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Optimal Step-Size Control with Bayesian Optimization for Correlation Integral Based Real Time Optimization

JingWei ZHAO[1], Zhong ZHAO[2]
Beijing University of Chemical Technology, College of Information Science and Technology, Beijing 100029, China

Abstract. Conventional real-time optimization (RTO) requires detailed process models, which may be challenging or expensive to obtain. Data-driven correlation integral based RTO method is an attractive alternative to circumvent the challenge of developing accurate process models. However, the searching step size in conventional correlation integral based RTO is set by trial-and-error. In order to improve the efficiency of the correlation integral based real-time RTO method optimiszation algorithm and enhance the applicability of the system, an Bayesian optimal optimisation step-size control strategy using Bayesian optimization based on correlation integral is proposed for the traditional correlation integral optimisation method applied in industrial systems. Based on the data-driven steady state model, the adaptive control of the step size is achieved by avoiding the change of the tuning step size through the trial-and-error method due to different working conditions during the real-time optimisation control. Based on the proposed method, the application software has been developed. The simulation and industrial application results have verified the feasibility and effectiveness of the proposed method.original real-time optimisation software is improved, and the practicality of the method is proved by simulation and industrial practical application.

Keywords. RTO; Correlation integral; Adaptive control; Bayesian optimizsation; Step-size control strategy

1. Introduction

For the steady-state optimization of production processes [1], the purpose of improving production efficiency can be achieved by changing the steady-state operating point without changing the existing production equipment, and traditional real-time optimization methods tend to determine the dynamic model of the system first [2-3], and the dynamic process is taken into account at the same time on the basis of steady-state tuning [4]. However, for complex industrial processes, their dynamic processes are often complex, and it is difficult to accurately model the dynamics of complex industrial processes. The data-driven correlation integral real-time optimization (RTO)

[1] JingWei ZHAO, Beijing University of Chemical Technology, College of Information Science and Technology, Beijing 100029, China; email: 1318093426@qq.com
[2] Corresponding author: Zhong ZHAO, Beijing University of Chemical Technology, College of Information Science and Technology, Beijing 100029, China; E-mail: zhaozhong@buct.edu.cn; Tel.: +86 136-7137-7301.

algorithm is a fast method [5-6] to estimate the steady-state cost gradient with dynamic operation data. Based on the above advantages, for complex large-scale chemical industrial processes, the method can perform feature extraction for nonlinear dynamic processes and based on this, it can optimize the operation of nonlinear complex processes that are difficult to establish accurate mechanism models.

However, the search step size of the traditional correlation integral RTO method is obtained by the trial-and-error method [7], and it often takes a lot of time to find the appropriate step size when facing different working conditions, which is inefficient and has certain limitations. For multi-input and multi-output systems, when the decision variables of the control system are in the local steady state [8], there exists a locally optimal objective function [9], however, the current locally optimal objective function value cannot be taken as the global optimal value of the control system's objective function, and it may be trapped in the local extreme value point.

Meanwhile, in order to efficiently perform global search and obtain the global optimal solution, some optimization algorithms that combine deterministic information [10] and stochastic information [11], i.e., modern optimization algorithms [12], have been proposed in recent years. Commonly used modern optimization algorithms include genetic algorithms [13], particle swarm optimization algorithms [14] and simple polygonal evolutionary algorithms (SCE-UA), etc[15-16]. The computational efficiency of the algorithms becomes a non-negligible issue when dealing with parameter optimization problems with complex models and large amounts of data, such as distributed models [17]. Although these automatic optimization algorithms perform relatively well in terms of computational accuracy, they still need to go through at least hundreds or even thousands of iterations to find a better set of parameter sets. As an effective solution for solving complex optimization problems that are non-convex, multi-peaked, and costly to evaluate, Bayesian optimization has gained wide attention in several fields in recent years [18]. The ideal solution can be obtained after only a few times of objective function evaluation, and the method has been widely used in the fields of system optimization, deep learning, environmental monitoring and life sciences [19-22], which provides a new way of thinking for solving complex system optimization problems. The core parts of the Bayesian optimization algorithm are the probabilistic agent model and the collection function. Commonly used probabilistic agent models include beta-Bernoulli model, linear model, generalized linear model, Gaussian process, random forest, and deep neural network. The acquisition function is generally constructed from the posterior probability distribution of the objective function, and the optimization algorithm selects the next evaluation node guided by maximizing the acquisition function to ensure that the total loss is minimized.

