Original Research Article

Comparison of different algorithms in typical process optimization of chemical industry

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Abstract: Complex problems in chemical processes often need to be transformed into optimization problems for solution, and intelligent optimization algorithms provide efficient strategies for this. Based on the Williams-Otto (WO) process and the crude oil atmospheric and vacuum distillation process, this study compares the performance of five optimization algorithms, including the Sequential Quadratic Programming (SQP) method, Particle Swarm Optimization (PSO) algorithm, etc., and evaluates them from dimensions such as running time, number of iterations, and the quality of results. The results show that the traditional gradient algorithm SQP is suitable for low-dimensional nonlinear problems, while heuristic algorithms exhibit better global search capabilities and robustness in the strongly coupled and multi-stable industrial process of crude oil atmospheric and vacuum distillation. It can be seen that different optimization algorithms have their own advantages and disadvantages, and a reasonable selection should be made according to specific problems.

Keywords: Atmospheric and vacuum process; Heuristic algorithm; Optimization algorithm; Algorithm model

With the advancement of the "dual carbon" strategy and the upgrading of the refined production requirements in the refining and chemical industry, the optimization of chemical processes has shifted to a data-driven paradigm. Currently, the energy efficiency of China's refining and chemical plants is 8%-12% lower than the international advanced level, and approximately 35% of the energy-saving potential in the process industry remains unexploited. Mathematical programming methods and intelligent optimization algorithms have become the key to breaking through the energy efficiency bottleneck.

In theoretical research, classical mathematical programming methods provide theoretical support. Huang Lingxiang [1] and others used the SQP algorithm to optimize the demethanization system of the cold box, reducing the consumption of high-pressure steam by 0.6% and decreasing the objective function value of the system's energy consumption and ethylene loss by 2.83%. Hwang [2] and Mortazavi [3] and their teams used a combination of GA and SQP to optimize the DMR and C3MR processes, reducing the power consumption by 34.5%. Heuristic optimization algorithms, on the other hand, can flexibly solve complex problems. Tian Peng [4] and others applied a variety of swarm intelligence algorithms to chemical engineering problems, significantly improving the optimization performance. Xu Yufei [5] and others optimized the parameters of residue oil hydrotreating using an improved whale algorithm. Osaba [6] and others used the discrete bat algorithm to solve the vehicle routing problem of pharmaceutical waste collection and distribution. However, there are two major problems in existing research: the algorithm evaluation system is "fragmented" and lacks a unified standard; a large number of studies focus on a single process, lacking process comparisons, making it difficult to reveal the relationship between algorithm performance and system complexity.

To address this, this paper constructs a multi-dimensional algorithm evaluation system. The WO process and the crude oil atmospheric and vacuum distillation process are selected as the test platforms, representing an idealized reaction system and an industrial-level complex process respectively. Taking the convergence speed, computational resource consumption, and the degree of achievement of the optimization objectives as indicators, the performance of algorithms such as SQP, GA, SA, PSO, and ACO is compared, aiming to improve the efficiency of resource utilization and provide a reference for the industry.

1. Optimization algorithms

1.1. Sequential quadratic programming (SQP) algorithm

The SQP algorithm [7] is an iterative method for efficiently handling nonlinear optimization problems. It solves the problem by transforming nonlinear constraints into a series of quadratic programming sub-problems and gradually approaches the optimal solution. It has the advantages of high computational accuracy, fast convergence speed, and good stability.

1.2. Genetic algorithm (GA)

The GA algorithm [8] is based on the mechanisms of natural selection and genetics. It simulates the operations of selection, crossover, and mutation in biological evolution. Without the need for a clear mathematical model, it is suitable for complex optimization problems, has strong global search capabilities, and can avoid getting trapped in local optima.

1.3. Particle swarm optimization (PSO) algorithm

Inspired by swarm behavior, the PSO algorithm [9] simulates the flight of particles and adjusts their positions according to their own experience and the best experience of the swarm. It is characterized by being easy to implement, having few parameters, and being highly efficient, which is conducive to achieving the global optimum. After initializing the particles, the velocity and position are updated by learning from the pbest (personal best) and gbest (global best).

1.4. Simulated annealing (SA) algorithm

The SA algorithm [10] draws on the annealing process of metals and adopts a probabilistic search method. After setting the initial temperature, it accepts solutions according to the Metropolis criterion. It does not require derivative information and has strong global search capabilities, but its computational efficiency is relatively low.

1.5. Ant Colony optimization (ACO) algorithm

The ACO algorithm [11] is derived from the foraging behavior of ant colonies. Ants release pheromones to mark paths, and through positive feedback, the path to the optimal solution is formed. The algorithm has the capabilities of distributed computing and global search, but it converges slowly and is prone to getting trapped in local optima.

This paper will systematically study the solution performance of these five algorithms in complex optimization problems in the chemical industry. **Table 1** lists the core information of the algorithms:

Table 1. Overview of algorithms.

Algorithm	Inspiration	Main Operations	Year
SQP	The idea of iterative optimization in quadratic programming	Transform nonlinear problems into quadratic programming problems and gradually approach the optimal solution	1975
SA	The annealing process of solid materials	Initialization, neighborhood search, acceptance criterion, cooling strategy	1983
ACO	Ant foraging behavior	Pheromone-guided path selection and dynamic update	1991

Algorithm	Inspiration	Main Operations	Year
GA	Theories of natural selection and crossover mutation	Selection, crossover, mutation, replacement	1992
PSO	The social behaviors of flocks of birds foraging and schools of fish swimming.	Track the individual and group optima, and iteratively update the positions and velocities of the particles.	1995

Table 1. *(continued)*

2. Case Studies of process systems

The evaluation of optimization algorithms for chemical processes needs to take into account both theory and practice. In this paper, the WO process and the crude oil atmospheric and vacuum distillation process are selected to construct a verification system: The WO process is a classic theoretical model, which can reveal the convergence characteristics of algorithms in continuously differentiable scenarios; the crude oil atmospheric and vacuum distillation process, as the core unit of the oil refining industry, can examine the global search capabilities of algorithms under complex constraints. The two complement each other in terms of the verification level and complexity.

