of powerful decision-aid methods that can be applied to a wide variety of multicriteria optimisation problems and provide the expert with the best possible compromised solution. There exist many multicriteria optimisation methods that have been proposed in the literature. These methods can be generally classified in two categories. The first category considers aggregating functions or methods that depend on the user's choice that must be known at the beginning of the process, so preference can bias the results (at early stages). This category of methods does not require the determination of the Pareto domain (Andres-Toro et al., 2002). Examples of such methods are techniques that deal with the multiple criteria by combining them, through a linear combination, to form a scalar objective function (such as the weighted sum of individual objectives) or a geometric average of the objective functions (multiplication of the objective functions). In some cases, these methods may focus on a single objective while transforming the others into constraints (Massebeuf et al., 1999). The second category, known as non-aggregating methods, requires the prior or simultaneous determination of the Pareto domain. These methods incorporate a domination criterion, they are considered to be more general and more accurate. The object is to find a non-dominated zone in which a decision-maker will be able to choose the best solution (Massebeuf et al., 1999). Net Flow Method (NFM) and Rough Set Method (RSM) belong to this category of methods. They essentially consist of determining the Pareto domain and then, using the conscious and intuitive preferences of the decision-maker, all Pareto-optimal solutions are ranked to obtain the optimal solution. The Pareto Domain (PD) is comprised of the set of all non-dominated solutions. Based on the Pareto domination criterion, a point dominates another if it is strictly better for at least one criterion and better or equal for the others (Deb, 2001).

The optimisation methods that are based on the Pareto domain usually consists of three main steps. First, a sufficiently comprehensive model of the process must be developed to represent the underlying phenomena that relate the input and output process variables.

Second, the decision space is reduced to circumscribe only the set of all non-dominated solutions (PD) using a sufficiently large number of solutions. Third, all these Pareto-optimal solutions are ranked using the knowledge and preferences of a human expert or decision-maker to identify the optimum solution. The most challenging step is often the third step since it depends on human judgment (Renaud et al., 2005). It is therefore necessary to have a robust procedure to extract the best possible information from the decision-maker to meet this challenge. This investigation is particularly interested in the Rough Set method (RSM). In RSM, the decision-maker is presented with a small subset of Pareto-optimal solutions and asked to rank this subset from the most preferred to the least preferred solutions. The ranking of the small subset is then transformed into a set of preference and non preference rules that are then used to rank all solutions that approximate the Pareto domain (Thibault et al., 2003).

Rough Set Method, originally proposed by Pawlak in early 1980s (Pawlak, 1982), has become a recognized and widely studied method. Despite the success of RSM in obtaining an optimum solution to multicriteria optimisation problems in different fields, there seems to be a major weakness that requires some attention to make the method more robust. This shortcoming arises from the way that the handful of Pareto-optimal solutions, presented to the expert for ranking, are selected. Since these points are normally selected randomly, once they are ranked, they do not guarantee the generation of all the rules or, at least, the most important ones. This situation occurs due to the duplication and elimination of rules which are performed after the rules are generated based on the small ranked subset of points (Thibault et al., 2003). In addition, if some objectives of different solutions within the subset are close to each other, a rule that would normally be located in the preference rule set may be classified as a non-preference rule. Therefore, the obtained optimum may be biased by a low number of rules and an inappropriate rule classification. As a result, every time a different subset of Pareto-optimal solutions is selected and ranked by the expert, different rules may be generated and a different optimum solution may be obtained.

In this paper, a new approach to RSM that provides a more reliable and robust method to optimize multiobjective problems is proposed and compared to the traditional RSM. The difference between the new and the traditional methods lies in the selection of the subset of points from the Pareto domain and the way it is presented to the expert. In the proposed scheme, points are selected two at the time while insuring that they are distant enough to generate a new and reliable set of rules each time. A modified batch method is also proposed which is expected to be more efficient in generating rules than the traditional RSM.

The paper is divided as follows. After a brief introduction of RSM, a detailed description of each of the three variants of RSM, the traditional RSM (RSM: Batch), RSM: Modified Batch and RSM: By Pair, is given. These methods are then implemented to find the optimal solution of three case studies and the results are presented and compared.

2. Rough Set Method

RSM has attracted considerable research interest and has become a powerful technique to identify the optimum zone of solution to multicriteria optimisation problems. It is used to rank the set of all Pareto-optimal solutions. Obtaining the PD is a common first step to the many multicriteria optimisation techniques and it is done without biased preference of an expert. On the other hand, the Rough Set theory relies on a tabular representation of the preferential information expressed by an expert. In the following sections, the "traditional RSM" or RSM: Batch is briefly described with an emphasis on major shortcoming of RSM which will set the path to proposing an alternative to render the method more robust and coherent.

2.1 Brief Description of the Traditional RSM (Batch)

In traditional RSM, to achieve the classification of the PD, the following procedure is carried out. A small subset of points is selected from different regions of the PD, most often randomly. This set of Pareto-efficient solutions is then presented at once (batch) to the expert who ranks the solutions from the most to least preferred. This ranking is based on the process knowledge of the expert and his/her preferences. Next, one must establish a set of rules that is based on the expert's ranked set such that a pairwise comparison of each point in the ranked set is performed in order to define rules of preference (P) and non-preference (NP). Each rule is a vector of dimension equal to the number of criteria, containing only binary numbers, i.e. 0 and 1. A value of one indicates that the first point is better than the second point with respect to a given criterion, while a value of 0 indicates that the criterion of the second point is better. In this process of creation of the rules, some rules may need to be eliminated due to the following two reasons. First, a rule needs to appear only once in P or NP set of rules, so when a rule appears more than once, only one copy of the rule is kept. Second, since a rule cannot appear in both P and NP rule sets, in case of this happening, both copies of the rule are eliminated. This is simply because the expert can not rank one point better than another point for the same reason that he considers a point worse than another point.

Once the elimination process is complete, the entire PD is ranked using the P and NP sets as follows: Each point in the PD is originally given a ranking score of zero. Then each point is compared to every other point within the PD. For each comparison, if a rule of preference is satisfied, the score of the first point is increased by one and the ranking score of the second point is decreased by one, and if a rule of "non-preference" is satisfied, the ranking score of the first point is decreased by one and that of the second point is increased by one. When a pairwise comparison leads to a rule that does not match one of the rules in the P nor the NP sets, the scores of the two points remain the same (Renaud et al., 2005).

Once the comparison process is complete, the PD points are ordered from the point with the highest score to the one with the lowest, and the optimum region is specified accordingly.

2.2 Problem involved with the traditional RSM (Batch)

The traditional RSM has been used successfully in obtaining optimum solution to multicriteria optimisation problems and has been shown to be a relatively robust method. For example, Thibault et al. (2003) used RSM to identify the optimal operating conditions associated with a thermomechanical pulping process. Despite some success in applying this method to solve mutiobjective problems, some shortcomings have been identified. The main problem is in the way that the points are selected and presented to the user. Indeed, a random selection of points within the Pareto domain does not guarantee that these points are discriminating enough to generate a representative set of rules. It is highly probable that the difference between some of the criteria will not be significant enough to allow the generation of a different and efficient number of rules, one that could be used reliably to order the entire PD. Also, some rules may be completely overlooked, since they may have appeared in both P and NP rule sets and therefore eliminated or did not initially appear in the expert's ranked subset. The eliminated rules or the rules that were not generated may be of significant importance to the outcome of the optimisation process; hence the results may not totally represent the actual optimum region. In the next section, an enhanced batch (or modified batch) representation of RSM is introduced in order to insure the generation of a larger number of rules and, hopefully, leading to a method that provides a more reliable optimum region.

2.3 RSM with modified batch approach

In the modified batch approach, instead of randomly selecting a small subset of points from the PD, two random points are first selected. The first selection, upon ranking by the decision-maker, will allow the generation of one preference (P) rule and one non-preference (NP) rule. One additional point is then selected randomly from the PD. This point is kept if, when compared to the other two previously selected points, leads to two new sets of rules, i.e. two P and two NP rules. Otherwise, a new third point is selected until this constraint is satisfied. If required, a fourth point is selected and compared with the previous three points while ensuring different rules are created. This process is continued until all or the desired number of P and NP rules is obtained. This approach prevents a rule to appear twice with the risk of being eliminated. However, when the number of criteria is large, it may become impossible to find a set of points that will provide the desired number of distinct rules, through all pairwise combinations. Moreover, the points are not selected in a systematic way in order to insure that the differences between criteria are distant enough from each other and, therefore, there is no guarantee that these points will generate representative rules. An additional feature that could easily be added to the modified batch approach is to incorporate a threshold of indifference in the selection of points to make sure there exists a significant distance between the various criteria to allow proper discrimination by the expert. The threshold of indifference, associated to each criterion, is defined as the range of variation of each criterion for which it is not possible to favor one criterion value over another value. Even though the threshold of indifference associated to each criterion may allow a more appropriate discrimination by the expert, the differences between criteria may still not be large enough to allow the generation of reliable set of rules. Moreover, the incorporation of the threshold of indifference may exacerbate the difficulty of identifying a set of points that will satisfy this additional constraint. The next section will present another RSM alternative to further tackle this problem.

