Optimization Techniques in Chemical Processes

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***Abstract*— In this paper, optimization techniques used in the chemical processes are explored. Chemical processes comprise of several multi-variable, non-linear and constrained blocks. The overall system performance depends on operating each block optimally. So every element has to be optimized in order to get an overall best possible outcome. This makes the choice of a good optimization algorithm very crucial. This survey includes the study of research done and implemented in the industry, perusing the variety of the optimization technique adopted, the details of the optimization algorithm, its advantages and shortcomings.**

***Index Terms*— Optimization, Chemical Processes.**

I. Introduction

THE chemical engineering has undergone significant changes during recent years due to the increased cost of energy, increasingly stringent environmental regulations, and global competition in product pricing and quality. One of the most important engineering tool addressing these issues is optimization. Modification in plant design and procedures have been implemented to reduce the cost and meet constraints. Various algorithms and methods have been developed to tackle the optimization problem that can be classified in three main categories: heuristics, mathematical programming and metaheuristic algorithms. euristics(of the classical kind) do not actually solve the optimization problem, but aim at finding good solutions by following a set of rules. In the chemical process design field, Douglas [1] and Siirola [2] have developed a method for hierarchical process synthesis that relies on sets of rules at different stages during process development. The computer-oriented implementation of such systems usually takes the form of an Expert System, as for example presented by Kirkwood $et.al.$ [3]. Such methods are good in finding quickly and reliably a good solution that can be used for example as starting point for more advanced metaheuristic algorithms. The mathematical programming methods (sometimes called exact methods) are optimization techniques aimed at solving the Linear, Nonlinear, Mixed Integer Non-Linear Problem (MINLP), constrained formulation of the design problem [4]. These techniques use usually algorithms derived from Branch and Bound or Outer Approximation, as discussed by [5]. A recent review of these methods has been published by [6].

The last category, the metaheuristic algorithms, are based on one (or several)initial solution(s) and a progressive (though not necessarily uniform) improvement of their quality. A popular example of metaheuristic is the genetic algorithm (GA) approach.

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The survey is focused on the use of mathematical and metaheuristic approaches used in the industry. The next section presents the mathematical programming followed by survey on metaheuristics.

II. Mathematical Programming

A. Integer Programming: Mixed Integer Programming (Linear and Nonlinear)

Many problems in plant operation, design, location and scheduling involve variables that are not continuous but instead have integer values. Decision variables for which the levels are dichotomy - to install or not install a new piece of equipment, for example termed “0 or 1” or binary variable. Other integer variables might be real numbers 0,1,2,3 and so on. Sometimes we can treat integer variables as if they were continuous, especially when the range of a variable contains a large number of integers, such as 100 trays in distillation column, and round the optimal solution to nearest integer value.

A problem only involving the integers is classified as *integer programming*(IP). The most general case is the *mixed integer programming* (MIP) problem, in which the objective function depends on two sets of variables x and y; x is a vector of continuous variables and y is a vector of integer variables. A special case of IP is *binary integer programming* where all the variables are either 0 or 1. Many MIP problems are linear in the objective function and constraints and hence are subject to solution by linear programming. These problems are called *mixed integer linear programming* problems. Problems involving discrete variables in which some of the functions are nonlinear are called *mixed integer nonlinear programming* problems. Some classical formulation of typical integer programming are:

- The knapsack problem
- The traveling salesman problem
- Blending problem
- Location of oil wells $etc.$

1) Boiler/Turbo-Generator System Optimization: Linear programming is often used in the design and operation of steam systems in the chemical industry. For instance the steam and power system for a small power house. The characteristics are mainly different flow rates of steam pressure in different valves. The system may be modeled as linear constraints and combined with a linear objective function. The objective is to minimize the operating cost of the system by choice of steam flow rates and power generated or purchased, subject to the demands and restrictions on the system.

