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Influence of Design Margin on Operation Optimization and Control Performance of Chemical Processes*

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Abstract Operation optimization is an effective method to explore potential economic benefits for existing plants. The maximum potential benefit from operation optimization is determined by the distances between current operating point and process constraints, which is related to the margins of design variables. Because of various disturbances in chemical processes, some distances must be reserved for fluctuations of process variables and the optimum operating point is not on some process constraints. Thus the benefit of steady-state optimization can not be fully achieved while that of dynamic optimization can be really achieved. In this study, the steady-state optimization and dynamic optimization are used, and the potential benefit is divided into achievable benefit for profit and unachievable benefit for control. The fluid catalytic cracking unit (FCCU) is used for case study. With the analysis on how the margins of design variables influence the economic benefit and control performance, the bottlenecks of process design are found and appropriate control structure can be selected.
Keywords design margin, operation optimization, control performance, bottleneck, fluid catalytic cracking unit (FCCU)

1 INTRODUCTION

Operation optimization is an effective method to explore potential economic benefits for existing chemical plants, while the economic benefits from operation optimization depend on the margins of design variables. According to the demand for optimal design of chemical process, the steady-state operating point of the optimal design generally lies on the boundaries of process constraints. In operations, process variables should be restricted within active constraints on condition that they are "hard". However, the effect of disturbances and uncertainties in real processes usually perturb the plant from the desired steady-state optimum operating point, violating some active constrains, so the plant can not run at the desired steady-state optimum operating point. To ensure operating feasibility and production goals, sufficient margins must be added on the design variables, then the operating point will move into the feasible region and there are proper distances between current operating point and active constraints. The magnitudes of the distances lead to the back-off of process economic performance but provide free space for operation optimization.

The margins of design variables will directly influence process operation and control performance. When process conditions change or disturbances occur, the process variables change with time dynamically, which are generally damped oscillation processes because of the process control system. The dynamic process must be considered in design margins, otherwise the process control system can not work. Xu and Luo [1–4] have pointed out that, for conventional proportional-integral-differential (PID) control or for model predictive control, design margins for control and operation must be considered and their sizes are related to process control system. The better control performance is requested, the more margins are required. Larger margin may bring more flexibility in operation and control, but requires larger equipment investment and operating costs.

A number of methodologies have been developed for addressing the interactions between process design and process control. Previous researches about margin analysis, operatability and control performance evaluation, and integration of process design and control are as follows.

(1) Process controllability assessment. When considering process uncertainty, the evaluation of open and closed-loop controllability indicators of different process designs allows the comparison and classification of alternatives in terms of operational characteristics, such as the metric of open-loop controllability [5], dynamic economic impact of disturbance and uncertain parameters [6, 7], and flexibility and resilience analysis [8–10].

(2) Simultaneous design and control. More systematic efforts are on the context of interactions of design and control to design economically optimal processes that could operate in an efficient dynamic mode within an envelope around the nominal point. Economics-based performance index and control performance are usually considered based on dynamic model, and possible disturbances and uncertainties are taken into account. Dynamic optimization is employed in order to determine the most economic process design and control system that satisfies all dynamic operability constraints. There are several aspects about the problem such as

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control algorithm, optimization algorithm, quantification of disturbances and parametric uncertainty. After years of development, control algorithms have extended from conventional PID control [11] to optimal control [12, 13], predictive control [14], and internal model control [15]. Optimization algorithms have developed from the conventional nonlinear programming [16] to the heuristic particle swarm optimization (PSO) algorithm [17], and the robust control tools based on Lyapunov theory and structured singular value analysis are used to estimate the bounds on process worst-case variability, process feasibility, and process stability [18–20]. The applied processes have extended from distillation column [21] to polymerization reactor [22–24]), crystallization reactor [25] and so on.

(3) Margin analysis and control design based on dynamic models. Xu and Luo [1–4] have integrated margin analysis methods into the optimized process and control design. It is found that the design margin should be divided into steady-state margin and dynamic margin, and the dynamic margin is necessary for control and is related to control system. In process design the control performance and design margins should be considered as a whole in order to fulfill process demand and achieve good control performance.

In the presence of design margins, the distances between current operating point and active constraints provide certain space for operation optimization. The steady-state operation optimization is often used for more economic benefit. However, there are various disturbances and process variables always vary in chemical processes, and some distances between the optimum operating point and process constraints must be reserved for dynamic regulations of control system, so the operation optimization can not fully explore the space from design margins and the benefit of the steady-state operation optimization can not be fully achieved. Only the benefit from dynamic operation optimization considering dynamic responses of process variables can be really achieved.

In this paper, steady-state optimization and dynamic optimization are used to evaluate the potential benefit of FCCU, which is divided into achievable benefit for profit and unachievable benefit for control. To explore how the margins of design variable influence the economic benefit and control performance, the bottlenecks of process design could be found and appropriate control structure could be selected.