2.4 Presenting solutions by pairs for a more robust RSM

To alleviate the problems of rule generation associated with the RSM: Batch, it is proposed, in a new RSM alternative referred to as RSM: By Pair, to present the expert with only one pair of points at a time instead of presenting a subset of points all at once. Since two points can only be associated to two rules, one P and one NP, the rules are automatically generated after the points are ranked by the expert. Then, another pair of points is selected in way to generate a different pair of rules, thus overcoming the duplication and elimination of rules. This process is continued until the desired number of rules or all possible rules are generated. When the number of criteria is large, the number of rules becomes excessively large, and it may be preferable to use only a fraction of the number of all possible rules. Therefore, if only a fraction of all possible rules is desired, the most frequently encountered rule and its complementary rule within the Pareto domain are first selected, and subsequently selecting Pareto-optimal points satisfying the next most frequent pair of rules, and so on until the desired number of rules are obtained. The selection of the two points to satisfy a given pair of rules can be performed in three different ways: strict random selection, random selection while insuring all the criteria are at least separated by the threshold of indifference, and the selection of the two points to insure that the differences for each of the criteria is sufficiently discriminative for the expert to decide unambiguously which point he/she prefers. In this investigation, in the latter approach, the pair of points was selected to ensure that the value of one criterion for one point was as close as possible to one quarter of the total range of the criterion and the value of the same criterion of the other point was as close as possible to three quarters of the total range. The pair of points that best meets this requirement for each set of rules is selected and presented to the expert. Any differences between the values of each criterion can obviously be used as long as two points are discriminative enough to generate consistent rules.

3. Optimisation Case Studies

In this paper, three multicriteria optimisation problems are examined. The optimum solutions to these problems were obtained by three RSM variants: RSM: Batch, RSM: Modified Batch, and RSM: By Pair.

Figure 1 shows a general schematic diagram of a model that applies to any optimisation process with 1 to m input variables (independent variables or decision space variables), represented as X_1 to X_m, and 1 to n output variables (dependent variables or criterion space variables), represented as C_1 to C_n.

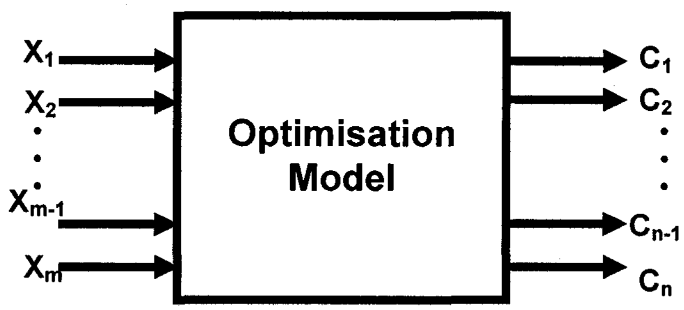


Fig. 1: m-input, n-output optimisation model

3.1 Case 1: 3-Criteria Cone problem

This problem represents a simple three-dimensional conic shape Pareto surface that is obtained by solving the system of equations given by Equations (1)-(3). This simple multicriteria optimisation problem has two input variables (X_1 and X_2) and three criteria (C_1, C_2, and C_3). It is required to maximize all three criteria. The ranges of variation for the input variables are presented in Table 1.

$$C_1 = (2 - 0.9X_1^{1/2}) \cdot X_2 \tag{1}$$

$$C_2 = 4 - 1.4(X_1 + X_2^2)^{1/2} \tag{2}$$

$$C_3 = (3.33X_1)^{1/2} \tag{3}$$

3.2 Case 2: High Yield Pulping Process

The second optimisation problem deals with the high yield thermo-mechanical pulping process of jack pine using an interstage sodium hydroxide treatment (Lanouette, 1998). Interstage NaOH treatment is an innovation that is designed in order to reduce extractive content of the resulting pulp (Thibault et al., 2003). This process is important because of the abundance and relatively low cost of jack pine (Lanouette et al., 1997). This process corresponds to a multicriteria optimisation problem with seven input variables (in this investigation) and numerous performance quality criteria. However, only four quality criteria were selected as the most important criteria for the optimisation process. Table 1 lists all the input and output variables used in the optimisation of this case study. It is desired to maximize both the ISO brightness (C_1) and the rupture length (C_4), while minimizing the specific refining energy (C_2) and the extractive content (C_3).

To develop a representative model for each of the four criteria, a D-Optimal experimental design was performed (Lanouette et al., 1998). A ten-level stacked three-layer feed forward neural network was used to model each objective criterion of the process. Each neural network used only six (X_1-X_6) of the input process variables.

3.3 Case 3: Enhancing Aroma Concentration in Beer Production

In brewing, during alcoholic fermentation where the yeast consumes sugars and amino acids of the wort, primary products such as ethanol, CO_2, biomass, and various secondary metabolites are produced. Some of the secondary products such as higher alcohols, esters, and vicinal diketones are flavor related and responsible for the taste of the final product. The concentration of six of these products that are known to be more significant to beer flavour based on their organoleptic threshold in beer (Titica et al., 1999), were selected as the six criteria of this process. A three-factor two-level factorial experimental design has been performed (Titica, 2000) to develop a model of the process. The three factors were the main operating variables: temperature, pressure, and yeast inoculum concentration. The operating range for these input variables and the desired concentration targets of the six criteria, as determined by taste experts, are presented in Table 1. From this information, kinetic models to account for the evolution of biomass, sugars, CO_2 and the six selected metabolite concentrations were derived (Titica, 2000). The models are used in this case study to optimize the fermentation process such that all aroma concentrations are as close as possible to their respective targets.

The goal is therefore to minimize the differences between the predicted values and the target values for the first five compounds and to ensure that the concentration of the last compound is less than 0.2 mg/L. These requirements represent the six individual competing objective functions (C_1 to C_6).

Table 1: Input and output variables and pertinent information for the three optimization case studies.

Case	Inputs		Outputs	
	Variables	Range	Variables	Objective/ Target
1	X_1	0 – 4	C_1	Max
	X_2	0 – 4	C_2	Max
			C_3	Max
2	**First refining stage**			
	Operating temperature(X_1)	115-135°C	ISO Brightness (C_1)	Max
	Plate gap (X_2)	0.7-1.0 mm		
	Interstage Treatment		Specific refining energy (C_2)	Min
	H_2O_2 charge (X_4)	1-5%		
	Temperature (X_5)	60-75°C		
	Retention time (X_6)	15-75min	Extractive contents (C_3)	Min
	Second refining stage			
	Consistency (X_3)	8-16%	Rupture length (C_4)	Max
3	Temperature (T)	10-16°C	Isomyl alcohol (C_1)	93.8
			Phenyl alcohol (C_2)	31.6
	Pressure (P)	50-800 mbar gage	Ethyl acetate (C_3)	23.6
			Isoamyl acetate (C_4)	2.04
	Yeast inoculum concentration	0.5 - 2.0($\times 10^7$) cells/mL	Ethyl hexanoate (C_5)	0.25
			Diacetyl (C_6)	<0.2

4. Results and Discussion

For each of the three case studies, the Pareto domain containing non-dominated solutions was first approximated by a large number of solutions that were obtained using a diploid genetic algorithm (Fonteix et al., 1995) for the second case study, and a uniform grid method for the first and third case studies (Halsall-Whitney and Thibault, 2006). For each case study, the three RSM variants (traditional batch, modified batch, and by pairs) will be compared. To rank the subsets of Pareto-optimal solutions in order to establish the preference and non-preference rules, it was decided to use the Net Flow Method (NFM) to act as the expert. The NFM is a fairly robust multicriteria optimisation technique that uses a relative weight and three thresholds (indifference, preference, and veto) for each criterion to rank the PD. The reader is referred to Thibault et al. (2002) for a more detailed description of NFM. The reason for choosing NFM to act as the expert is to have an expert that will consistently resort to the same thinking process to rank the small Pareto-efficient data set for the three processes studied

4.1 Case 1: 3-Criteria Conic Surface

In this case study, there are three conflicting criteria that should be maximized simultaneously. The Pareto domain for this case contained 1681 solutions that were ordered from best to worst using the three RSM variants. Figure 2 shows the Pareto domain ranked by RSM: By Pair. Figure 2(a) presents the decision space whereas Figures 2(b) and 2(c) show the three-dimensional criterion space projected onto two two-dimensional spaces. The light grey points correspond to the best 10% of the ranked PD, the dark grey points represent the subsequent 40%, and the black points show the last

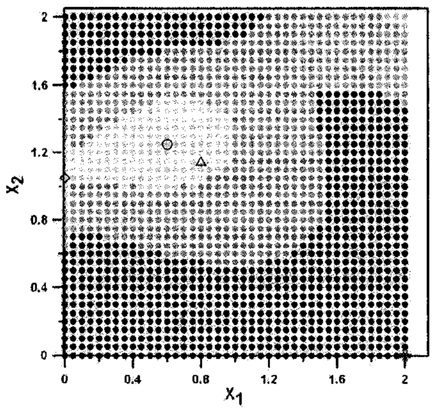
50%. The best points (optimums) obtained by NFM (the expert) and the three RSM variants are also shown on each plot.

The best solutions obtained by the three RSM variants were compared to the optimum obtained by NFM and, as it is shown on the graphs (Figure 2), the optimum obtained by RSM: By Pair is much closer to the optimum of NFM (expert). The three RSM variants were ordered from best to worst in comparison to the expert's optimum, and the results are presented in Table 2 along with the input and output values obtained by each method.

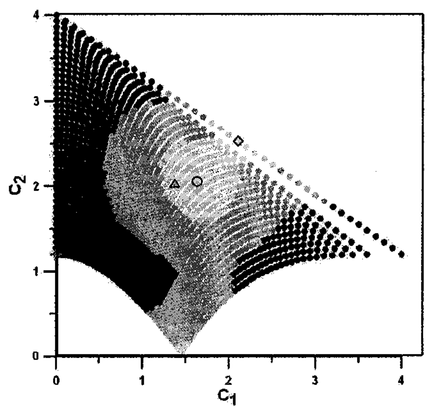
Table 2: 3-Criteria cone problem: The optimum points obtained by the four methods and ranks assigned to RS methods compared to NFM.

