

Optimization and Decision Making in Chemical Engineering Problems

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Abstract-The applications of Multiple Criteria Decision Making (MCDM) in dealing with the chemical engineering optimization problems are rapidly increasing. It has been inspired by increased computational resources and the effectiveness of the methods for solving the Multiple Objective Optimizations (MOO). Meanwhile the number of objectives in MOO of chemical applications, due to the inclusion of the new economical and environmental objectives to the processes, is increasing. As a result, the most recent utilized MOO methods cannot effectively deal with this expansion. However it is important that when selecting a method, the pros and cons set by the method are understood. Otherwise, the optimal results may not deliver the true impression about the problem. In this situation this paper aims to widen the awareness of the readers of the existence of interactive methods, in particular the NIMBUS method, which are capable of handling MOO problems with more than two objectives. For this reason some encouraging experiences and advantages of the NIMBUS method in recent chemical engineering applications are briefly reviewed following a brief introduction to the whole subject.

Keywords- Interactive Methods, Optimization, Decision-Making Chemical Engineering

I. INTRODUCTION

Optimization, in general, is the process of obtaining the value of decision variables, which provides the optimal of requested objectives. Optimization tools in chemical applications now exists more than the past especially, with the ever changing economic, energy and environmental situations which leads to the better design of chemical systems.

Optimization has wide applications in chemical and its related industries, e.g., mineral processing, petroleum, oil and gas refinery, pharmaceuticals. The study of the chemical engineering applications of optimization in literature, for instance (Tawarmalani and Sahinidis, 2002; Diwekar, 2003; Reklaitis et al., 2006), shows that optimization of the chemical processes has been an interesting field of study for many decades. Moreover up until the 1980s the problems in chemical engineering were optimized utilizing just the single-objective functions. However, real life chemical engineering problems require the simultaneous optimization of several objectives which cannot be solved by single-objective functions. Practical applications of chemical engineering can include many objectives such as cost, profit, selectivity, quality, recovery, conversion, energy required, efficiency, safety, hazard analysis, control performance, environmental quality, economic efficiency, complexity, speed, robustness, etc.

The MOO refers to the simultaneous optimization of multiple, often conflicting objectives, which produces a set

of alternative solutions called the Pareto-optimal solutions (Deb, 2001). Many methods are available for solving the MOO problems but the main attention of optimization of chemical processes so far has been single-objective optimization or handling multiple objectives by combining them suitably into one objective. The MOO problems in chemical engineering presented by Seinfeld and MacBride (1970), Shieh and Fan (1980), Umeda et al., (1980) and Grossmann et al., 1982 have been solved by single-objective optimization. Yet, according to (Chankong and Haimes, 1983; Haimes, 1977) by combining the multiple objectives in a single objective function, some optimal solutions might be lost.

Problems containing multiple conflicting objectives are known as multiple criteria decision making (MCDM) problems. In the MCDM, solving the related MOO problem assists the Decision Maker (DM) in finding the right Pareto-optimal solution (Miettinen, 1999). Additionally the solution process needs some involvement of the DM by providing some preferences. Several techniques are available to generate the Pareto-optimal solutions. Extensive researches on the algorithms used for the generating of Pareto-optimal solutions are described in several books and articles (Zeleny, 1982; Cohon, 1978; Steuer, 1986; Clark and Westerberg, 1983, Srinivas and Deb, 1995).

MOO has attracted the researchers in chemical engineering, particularly in the past decade and has received wide attention in the literature and additionally according to Rangaiah (2009) the effectiveness of MOO in chemical engineering problems is increasing by applying the new effective methods.

In the complex chemical processes, finding the optimum operating points of the multiple conflicting objectives given the various economical and environmental constraints is very important for the profitability of chemical plants. For this reason, MOO has been applied to many chemical process optimization problems. In this regard the motivation for this paper is to show that a variety of methods and approaches exists. In this way, people solving different problems are able to use the most appropriate approaches in the given situation. The new generation of chemical engineering problems requires better methods which can handle more than two objectives utilizing the minimum computation efforts.