2) Optimization of a Thermal Cracker via Linear Programming: Reactor systems that can be described by a “yield matrix” are potential candidates for the application of linear programing. In these situations, each reactant is known to produce a certain distribution of products. When multiple reactants are employed, it is desirable to optimize the amounts of each reactant so that the products satisfy flow demand constraints. Linear programming has become widely adopted in scheduling production in olefin units and catalytic crackers. The “yield matrix” is structured on various feeds and corresponding product distribution for a thermal cracker that produces olefins. The possible feeds include ethane, propane, debutanized natural gasoline and gas oil, some of which may be fed simultaneously [7].

3) Optimal Design of a Gas Transmission Network: A gas-gathering and transmission system consists of sources of gas, arcs composed of pipeline segments, compressor stations and delivery sites. The design or expansion of a gas pipeline transmission systems involves capital expenditures as well as the continuous operating cost of operation and maintenance. Many factors have to be considered. This include the optimum number, locations and initial construction dates of compressor stations. Different optimal dimensions of the compressors and pipes and optimal pressures.

The criterion for the design is the minimum total cost of operation including capital, operation and maintenance costs. This problem is solved using the MINLP technique in [8].

4) Optimal Design and Operation of Distillation Column: Distillation is probably the most widely used separation process in industry. Various classes of optimization problems for steady-state distillation are, in increasing order of complexity.

- Determine the optimal operating conditions for an existing column to achieve specific performance at minimum cost (or minimum energy usage) given the feed(s). Usually, the manipulated (independent) variables are indirect heat inputs, cooling steam inputs, and product flow rates. The number of degrees of freedom is most likely equal to the number of product streams. Specific performance is measured by specific components concentrations or fractional recoveries from the feed (specification leading to equality constraints) or minimum (or maximum) concentrations and recoveries (specification leading to inequality constraints). The optimization problem is a nonlinear programming problem often with implicit nested loops for calculation of physical properties. If the number of degrees of freedom is reduced to zero by specifications placed on the controlled variables, the optimization problem reduces to the classical problem of distillation design that requires just the solution of a set of nonlinear equations.
- A more complex problem is to determine not only the values of the operating conditions as outlined in the last case but also the minimum number of stages required for the separation. because the stages are discrete, the problem becomes nonlinear mixed integer programming problem. In this form of the design problem, the costs include both capital costs and operating costs. Capital costs increase with the number of stages and internal column flow rates, whereas operating cost decrease up to a certain point.
- An even more difficult problem is to determine the number of stages and the optimal locations for the feed(s) withdrawal. Fortunately, the range of candidates for the stage locations for feed and withdrawals is usually small, and from a practical viewpoint the objective function is usually not particularly sensitive to a specific location within the appropriate range.

Optimization of distillation columns using mathematical programming, as opposed to other methods, has been carried out using many techniques, including search methods such as Hooke and Jeeves [9], MINLP [10], GAs [11] and successive quadratic programming [12].

5) Robust MILP: In a recent paper Lin *et.al.* [13] presented a robust optimization methodology, which when applied to MILP problem produces “robust” solutions which are in a sense immune against bounded uncertainty. The robustness is considered for all the coefficients of the objective function, equalities and inequalities. By introducing a small number of auxiliary variables and constraints, a deterministic robust counterpart problem is formulated to determine the optimal solution given the relative magnitude of uncertain data, feasibility tolerance and reliability level when a probabilistic measurement is applied. For each inequality constraint that involves uncertain coefficients and/or right hand side parameters, an additional constraint is introduced to incorporate the uncertainty and maintain the relationships among the relevant binary and continuous variables under the uncertainty level and the given infeasibility tolerance.

B. Quadratic and Sequential Quadratic Programming

A quadratic programming (QP) problem is an optimization problem in which a quadratic objective function is minimized subject to linear inequality or equality constraints. A convex QP is the simplest form of a nonlinear programming problem with inequality constraints. A number of practical optimization problems, such as constrained least squares and optimal control of linear systems with quadratic cost functions and linear constraints, are naturally posed as QP problems.

