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Multiobjective optimization of industrial petroleum processing units using Genetic algorithms

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Abstract

For many years most of refining processes were optimized using single objective approach, but practically such complex processes must be optimized with several objectives. Multiobjective optimization allows taking all of desired objectives directly and provide search of optimal solution with respect to all of them. Genetic algorithms proved themselves as a powerful and robust tool for multi-objective optimization. In this article, the review for a last decade of multi-objective optimization cases is provided. Most popular genetic algorithms and techniques are mentioned. From a practical point it is shown which objectives are usually chosen for optimization, what constraint and limitations might impose multi-objective optimization problem formulation. Different types of petroleum refining processes are considered such as catalytic and thermal.

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Keywords: multiobjective optimization; petroleum refining, genetic algorithm

1. Introduction

It is hardly possible to diminish importance of the key roles of petroleum refining in modern chemical industry. It produces different types of fuels (e.g. gasoline, diesel, furnace fuel, etc.) or wide variety of valuable chemicals which constitutes significant part of global market. Due to its importance, optimization of refining processes is essential. Capacities of modern units are high, and hence, even small performance improvements might lead to significant economical profits.

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Conventional methods of optimization for many years had been based on formulation of single objective function and search of its minimum (or maximum). In case of complex industrial processes either most important objective was chosen or single objective function in some way related to economic effect (e.g., profit maximization or cost minimization). Practically solution of such optimization problem yields single-point solution. This approach has some obvious disadvantages. Optimization of only one objective while disregarding the others might lose some practically meaningful solution and at times solution may be practically irrelevant. Nevertheless, sometimes relation between real objectives and their economic effect is not clear which makes difficult formulation of single objective function. Moreover, cost or profit functions are site-specific and time-specific and solution may not be useful.

Multi-objective optimization with its concepts and methods allow overcoming issues mentioned above. Applying multi-objective approach for solving real-life optimization problems, it becomes possible to take into account all of desired objective functions and treat them directly regardless of any explicit relation to economic efficiency. It is especially important for petroleum refining processes due to its complexity, i.e. variety of components in feedstock and products, diversity of chemical reactions, number of units included into processing scheme. Such nature of oil refining processes makes multi-objective optimization “a more advanced” tool in a search of optimal solution(s).

2. Solution of multiobjective optimization problem

Any multi-objective optimization (minimization) problem (MOO), regardless of area of application, is formulated as following:

$$\text{Minimize } \mathrm{I(x)} = [\mathrm{I}_1(\mathrm{x}), \mathrm{I}_2(\mathrm{x})...\mathrm{I}_n(\mathrm{x})] \tag{1}$$

$$\text{Subject to:}$$
$$\mathrm{x} \in \mathrm{S}$$
$$\mathrm{g}_k(\mathrm{x}) \le 0, \mathrm{i} = 1, 2...\mathrm{K}$$
$$\mathrm{h}_j(\mathrm{x}) = 0, \mathrm{j} = 1, 2...\mathrm{J}$$

where n is a number of objectives, g_k and h_j are inequality and equality constraints quantities of K and J respectively, x - set of decision variables, S - decision domain for x. However, optimization might include both minimization and maximization of objectives, for the sake of simplicity we will consider minimization problem. All the ideas and approaches can be easily extended for maximization problems.

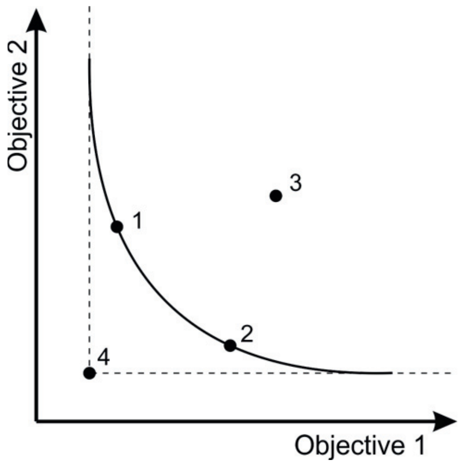

Fig. 1 Pareto front for two-objective optimization problem in objective domain

Unlike in case of single objective optimization, the non-trivial solution for problem (1) is not a single point, but a number of points called Pareto-optimal solutions.