Method	Rank Compared to the Expert	X_1	X_2	C_1	C_2	C_3
NFM	Expert	0.8	1.15	1.37	2.04	1.63
RSM: By Pair	1	0.6	1.25	1.73	2.15	1.12
RSM: Traditional Batch	2	0	1.05	2.1	2.53	0
RSM: Modified Batch	3	2.0	0	0	1.2	2.58

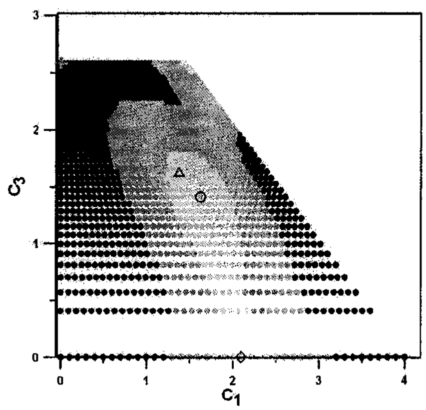
In this case, the ideal optimum would be the one that gives maximum possible values for all criteria. Results of Figure 2 and Table 2 show that a good compromise amongst the three criteria is achieved by RSM: By Pair. RSM: Traditional Batch leads to ideal values for criteria 1 and 2 but sacrifices criterion 3 completely, where its minimum value was obtained. RSM: Modified Batch acted in a similar manner by sacrificing C_1 completely, achieving the maximum value for C_3 and an intermediate value for C_2.



(a)



(b)



(c)

Fig. 2 Ordered Pareto Domain by RSM: By Pair for 3-criteria problem (a) Input space, (b) and (c) Output Space. (o Best point RSM: By Pair; ◇ Best point RSM: Traditional Batch; ✚ (gray) best point Modified Batch; Δ Best point NFM)

The results point to an interesting issue that must be addressed. Since both RSM: By Pair and Modified Batch generated all possible rules (Table 3) and no rules were eliminated, one would expect the two methods should provide similar results. In fact, the opposite is observed. On Figure 2, results show that the optimum obtained by RSM: Modified Batch appears at almost the extremes of the last 50% ranking of RSM: By Pair. From the location of this optimal point (compared to the other points) on criteria plots, it is observed that C_1 is totally sacrificed ($C_1 = 0$), and C_2 is positioned at a relatively low

Table 3 - Case 1: P and NP rules obtained by RSM: By Pair, RSM: Modified Batch and RSM: Batch

		C_1	C_2	C_3	FO%
P Rules:	**By Pair**	1 1 0	0 1 1	1 0 1	19.6 18.6 13.1
	Modified Batch	1 0 0	0 0 1	1 1 1	19.6 18.5 13.1
	Batch	1	1	0	18.6
NP Rules:	**By Pair**	0 0 1	1 0 0	0 1 0	18.4 18.5 11.9
	Modified Batch	0 1 1	1 1 0	0 0 0	18.4 18.6 11.9
	Batch	0	0	1	18.5

value (1.2) compared to most of the other points. Only C_3 displays an excellent value (2.58). Clearly this point is represented by the preference rule (001). This rule has a high frequently of occurrences (FO = 18.5%). It appears as a preference rule in RSM: Modified Batch and as non-preference in RSM: By Pair. As shown in Table 3, this rule is the only inversion between the two sets of rules and led to the significantly different results. Rule (001) in the preference set implies that both criteria C_1 and C_2 can be sacrificed for the sake of achieving good values for C_3. The appearance of this particular rule in the preference rule set of RSM: Modified Batch is equivalent to reducing the three criteria optimisation problem to a single objective optimisation problem. It is due to the random selection of the first pair of points where there is no guarantee that some of the criteria are distant enough to generate representative rules. The preference rule (001) was generated by randomly selecting points (0.3998, 3.123, 1.353) and (0.5146, 3.557, 0.5771). C_1 and C_2 for this pair of points are very close to each other and did not provide sufficient discrimination to generate a representative rules. In this study, no systematic method was used by RSM: Modified Batch for selecting the points, as far as the distance between their criteria is concerned. This problem is obviously more critical when the number of criteria (number of rules) is low as one inversion in the rule sets has a more profound impact on the ranking of the Pareto domain. Comparing the results obtained by the three RSM variants, it is clear that only RSM: By Pair provides a good optimum (Figure 2 and Table 2).

In Figure 2, there are a number of points that belong to the best 10% region (light gray) for RSM: By pairs, even though they are disjoint of the bulk of the optimal zone. These points are located at the extreme edge of the input space (X_1=2.0, X_2=2.0) and in the vicinity of (C_1=1.5, C_2=~0.05, and C_3=2.65). Based on NFM (not shown), these points were ranked very low. Although the number of points in that situation is not significant, it creates a contradiction between the two methods. This contradiction arises from the intrinsic ranking scheme of the two methods. In NFM, the knowledge that the decision-maker has on his process and his preferences are expressed using four sets of parameters:

the relative weight and three thresholds for each criterion. One important parameter is the fourth parameter, referred to as the veto threshold. This parameter serves to ban a point relative to another if, in a pairwise comparison, the difference between the values of a given criterion exceeds a tolerable limit. A point is banned if the veto threshold is violated for at least one of the criteria even if the other criteria are acceptable, and thereby prevent an extreme solution to dominate the ranking. RSM does not have this capability, and in fact it operates in an opposite manner. RSM ranking favors solutions that are almost at extreme of each criterion such that a given rule could dominate pairwise comparisons in search of the best compromise. Due to this difference in the ranking scheme, some points that were identified to be in the best 10% of the ranked PD by RSM: By Pair were banned from the same zone when NFM was used (results are not shown). Some examples of these points are (2.3, 2.39, 0), (2.5, 2.25, 0), (1.49, 0.089, 2.55), and (1.45, 0.04, 2.58). The first two points are represented by the preference rule (110) and the last two by the preference rule (101). It can clearly be seen that one criterion is totally sacrificed for the sake of obtaining very good values (almost at the extremes) for the other two. Indeed, NFM penalizes excessive differences between the values of the objective functions whereas RSM rewards large differences by favoring objective functions located at extremes of their ranges. RSM guarantees that some criteria are well satisfied at the cost of completely sacrificing the others.

In NFM, the information is in the form of a sensitivity of the differences of each criterion to the target values whereas for RSM, the information is indirectly obtained by forcing the expert to make a choice between solutions taken from the PD. RSM strongly relies on the ability of the method to select representative solutions that are presented to the expert to decide which point is better within a pair (By Pair) of points or a small set of points (Batch). In previous investigations with RSM: Batch, the rules were established with the risk of obtaining duplicate rules, not accounting for some rules that could play an important role in final ranking of the set. RSM: By Pair prevented the presence of duplicate rules such that a pair of points was selected in order to generate two new rules each time, so there is no duplicate set of rules generated, hence, there is no need for elimination.

In Case Study 1 with 3-criteria, a maximum of 6 distinct rules exist, i.e. 2^3-2. The minus two accounts for the rules (000) and (111) that can not be part of the PD since they correspond to a dominated point and a point that dominates another point, respectively. Every time a pair of points is selected, two complementary binary rules are generated (Ex.: 110 and 001). Table 3 shows the rules obtained and used to rank the PD by RSM: By Pair, RSM: Modified Batch and RSM: Batch. The percentage of occurrences of each rule within the PD is also included in this table.

These results clearly show that RSM: By Pair, by making sure to generate the desired number of rules and insuring a discriminative distance between the different criteria, is superior to the other two variants of RSM.

4.2 Case 2: High yield Pulping Process with NaOH Treatment

The set of all non-dominated solutions, the PD, contained 6000 points. This set was ordered in the same manner as Case Study 1 by the three RSM variants, and NFM acting as the expert. The resulted optimums are presented in Table 4. The ranked PD is plotted as three two-dimensional input vs. input plots and two two-dimensional output vs. output plots (Figure 3). The color coding is identical to the one of Case Study 1. Table 5 presents the rules obtained by three RSM variants.

