Optimal controlled variable selection using a nonlinear simulation-optimization framework

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Abstract

In feedback control, controlled variables are those process variables which are measured and fed back to controllers. Then in the presence of disturbances, controllers by the means of manipulating the inputs aim to maintain the controlled variables at their setpoints. The objectives for the selection of controlled variables can be conflicting and competing. These objectives include minimization of (1) economic losses, (2) input manipulations, (3) output variations and (4) changes in process states. This research aims to present a systematic framework for optimal selection of controlled variables. Each of the above-mentioned objectives is defined within a multi-objective function. In addition, the reasoning behind the selection of nonlinear steady state model is explained. The proposed methodology is benchmarked on an industrial distillation train. Optimization programming is presented and the paper discusses how the size of the optimization problem can be reduced by means of engineering insights and addressing the concerns regarding feasibility of the developed control structure. The methodology is scalable to large industrial problems, while maintaining its rigour. The results confirm that a very good trade-off is established between different objectives.

Keywords: controlled variables, optimal control, simulation-optimization, profitability.

1. Introduction

Some process variables are more important than others, in that if they are optimally controlled, they ensure optimal operation of the process (Morari, 1980). The decision regarding optimal selection of controlled variables is at a higher level than pairing controlled and manipulated variables. The optimal controlled variable benefits an on-line optimizing control structure in that maintaining these controlled variables at their setpoints maximizes profitability and minimizes the requirement for setpoint manipulation. In addition, in a control structure with constant setpoint policy, optimal controlled variables induce a self-optimizing framework, (Skogestad, 2000).

This paper presents a simulation-optimization framework for the optimal selection of the controlled variables. Its novel contributions are: (i) it explicitly establishes a trade-off between conflicting and competing desirable properties of controlled variable, (ii) operability of the process is ensured through nonlinear modelling. As a result, the method is not limited to linearization region, and (iii) engineering insights are used to reduce the size of the problem. Thus, although the methodology systematically addresses the problem, the formulation is manageable and practicable.

The paper is organized as follows. Section 2. discusses the selection of optimization variables, mathematical statement of the problem, and the reasoning behind the selection of the type of model. Optimal selection of controlled variables for an
industrial distillation train is presented in Section 3. It is explained how engineering insights are employed to reduce the problem size. The results are discussed in Section 4.

2. Problem formulation

This section discusses the methodology for formulating the optimal selection of controlled variables as an optimization problem.

2.1. Selection of which controlled variables are going to be optimized

Two categories of controlled variables are imposed by the process and are exempt from the economic optimization. Firstly, as discussed by Luyben (1998), control structure selection must ensure consistency and feasibility of the process operation such as setting throughput, ensuring total and component mass balances (i.e. inventory controls), and energy management. Secondly, during process optimization some inequality constraints become activated. An example is the reactor temperature, limited by catalyst tolerance. Such a variable cannot be included in economic optimization because higher values invoke technical concerns and lower values involve degradation of the profitability. Therefore, there is no choice of whether to control or not, because it must be controlled.

2.2. Mathematical statement

The following mathematical statement of the problem is adopted from Halvorsen (2003), but is not restricted to the linear case. The overall objective function can be expressed in terms of maximization of profits or minimization of losses:

\[ y = \text{arg}(\min Z(u, x, d)) \quad \text{subject to: } g_1(u, x, d) = 0, \ g_2(u, x, d) \leq 0 \]  

In the above, \( u \) is a vector\(^1 \) of manipulated variables (also called inputs), \( d \) is a vector of disturbances that independently influence the process. Vector \( x \) represents state variables. Some state variables can be measured directly, but the rest, if needed, must be estimated. Vector \( y \) represents the vector of controlled variables (also called outputs) which is selected from the measurable state variables. Vector \( g_1 \) represents equality constraints such as the process model and vector \( g_2 \) represents inequality constraints, such as technical, safety or environmental concerns. State variables can be calculated from equality constraints, in terms of disturbance and input variables:

\[ y = \text{arg}(\min Z(u, d)) \quad \text{subject to: } g_2(u, d) \leq 0, \ x = g_3(u, d) \]  

As discussed above, when an inequality constraint becomes active during optimization of the process, it changes to an equality and therefore removes a degree of freedom. Consequently, the initial set of manipulated variables \( u \) will be reduced to \( [u^r] \in [u] \):

\[ y^r = \text{arg}(\min Z(u^r, d)) \quad \text{subject to: } g_2^r(u^r, d) = 0, \ x = g_3(u, d) \]  

where superscript \( r \) represents the reduced search space. More insights can be achieved about the problem [3] by examining the fact that disturbances occur independently, while the inputs will be determined by solving the optimization problem. Therefore, the value of objective function depends on the value of disturbances only, and is a function only of disturbance variables:

\[ Z_{\text{opt}} = Z^r_{\text{opt}} = Z(d) \]  

2.3. Objective functions and optimization variables

This sub-section discusses optimization objectives, i.e. which indices can measure the fitness of candidate controlled variables. The proposed objective functions are listed in Table 1 and will be discussed in the following.