Aiming at the multi-peaks and inefficiency waiting to be solved in the tuning process, this paper proposes a data-driven correlation-integral Bayesian optimization step-size control method based on the gradient relationship between the decision variables and the objective function calculated by correlation-integration, and the step-size parameter formula and the objective function as the Bayesian optimization framework, which allows us to search for the globally optimal objective function value of the control system when the system is faced with different working conditions. The improved method greatly enhances the original algorithm. The improved method greatly enhances the applicability of the original algorithm and improves the efficiency of real-time optimization of the control process.

This paper describes the principle of gradient extraction of the traditional correlation integral algorithm and presents the defects of the correlation integral algorithm in Section 1; in Section 2 the adaptive step-size control method with Bayesian optimisation as the core is illustrated; Section 3 describes the development of a real-time optimisation software to apply the improved method and simulation is performed to validate the feasibility of the method; and the tuning of a real industrial model after the improvement of the method is performed in Section 4 to improve the economic efficiency; The main conclusions are given in Section 5.

2. Problem Describes the Flaws in the Relevant Integral Algorithm

The inefficiency of the step-size trial patch that exists in the traditional real-time optimization of correlation integrals is addressed as follows:For the steady-state optimisation of dynamic processes in multi-input multi-output systems, stochastic dynamic models are required:

$$\begin{cases} \dot{\tilde{x}}(t) = f(\tilde{x}(t), \tilde{u}(t)) + \tilde{w}(t) \\ \tilde{J}(t) = g(\tilde{x}(t), \tilde{u}(t)) + \tilde{v}(t) \end{cases} \tag{1}$$

where each variable in Eq. is defined as follows, $\tilde{u}(t)$, $\tilde{x}(t)$, $\tilde{J}(t)$ are the input variables, state variables and output variables of the system (1), respectively, and $\tilde{w}(t)$ 、 $\tilde{v}(t)$ are zero-mean Gaussian white noise.The objective function of the system is expressed as:

$$\tilde{J}(t) = J(\tilde{u}(t), \tilde{w}(t), \tilde{v}(t), t) \tag{2}$$

The tuning process needs to find the extremes of the objective function

$$\tilde{J}^*(t) = \max_{E(\tilde{u}(t))} J(E(\tilde{u}(t)), \tilde{w}(t), \tilde{v}(t), t) \tag{3}$$

In equation (3) $\tilde{J}^*(t)$ is the optimal value of the optimisation objective function and $E(\tilde{u}(t))$ is the mean value of the tuning variables. By finding the gradient between $\tilde{u}(t)$, $\tilde{J}(t)$ that is, the gradient relationship between the decision variable and the target expectation, the use of correlation and integration method to drive the gradient between the two to 0, that is, the local extreme value of the objective function.

Lemma 2-1 [6] Let the system (1) be able to stabilise around the interval around time $u_0 = E(\tilde{u}(t))$, then when time $\tilde{u}(t) \to u_0$

① The partial derivative of the optimisation objective function with respect to the mean value of the tuning variable is equal to the infinite integral of the linearised impulse response function:

$$\frac{\partial J(E(\tilde{u}(t)), \tilde{w}(t), \tilde{v}(t), t)}{\partial E(\tilde{u}(t))} = \int_0^\infty \tilde{h}(t)dt \tag{4}$$

② The necessary condition for the optimal value of the optimisation objective function is:

$$\int_0^\infty \tilde{h}(t)dt = 0 \tag{5}$$

Lemma 2-2 [6] When the system (1) converges to the steady state operating point u_0 and the tuning variable converges to the mean value of the tuning variable

$$\frac{\partial J(E(\tilde{u}(t)),\tilde{w}(t),\tilde{v}(t),t)}{\partial E(\tilde{u}(t))} = \frac{\partial J(u_0,\tilde{v}(t))}{\partial u_0} \tag{6}$$