2 OPERATION OPTIMIZATION AND DESIGN MARGIN

An ideal process should be designed to achieve optimal economic performance while meeting all process constraints. The optimal design is given by

$$\min F(\boldsymbol{x},\boldsymbol{d},\boldsymbol{u}) \tag{1a}$$

$$\text{s.t.}\quad \boldsymbol{f}(\boldsymbol{x},\boldsymbol{d},\boldsymbol{u})=0 \tag{1b}$$

$$\boldsymbol{g}(\boldsymbol{x},\boldsymbol{d},\boldsymbol{u})\leqslant 0 \tag{1c}$$

where vector $\boldsymbol{x}$ represents the state variables, $\boldsymbol{d}$ represents the design variables, $\boldsymbol{u}$ represents the manipulation variables, $\boldsymbol{f}(\cdot)$ the equations of process model, $\boldsymbol{g}(\cdot)$ the equations of process constraints, and F is the objective function of optimal design, involving equipment investment cost and operating cost. With the steady-state optimization, the optimal design ($\boldsymbol{x}^*$, $\boldsymbol{d}^*$, $\boldsymbol{u}^*$) can be obtained.

To solve the optimal design problem, we define the Lagrange function as

$$L(\boldsymbol{x},\boldsymbol{d},\boldsymbol{u})=F(\boldsymbol{x},\boldsymbol{d},\boldsymbol{u})+\boldsymbol{\lambda}^{\mathrm{T}}\boldsymbol{f}(\boldsymbol{x},\boldsymbol{d},\boldsymbol{u})+\boldsymbol{\mu}^{\mathrm{T}}\boldsymbol{g}(\boldsymbol{x},\boldsymbol{d},\boldsymbol{u}) \tag{2}$$

where $\boldsymbol{\lambda}$ is the Lagrange multiplier vector of equality constraints and $\boldsymbol{\mu}$ is the Lagrange multiplier vector of inequality constraints.

Let i and j represent the active set and non-active set of inequality constraints respectively. For the active set, the optimal solution is on the boundaries of process constraints $g_i(\cdot)=0$, with corresponding Lagrange multiplier $\mu_i\geqslant 0$. For the non-active set, the optimal solution is within the boundaries of process constraints $g_j(\cdot)<0$, with corresponding Lagrange multiplier $\mu_j=0$.

According to the first-order necessary conditions of local extremum for constrained nonlinear programming, a sensitivity analysis is carried out on ($\boldsymbol{x}^*$, $\boldsymbol{d}^*$, $\boldsymbol{u}^*$),

$$\frac{\partial F(\cdot)}{\partial \boldsymbol{x}}\Delta\boldsymbol{x}+\boldsymbol{\lambda}^{\mathrm{T}}\frac{\partial \boldsymbol{f}(\cdot)}{\partial \boldsymbol{x}}\Delta\boldsymbol{x}+\boldsymbol{\mu}^{\mathrm{T}}\frac{\partial \boldsymbol{g}(\cdot)}{\partial \boldsymbol{x}}\Delta\boldsymbol{x}=0 \tag{3a}$$

$$\frac{\partial F(\cdot)}{\partial \boldsymbol{d}}\Delta\boldsymbol{d}+\boldsymbol{\lambda}^{\mathrm{T}}\frac{\partial \boldsymbol{f}(\cdot)}{\partial \boldsymbol{d}}\Delta\boldsymbol{d}+\boldsymbol{\mu}^{\mathrm{T}}\frac{\partial \boldsymbol{g}(\cdot)}{\partial \boldsymbol{d}}\Delta\boldsymbol{d}=0 \tag{3b}$$

$$\frac{\partial F(\cdot)}{\partial \boldsymbol{u}}\Delta\boldsymbol{u}+\boldsymbol{\lambda}^{\mathrm{T}}\frac{\partial \boldsymbol{f}(\cdot)}{\partial \boldsymbol{u}}\Delta u+\boldsymbol{\mu}^{\mathrm{T}}\frac{\partial \boldsymbol{g}(\cdot)}{\partial \boldsymbol{u}}\Delta\boldsymbol{u}=0 \tag{3c}$$

For the process state equation $\boldsymbol{f}(\cdot)$, the first-order Taylor expansion is implemented at the steady-state optimal design point ($\boldsymbol{x}^*$, $\boldsymbol{d}^*$, $\boldsymbol{u}^*$),

$$\frac{\partial \boldsymbol{f}(\cdot)}{\partial \boldsymbol{x}}\Delta x+\frac{\partial \boldsymbol{f}(\cdot)}{\partial \boldsymbol{d}}\Delta\boldsymbol{d}+\frac{\partial \boldsymbol{f}(\cdot)}{\partial \boldsymbol{u}}\Delta\boldsymbol{u}=0 \tag{4}$$

Adding Eqs. (3a), (3b) and (3c), we obtain

$$\Delta F+\boldsymbol{\mu}^{\mathrm{T}}\Delta\boldsymbol{g}=0 \tag{5}$$

For non-active constraints, there is Lagrange multiplier $\mu_j=0$. The non-active constraints can be removed from Eq. (5),

$$\Delta F+\sum_i \mu_i\Delta g_i=0 \tag{6}$$

The steady-state operating point of the optimal design generally lies on the boundaries of some process constraints, which are active constraints $g_i(\cdot)=0$. Because these active constraints are "hard", process variables should be restricted within them when process runs. Since some uncertainties may violate active constrains, the margins $\Delta\boldsymbol{d}$ must be added to the design variables $\boldsymbol{d}^*$, then the operating point will move