Pareto-optimal point: a point $x \in S$ is called Pareto optimal point if and only if there is no other point $x' \in S$ such that $I_i(x') < I_i(x)$ for all objectives simultaneously.

Set of Pareto-optimal points for problem (1) is called Pareto front and represents a solution of multi-objective optimization problem. Let's consider simple two-objective problem (Fig. 1). Here solid line is a Pareto front. Points 1 and 2 are two representative points belonging to Pareto front. If we move from point 1 to 2, objective 2 is improving (decreasing) while objective 1 is worsening (increasing). Hence, point 1 and 2 are equally-good non dominated points. Point 3 is not Pareto optimal point since it has both objective values "worse" than any of points from Pareto front. Point 4 is imaginary point where both objectives 1 and 2 have minimum values. This point is unreachable due to conflictive nature of objectives and equality and inequality constraints from (1) which might introduce limitation to search space.

3. Use of Genetic algorithms for multiobjective optimization

There's a number of different method for solving MOO, i.e. search of Pareto-optimal solutions[1,2]. In last several years, numerous of modifications on methods based on genetic algorithms (GAs) experienced a significant growth in popularity for solving MOO problems. Original concept of genetic algorithm was established by Holland[3] and evolved further by Goldberg[4]. Nowadays many of different adaptations of GAs exist but all of them have the same basic principles, which are:

- GA works with number of decision points (called chromosomes) instead of single one
- Doesn't use derivatives of objective functions in MO search
- GA operators are probabilistic in nature

GAs have proved themself as a very robust optimum search methods. First of all, it is a global optimum search procedure, which overcome the drawbacks of majority of derivative-based methods. GAs can treat continuous or discrete functions (or decision variables); they can find optimum for multi-modal functions or converge to non-convex Pareto front[5].

To understand GA's main principles, one should consider Simple Genetic Algorithm (SGA). It is necessary to notice that SGA deals with coded variables. Any discrete or continuous variable is represented in a form of binary string (i.e. sequence of 0's and 1's). More detailed description about mapping of real variable into binary can be found elsewhere[4]. SGA first initializes a random set of N solutions (called "population").

Each member of the set (called "individual") represents a single set of decision variable with corresponding value of objective function(s). After population is created, SGA form a "mating pool"– an intermediate population, members of which are copied from original population - through reproduction. The chance of an individual to be chosen for mating is proportional to its objective function value; the lower the value, the higher the probability. In other words, the mating pool will be inhabited more with individuals who have lower objective values.

When mating pool is formed, SGA performs genetic operation over its individuals. The nature of these operators is not similar to any mathematical operators. Like the reproduction, they mimic the behavior of real genetic operators in nature. That's what makes GA an outstanding search procedure from any other mathematical techniques. Firstly, SGA choses two strings to carry out a crossover operator with probability $p_{crossover}$ (~0.5-0.7). Single-point crossover operator choses a random position at binary sequence and swap subsequences of two individuals (Figure 2). Another following conventional GA operator is mutation. It simply alters single bit (from 1 to 0 or vice versa) in binary sequence with probability $p_{mutation}$ (~0.01-0.1).

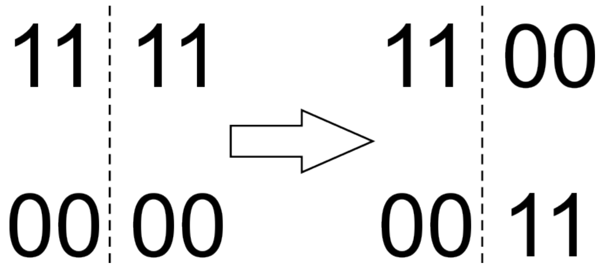

Fig.2 Single-point crossover operation

After these operations are done, one has a new generation of individuals. The reproduction, crossover and mutation are carried out once again. This drives the optimization search to an optimum until some termination criteria is satisfied. Usually it is a number of generations (practically around ~250-1000).