In the above equation, when $\tilde{v}(t) = 0$, $J(u_0,0)$ is the static relationship between the optimisation objective function of system (1) and the decision variables. Then, from Lemma 2-2, when the fluctuations and disturbances of the decision variables are small enough, the mean values of the decision variables are equivalent to the static tuning of the system. Therefore, the above dynamic process steady-state optimisation problem is transformed into changing the set values of the decision variables so that the static gain of the optimisation objective function on the decision variables tends to 0. However, since the specific form of the objective function is unknown, the gradient information cannot be obtained directly according to Eq. (6). And the static gain of the tuning variable for the optimisation objective function is related to the autocorrelation integral of the tuning variable and the cross-correlation integral of the tuning variable and the optimisation objective function.

$$k_{\tilde{u}\tilde{J}}(T,M) = k_h k_{\tilde{u}\tilde{u}}(T,M) + k_{\tilde{u}\tilde{w}}(T,M) \tag{7}$$

where $k_h = \int_0^\infty \tilde{h}(t)dt$, is the static gain of the system (1), $k_{\tilde{u}\tilde{J}}(T,M)$ is the cross-correlation integral between the tuning variables and the optimisation objective function in finite time, $k_{\tilde{u}\tilde{u}}(T,M)$ is the autocorrelation integral between the tuning variables in finite time, $k_{\tilde{u}\tilde{w}}(T,M)$ is the correlation integral between the tuning variables and the disturbances, and T, M are the integration constants. Then, the real-time gradient information can be obtained indirectly from the real-time data of the tuning variables as well as the optimisation objective variables that can be obtained in real-time.

There are in the range of $(-T-M+t_0, T+M+t_0)$:

$$k_{\tilde{u}\tilde{u}}(T,M,t_0) = \int_{-M}^{M} \frac{1}{2T}\int_{-T}^{T} \tilde{u}(t+t_0)\tilde{u}(t+t_0-\tau)dtd\tau \tag{8}$$

$$k_{\tilde{u}\tilde{J}}(T,M,t_0) = \int_{-M}^{M} \frac{1}{2T}\int_{-T}^{T} \tilde{J}(t+t_0)\tilde{u}(t+t_0-\tau)dtd\tau \tag{9}$$

where t_0 is the central locus during the data period.

From equation (7), it can be seen that the static gain k_h can be estimated from the computed data of $k_{\tilde{u}\tilde{J}}(T, M, t_0)$ as well as $k_{\tilde{u}\tilde{u}}(T, M, t_0)$ using the least squares algorithm.

After obtaining the static gain k_h, the conventional correlation integral optimisation algorithm uses the following iterative algorithm to change the set values of the tuning variables:

$$\tilde{u}_{sp}(i+1) = \tilde{u}_{sp}(i) + \lambda k_h(i) \tag{10}$$

The parameter that controls the tuning step size as well as the direction is the parameter λ in the above equation

$\tilde{u}_{sp}(i+1)$ is the set value of the tuning variable at the next optimisation moment, and λ is the constant of the weighting coefficients, with the sign of λ being determined by whether a very small or a very large value is sought. The sign of λ is determined by whether the value is extremely small or extremely large. If an extremely large value is sought, then λ takes on a positive value; if an extremely small value is sought, then λ takes on a negative value. The value of the parameter is also problematic, when the value of the λ weight coefficient constant is large, it will lead to the tuning of the system's objective function to skip the local optimum, and when the value of the λ weight coefficient constant is small, it will lead to the tuning of the system's objective function to search for the global optimum in a very slow and inefficient process . Therefore, the value of the parameter is very important, the traditional correlation integral real-time optimization method, when facing the optimization under different working conditions, can only take the value of the step-size parameter through the trial-and-error method, and can't achieve the effect of adaptive to the working conditions, according to the above description of the problems, this paper proposes the Bayesian parameter optimization as the core of the variable step-size control strategy on the basis of the original correlation integral algorithm.

3. Improved Correlation Integral Bayesian Optimal Step-size Control Strategy

Bayesian optimisation transforms complex optimisation problems into optimisation functions to be solved as follows:

$$X^* = \arg\max_{x \in V \subseteq R^d} J(x) \tag{11}$$

Where, x denotes a d-dimensional decision vector, V denotes the decision space, $J(x)$ denotes the objective function, and the exact form of $J(x)$ may not be known and is a black-box function. But the value of $J(x)$ can be observed using experiments.