Successive or sequential quadratic programming (SQP) methods solve a sequence of quadratic programming approximations to a nonlinear programming problem. The constraints are linearizations of the actual nonlinear constraints about the selected point. The objective is a quadratic approximation of the Lagrangian function of the original objective augmented with the weighted difference of violation of the constraints.

1) Optimization of Sulfolane Extraction Plant: The sulfolane extraction process is widely used in benzene-toulene-xylene (BTX) plants to separate aromatics from hydrotreated feedstocks. The optimization of the extraction plant is by far the most important aspect to improve the economics of the BTX plant. In [14], optimal operating conditions of the sulfolane plant were identified based on modeling and simulation of the actual plant. From the results of simulations based on rigorous plant models, parametric models for each plant unit were developed, which, in turn, were employed in the SQP method to optimize the operation of the extraction plant.

C. Gradient Descent Approach

The gradient descent approach is also used in the optimization of chemical process. This approach is based on minimizing a cost function that is some kind of a performance index for the system and a function of system parameters. The parameters are updated iteratively in the negative direction of the gradients of the performance index, such that the performance index is optimized.

1) Heat Transfer in Glass Forming Process: This paper [15] addresses a method for estimating a number of unknown heat transfer coefficients in solving the heat conduction problem of the glass forming process. These coefficients can be found if there are proper data measured from the process in the operation. A sum of normalized squared errors is used as the objective function that is a function of values depending upon the estimated coefficients and the measure values, subject to an equality constraint that is itself a function of the coefficients and measured values. This objective function is minimized if the coefficients represent the true or near true values of the system.

III. Metaheuristic Approaches

Recently, SA, GA and TS have been designated by the Committee of Next Decade of Operations Research as “extremely promising” for the future treatment of practical applications. The most recent papers show this clear trend in using the metaheuristic approaches for the optimization in chemical processes.

A. Simulated Annealing

Simulated Annealing (SA) developed by Kirkpatrick *et. al.* [16], is a general adaptive heuristic approach which belongs to the class of nondeterministic iterative algorithms [17]. SA is also a non-deterministic algorithm that accepts bad moves in the search space with certain probability. This feature enables SA to escape from local minima. The probability of accepting bad moves depends on a parameter named temperature, that is initialized to a high value, then gradually decreased with a rate specified by another parameter called cooling rate. The lower the temperature, the lesser is the probability of accepting bad moves. The algorithm starts with initial solution. A neighbor solution is generated in each iteration, if the cost of neighbor solution is better than the cost of the current solution then it is accepted, otherwise it is selected with some probability. This probability depends upon the temperature (T). Initially probability of selecting bad solution is high, that gradually decreases with some predetermined strategy. After considerable number of iterations, probability of selecting bad solution is very near to zero.

1) Applying SA to Separation Sequence Synthesis: Floquet $et.al.$ [18] applied SA to problems of separating a mixture of n components into pure products at minimal annual investment plus operating costs. The assumptions were:

- Each component of the feed stream exits in exactly one output stream of a separator. This is called $sharpseparation$.
- Only one input/two output (simple) or one input/three output (complex) sharp separators are used.

Under these assumptions, the problem is to select the separators to be connected and the way they will be connected. Floquet show how to encode the possible separation sequences as vectors containing the entries -1, 0, 1, which satisfy appropriate restrictions, and how to transform such vectors into neighboring sequences. For example, some transformations correspond to the insertion or deletion of a complex separator. Given this definition of a solution **x** and its neighborhood $N(\mathbf{x})$, and given fixed and operating costs for each type of separator that defines the objective function $f(\mathbf{x})$, the author applied simulated annealing to find the cheapest separation sequence. In solving problems with 5, 10 and 16 components with known optimal solutions, their SA algorithm found optimal solutions for all cases and less than 2% of the feasible sequences were evaluated when the best solution was found.