The following procedure describes the basics of GA. Multi-objective genetic algorithms utilize the same principles combined with MOO concepts of Pareto optimality. Modern GAs are more complex than SGA. They utilize modified genetic operator (e.g. two-point crossover), might treat real variables directly or implement different selection algorithms, but still principles remain the same. Here is the list of some of the modifications and adaptations: Multi-objective GA (MOGA)[6], Vector Evaluated Genetic Algorithm (VEGA)[7], NSGA-II[8], Differential Evolution[9] and many others.

Based on literature review over the last decade authors would like to emphasise that practically many of chemical engineering optimization problems were solved using NSGA-II. This algorithm has proved itself as very powerful tool for MOO. Detailed description of NSGA-II can be found in original source[8].

The main advantages of NSGA-II among other multi-objective GAs are notable and they are:

- relative simplicity of algorithm
- provides better convergence to a Pareto front
- provides wider distribution of solutions along Pareto front
- uses concept of *elitism*, which allow to carry individuals with better objective values through generations
- relatively low computational cost due to *Non-domination Sorting Approach*
- with *Constrained tournament method* it is possible to treat constraints directly without increasing computational time.

4. Multiobjective optimization of petroleum refining processes

Petroleum refining processes might be considered on different levels. Usually feedstock for refining unit includes variety of components which yields to multi-product outflow containing desired and undesired components. Commonly units operate under high temperature and pressure, which significantly contributes to cost of final product and impose restrictions to process operation parameters. Majority of processes utilize heterogeneous catalysts, which are also sensitive to process conditions. Nevertheless, typical refining process consists of many auxiliary units, the performances of which can significantly affect optimal conditions. All of these increases complexity of refining process.

In such scenario, application of multi-objective optimization becomes essential for improvement of unit performances. To carry out MOO of refining process it is vital to formulate real-life objectives in addition to implementation of relevant constraints.

Critical literature review showed a growing interest for use of genetic algorithms in multi-objective optimization of petroleum refining processes in the last several years.

In Bhutani et al.[10] authors performed a multi-objective optimization of an industrial hydrocracking unit, which is used to process heavy distillates to valuable products in presence of hydrogen. The unit considered mainly consisted of two reactors in series – a hydrotreater (HT) and a hydrocracker (HC). Both are packed bed reactors with 2 and 4 beds respectively.

Authors utilized a simplified model for HT and first-principle model for HC. Reaction products were lumped into 8 components (e.g. liquefied petroleum gas (LPG), light naphtha, heavy naphtha, etc.). Kinetic scheme were developed for these pseudo components. The HC modeling was based on the following assumptions: plug-flow reactor without axial diffusion, adiabatic, steady state operation.

Objectives were chosen based on industrial priorities and they were applied to maximize diesel, kerosene and naphtha production and to minimize off-gases, LPG production and hydrogen consumption. Due to many important objectives MOO problem was divided into 3 two-objective cases for simplicity:

- Maximization of kerosene flow rate and minimization of hydrogen consumption
- Maximization of diesel flow rate and minimization of hydrogen consumption
- Maximization of high-value end products (“HE” which is sum of all products except LPG) and minimization of low-value end products (“LE” which is sum of light components)

Additional constraints were introduced into MOO problem formulation. HC bed’s inlet and outlet temperatures were limited with upper value to ensure stable HC operation. Liquid hourly space velocity in the reactor was bounded to guarantee proper hydrodynamic regime in the reactor. Also, conversions of feed per one pass and overall throughput of the reactor was imposed to lie within certain range to maintain unit operation on reasonable level.

MOO was carried out using real-coded NSGA-II with 50 individuals (chromosomes) and for 200 generations. Each optimization case yielded in Pareto optimal front. Solutions were represented in two-dimensional objective domain with corresponding values for (optimum) decision variables.

