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Real-time optimization of converter inlet temperature in acid production with flue gas

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ABSTRACT

The conversion rate of SO_2 is of great significance to the efficiency of sulfuric acid production with flue gas. However, the existing optimization methods for SO_2 conversion rate can hardly achieve the optimal effect, because the parameters change and the working conditions fluctuate during the production process. Therefore, we propose a modifier-adaptation strategy with regulatory factors for real-time optimization of SO_2 conversion process in this paper. We first establish the optimization model of converter inlet temperature. Then, considering that the plant-model mismatch during the process of sulfuric acid production with flue gas is mainly caused by the change of initial oxygen concentration, initial SO_2 concentration, gas flow rate, catalyst activity and other factors, we study a modifier-adaptation strategy for real-time optimization with regulatory factors, designing and ameliorating the modifier term. We use the measurement values and gradient information in the real industrial process to revise the original optimization problem continuously, so that the solution will converge to the optimal set point of the real industrial process. The simulation results show that both the convergence rate of the proposed optimization strategy and the total conversion rate of SO_2 have been improved.

1. Introduction

Acid production with flue gas is an important way to produce sulfuric acid. It has advantages over acid production with pyrites or sulfur, because it can make full use of resources, keep the environment away from pollution, and increase economic benefits for enterprises (Zhang et al., 2012). Conversion process is an important part of sulfuric acid production process with flue gas. Off-gas from the smelter first flows into the purification process, and then flows into the conversion process. Through the effect of catalyst, SO_2 in flue gas reacts with oxygen to form sulfur trioxide under certain temperature (Bal'zhinimaev et al., 2001). The converter is the core equipment of the conversion process, and the core objective is to maximize the conversion of SO_2. In order to ensure the conversion rate of SO_2 stable at a high level, entrance temperature in each layer of the converter must be set reasonably. It is usually necessary to determine the set value of entrance temperature in each layer of the converter which can maximize the total conversion rate of SO_2, so that the process of SO_2 conversion can achieve the best operating state. The problem was studied by Yu (2009), in which genetic algorithm was used to optimize the setting, but the model mismatch problem was not considered.

The premise for the optimization of SO_2 conversion process is to establish an accurate process model. The mechanism model of SO_2 conversion process is composed of the thermodynamic and kinetic reaction rate model during SO_2 conversion reaction. Because of the limitation of actual production, there is uncertainty with the model parameters, which makes it quite difficult to establish the model which is completely matched with the actual acid production process. There are two main causes for the uncertainty. First come the uncertainty, randomness and unpredictability of object features. In the process of SO_2 conversion, the activity of the catalyst will change during the reaction, but it is difficult to be described quantificationally. Poison correction coefficient is a quantity related to the activity of the catalyst with uncertainty. The second one derives from fitting a complex process system with a simple model. Additionally, the model fitting become more complex because data are often noisy and it is always

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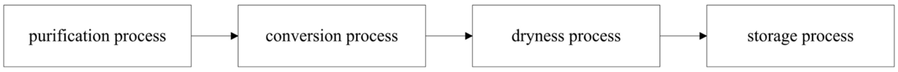

Fig. 1 – The process of acid production with flue gas.

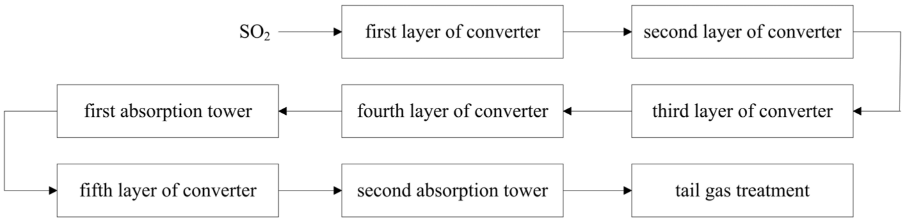

Fig. 2 – The SO_2 conversion process in the production process of gas acid-making.

hard to identify the process with signals that carry little information. Therefore, by the use of imprecise model, we may get suboptimal results, even infeasible results when there are constraints.