The iterative relationship in Eq. (10) reflects the relationship between the decision variables and the tuning step parameter and the decision variables and the optimisation objective function gain at the current and next moments. In the next section of the paper, the real-time optimization software will be used to change the set values of the decision variables according to the iterative relationship in the above equation to find the decision variables of the local optimal steady state operating point, and then analyse the optimal objective function value of the optimal steady state operating point. For control parameter λ, when its value is large, it means that the step size is large, and vice versa. When the system decision variables and objective function values are close to the optimal operating point, the system should adaptively reduce the step size, so as to gradually approach the optimal operating point, and obtain more accurate critical point calculation results. According to the above analysis, the optimal step-size control strategy should be adaptive in order to ensure that the system is optimised to the precise optimal objective function value and at the same time improve the computational performance.

Bayesian optimisation is a very effective global optimisation algorithm, and the goal is to find the global optimal solution in Eq. (11). In order to overcome the multi-peak situation of the optimisation objective function, the step-size control strategy can directly find the global optimal objective function value, so that the step-size can be adjusted adaptively with the slope size of the objective function curve, in the region of the curve with a larger slope to control a smaller step-size, in the region of the curve with a smaller slope to control the step-size is relatively large, then it can be ensured that the step-size is more appropriate throughout the optimisation of the objective function curve, thus avoiding the multi-peak situation . This can avoid the situation of multiple peaks in the curve. The slope of the optimisation objective function curve can be expressed by equation (12):

$$k_h = \frac{dJ}{du} \tag{12}$$

In order to enable the step size to follow the optimisation objective function for adaptive adjustment, the Bayesian parametric optimal step size control strategy is proposed viz:

$$\lambda = a \cdot e^{-b|k_h|_{\max}+c} + d \tag{13}$$

Where $|k_h|_{\max}$ is the maximum value of the slope of the optimisation objective function curve and $|k_h|$ can be taken by the following equation

$$|k_h| = \frac{\partial J(u_0, \tilde{v}(t))}{\partial u_0} = \begin{cases} -\dfrac{\partial J(u_0, \tilde{v}(t))}{\partial u_0}, u_0 < u_{sp} \\ \dfrac{\partial J(u_0, \tilde{v}(t))}{\partial u_0}, u_0 > u_{sp} \end{cases} \tag{14}$$

The parameters in Eq. (13) mainly include four, a, b, c, d are the parameters controlling the calculation of step size, which can be calculated according to the

Bayesian optimisation method. From the image of the exponential function of e, it can be seen that at the beginning of the calculation, the size of the step size is mainly determined by a, c, at this time it is necessary to set the appropriate value to make the step larger; after the calculation is carried out for a period of time, the slope gradually increases, and the influence of the parameters a, b gradually increases, and the influence of the value of c gradually decreases. When approaching the critical point, the step size needs to become smaller, and at this time the step size is determined by the constant d.

The collection function of Bayesian optimisation is the basis for purposefully searching the next evaluation point from the parameter space, and there are mainly three kinds: PI, EI, and UCB, in this paper, PI (Probability of Improvement) is selected as the collection function. PI indicates the possibility that the next sample point of the collection may improve the optimal objective function, as shown in the following equation:

$$\alpha_t(x;D_{1:t}) = p(J(x) \le v^* - \varsigma) = \varphi(\frac{v^* - \varsigma - \mu_t(x)}{\sigma_t(x)}) \tag{15}$$

Where v^* is the optimal value of the current objective function; $\varphi(\bullet)$ is the standard normal distribution cumulative density function; ς is the balance parameter, by adjusting the size of ς can avoid falling into the local optimum, to achieve the global search for the optimal value.