Figure 3 illustrates Pareto front for maximization of HE and minimization of LE case. One can see from the plot, objectives are competing (conflicting). It is impossible to satisfy both objectives simultaneously. The resulted Pareto from is given to a decision maker (a unit manager, engineer, researcher), who can pick a certain desired point to operate industrial HC. There’s no better points beside provided in the Pareto solution.

It is be noted that real industrial operating point (represented by a solid square) are far from all optimum solutions (hollow squares). The results clearly show that some improvements are possible to make just by changing process operating condition to improve its performance.

In the work of Kasat et al.[11], MOO of industrial Fluidized Catalytic Cracking (FCC) unit was performed. Authors utilized lumped kinetic scheme with empirical reactor model to simulate FCC unit behaviour. They formulated three multi-objective cases to solve: a) maximization of gasoline yield and minimization of CO in a flue gas with constraints limiting amount of coke on catalyst, b) maximization of gasoline yield and minimization of air feed rate in regenerator with constraints limiting amount of CO in flue gas and c) maximization of gasoline yield, minimization of air feed rate in regenerator and minimization of CO amount in a flue gas with constraints like in previous two cases.

NSGA-II was used as a multi-objective optimization method. Authors obtained two and three dimensional Pareto fronts. They reported that varying constraints and choosing different objective functions it is possible to adapt proposed approach to any existing FCC unit to improve its performance. Later Kasat and Gupta[12] carried out the same MOO case as in Kasat et al.[11], but they introduced an improved genetic operator called jumping gene (JG) (for a description of JG principles one can refer to original source). Authors reported a better distribution of individuals along the Pareto front as well as faster convergence of modified algorithm. Faster convergence might be beneficial for MOO, since majority of industrial units’ simulations has high computational cost.

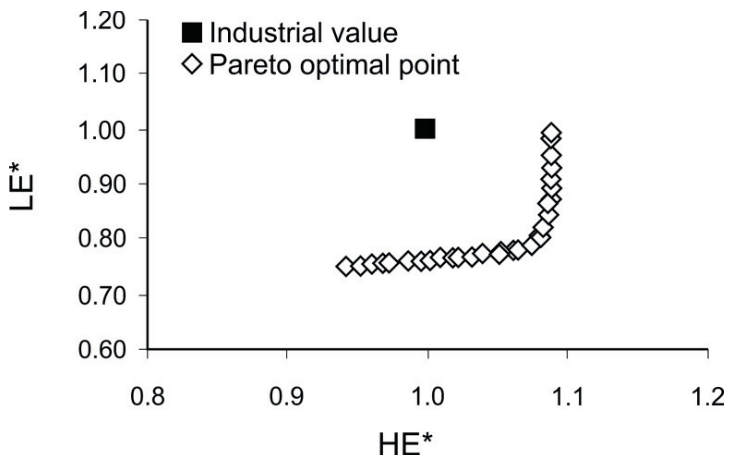

Fig.3 Pareto optimal front for two-objective optimization problem for industrial hydrocracking unit: Maximization of high-value end (HE) products and minimization of low-value end (LE)

Note: values are given in dimensionless form due to proprietary reasons. (Adapted with permission from Ind. Eng. Chem. Res. 45(4) N. Bhutani, A. K. Ray and G. P. Rangaiah, "Modeling, Simulation and Multi-objective Optimization of an Industrial Hydrocracking Unit", p1354-1372. Copyright 2006 American Chemical Society)

Weifeng et al.[13] proposed a multi-objective optimization of naphtha catalytic reformer. The fixed bed unit with 4 radial-flow reactors was studied in the proposed research. Unit was mainly operated for production of aromatics. The radial flow model combined with lumped kinetics was utilized assuming no axial or radial dispersion effects in the reactor. In addition to reactor, models of auxiliary units were also included (e.g. separator, heat-exchangers). Formulation MOO problem authors chose to a) maximize aromatics yield and b) minimize yield of heavy aromatics. Main process variables affecting these objective values were taken as each reactor inlet temperatures, process pressure, and hydrogen/hydrocarbon molar ratio. Objective values and decision variables were bounded based on industrial practice.