Table 4: Pulping Process: The optimum points obtained by the four methods and relative ranking assigned to RS methods compared to NFM

Method	**Net Flow**	**RS: By Pair**	**RS: Batch**	**RS: Modified Batch**
Score vs NFM	Expert	1	2	3
X_1	117	116	122	123
X_2	0.977	0.975	0.989	0.971
X_3	10.1	11.9	8.98	9.87
X_4	4.8	4.8	4.64	4.0
X_5	74.4	74.9	72.2	65.4
X_6	70.3	70.6	57.8	65.2
C_1	68.3	68.4	67.5	65.1
C_2	8.24	8.53	7.68	6.0
C_3	0.161	0.148	0.189	0.119
C_4	4.23	4.34	3.79	3.69

In Figure 3, the best point obtained by RSM: By Pair is located at a far superior position compared to RSM: Batch, RSM: Modified Batch, and even the expert NFM (Table 4). Akin to case study 1, the optimum obtained by RSM: Modified Batch is positioned far away (almost opposite) from the one obtained by the RSM: By Pair. RSM: Modified Batch satisfies C_2 and C_3 extremely well whereas C_1 and C_4 assumed relatively low values. This is due to the different preference and non-preference rule sets used by the two methods. A highly frequent preference rule that is generated by one method, appearing as a non-preference rule for the other method, results in obtaining different

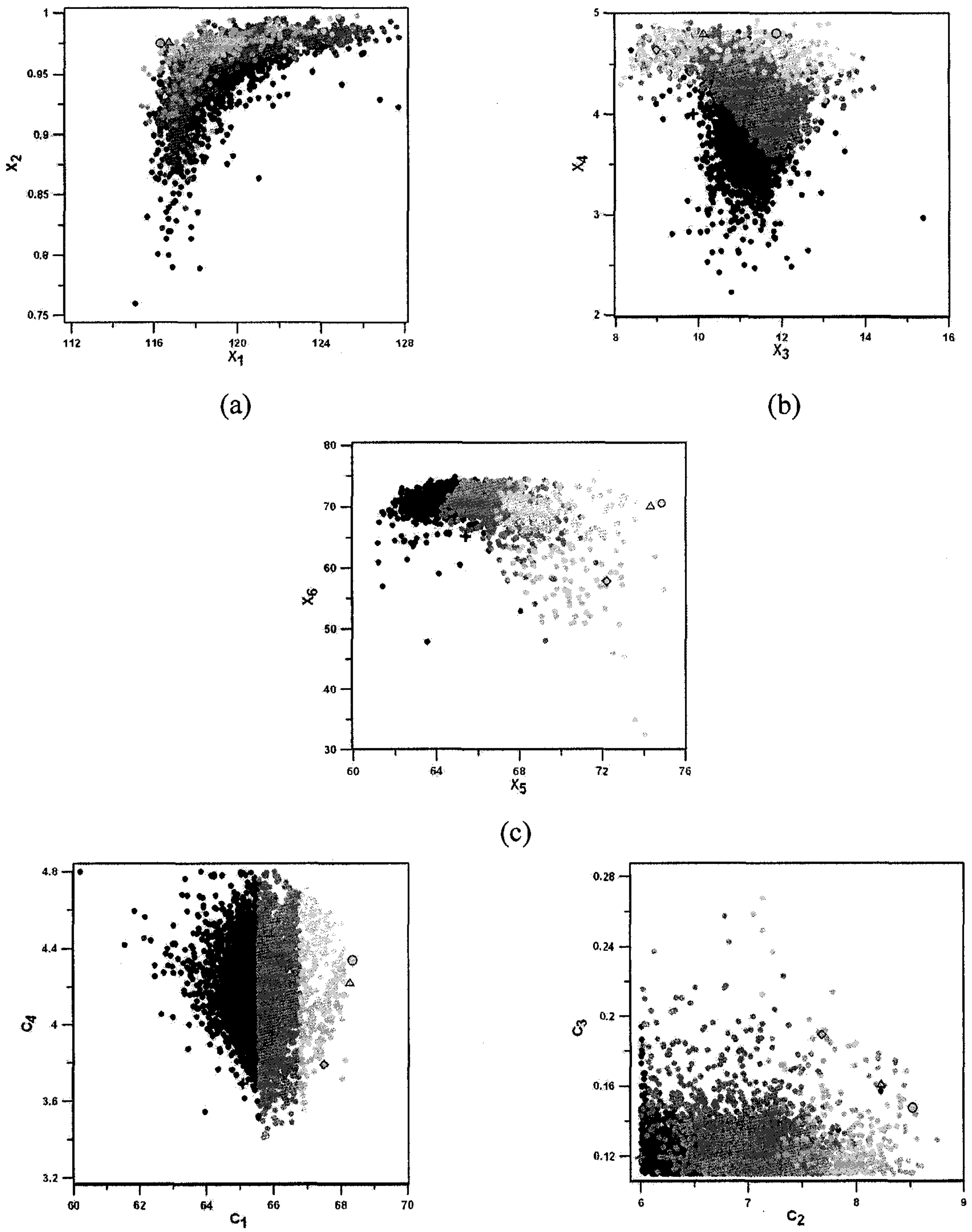


Fig. 3 Pulping Paper: Ordered PD using RS: By Pair, (a), (b) and (c) Input space; (d) and (e) output space. (○ Best point RSM: By Pair; ◇Best point RSM: Batch; Δ Best point NFM; ✚ (in white, gray or black) best point modified Batch)

optimum solutions. For instance, the preference rule of (1001) (Table 5) in RSM: By pair with the highest frequency of occurrences (12.9%) is the highest occurring non-preference rule in RSM: Modified Batch. The preference rule (0110) for the RSM: Modified Batch does indeed favor C_2 and C_3 to be better satisfied at the expense of the other two criteria.

Table 5 clearly shows that RSM: By Pair is a more reliable and robust method than the other two RSM variants. In addition, RSM: By Pair has generated all possible 14 rules associated to this problem whereas RSM: Modified Batch generated 12 rules and 10 for RSM: Batch. It is important to note that a different set of solutions for RSM: Batch or RSM: Modified Batch, selected from the PD and ordered by the expert, could result in a different P and NP sets of rules and, as a result, to a different PD ranking.

4.3 Case 3: Beer Aroma Production

The PD for this six-criterion optimisation problem was approximated by 5000 points. As in the previous two case studies, the ranking was done by all three methods. The ranked PD by RSM: By Pair is presented by projecting the three-dimensional input space onto two two-dimensional plots (Figures 4(a) and 4(b)) and the six-dimensional criterion space onto three two-dimensional plots (Figures 4(c), 4(d) and 4(e)). The color coding is identical to previous cases. The desired target for each criterion is indicated using horizontal or vertical lines.

Figures 4(c), 4(d) and 4(e) show that the best 10% PD satisfies five of the six criteria. The only criterion with a ranking pattern contrary to the desired one is C_1 where the optimal zone is farthest from the desired target value. Of course, it is not possible to satisfy all the criteria simultaneously. In this case, the quality of criterion C_1 is sacrificed

Table 5 Case 2: P and NP rules obtained by RSM: By Pair, RSM: Modified Batch and RSM: Batch

		C_1	C_2	C_3	C_4	FO%
P Rules	**By Pair (7 rules)**	1	0	0	1	12.9
		1	0	1	1	11.6
		:	:	:	:	:
		1	1	1	0	4.71
		1	1	0	1	0.037
	Modified Batch (6 rules)	0	1	1	0	11.7
		1	1	0	0	11.5
		:	:	:	:	:
		1	1	1	0	5.41
		0	1	0	1	4.74
	Batch (5 rules)	1	0	1	1	12.9
		1	0	0	1	11.6
		1	1	0	0	8.31
		1	0	0	0	7.65
		1	1	1	0	4.71
NP Rules	**By Pair (7 rules)**	0	1	0	0	12.6
		0	1	1	0	11.8
		:	:	:	:	:
		0	0	0	1	4.56
		0	0	1	0	0.031
	Modified Batch (6 rules)	1	0	0	1	11.9
		0	0	1	1	7.74
		:	:	:	:	:
		1	0	1	0	4.74
		0	0	0	1	3.93
	Batch (5 rules)	0	1	0	0	12.6
		0	1	1	0	11.8
		0	0	1	1	8.22
		0	1	1	1	7.75
		0	0	0	1	4.56

in order to obtain relatively good solutions for all the other five criteria. The trade-off that must inevitably exist between some criteria is very well illustrated in Figure 4(d) where criterion C_4 is plotted as a function of C_3. An increase in C_3 must also be accompanied by an increase in C_4 to remain in the optimal region and vice-versa. This highlights the advantage of using a multicriteria optimisation technique that uses the entire PD, because it provides valuable information on the interrelationship that exists between the various criteria, in contrast with traditional optimisation where a unique solution is obtained.

Figure 4(e) shows that the best 10% for criterion C_5 is located closest to the target value. However, no solutions within the domain of exploration that meet the target were obtained. The target was established by experts through tasting trials but, assuming that the model predictions are accurate, the target value for C_5 can not be obtained with the current range of experimental operating conditions. In addition, it is necessary for criterion C_6 (concentration of dactyls) to be lower than 0.2. This objective was achieved for all points in the Pareto domain. In the current investigation, this criterion was however minimized, i.e. a value of C_6 closest to 0 was desired.

Table 6 shows the best solutions from the ranked PD using the three RSM variants and NFM along with the target values. A score (Table 6, column 2) was given to each RSM variant based on the number of criteria, C_1 to C_6, that are closer to the target values. It is clear that RSM: By Pair provides the best compromise considering that there are three out of the five criteria that are closest to the target values. RSM: Modified Batch provides the poorest results compared to the other methods. This method largely sacrifices three (C_3,

C_4 and C_5) out of the first five criteria and obtains the highest concentration for C_6 compared to the other methods. This poor performance is associated with the lowest allowable temperature (10°C) and the highest inoculum concentration (2.0×10^7 cells/ml).

Table 7 presents the P and NP rules that were obtained for the three RSM variants. It is interesting to note that the two most frequent preference rules in RSM: By pair, (011110) and (001111), are the two most frequent non-preference rules in RSM: Modified Batch. This explains the location of optimum obtained by RSM: Modified Batch and why it performs almost opposite to RSM: By Pair. The best points obtained by these two methods are represented by these rules. Again this difference is due to the separation between the criteria of the selected points.

Table 6: Beer Aroma Production: The optimum points obtained by all the methods and scores assigned to RS methods compared to NFM, highlighted values are the closest to the targets for each method.