A. Classification the MOO Methods

Your Examples of surveys of MOO methods are available in Chankong and Haimes (1983), Marler and Arora (2004), Miettinen (1999), Sawaragi et al. (1985), Steuer (1986) and Vincke (1992). However the dimension of existing MOO methods still remains a major challenge because of the conflicting nature of the multiple objectives. On the other hand it is very important that at the time of the selecting a method its pros and cons are understood. Otherwise, the

optimal results may not deliver the true impression about the problem. In this regard studying the methods would help to give an overview of the existing approaches to chemical process engineers Rangaiah (2009).

The available methods for MOO can be classified in different ways. One way is based on whether the Pareto-optimal solutions are generated or not, and the further role of the DM in solving the MOO problem. This particular classification has been applied by Diwekar (2003), Hwang and Masud (1979), Miettinen (1999), and Rangaiah (2009). Based on this classification method the MOO methods are divided into two main groups: *Generating* methods and *Preference-based* methods. The *Generating* methods generate one or more Pareto-optimal solutions without any inputs from the DM. On the other hand, preference-based methods use the preferences provided by the DM in solving the MOO problem. Figure 1 shows the classification of the MOO methods.

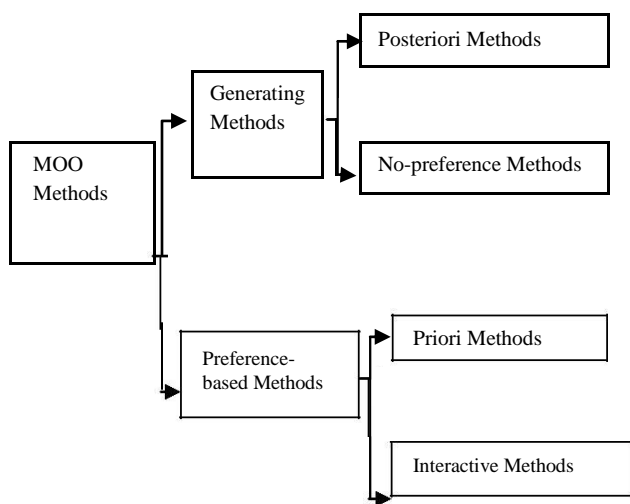


Figure 1. The classification of the MOO methods.

The group of Generating methods is also divided into two groups of No-preference methods and Posteriori methods. If there is no DM involved but the preference information available, it is possible to use No-preference methods which find some neutral compromise solution without any additional preference information. On the other hand in the Posteriori methods, a representative set of Pareto-optimal solutions is generated and then the DM must select the preferred one. In this way, the DM gets an overview of the problem over the visualization on a two-dimension plane involving two objectives. Furthermore, generating the set of Pareto-optimal solutions may be computationally expensive. Evolutionary MOO (EMO) algorithms and GA-based methods belong to this class.

The preference-based methods are also divided into two main groups of the Priori methods and the Interactive methods. In the Priori methods, the DM first gives preference information and then the method looks for a Pareto optimal solution satisfying the objectives.

There are lots of interactive methods available but they are not still widely known among people solving real applications. In interactive approaches, a solution pattern is created and the DM can specify the preference of each

interaction. The main specification of this method is its ability to deal with more than three objectives.

From the existed interactive methods, using the interactive approach of NIMBUS (Miettinen, 1999; Miettinen and Makela, 2006) is suggested where the role of a DM is well emphasized and the method is able to satisfy more than two objectives by utilizing minimum computational efforts for the real-life chemical engineering applications which involve more than three objectives.

However, a general MOO method suitable to all type problems does not yet exist, and the results from current methodologies can vary significantly in terms of the achieved Pareto-optimal solutions. For this reason, many standard benchmark test cases such as (Deb, 2001; Kursawe, 1990; Poloni et al., 2000; Silva and Biscaia, 2003; Viennet et al., 1996) have been developed to allow researchers to compare their techniques to others.