The parameter optimisation process is shown in Figure1:

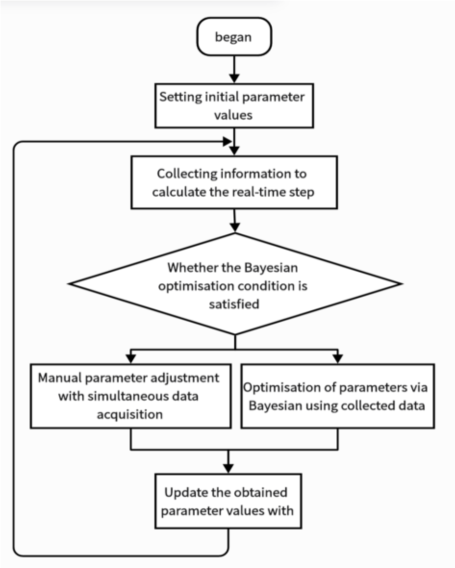

Figure 1. Bayesian optimisation flowchart

Its corresponding optimisation process is:

①The real-time gradient information of the objective function and the decision variable is extracted by correlation integration, and the initial value of the step function parameter is set, so that the initialised objective function distribution and sampling can be obtained.

② The next evaluation point is actively selected, which can make the collection function maximised.

③Add the newly collected samples to the historical sampling set.

④ When the objective function reaches the local optimum, determine whether it is the global optimum and update the parameters to continue tuning.

4. Verification of The Developed Software with Simulation

The full name of the developed software is: "CIM-Tuner Multivariate Optimization Control Software". which is shown in figure 2. This software mainly constructs CIM optimization controller to control the controlled object based on Correlation Integral Algorithm (CIM), and Bayesian optimization method. The control process controls the controlled object through OPC. When controlled by OPC, the controlled object can be the DCS system of the actual industrial plant, or a simulation system built by Simulink and other simulation software on the local or remote computer. In this paper, the simulation is chosen to construct the control system by building simulink model, and real-time optimization is carried out under the premise of multiple peaks of the objective function, aiming at avoiding the emergence of multiple peaks through the improved Bayesian optimization with variable step-size control strategy, so as to realize one-time tuning to find the global optimal value of the objective function.

① is the main menu of software operation, Controller: initialization of the controller; Simulation: offline testing of the controlled system; OPC: the DMC controller through the OPC role in the controlled object;

② is the trend graph of optimization variable (PV).

③ is the trend graph of operation variable (MV)

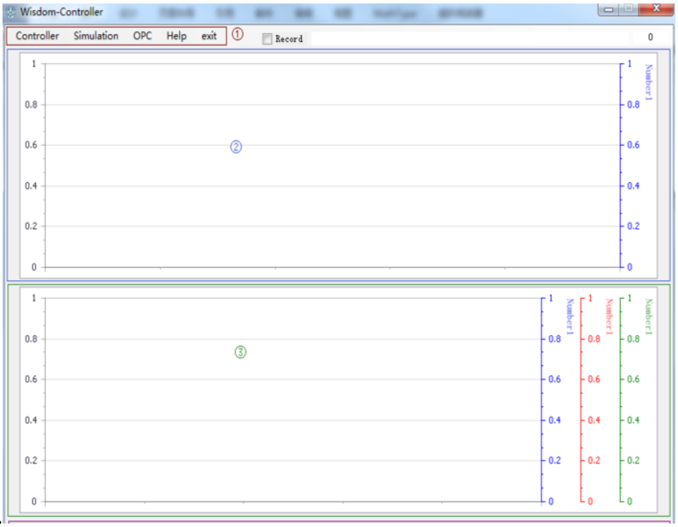

Figure 2.CIM-Tuner software interface

The figure 3 builds the control system through simulink, connects to CIM-Tuner through the universal OPC server platform MatrikonOPC Explorer, and realises the target optimisation through CIM-Tuner.