2) Simulated annealing for the optimization of batch distillation processes: Batch distillation processes are widely used in the chemical industry. The interest on the simulation and optimization of batch processes is growing since such processes have a number of advantages over continuous processes: they are useful for the simultaneous separation of different species with a single column, they are more flexible, and they are necessary for the production of very pure chemicals.

In [19], an investigation is done on the applicability and the limitations of the simulated annealing method for solving the optimal operation problems of batch distillation processes. Considering that the algorithm uses only the values of the cost functional, the simulation package that are now well developed for these industrial cases, can be used as a black box. In addition, the method converges towards a global minimum (in probability), though due to the stochastic nature of the method the speed of convergence can be very slow.

B. Genetic Algorithm

GA is an elegant search technique that emulates the process of natural evolution as a means of progressing towards the optimal solution. GA uses an encoded representation of solution in the form of a string made up of symbols called genes. The string of genes is called chromosome. The algorithm starts with a set of initial solutions called population that may be generated randomly or taken from the results of a constructive algorithm. Then, in each iteration (known as generation in GA terminology), all the individual chromosomes in the population are evaluated using a fitness function. Then, in the selection step, two of these chromosomes at a time are selected from the population and different operators namely crossover, mutation, and inversion act on the selected individuals for evolving new individuals called offsprings. One important genetic operator is crossover. It is applied on two individuals to generate an offspring. The generated offspring inherits some characteristics from both its parents in a way similar to natural evolution. There are different crossover operators namely simple, order, partially mapped, and cycle. The simple crossover operation for instance, works by choosing a random cut point in both parent chromosomes (the cut point should be the same in both parents) and generating the offspring by combining the segment of one parent to the left of the cut point with the segment of the other parent to the right of the cut [17]. (For description of other crossover operators see [17], [20], [21]). The Mutation operator is used to introduce new random information in the population. It is usually applied after the crossover operator. It helps in producing some variations in the solutions so that the search does not get trapped in local minima. An example of mutation operation is the swapping of two randomly selected genes of a chromosome. The importance of this operation is that it can introduce a desired characteristic in the solution that could not be introduced by the application of the crossover operator alone. However, mutation is applied with a low rate. The quality of the solution obtained from GA is dependent on the choice of certain parameters such as population size, crossover and mutation rates and also the type of crossover used. The selection of values for these parameters is problem specific and is left to the conception and intuition of the person applying GA to a specific problem.

1) Optimization of fed-batch bioreactors using genetic algorithm: multiple control variables: The usual objective in optimal control of a fed-batch bioreactor is to maximize the biomass and/or the metabolite production. The optimization has been traditionally sought with respect to substrate feed rate. Determination of optimal substrate feed rate is a problem in singular control since the control variable appears linearly both in the dynamic equations describing the process and/or in the performance index which is to be optimized. The optimization in this paper [22] is the maximization of the product quantity. Taking into account all the limits the chromosome appears to be in three parts. The pattern (feeding sequence), the coefficients for the correction term, and the switching times. Each part indicating the maximum feed, the singular feed by 2, and the minimum feed by 3. The constraints are handled by penalizing them in the objective function.

2) Optimization of shape and process parameters in metal forging using GAs: In this paper [23], an evolutionary GA is proposed to calculate the optimal work-piece shape geometry and work-piece temperature. The authors have optimized two objectives at a time that are the total energy of the system and the difference between the current and desired shape. These functionals are dependent on the parameters subject to upper and lower bounds alongwith the temperature constraint limiting current temperature not exceeding the maximum allowed. The ease of using the GA can be seen in the fact that all the parameters in this process are not similar quantities with similar units. The other governing equations are the heat content equation, and the pressure and velocities.