Method	Score	T(°C)	P(mbar)	$X_0\times10^{-7}$ (cells/mL)	C_1	C_2	C_3	C_4	C_5	C_6
Target	Target	10-16	50-800	0.5-2.0	93.8	31.6	23.9	2.04	0.25	<0.2
NFM	Expert	14.9	425	0.5	88.2	37.8	15.9	1.8	0.15	0.04
RSM: By Pair	1	13.4	50.0	0.5	73.4	31.5	22.6	2.62	0.21	0.06
RSM: Batch	2	16.0	472	0.5	92.3	40.6	15.8	1.81	0.15	0.03
RSM: Modified Batch	3	10.0	378	2.0	84.3	31.8	6.32	0.30	0	0.18

The top points ranked by NFM (expert), RSM: Batch and RSM: By Pair are also shown on the input and output graphs on Figure 4. RSM: By Pair provides the best result compared to the other methods and performs very well by sacrificing only one criteria and obtaining excellent values for the others.

For a six-criterion problem, there are a maximum of 62 distinct rules. All these rules were used by RSM: By Pair to rank the entire PD (Table 7), whereas only four rules were used by RSM: Batch. Naturally, some rules are more frequent than others. The rules in Table 7 are ordered from most to least frequent for both preference and non-preference sets. The most frequent rules are not present for RSM: Batch; they were either eliminated during the elimination process or never appeared in the selected subset of PD points that were ranked by the expert (NFM). This observation points to the importance of properly selecting a subset of Pareto-optimal solutions that is presented to the expert for ranking. It is obvious that RSM: By pair is far superior to the other two RSM variants.

Another important issue that exists with RSM: Batch is that the obtained optimum may change each time that a different subset of random points are selected and presented to the expert for ranking. This is because for each different subset, different rules and a different number of rules may be generated. These rules could be completely different from the rules that are generated by another random seed or they could be partially different. Table 8 shows four different optimum solutions obtained with different random seeds. As shown, for each trial a different number of rules are generated to rank the PD. With different sets of rules, the ranking of the PD is obviously different, thus leading to a different optimum.

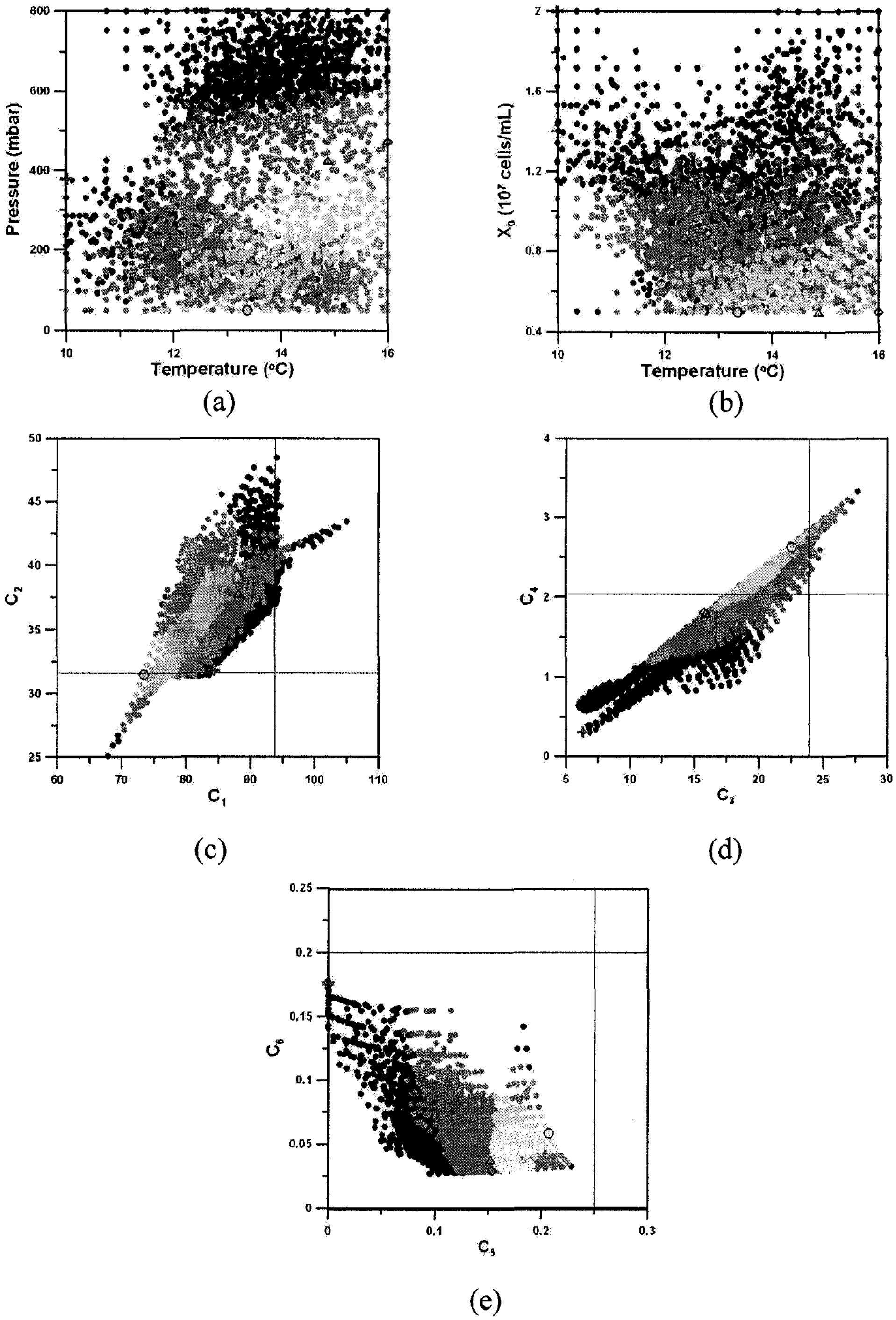


Fig. 4 Ordered Pareto Domain by RSM: By Pair for beer aroma production (a) and (b) Input space; (c), (d) and (e) output space. (○ Best point RSM: By Pair; ◇Best point RSM: Batch; Δ Best point NFM; ✚ (in grey) best point modified Batch)

Table 7 Case 3: P and NP rules obtained by RSM: By Pair, RSM: Modified Batch and RSM: Batch

		C_1	C_2	C_3	C_4	C_5	C_6	FO (%)
P Rules	**By Pair (31 rules)**	0 0 : 1 1	1 0 : 1 1	1 1 : 1 1	1 1 : 0 1	1 1 : 1 0	0 1 : 0 1	10.5 9.21 : 0.0021 0.0016
	Modified Batch (10 rules)	1 1 : 1 0	0 1 : 0 0	0 0 : 0 1	0 0 : 1 0	0 0 : 1 0	1 0 : 1 0	10.35 9.23 : 0.77 0.104
	Batch (2 rules)	1 1	0 0	1 0	1 1	1 1	1 1	8.58 0.7824
NP Rules	**By Pair (31 rules)**	1 1 : 0 0	0 1 : 0 0	0 0 : 0 0	0 0 : 1 0	0 0 : 0 1	1 0 : 1 0	10.4 9.21 : 0.0021 0.0016
	Modified Batch (10 rules)	0 0 : 0 1	1 0 : 1 1	1 1 : 1 0	1 1 : 0 1	1 1 : 0 1	0 1 : 0 1	10.53 9.18 : 0.798 0.108
	Batch (2 rules)	0 0	1 1	0 1	0 0	0 0	0 0	8.55 0.7853

Table 8: Beer Aroma Production: Results obtained for every different set of feed

points that was presented to the expert for ranking and generation of rules.

Feed	Task	T	P	X_0	C_1	C_2	C_3	C_4	C_5	C_6
1	Optimum	16	472	0.5	92.3	40.6	15.8	1.81	0.154	0.029
	# of pts	6								
	# of Rule Sets	2								
2	Optimum	12.7	193	0.534	76.7	31.5	18.7	2.09	0.171	0.069
	# of pts	6								
	# of Rule Sets	9								
3	Optimum	11.1	50	0.594	72.7	28.3	18.8	2.06	0.174	0.108
	# of pts	4								
	# of Rule Sets	4								
4	Optimum	11.9	50	0.688	76.6	31.3	19.3	2.08	0.166	0.085
	# of pts	4								
	# of Rule Sets	6								

5 Conclusion

In this investigation two new approaches to RSM were introduced. In these new approaches, the method of selecting the points that are presented to the expert for ranking is different than the traditional RSM (RSM: Batch). For RSM: By Pair, the points are selected two at the time to guarantee the generation of a new pair of rules each time. It is therefore possible to generate the maximum, or the desired, number of rules. This method guarantees that no rules are overlooked. Also, since the points in each selected pair are chosen to be discriminative enough, the PD can be more reliably ranked using the generated rules from the pairwise comparison of these points. In RSM: Modified Batch, the first pair of points is selected randomly to generate a pair of rules and the third point is selected such that it generates a new pair of rules with each of the points of the previous pair. This method did not perform as well as expected, in obtaining the desired results. The poor performance is associated to the confusion in generating rules when a given criterion of two points in the small PD subset presented to the expert, is not sufficiently distant for the expert to make a clear choice.

In this study, NFM was used as the expert. This method was used to rank the entire PD for all three case studies. RSM: By Pair, RSM: Modified Batch and the RSM: Batch were used to rank the PD of the three case studies. The results obtained for each case were compared with the results obtained by NFM. Based on these comparisons, it was found that the RSM: By Pair is far superior and more robust compared to both RSM: Batch and RSM: Modified Batch.