II. REVIEW

According to the knowledge of the author of this paper there have been five reviews of the MOO made so far in the area of chemical engineering, including applications in process design and operation, biotechnology and food industry, petroleum refining and petrochemicals, pharmaceuticals polymerization. Bhaskar et al. (2000) presented the background of MOO, different methods and their applications until the year 2000 by reviewing the 30 journal publications covering most of areas in chemical engineering. MOO applications in polymerization are included in the

review of genetic algorithm (GA) applications in polymer science and engineering by Kasat et al. (2003). Applications of GA-based MOO optimization in chemical reaction engineering were reviewed by Nandasana et al. (2003). In addition nearly a hundred applications in chemical engineering were studied by researchers and reported in more than 200 journal publications so far which have been thoroughly reviewed by Masuduzzaman and Rangaiah (2008) and Rangaiah (2009).

According to Rangaiah(2009) on average, about 15 new applications of MOO in chemical engineering have been reported every year since 2000. These applications are from several industrial sectors and areas of interest to chemical engineers. Many of them were modeled using first principle models and employed two, to maximum, three objectives. Moreover most of the studies in chemical engineering focused on finding Pareto-optimal solutions and only a few studies considered ranking and selecting one or a few Pareto-optimal solutions for implementation. However more emphasis and studies on ranking and selection from among the Pareto-optimal solutions are expected in the future.

The above mentioned excellent reviews indicate that optimal design of chemical processes e.g., selectivity, productivity and simple profit are mostly used alone in a single-objective for optimization. On the other hand environmental objectives as well as advanced economical objectives are gaining importance due to the increasing emphasis on environmental protection and sustainability, for more proof see chapter two of Rangaiah(2009). As the result of this fact, in the future we are expecting to face more objectives as well as complicated plants, dynamic optimization, and more uncertain parameters.

The above reviews show EMO approaches (which belong to posteriori approaches), in particular GAs, have been most popular for solving the chemical engineering applications mostly in two-objective optimization problems. EMO-based methods have been applied for more than 60% of the reviewed cases. Apart from the above reviews the recently solved chemical engineering problems, for instance Rajesh et al., 2001; Roosen et al., 2003; Subramani et al., 2003; Tarafder et al., 2005; Zhang et al., 2002 which are not included into the five mentioned reviews, also indicate that EMO methods have become very popular, but still only two or maximum three objectives have been considered due to the limitations of EMO approaches to visualize multiple objectives.

By the increasing number of MOO problems in chemical engineering, interactive methods could be utilized as the alternatives to EMO. Moreover the interactive methods complement evolutionary approaches. More details about the relationship of the MCDM and EMO fields are available in Branke et al. (2008).

III. INTRODUCTION TO INTERACTIVE METHOD

Interactive MOO methods have significant advantages over the methods mentioned above. For instance they overcome weaknesses of the Priori and Posteriori methods as the process avoids setting cognitive overload on the DM, which the comparison of many solutions typically implies. This causes the minimization of computational costs, which is a significant advantage. However, they have been used very rarely in chemical engineering applications which are briefly mentioned in surveys of Andersson (2000) and Bhaskar et al. (2000), and Rangaiah (2009). As Rangaiah (2009) mentions this might be because of the lack of the knowledge about the available methods or the lack of suitable packages. Also a few examples of interactive MOO methods and their applications in chemical engineering are available in Grauer et al. (1984) and, Umeda and Kuriyama (1980).

The statements of interactive methods have been presented in Miettinen (1999); Stewart (1992); Vanderpooten and Vincke (1989); Haimes et al. (1990). In this kind of MOO method, a solution pattern is created and the DM specifies preference information progressively during the solution process. In other words, the solution process is iterative and the phases of preference elicitation and solution generation alternate. In brief, the main steps of a general interactive method according to Miettinen (1999) are the following: (1) initialization, (2) generate Pareto-optimal solutions, (3) ask for preference information from the DM, (4) generate new Pareto-optimal solution according to the preferences (5) If several solutions were generated, ask the DM to select the best solution (6) stop, or if the DM wants to do otherwise, go to step (3). In each interaction some information about the problem or solutions available are collected by DM and then it is supposed to answer some questions in order to provide adequate information. New solutions are generated based on the information specified. In this way, the DM directs the solution process towards such Pareto-optimal solutions that DM is interested in and only those solutions are generated.