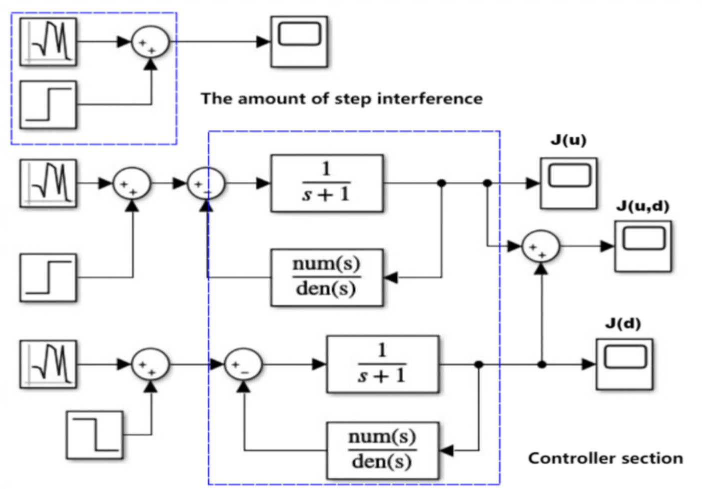

Figure 3. Built simulink simulation control system

The figure 4 shows the multi-peak optimisation objective function of the system, it can be seen that multiple extremes occur in different intervals during the tuning process, and due to the fixed step size, adaptive control is not implemented, which leads to the system tuning process can not directly find the global optimum value of the objective optimisation function.

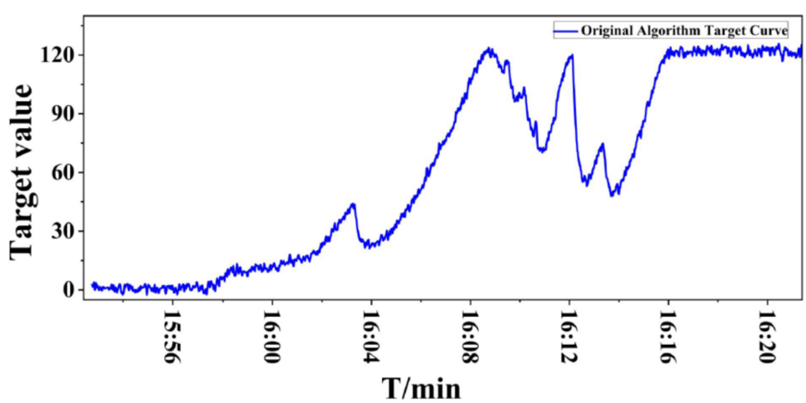

Figure 4. CIM-Tuner simulation of the original algorithm optimisation objective function curve

The figure 5 shows the tuning process of optimising the objective function through the Bayesian optimisation with variable step size control strategy. As can be seen from the figure, due to the adaptive adjustment of the tuning step size, there is no multi-polar values in the interval of the objective optimisation function during the tuning process, and it is possible to find the global optimal value of the objective optimisation function directly.

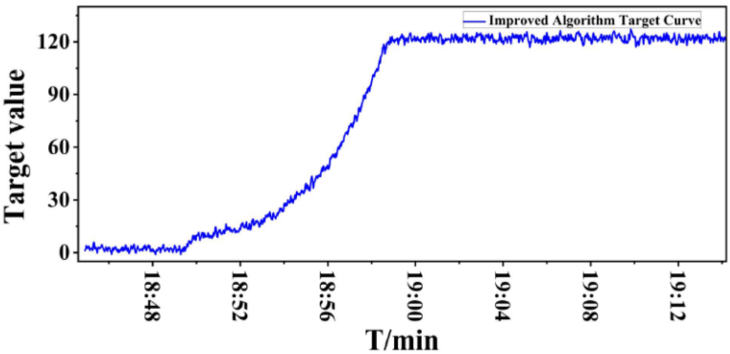

Figure 5. Optimisation objective function curve of CIM-Tuner simulation improvement algorithm

5. Industrial Application

The process flow based on this paper is the ethane recovery project procedure of Xinjiang Bazhou Tarim Energy Co., Ltd. which adopts advanced "propane pre-cooling + expander refrigeration + double reflux ethane recovery" technology for ethane recovery, and produces ethane, liquefied gas and stabilized light hydrocarbons as main products. The gas from Dirun line, Yinglun line, Tirun line and Kirun line enters into the pipe cleaning device after summarization, and then enters into two dehydration and mercury removal devices in two rows after dust removal and metering; the wet gas removes the small amount of solid particles and liquids entrained therein, and then enters into the mercury removal tower from top to bottom, and then the wet gas after mercury removal is dewatered; the dewatered dry gas filters out molecular sieve dust and then enters into the cold box of the ethane recovery device. Through the cold box D line pre-cooling into the cryogenic separator gas-liquid separation, liquid phase throttling down pressure into the 21st layer of the tower plate of the upper demethanization tower; the gas phase into the expansion end of the expander expansion, cooling down into the 16th layer of the tower plate of the tower of the demethanization tower tower tower tower top gas by the cold box A line reheat into the expander compression end, compression, pressurization and cooling, to the separation of metering equipment; the bottom of the tower of the tower of the demethanization liquid phase throttling down pressure into the middle of the tower of de-ethane; the tower of the ethane recycling device cold box. The liquid phase at the bottom of the deethane tower is throttled and depressurized, and then enters the middle of the deethane tower; the gas at the top of the deethane tower is cooled by the condenser at the top of the deethane tower and then enters the reflux tank of the deethane tower to carry out gas-liquid separation, and the liquid phase is pressurized by the reflux pump of the deethane tower and then goes to the top of the deethane tower to serve as a return flow.