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Chapter 3

Paper 2

Muticriteria Optimisation of Beer Quality Using the Rough Set Method

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Abstract

Volatile compounds like higher alcohols and esters contribute to beer's organoleptic profile. Most of these compounds are produced during alcoholic fermentation and operating conditions play an important role on their formation. In this study, a multicriteria optimisation method, the Rough Set Method (RSM), is successfully used to determine the optimal region of fermentation conditions (temperature, pressure and initial yeast concentration) with respect to a specified beer aroma profile.

Keywords: multicriteria optimisation, rough set method, beer fermentation process.

1. Introduction

The complexity of multicriteria optimisation problems in different fields of medicine, systems science, biotechnology and many more, has spurred the need to develop powerful methods that can be easily applied to solve different types of complex problems and provide the decision maker with an acceptable compromised solution.

The optimisation of complex processes normally involves minimizing and/or maximizing numerous conflicting objectives; in cases like these, there is no unique solution that can provide the optimal values for all the objective criteria simultaneously. Therefore the decision maker must find a reasonable compromise. In a previous study, the optimisation of brewing process with respect to the beer's organoleptic profile has been formulated as a multicriteria optimisation problem (Titica et al., 2001; Trelea et al., 2004). The beer quality has been defined in terms of flavour-active components content. Six aroma compounds have been selected with respect to their organoleptic threshold: two higher alcohols (isoamyl alcohol and phenyl ethanol), three esters (ethyl acetate, ethyl hexanoate and isoamyl acetate) and one vicinal diketone (diacetyl). These components are mainly produced during alcoholic fermentation and operating conditions play an important role on their formation. Thus, the optimisation of the operating conditions like temperature, pressure and initial yeast concentration in the fermentation tank, has been proposed as a way to modify beer organoleptic profile and to guarantee its regularity. The best compromise of operating temperature, pressure and yeast inoculum's size will ensure the best quality beer. The selection of the optimal operating conditions by the decision maker is a very complex task. To cope with these complex problems multicriteria optimisation methods can be used, such as the Net Flow Method (NFM) and the Rough Set method (RSM) that can capture the knowledge that the decision maker has on the fermentation process in order to locate the optimal zone of operation.

In this paper, the aroma production model is first presented. Then, the optimisation protocol involving the RSM is presented. Finally, the RSM is used to determine the optimal concentrations of the six major aromatic compounds responsible for the organoleptic properties of beer and to specify the optimal fermentation operating conditions. Results are compared with those obtained with the NFM and least squares methods.

2. Aroma Production Model

In brewing, during the alcoholic fermentation where the yeast consumes sugars and amino acids of the wort, primary products such as ethanol, CO_2, biomass and various secondary metabolites are produced. Some of the secondary products such as higher alcohols, esters, and vicinal diketones are flavour related and are responsible for the taste of the final product. In this study six of these products, as listed in the introduction, that are known to be more significant for beer flavour were selected based on their organoleptic threshold in beer (Titica et al., 2001). A three-factor 2-level full factorial experimental design has been performed (Titica, 2000). The three factors were the main three operating variables: temperature ($T \in 10\text{-}18^{\circ}C$), pressure (50-800 mbar gage), and yeast inoculum concentration (0.5-2.0 cell/mL). From this information, kinetic models to account for the evolution of the biomass, sugars, CO_2 and the six selected aroma compound concentrations were derived. These models were used in this investigation to optimise the fermentation process.

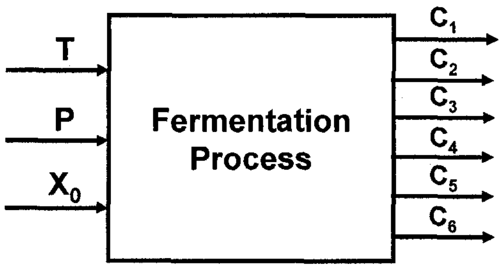

Fig. 1 3-input 6-output optimization model

In terms of optimisation, the fermentation process can be schematically represented by Figure 1. Given a set of input variables, the concentration of the six selected beer flavour products can be predicted. It is desired to have all of these products as close as possible to their defined targets. The target values for each compound, as determined by a group of experts, are given in Table 1. It is therefore desired to minimize the difference between the predicted values and target values for the first five compounds and to ensure that the concentration of the last compound is less than 0.2 mg/L. These requirements represent the six individual competing objective functions and will be referred as C_1 to C_6.

Table 1: Concentration target for each product

Criteria	Compound	Target [mg/L]
C_1	Isoamyl alcohol	93.8
C_2	Phenyl alcohol	31.6
C_3	Ethyl acetate	23.9
C_4	Isoamyl acetate	2.04
C_5	Ethyl hexanoate	0.25
C_6	Diacetyl	< 0.2

3. Optimization Method Used for Beer Aroma Production

In this investigation, a multicriteria optimisation method, known as Rough Set Method (RSM), is used to determine the optimal operating region of the beer fermentation process. A flow chart of the typical procedure for the multicriteria optimisation of a process is presented in Figure 2. After obtaining a proper model of the process, the optimisation method boils down to: (1) circumscribing the Pareto domain approximated by a sufficiently large number of non-dominated solutions, and (2) ranking the entire Pareto domain by order of preferences. The Pareto domain (PD) represents the collection of solutions taken from the total solution set that are not dominated by any other solution within this set. In this respect, a point is said to be dominated by another point if the values of all optimisation criteria (six in this investigation) are worse than those of the second point (Thibault et al., 2002b). A genetic algorithm is often used to obtain the desired number of non-dominated points in order to adequately represent the entire Pareto domain (Halsall-Whitney and Thibault, 2006; Viennet et al., 1996). This first step is common to the majority of multicriteria optimisation techniques and is performed in absence of any biased preference of an expert or decision maker. It is only required to know if a given criterion should be minimized, maximized or as close as possible to a target value.

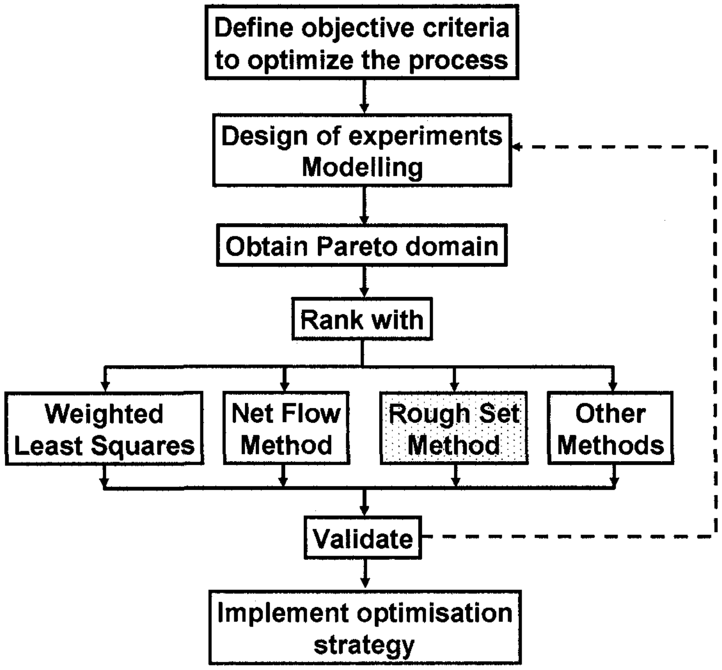

Fig. 2 Flow chart of multicriteria optimisation

The second step consists of ranking the entire Pareto in order of preferences based on the conscious, and sometimes unconscious, knowledge that an expert has on his/her process. There exist many multicriteria optimisation methods such as Rough Set method (RSM), Net Flow method (NFM), Least Square method. In this study, the method of interest is RSM.

The Rough Set method is able to transform the preferences of a human expert, who ranks a small set of possible solutions extracted from different regions of the PD, to a simple set of rules for ranking the entire domain (Yanofsky et al., 2005). In the traditional RSM, the set of selected points are presented to the expert all at once (batch). Thibault et al. (2002b) used the traditional RSM to classify the PD for the optimisation of a thermomechanical pulping process. They presented the expert, who had a profound knowledge of the process, with seven points all at once, taken randomly from different regions of PD. This set was then ranked by the expert from the most preferred to the least preferred points. From this classified ranked set, rules were established and these rules were used to rank all the members of the PD.

In RSM, rules are established based on the expert's ranked set and the range of indifference for each criterion which is defined as the difference between two values of that criterion that is not considered significant enough to rank one value as preferred over the other; these are also established by the expert. To obtain a rule, each point is compared to every other point within that set in order to define "rules of preference" (P) and "rules of non preference" (NP). A rule is represented in the form of a binary set of values (i.e. 0 or 1), one for each criterion. A value of 1 indicates that the first point is better than the second point, while a value of 0 indicates that the first point is equal, worse than, or not significantly different than the second point with respect to a particular criterion (Thibault et al., 2002b).

Once all possible rules from the expert's ranked set have been established, some rules need to be eliminated. This elimination is necessary for two reasons. First, if two preference or non preference rules are identical, only one copy of the rule is retained. Second, if a preference rule is identical to a non-preference rule, they are both eliminated since the expert cannot rank one point better than another point for the same reason that he considers a point worse than another point.

One perceived problem with the RSM is the selection of the small random set of points that are presented to the expert. These points must be discriminative enough to allow the generation of a representative set of rules (Renaud et al., 2005). This cannot be guaranteed since the points are selected randomly and it is very much possible that there is not enough distance between some of the criteria of these points to allow the generation of different and efficient number of rules, i.e. a set that one could use to reliably order the entire Pareto domain.