The advantage of interactive methods is that the DM can qualify the preferences during the solution process which is a very important state of interactive methods. Actually, finding the final solution is not always the only task but it is

also notable that the DM gets to know the problem with its all conditions.

According to the reviewed applications, the interactive MOO methods have been shown to be well-suited for chemical process design problems because it takes the preferences of the DM into account that enables a focused search for the better Pareto-optimal solution, which is the best compromise between the conflicting objectives. For this reason, only those solutions that are of interest to the DM are generated which deliver computational efficiency to the workflow.

Many interactive methods exist e.g., reference point approaches, classification-based methods, satisfying trade-off method, interactive surrogate worth trade-off and the NIMBUS method. However none of them is preferable to the others but some methods may suit some particular types of applications better than others. Methods may differ from each other according to the style of included interactions and the technical matters, the given quality of information to the DM, the specified form of preference information by the DM, the condition of the scalarizing function and generally the Pareto-optimal solutions which are used (Miettinen, 1999).

IV. NIMBUS METHOD

The NIMBUS method of the MOO is available on the WWW-NIMBUS system (Miettinen and Makela, 2000, 2006) and has been operating via the internet at <http://nimbus.it.jyu.fi> since 1995. It can be used free of charge for teaching and academic purposes, just by applying a browser. All the computation is carried out on the server computer at the University of Jyväskylä.

Several variants of NIMBUS method exists. But here it is concentrated on the latest online available version, the synchronous version, (Miettinen and Makela, 2006), where several scalarizing functions can be used based on a classification once expressed.

After creating an account it would be possible to save the defined problem as well as the resulted solutions on the system. The WWW-NIMBUS takes the user from one web page to another. The modeled problem can be initialized by filling in a web form. It first asks for the name and the dimensions of the problem. On the second web page, the user can type in the formulas of each objective and constraint function as well as the variables. Later on the interactive nature of NIMBUS method solution process naturally tries to set its own essential condition. The system also has a useful tutorial that guides the user through the different phases of the interactive solution process. In addition, each web page provides individual help as well.

As mentioned earlier by applying the NIMBUS, more than three objective functions can be easily considered only in the presence of more visualization efforts. As long as the comparison and evaluation of the solutions are concerned, the visualizations process is very important as the obtained solutions are presented to the DM via its capabilities. Therefore a good graphical interface tool is necessary in order to enable the interaction between the DM and the method. (Hakanen, 2006).

The modeled MOO problem is initially converted into a scalarized problem using the classified information. Then the solved problem attempts to satisfy the goals which are

defined in the classification. (Miettinen, 1999; Miettinen and Makela, 2006)

Once the DM has classified the objective functions, DM can decide how many Pareto-optimal solutions need to be compared. Then many scalarized problems are solved and the new solutions are shown to the DM. If the DM has found the most preferred solution, the solution process stops. Otherwise, the DM can select a solution as a starting point of a new classification. The DM frequently learns about the possible solutions available for the relevant problem. In other words the DM can learn much more about different solutions satisfying the objectives which best follows the preferences because they take the preference information into account in slightly different ways. (Miettinen and Makela, 2000)

Unlike some other classification based methods, the favorable outcome of the solution processes are not dependent completely on the DM in managing the classification and the appropriate parameter values but

partly on the process. This means the classification is a dynamic kind and the DM is free to explore the intermediate points.

V. NIMBUS FOR CHEMICAL ENGINEERING APPLICATIONS

The MOO package of NIMBUS can successfully be applied in chemical process design problems. The researches on the application of NIMBUS in chemical engineering problems such as encouraging experiences related to papermaking and sugar industries have been reported in Hakanen (2006), Hakanen et al. (2004, 2005, 2006, 2007 and 2008) and Rangaiah (2009). These successful cases are described and summarized in Table 1. These studies have focused on offering the chemical engineering community an efficient and practical way of handling all the necessary objectives of the problem. In this regard NIMBUS method has delivered the ability of considering several conflicting objectives that affect the behavior of the problem.