The SEPSim Tarim optimization algorithm test model was used for experimental validation of industrial applications, Figure 6 shows the SEPSim model building interface, where the unit gain OBJ_BM was set as the optimization objective value, the separator top temperature AIC-TV111_1, the expander outlet temperature AIC-Q-JT-1, and the deethanization tower top C2 control AIC-C2, were set as the three decision variables for tuning.

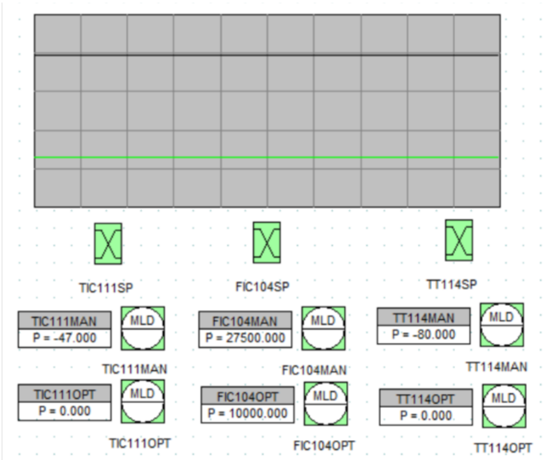

Figure 6. Test model of the Tarim optimisation algorithm

The model's plant revenue OBJ_BM unit is billion/year, by tuning the model's dynamic process steady-state optimisation can increase the plant revenue from 8.326 million/year to 8.708 million/year,increasing the revenue by 0.382 billion/year. The figure 7 shows the multi-peak situation of the device revenue tuning curve, from the figure can be seen due to the optimisation objective function there is a multi-peak situation, the tuning process is not strictly convex optimisation, there may be a short-lived tuning in the opposite direction, the fundamental reason is that the tuning step is set to be unchanged, giving a fixed value of the tuning step is unreasonable, and should be adapted along with the control system objective optimisation function of the steady state optimisation:

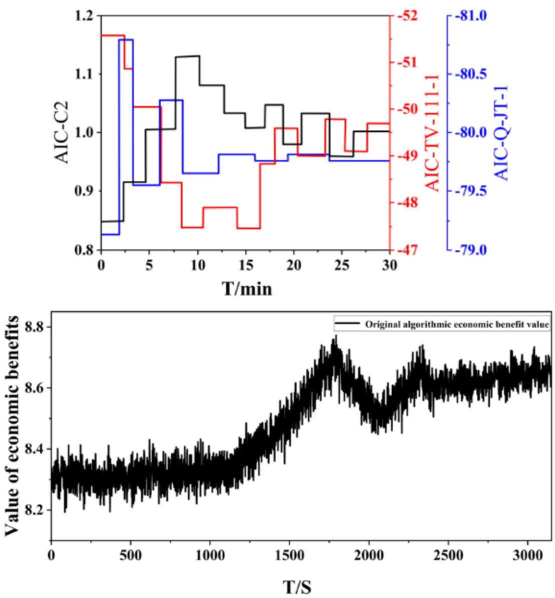

Figure 7. Optimisation curve of decision variables and objective function of the original algorithm for Tarim model

The results of the steady state optimisation of the dynamic process of the target device benefit by the Bayesian optimal step size control strategy are shown in the figure 8, which shows that the optimisation curve of the target function OBJ_BM does not have the phenomenon of multiple peaks, and due to the adaptivity of the tuning step size, it makes that the OBJ_BM can be tuned to the global optimum directly, avoiding multiple times of tuning, which improves the efficiency of the tuning.The tuning step size of the Bayesian optimization method is adaptive as shown in Table 1.