The method that is suggested and implemented in this paper for selection of points that were presented to the expert, to optimise the beer quality, seems to have effectively resolved the problem involved with the RSM. In this method, instead of presenting a subset of points from the PD to the expert all at once, the points were presented two at a time. Since two points can only be associated to two rules, one preference and one non preference, the rules are automatically generated after the points are ranked by the expert. Then, another pair of points is selected in a way to generate a different pair of rules, thus overcoming the duplication and elimination of rules. This process is continued until the desired number of rules or all possible rules are generated. If only a fraction of all possible rules is desired, the selection process would start with the most frequently encountered rule and progress towards the least frequent rules contained in the PD. It is important that all criteria of the selected pairs of points be sufficiently spaced to allow proper discrimination between the two points. In this investigation, the pair of points was selected in such a way that the value of one criterion for one point was as close as possible to one quarter of the total range of the criterion and the value of the other point was as close as possible to three quarter of the total range. The pair of points that best met this requirement for each set of two rules was selected.

In this investigation, we did not have readily access to an expert. It was therefore decided to use the Net Flow Method as the expert such that the ranking obtained with NFM was used as the expert's ranking. The NFM is a fairly robust multicriteria optimisation technique that uses the relative weighting of each criterion along with three thresholds for each criterion (indifference, preference and veto) to rank the entire PD. The reader is referred to Thibault et al. (2002a) for more details on the NFM.

4. Results

The Pareto domain for the six-criterion beer fermentation process was approximated with 5000 Pareto-optimal solutions. The existence of multiple Pareto-optimal solutions only occurs when the objectives are conflicting to each other. Otherwise a unique solution is obtained. The PD only contains non-dominated solutions, i.e. in a pairwise comparison there is at least one criterion for each point in the PD that is better than one of the criteria for all the other points. When several criteria are considered simultaneously there is no unique optimal solution but a set of mathematically equivalent Pareto-optimal solutions. According to Pareto, a solution is optimal if no criterion can be improved without impairing some other criterion. This reduced search space was then ranked using the RSM.

The PD for the six criteria is graphically represented by projecting the six-dimensional criterion space onto three two-dimensional spaces as shown in Figures 3 to 5. On each plot, the black points correspond to the best 10%, the dark grey area represents the subsequent 40% and the light grey area shows the last 50% of the ranked PD. The intended target for each criterion is shown as a horizontal or vertical line on each plot.

As clearly shown in Figures 3 to 5, the solutions circumscribed by the best 10% satisfy very well five out of the six criteria. The only criterion that has a ranking pattern that is contrary to the desired one is C_1 where the optimal zone is the farthest from the desired target value. It is important to remember that all these criteria are competing and it is not possible to satisfy all criteria simultaneously. The optimisation procedure has undoubtedly compromised the quality of the C_1 solution to obtain relatively good solutions for all the other criteria. The trade-off that must inevitably exist between some criteria is very well illustrated in Figure 4 where the criterion C_4 is plotted as a function of C_3. An increase in C_3 must also be accompanied by an increase in C_4 to remain in the optimal region and vice-versa. This highlights the advantage of using a multicriteria optimisation technique that uses the entire PD because it provides valuable information on the interrelationship that exists between the various criteria, in contrast with traditional optimisation where a unique solution is obtained.

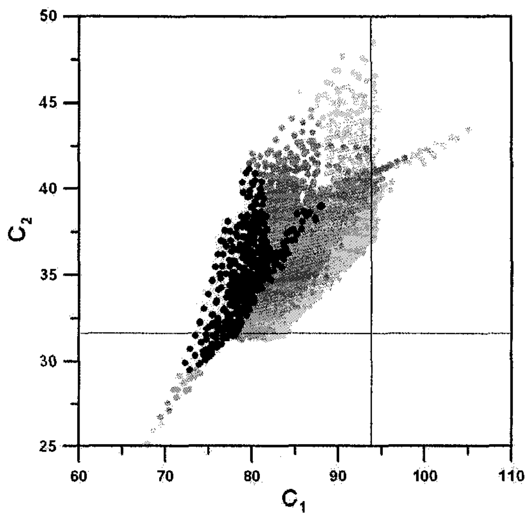

Fig. 3 Rough Set Method C_2 vs. C_1

Figure 5 shows clearly that the best 10% for criterion C_5 is located the closest to the target value. However, no solutions within the domain of exploration were able to satisfy the target. The target was established by experts through tasting trials but, assuming that the model predictions are accurate, the target value for C_5 cannot be obtained with the current range of experimental operating conditions. For criterion C_6, it is necessary for the concentration of diacetyl to be lower than 0.2 which was achieved for all points in the Pareto domain. In the current investigation, this criterion was however minimized, i.e. a value of C_5 closest to 0.

It is believed that the RSM has successfully identified the zone corresponding to the best 10% of all solutions in the PD. It is now important to examine the operating condition space that has given rise to the ranked PD. Figures 6 and 7 present the operating conditions corresponding to the PD using the same colour coding used in Figures 3 to 5. The operating conditions corresponding to the optimal region (best 10%) are in the following ranges: T∈[12-16°C], P∈[60-310 mbarg] and X_0∈[0.5-0.75 cell/mL]. To achieve the best 10% of all Pareto-optimal solutions, low pressure and low initial inoculum, compared to the initial range of operation, should be used whereas the temperature spans over a larger range of operation.

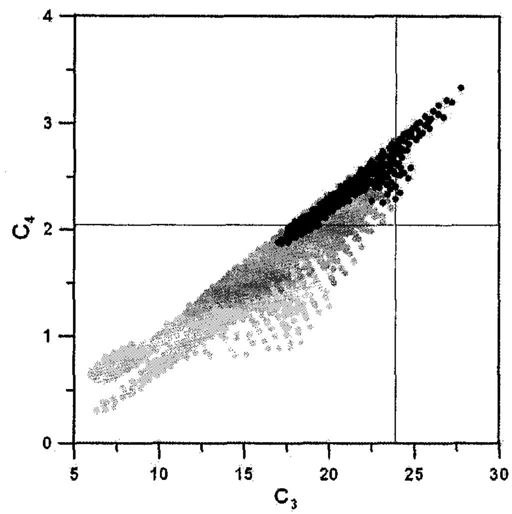

Fig. 4 Rough Set Method C_4 vs. C_3

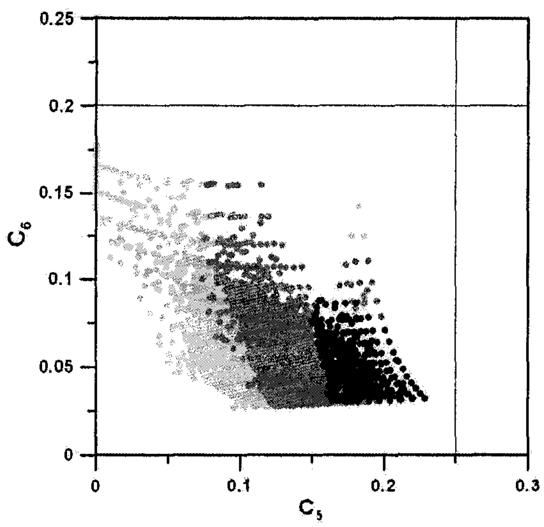

Fig. 5 Rough Set Method C_6 vs. C_5

Table 2 shows the operating conditions and the solution that ranked first amongst all Pareto-optimal solutions using the RSM. The results, obtained with the NFM and the weighted Least Squares method (LSQ), are also presented for the purpose of comparison. Each criterion closer to the target is identified in bold characters. For the LSQ, the solutions in the PD were ranked according the following global objective function:

$$J_{LSQ} = \frac{1}{6}\sum_{n=1}^{6}\left(\frac{\delta_n}{\delta_{n,max} - \delta_{n,min}}\right)^2 \tag{1}$$

$$\text{with } \delta_n = \left|C_n - C_{n,\ target}\right|$$

In the LSQ, equal weights were used for all criteria. Comparing the criteria of the optimal points (presented in Table 2) obtained by the three methods, for the first five criteria the RSM optimum was closest to the desired target for three criteria, whereas the optimum obtained by the NFM was closest to the target values for two criteria and the one by LSQ for none. All methods obviously satisfied criterion C_6 and identified a relatively low value.

In this investigation, the Net Flow method played the role of the expert to rank each selected pair of points. The preference and non preference sets of rules were determined from the small ranked set. The two methods rank the entire Pareto domain using the information from an expert or decision maker. In the NFM, the information is in the form of a sensitivity of the differences of each criterion to the target values whereas for RSM, the information is indirectly obtained by forcing the expert to make a choice between solutions taken from the PD. It is therefore interesting to see how well the RSM was able to capture the information portrayed by the NFM. Figure 8 presents the parity plot of the

Rough Set ranking as a function of the NFM ranking, from 1 to 5000 corresponding to best to worst PD points (respectively) for both methods. It is clear that the best 10% is more or less the same as the best solutions are gathered in the lower left-hand corner of the plot. The correlation coefficient between the rankings of the two methods is 0.925 even though it is much lower for the best 10%. For comparison, the correlation coefficient between the RSM and LSQ is 0.895. The LSQ becomes identical to NFM when the three thresholds are equal to zero.