There are mainly two kinds of optimization methods used to deal with uncertainty (Chachuat et al., 2009). The main difference lies in whether to use measurement information in the calculation of the optimization strategy. Robust optimization is often used when measurement information is not available, and the feasibility for the whole range of the expected change is guaranteed by introducing conservatism. When measurement information is available, the adaptive optimization, also known as real-time optimization (Mark et al., 2011), can help to adapt to the process change and disturbance, so as to reduce the conservatism (Chachuat et al., 2009). In recent years, some scholars have studied the optimization problem of mismatched model. Here are some examples. An integrated batch-to-batch and within batch optimization approach was proposed for real-time optimization of uncertain batch processes by Ye et al. (2014). According to the different forms of input variables, parameters were transformed into a number of scalar sub trajectories and decision variables. Within batch optimization strategy was used for gradient trajectories, while batch-to-batch optimization strategy was used for active terminal constraint and real-time optimization was realized by feedback control approach. In one study of Zhu and Ma (2014), a robust optimization method of improved EOQ model based on the Kriging model was proposed considering the uncertainty of the purchase cost in the classical EOQ (economic order quantity) model, combining the idea of robust parameter designing with Kriging model method. In one study of Zhang et al. (2014a,b), a constrained programming model with two layers of random chance under the influence of parameter uncertainties was established, and the intelligent optimization algorithm was designed. However, the methods mentioned above are not suitable to solve the problem in this paper, as they have a strong pertinence to their own research objects. Real-time optimization method is a kind of optimization method with general adaptability, which has been paid more and more attention by researchers in recent years. In one study of Zhang et al. (2014a,b), the effect of model uncertainty on the optimization results was reduced by the modifier-adaptation method for real-time optimization. The scheme not only converged to the KKT (Karush–Kuhn–Tucker) point (François and Bonvin, 2013; Marchetti and Basualdo, 2012; Marchetti et al., 2009) of the practical model of the plant, but also showed a faster convergence rate. It provides good ideas to solve the optimization problem of SO_2 conversion process in the case that the parameters are mismatched.

This paper focuses on a modifier-adaptation strategy with regulatory factors for real-time optimization of SO_2 conversion process during the acid production process with flue gas, taking full consideration of the plant-model mismatch. It is organized as follows. Sulfuric acid production process with flue gas and the SO_2 conversion process are introduced in Section 2. Section 3 describes the modifier-adaptation approach. The optimization problem for converter inlet temperature is given. The modifier-adaptation method is tested in sulfuric acid production process in Section 4, and conclusions are presented in Section 5.

2. Process of SO_2 conversion

2.1. *Technological process*

The process of acid production with flue gas is shown in Fig. 1.

In the process of acid production with flue gas, off-gas from the smelter flows into the purification process firstly. After dust, acid mist, arsenic, fluoride and other harmful impurities in the flue gas are removed in this process, the off-gas flows into the conversion process. Under certain temperature, SO_2 in flue gas reacts with oxygen to form sulfur trioxide through the catalytic effect of catalyst. Sulphur trioxide produced in the conversion process reacts with water in concentrated sulfuric acid to generate sulfuric acid.

As we can see in Fig. 2, the SO_2 conversion process in the production process of gas acid-making for a smelting plant is investigated in this paper. The technology of '4 + 1' and double conversion is used in the conversion process in which there is a total of five layers (Yu, 2009). Flue gas from smelters is absorbed in the first absorption tower for the first time after getting through the first four layers of converter. Then it enters the fifth layer of converter, and is absorbed in the second absorption tower for the second time. The conversion of SO_2 is an exothermic reversible reaction. The reaction equation is shown in formula (1) (Schwämmle et al., 2013).

$$SO_2 + \frac{1}{2}O_2 \overset{catalyst}{\leftrightarrow} SO_3 + Q \tag{1}$$

2.2. *Mechanism model*

(1) Equilibrium conversion

Under certain reaction conditions, such as the temperature, the concentrations of SO_2 and O_2, and so on, the maximum conversion rate of SO_2 is known as the equilibrium conversion rate. Equilibrium conversion rate can be expressed as

$$X_T = \frac{K_P}{K_P + \sqrt{\frac{100-0.5aX_T}{b-0.5aX_T}}} \tag{2}$$

where a, b are the concentrations of SO_2 and O_2 in the mixture of the original gas in volume fraction, %; X_T indicates the equilibrium conversion rate, %; K_P is the equilibrium constant.

(2) Reaction rate of SO_2