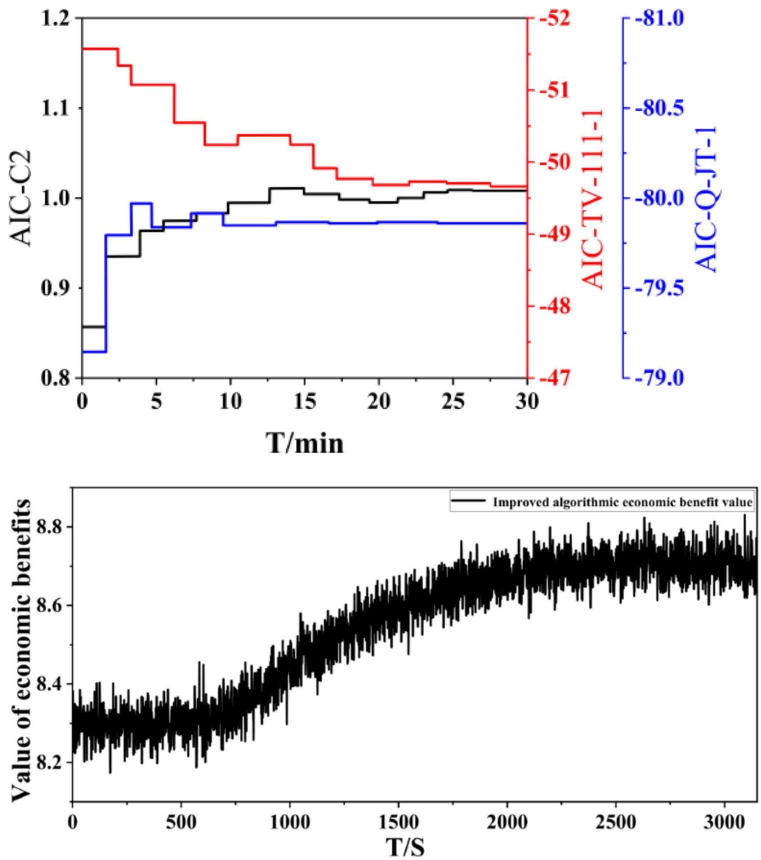

Figure8. Optimisation curve of decision variables and objective function of the improved algorithm for the Tarim model

Table 1 Variable step size control process data

Step i	λ	a	b	c	d
1	0.02	0.3025	1.824	2.464	-0.8283
2	0.05	0.2209	2.765	3.650	-0.5361
3	0.3	0.1867	3.5023	5.126	-0.1953
4	0.45	-1.426	3.886	0.033	0.9602
5	0.5	-1.551	4.231	0.027	1.0262
6	0.1	0.1072	1.862	2.881	-0.0774
7	0.05	0.2209	2.765	3.650	-0.5361

6. Conclusions

This paper focuses on the inefficiency of the algorithm and the weak applicability of the working conditions due to the trial-and-error method used in the traditional correlation-integral real-time optimization method for tuning the step size, as well as the multi-peak phenomenon in the real-time optimization and tuning of the objective function of the steady-state optimization of the dynamic process, and further analyzes the phenomenon of multiple peaks, which is due to the irrational setting of the tuning step size parameter. On the basis of the original correlation integral real-time optimisation algorithm, combined with the Bayesian optimisation method, an adaptive variable step-size control strategy is obtained, and an improved algorithm is obtained to obtain the fitting parameters for variable step-size tuning. Based on the ethane recovery project process operation procedure of Tarim Energy Limited Liability Company, using the Tarim optimization model test algorithm of SEPSim, the original algorithm and the improved Bayesian optimization step-size control algorithm based on correlation integral were used to make a comparative analysis of the optimization target economic benefit OBJ_BM curve, respectively. The analysis results show that the improved algorithm can adaptively adjust the step size in different time periods to avoid the emergence of multi-peak situations, and can directly tune the objective optimisation function to the global optimum. It improves the efficiency of the algorithm and brings certain economic benefits.

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