Neighbourhood and archived genetic algorithm (NAGA) was used to solve the problem; Pareto-optimal set of solutions was obtained. Authors noted that among all decision has conflicting effect for chosen objectives, but inlet temperature in fourth reactor which allows increasing aromatics yield while decreasing heavy aromatics.

Rahimpour et al.[14,15] carried out similar multi-objective cases for non-conventional type naphtha catalytic reformer with 3 reactors in series, where each reactor in coupled with heat-exchanger, thereby excluding the necessity of inter-stage heating. They maximized production of aromatics, hydrogen and aniline. Notable point is that they included a catalyst distribution between reactors as a decision variables, unlike to Weifeng et al.[13].

MOO problems were solved using objectives sum method with differential evolution. Authors came up with single-point optimal solution and optimal profiles for operating conditions along reactors length. It was reported significant increase in objective values for all chosen objectives. Also, results were compared with performance of conventional naphtha reformer; advantages of a new reactor were shown.

Iranshahi et al.[16] performed design and operation stage MOO of combined tubular membrane (refereed as “M”) and radial-flow spherical (referred as “S”) for two different unit arrangement in series (called as SMS and SMM). Authors chose hydrogen and aromatic production as objective function. Problem was constrained by hydrogen-to-hydrocarbons ratio.

Like in two previous works, differential evolution genetic algorithm was used to maximize sum of objectives. Constraints were handled in a form of penalty function. Single optimal solution for each of proposed reactor arrangements and results were compared. Show that optimization allowed improving performance of both reactor arrangements, however drew up a conclusion that SMS arrangement performs better comparing to SMM.

Work of Wang and Tang [17] utilizes data-based model to simulate and optimize performance of industrial naphtha pyrolysis unit. Authors used multi-objective genetic algorithm based on differential evolution approach called MOPDE-CES. Pyrolysis mainly is used for decomposition of higher hydrocarbons into light products, especially gases. The objectives for MOO were chosen as: maximize a) ethylene and b) propylene yield and no constraints were introduced. The number of Pareto-optimal solutions was obtained. Additionally, performance of MOPDE-CES and NSGA-II for solving the same MOO case was compared. Authors reported good convergence of MOPDE-CES to Pareto front comparing to NSGA-II with less computational cost.

Bayat et al.[18] performed MOO of paraffin dehydrogenation unit (PacolTM process), which is a part of linear alkylbenzenes (LAB) plant. The process is aimed for conversion of C10-C14 paraffins into corresponding olefins for further benzene alkylation. The dehydrogenation reactor is a fixed-bed radial flow reactor. To simulate its behaviour authors developed non-steady-state (to take into account catalyst deactivation) one-dimensional homogeneous model including mass and heat balance over the reactor. Objectives chosen for MOO were: maximize a) production and b) selectivity of olefins.

MOO was carried out using NSGA-II. Solution of optimization problem yielded into several Pareto fronts with respect to time. It was shown how do Pareto-optimal solution are shifting due to catalyst deactivation. Also one solution of entire Pareto front was proposed as “the most acceptable” to operate the industrial unit.

5. Conclusions

Conventional refinery consists of processes of different types – heterogeneous and homogeneous catalytic, thermal, physical (such as distillation or mixing), and genetic algorithms for MOO might be applied to any type them. They differ in the nature of reactions, products, unit arrangements or technologies applied.

In this light, to account all of these, the importance and significance of MOO for petroleum refining processes is evident. Multi-objective genetic algorithms are very robust technique to carry out MOO of industrial processes. They allow taking into account all complexity of considered problem and finding optimal solution(s). Genetic algorithms can easily treat several objectives and constraints simultaneously. This is often vital for industrial cases since solution provided by single-objective optimization methods might be irrelevant in real life.

However, use of genetic algorithms in optimization of industrial oil refining processes is relatively new field of research comparing to other fields in chemical engineering. It makes it an attractive field for further investigations.

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