2.1. Williams-Otto reactor problem

2.1.1. Description of the WO process

The Williams-Otto reactor [12] is a continuous stirred tank reactor (CSTR). Three irreversible reactions occur inside it. The flow rate of raw material B, FB, and the reaction temperature, TR, are taken as the operating variables to maximize the yields of products P and E.

2.1.2 Objective function, decision variables and constraints

FA is the known feed flow rate, and FB and TR are the decision variables. The constraints limit the ranges of temperature, flow rate and the concentrations of various components. The objective function is to maximize the difference between the sales profit of products E and P and the cost of raw materials[13].

2.1.3 Setting of optimization parameters

For the SQP, PSO, ACO, SA and GA algorithms, parameters such as the population size and the number of iterations are determined. The experimental hardware is an Intel Core i9-12900HX at 2.3GHz with 16GB of RAM.

2.1.4 Optimization results of the wo process

The SQP algorithm performs the best. The optimization result is 0.0011%, 0.0016%, 0.000970% and 0.0015% higher than those of the PSO, ACO, GA and SA algorithms respectively, and its calculation time is also the shortest. This algorithm shows its advantages in low-dimensional nonlinear problems.

2.2. Problem of crude oil atmospheric and vacuum distillation process

2.2.1. Description of the crude oil atmospheric and vacuum distillation process

The crude oil atmospheric and vacuum distillation unit consists of three steps: pretreatment, atmospheric distillation and vacuum distillation. The WO process can be directly modeled mathematically, while the crude oil atmospheric and vacuum distillation unit needs to use Aspen HYSYS and select the Peng-Robinson physical property package to construct a high-fidelity model.

2.2.2. Objective function, decision variables and constraints

The steam flow rate F16 of the atmospheric tower and the steam flow rate F17 of the vacuum tower are selected as the decision variables. Their flow rate ranges are constrained, and the objective function is to maximize the difference between product sales and costs.

2.2.3. Optimization parameter settings

The selection of optimization parameters is the same as that of the above-mentioned WO process. For other optimization algorithms, the specific parameter settings are as follows:

Sequential Quadratic Programming (SQP) algorithm: The initial value x0 = [7000 600], the step size tolerance is 10 to the power of negative 6, the finite difference step size is 10 to the power of negative 4, and the maximum number of iterations is 100.

Particle Swarm Optimization (PSO) algorithm: The population size NP = 20, the inertia weight w ranges from 0.2 to 0.9, the learning factor c = 2, and the maximum number of iterations is 100.

Genetic Algorithm (GA): The population size NP = 20, the crossover probability is 0.82, the fitness tolerance is 10 to the power of negative 6, and the maximum number of iterations is 100.

Ant Colony Optimization (ACO) algorithm: The population size NP = 20, the pheromone concentration a = 1, the heuristic factor b = 5, the evaporation coefficient r = 0.2, the pheromone intensity Q = 100, and the maximum number of iterations is 60.

Simulated Annealing (SA) algorithm: The initial temperature InitialTemperature = 100, the reheating interval is 100, the function value tolerance is 10 to the power of negative 5, and the maximum number of iterations is 500.

The curves showing the number of iterations and the convergence of the optimization results of all these five algorithms depict the convergence trends of the optimization results of each algorithm as the number of iterations increases during the optimization process of the crude oil atmospheric and vacuum distillation unit.

2.2.4. Optimization results of the crude oil atmospheric and vacuum distillation unit

The optimization result of the ACO algorithm is the best, which is 0.67%, 0.0142%, 0.0481% and 0.0237% higher than those of the SQP, PSO, GA and SA algorithms respectively; the PSO algorithm has the shortest calculation time. In the high-dimensional non-convex space of the crude oil atmospheric and vacuum distillation unit, ACO and PSO are more valuable for industrial applications in terms of accuracy and efficiency.

3. Conclusions

This study compares and analyzes the performance of five optimization algorithms in the WO process and the crude oil atmospheric and vacuum distillation unit. In the low-dimensional and continuously differentiable WO process, the SQP algorithm performs excellently in terms of solution accuracy and calculation speed, far surpassing heuristic algorithms; while in the high-dimensional non-convex scenario of the crude oil atmospheric and vacuum distillation unit, due to its dependence on local gradients, the SQP algorithm is prone to falling into suboptimal solutions. Heuristic algorithms such as PSO and ACO have more advantages in convergence accuracy by virtue of swarm cooperative search. The results show that SQP is suitable for low-dimensional nonlinear systems, and heuristic algorithms have more potential in complex industrial processes.

There are still limitations in this study: insufficient sensitivity analysis of key parameters, failure to consider the impact of dynamic factors on the robustness of the algorithms, and lack of adaptability evaluation under different hardware environments. Future research can be deepened in many aspects: expand the comparison of algorithms to more complex chemical units; develop hybrid optimization strategies; use machine learning to achieve adaptive parameter adjustment; and improve the industrial-level verification and multi-objective evaluation system. The selection of optimization algorithms needs to be combined with the characteristics of the problem and industrial requirements, and a better solution for chemical process optimization should be provided through the integration of multiple disciplines.

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