The RSM strongly relies on the ability of the method to select representative solutions that are presented to the expert to decide which of the two points is better. In previous investigations, a small set of points were presented in batch to the expert and then the rules were established (Thibault et al., 2002b) with the risk of obtaining duplicate rules, not accounting for some rules and finding rules in both the preference and non preference sets. The method proposed in this investigation, for selecting points presented to the decision maker, prevented the presence of duplicate rules as a pair of points was chosen in order that each time two new rules were generated. For a system with six criteria, there exists a maximum of 62 distinct rules, i.e. 2^6-2. The minus two accounts for rules (000000) and (111111) that cannot be part of the PD because of the domination constraint. Each time a pair of points is chosen, two complementary binary rules are generated (Ex.: 110011 and 001100). In the current PD, all 62 rules were present such that it was necessary to select 31 pairs of points in the PD to generate all possible rules. Naturally, some rules were more frequent than others. The most frequent set of rules was {(011110);(100001)} with 21% occurrence, whereas the least frequent set was

{(111101);(000010)} with 0.0032%. Some of the rules along with their frequency of occurrences (FO) are presented in Table 3. The rules in Table 3 are ordered from most to least frequent for both the preference and non preference sets. The 31 pairs of rules were used to rank all points of the PD as shown in previous Figures 3 to 5.

Table 2: Optimal point for each method

	LSQ	NFM	RSM
T (°C)	15.3	14.87	13.37
P (mbarg)	284	425	50
X (10^7 cell/mL)	0.5	0.5	0.5
C_1	84.0	**88.18**	73.42
C_2	37.4	37.81	**31.49**
C_3	20.0	15.93	**22.55**
C_4	2.33	**1.795**	2.624
C_5	0.181	0.1523	**0.2069**
C_6	**0.0357**	**0.0377**	**0.05816**

To present 31 pairs of points to the decision maker to account for all possible rules is undoubtedly excessive as it represents a large human effort. In batch mode if 7 points are presented to the expert, a total of 21 point-to-point comparisons must be made simultaneously, which may be overwhelming for the expert. However, it is believed that selecting a reduced number of pairs of points representing the most frequent rules could be sufficient to provide an equivalent ranking of the PD. In the present optimisation

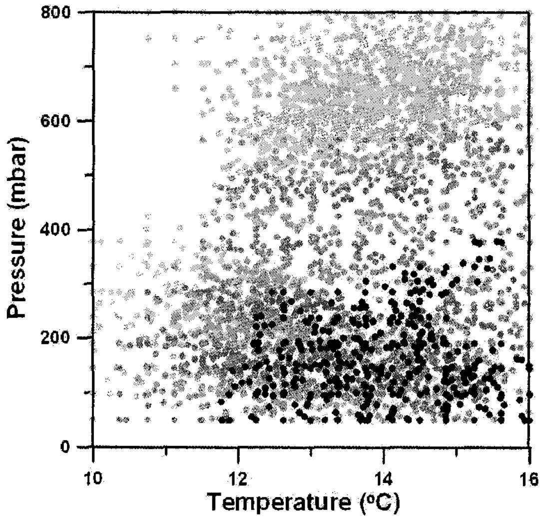

Fig. 6 Rough set Method P vs. T

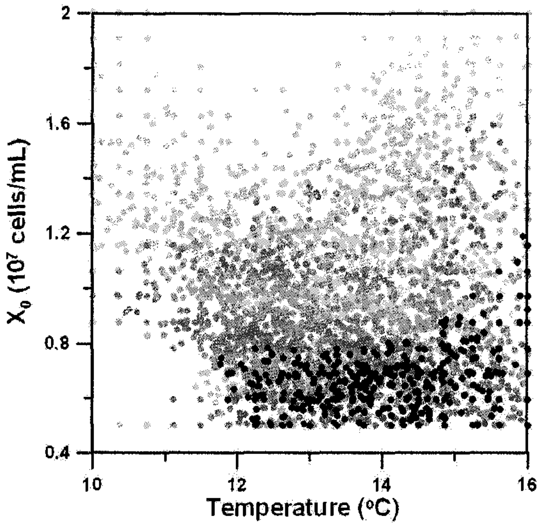

Fig. 7 Rough Set Method X_0 vs. T

problem, if five pairs of points are chosen to represent the ten most frequent rules, 92% of all pairwise comparisons within the PD would be accounted for. This percentage increases to 97% if 10 pairs of points are presented to the expert. The last 30 rules (last 15 complementary pairs) account for only 3% of the total number of occurrences. To test this hypothesis, the ranking of the PD was performed from a reduced number of rules and

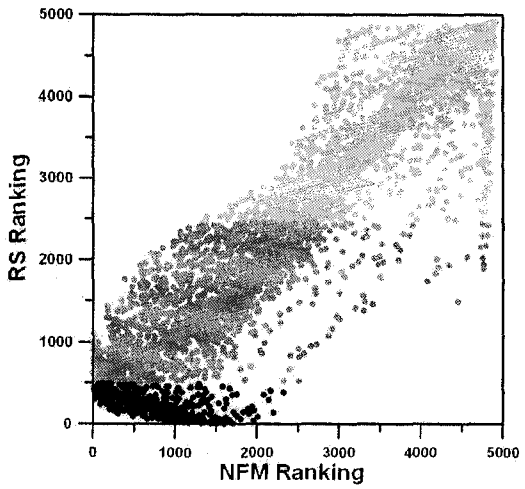

Fig. 8 Ranking comparison between NMF and RSM (from 1 to 5000, corresponding to the best to worst PD points, for both methods)

the results are presented in Figure 9. The ranking with a reduced number of rules is compared in terms of the regression coefficient (R^2) with the NFM ranking and the ranking using all 31 sets of rules. It is obvious that in the present case, using approximately 10 sets of rules leads to an equivalent results than for the 31 sets of rules, and a result, the experts has to examine a much lower number of points for an identical final result.

Another important aspect of the present optimisation problem is the uncertainty whether or not the experts would be able to assess the quality of beer based on the values predicted by the model since they usually assess the quality of beer through actual testing. The expert needs to associate a given aroma concentration with an actual tasting of beer, which may represent a significant challenge. It is believed that if the model is good, using a robust multicriteria optimisation method will lead to acceptable results. It is required to finally perform a validation experiment at the optimal operating conditions where the experts would actually test the final product.

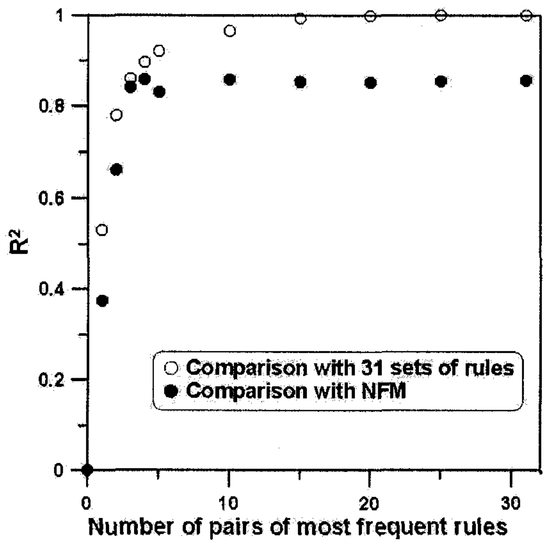

Fig. 9 Performance of RSM using a reduced number of rules from most to least frequent rules.

Table 3: P and NP rules with frequency of occurrences (FO)

	C_1	C_2	C_3	C_4	C_5	C_6	FO (%)
P Rules	0	1	1	1	1	0	10.5
	0	0	1	1	1	1	9.21
	…	…	…	…	…	…	…
	1	1	1	0	1	0	0.0021
	1	1	1	1	0	1	0.0016
NP Rules	1	0	0	0	0	1	10.4
	1	1	0	0	0	0	9.21
	…	…	…	…	…	…	…
	0	0	0	1	0	1	0.0021
	0	0	0	0	1	0	0.0016

5. Conclusion

This investigation has considered the use of the Rough Set method for selecting the operating conditions that would optimize the quality of beer. The RSM was able to clearly identify an operating zone for which the concentrations of the six most important metabolites, responsible for the organoleptic quality of beer, would be as close as possible to their estimated target values.

The RSM can be very useful for multicriteria optimisation to capture in a very natural way the conscious and, sometimes unconscious, knowledge that the expert has on his/her process. This knowledge is not always efficiently captured by traditional optimisation methods.

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Chapter 4

Conclusion

This research focused on a particular multicriteria optimisation technique, the Rough Set method. The modification of the traditional Rough Set towards development of a new and more reliable technique that provides the user with a better optimum solution for optimisation processes was the main concern of this work.

In Paper 1, Selection of Pareto-Optimal Solutions for Process Optimisation Using Rough Set Method: A New Approach, two new Rough Set methods with new approaches for selection of subset of points from the PD, that are presented to the expert for ranking are suggested. These approaches are different than the traditional RSM approach. The robustness of the new RSMs was studied using three case studies. The Pareto domains for these optimisation processes were obtained using a uniform grid method for the first and third case studies and a diploid genetic algorithm for the second case study. In this comparison process where the results obtained by the three Rough Set methods (Traditional Batch, By pair and Modified Batch) were compared to the results obtained by Net Flow method, it was found that the RSM: By Pair is far superior and more robust compared to both RSM: Batch and RSM: Modified Batch. This method was used in the subsequent paper to optimize the multicriteria problem of beer quality.

In paper 2, Multicriteria Optimisation of Beer Quality Using the Rough Set Method, the optimistaion strategy, Rough Set: By Pair, suggested in Paper 1, was used to determine the optimal operating conditions for the beers organoleptic profile, which resulted in a better compromise (closest to the target values) between the conflicting objectives when compared to results obtained by Least Squares and Net Flow methods. The RSM: By Pair was able to clearly identify an operating zone for which the concentrations of the six most important metabolites, responsible for the organoleptic quality of beer, would be as close as possible to their estimated target values.