Table 1. Applications of NIMBUS in chemical engineering problems

No	Application	Objectives	Reference(s)
1	Heat recovery system design in a paper mill	Minimization of (1) steam needed in summer, (2) steam needed in winter, (3) area of heat exchangers and (4) cooling/heating needed for the effluent.	Hakanen et al. (2005 and 2006) Miettinen et al 2009
2	A co-generation plant to produce shaft power and steam	Minimization of energy loss and total cost while maximizing shaft power.	Hakanen et al. (2006)
3	Glucose-Fructose separation using Simulated Moving Bed and Varicol Processes	Four objectives: (1) maximization of throughput, (2) minimization of solvent consumption in desorbent stream, (3) maximizing product purity, and (4) maximizing recovery of valuable component in the product stream.	Hakanen et al. (2007)
4	Water Allocation Problem	Three objectives : the goal is to minimize the amount of fresh water taken into the process and also to minimize the amount of dissolved organic material in critical parts of the process by determining the right recycling of water	Hakanen et al. (2007), Miettinen et al (2009)
5	Simulated Moving Bed Processes	Four objectives: (1) functions represented throughput, (2) consumption of desorbent, (3) purity and (4) recovery	Miettinen et al (2009)

The solution of the *Simulated Moving Bed* design problem described in Hakanen *et al.* (2007) and Miettinen et al (2009), including four highly conflicting objective functions, is a novel approach. However, previously only two or maximum three objective functions could be considered (Subramani et al., 2002 Zhang, Z., 2003). This enabled full utilization of the properties of the problem without any unnecessary simplifications. In addition, the DM via NIMBUS gained more understanding of the considered objectives' interactions and therefore learned more about the problem.

The solution for the *Water Allocation* problem, as it is represented in Hakanen *et al.* (2007) and Miettinen et al (2009) is a MOO problem by nature. The other available approaches can produce only one solution at a time corresponding to the upper bounds set for the new inequality constraints. It is also difficult to set correct upper bounds to find the most desirable solution without knowing the

behavior of the problem and the roles of the objective functions and the constraints. In this condition according to the preferences of the DM and the study of the interrelationships of the different objective functions by utilizing the NIMBUS design tool, different solutions can be generated. The NIMBUS in Hakanen *et al.* (2007) and Miettinen et al (2009) first of all provided a better understanding of the interrelationships of the objective functions when compared to the previous solutions and secondly dealt with more objectives utilizing less computational resources.

In the other application, *heat recovery system design*, there are four objective functions involved. Solving it doesn't cause any troubles for an interactive method like NIMBUS. In a detailed description of the interactive solution process presented by Hakanen et al. (2005, 2006) a new insight into the problem obtained and a satisfactory solution found.

VI. CONCLUSION

The interactive methods, in particular NIMBUS, for reason of solving the MOO problems of the MCDM in chemical engineering applications have introduced and following it the advantages of applying the NIMBUS in such applications were discussed.

Interactive approaches in general allow the DM to learn about the problem considered and the interrelationships in it. As the result, deeper understanding of the phenomena in question is achieved. Because the DM can manage the search for the most preferred solution, only interesting solutions are generated which means savings in computation time which is a significant advantage. For taking the true nature of the problem into account specially by including the environmental and economical objectives into the process the interactive methods can easily be applied.

However, when the problem has more than two objectives, the visualization is no longer simple. In this situation the interactive approaches offer a viable alternative to solve the problem without artificial simplifications.

Because interactive methods rely heavily on the preference information specified by the DM, it is important to select such a user-friendly method, NIMBUS, where the style of specifying preferences is convenient for the DM. The presented applications have shown how interactive MOO can be utilized in chemical process design by demonstrating of their benefits. In all the cases, it was possible to solve the problems in their true multi-objective character and an efficient tool was created to support the DM in the decision making problem.

VII. REFERENCES

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