3) Use of genetic algorithms and gradient based optimization techniques for calcium phosphate precipitation: Phase equilibirium calculations constitute an important class of problems in chemical engineering applications. The calcium phosphate precipitation is dealt in [24]. Calcium phosphate precipitation involves many parameters: calcium and phosphate ion concentrations, supersaturation, ionic strength, temperature, ion types, pH and also time. The process studied in this paper is based on calcium phosphate solution with calcium ions and a base. During this precipitation, the aqueous species considered are different calcium and phosphate ions with corresponding calcium salts. The concentrations of calcium and phosphate ions are subject to mass balance constraints for calcium and phosphates. The function to be optimized is the minimization of Gibbs free energy of the system expressed as a linear combination of the chemical potential of each component. Formulation of GA is based on encoding the concentrations of calcium and phosphate ions in a binary string.

4) Environmentally Conscious Chemical Process Design: This paper presents a systematic and hierarchical approach for incorporating environmental considerations into all stages of chemical process design [25]. The complexity of the environmental and economic assessments increases as the design proceeds. Changing some continuous variables while keeping others constant can cause structural changes to the design. Examples of structural changes would be repositioning of a heat exchanger network or changing the size of some pieces of equipment. Structural optimization is performed manually in this study on those variables having substantial influences on the structure of the process. The next step is to set up a multiobjective function including economic and environmental indicators and perform optimization using the reduced set of key design variables. These key design variables are considered manipulated variables prior to the performance of parametric optimization. The objective function combines two different types of performance measures, an economic index, net present value (NPV), and an environmental index, process composite environmental index.

Genetic algorithm is used in this work to perform the optimization because it provides a flexible, relatively efficient, and effective method for handling the black-box, discontinuous, and nondifferentiable objective functions and can often find the global optimum.

C. Tabu Search

A third metaheuristic method is the Tabu Search (TS), developed by Glover [26]. Tabu search is an iterative heuristic that has been applied for solving a range of combinatorial optimization problems in different fields [17]. Tabu search starts from an initial feasible solution and carries out its search by making a sequence of random moves or perturbations. A Tabu list is maintained that stores the attributes of a number of previous moves. In each iteration, a subset of neighbor solutions is generated by making a certain number of moves and the best move is accepted, provided it is not in the Tabu list. Otherwise, if the said move is in the Tabu list, the best solution is checked against an aspiration criterion and if satisfied, the move is accepted. Thus, the aspiration criterion can override the Tabu list restrictions. It is desirable in certain conditions to accept a move even it is in the Tabu list, because it may take the search into a new region due to the effect of intermediate moves. The behavior of Tabu search heavily depends on the size of Tabu list as well as on the chosen aspiration criterion. The aspiration criterion determines the extent to which the Tabu list can restrict the possible moves. The detailed description of Tabu search can be found in [17][45]. In contrast with GA, TS uses single solution and tries to optimize it with iterations. The unique feature of TS is its memory element, that is used to record some characteristics of a certain number of previous moves. The number of moves whose characteristics can be recorded depends on the size of this list. This feature prevents the search process from cycling (i.e. revisiting a point) in the search space.

1) Multi-objective process design: To our knowledge TS has been used only twice in the field of batch process design. Wang, Quan, and Xu [27] used TS for the problem of the grassroot design of multiproduct batch processes. Cavin $et.al.$ [28] used TS with a multi objective process design in multi purpose batch plants.

For the latter one, the goal was to enable the use of external batch simulation programs (black-box optimization). Black-box models are exceedingly difficult to handle in conjunction with mathematical programming approaches, therefore making it attractive to employ a metaheuristic algorithm. Gross and Roosen (1998) have tackled a similar problem (continuous process design with a black-box external simulation package) and have chosen a genetic algorithm. However, GA approaches have encountered significant difficulties when confronted with problems that contain complex constraints, which are a pre-dominant feature in the problems faced. The limitation of GAs in these settings arises from the inability to implement crossover operations that generate valid designs. Recourse to penalty approaches and ad hoc repair operators as an attempted remedy entails a risk of spending most of the computational effort in handling invalid solutions, making GAs unsuitable for this application.

D. Other Metaheuristic Approaches

Recently Swarm Intelligence (SI) techniques, Particle Swarm optimization (PSO) and Ant Colony Optimization (ACO) techniques are gaining more importance. They are used to solve the combinatorial optimization problems, due to its simplicity in coding and consistency in performance. These techniques use swarm behavior to solve the problem, (i.e.) they use the concept of group intelligence along with individual intelligence. PSO technique is used to solve continuous combinatorial optimization problems [29], [30]. PSO is developed through simulation of bird flocking in two-dimensional space. The position of each agent is represented in XY plane with position (s_x, s_y), v_x (velocity along X-axis), and v_y (velocity along Y-axis). Modification of the agent position is realized by the position and velocity information.

Bird flocking optimizes a certain objective function. Each agent knows its best value so far, called Pbest, which contains the information on position and velocities. This information is the analogy of personal experience of each agent. Moreover, each agent knows the best value so far, in the group Gbest among Pbests. This information is the analogy of knowledge, how the other neighboring agents have performed. Each agent tries to modify its position by considering current positions (s_x, s_y), current velocities (v_x, v_y), the individual intelligence (Pbest), and the group intelligence (Gbest)[31].

Another evolutionary approach, path relinking, offers a greater capability for handling constraints. This approach is often coupled with TS and in fact emerged from the same origin as TS [28].

IV. MISCELLANEOUS TECHNIQUES

A. Combination of global and local search

A combination of direct global and local search optimization technique is presented in [32]. The authors have presented this method as a replacement to other meta-heuristic techniques like GA and TS for the case of expensive evaluation of the cost function.

The natural complex and apparently unsolvable problem is subdivided into smaller problems, which can be solved by already existing solution methods. This well-known principle of divide and conquer is also applicable to solve np-hard problem of global optimization, which can be sub-divided into two phases: pre- and fine optimization. The task of pre-optimization is to explore the search space in order to find regions comprising global optimum points. These regions are called promising regions. To keep the computational effort low, this task should be performed as roughly as possible. Outgoing from the results of the pre-optimization, the task of fine-optimization is to efficiently nd exactly localize the optimum point of a promising region.

B. SUPRA

In this paper [33], the authors have proposed a new query optimization method named SUPRA (sampling unit preservation method) which preserves he sampling unit during the optimization of the sampling operations. This method enables preservation of the sampling unit by adopting a special sampling operation in which all the records specified as included in the same sampling unit and he randomness of data extraction through is query optimization. When the cube-creating sampling queries are issued to the database, the query optimized module of the database system automatically identifies the sampling units of the queries and transforms them into equivalent ones in the application point of the sampling operations have been moved forward.

C. Optimization of Gas-Sensitive Polymer Arrays

A very simple technique for optimizing an array of conducting polymer gas sensors for sensing one of five analytes in the presence of up to four interferents is presented [34]. The optimized array consists of subarrays of homogeneous (like) sensors contributing to a larger heterogeneous array of up to ten points (unlike sensors) in multidimensional sensor space. The optimization techniques presented are linear, since the polymer sensors in their useful (low concentration) operating range exhibit linear and additive response characteristics.

Optimization is performed using a metric depending upon the average multidimensional distance from the cluster mean. Since the clusters are linearly separable, this technique is intuitive.

V. CONCLUSIONS

Optimization in chemical processes is a critical step to get the best results. The choice of optimization technique is equally crucial to best match the actual process and objective. A number of different optimization techniques adapted in the chemical engineering are discussed mainly focusing the mathematical and metaheuristic approaches. A strong bias towards the heuristic approaches is observed in the recent literature due to the fact that they are simple, unstraining the mathematical hassle.

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