The implication of the first objective, \( f_1 \), is that maintaining the candidate controlled variables at their setpoints must guarantee the specification of products. The second objective, \( f_2 \), aims to minimize changes in manipulated variables, in order

\(^1\) In this paper, the **bold** case is reserved for vectors and scalar values are shown by *italics*. 
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to avoid valve saturation (thus, maintaining controllability), to reduce the interaction between process variables, to minimize the consumption of inputs, and to minimize the required time for disturbance rejection, (Qin, 2003; McAvoy, 1999).

The third objective $f_3$ measures the resistance of the closed loop process against disturbances when the controlled variables are maintained at their setpoints. An example of this objective is the changes in the temperature profile of a distillation column when flow or composition of feed is disturbed. The implication of the above three objectives is to minimize trajectories between ultimate steady states of the process, hence minimizing the required control time and efforts.

The fourth objective concerns operational loss, i.e. decrease in profitability due to disturbances. The origin of this objective refers to the notion of self-optimizing control and its implication is that maintaining the optimal controlled variables at their setpoints must minimize losses in the presence of disturbances, (Skogestad, 2000).

2.4. The simulation-optimization framework

The equality constraint of Problem [2] in the linear form, is as below:

$$ y = G_2 \times u + G_{3,d} \times d \rightarrow u = G_2^{-1} \times y - G_{3,d}^{-1} \times G_{3,d} \times d \quad [5] $$

where $y$ is subset of state variables which are selected as controlled variables. The implication of equation [5] for optimal selection of controlled variables is that for each set of controlled variables a specific linearized model $G_3$ must be constructed and the model matrix must be inverted, $G_3^{-1}$. This model matrix, however, is not always invertible or a good approximation, resulting in inoperable designs. Therefore, a nonlinear model is employed, in which inverse model is replaced by the simulation.

Figure 1 shows the proposed simulation-optimization framework. The simulator is based on the first principle laws. The disturbance model represents the uncertainty associated with independent exogenous variables which affect the process, such as changes in the flow or composition of the feed. When the selected controlled variables, decided by the optimizer, are set in the simulation software, the disturbance scenarios are imposed to the model and then the consequence of controlling these choices of controlled variables will be evaluated through the objective functions. The result will be reported to the optimizer.

3. Case study

This section discusses process description and engineering insights regarding the benchmarking problem.

3.1. Process description of pyrolysis gasoline hydrogenation (PGH) plant

The case study is adapted from the olefin plant of Arak Petrochemical Co. The process
description for the overall olefin plant is available in the literature (e.g. Othmer 2007). In the products of olefin plant, there is a blend with properties very similar to gasoline. The disadvantage of this product is that the dissolved light olefins are highly reactive with risk of polymerization, if are stored untreated. Therefore, this blend must be saturated by hydrogenation reactions. Then, a sequence of three distillations will separate \( C_5, C_6, C_7 \) and heavy-ends products. The process schematic is shown in Figure 2. The distillation train, studied in this research, is enframe on the lower right hand side of the Figure 2. The first column, depentanizer, has three products. The column has a partial reflux configuration and the gaseous overhead product is mostly hydrogen. The main product is \( C_6 \) cut, and is withdrawn as the side stream. The bottom stream is fed to the dehexanizer column. The \( C_6 \) cut is produced as the top product and the bottom stream is fed to a vacuum (last) column to be resolved to \( C_7 \) and heavy-ends.

The required computational effort of simulating the process is relatively high because the pyrolysis gasoline must be estimated by 34 components. The modified Peng-Robinson equation of state is applied for thermodynamic calculation (Aspen-HYSYS(V7.1)). The simulation is performed using Aspen-HYSYS® and the optimization algorithm is GA® toolbox of MATLAB® which is linked to Aspen HYSYS using COM® automation interface as the client. The feed stream to the depentanizer column is assumed as disturbance. The feed can be interpreted as the mixture of four products: \( C_6, C_6, C_7 \) and heavy-ends cuts. Assuming ±5% disturbance in each of these cuts, there are sixteen disturbance scenarios in flowrate and composition of the feed.

3.2. Reducing the size of optimization problem
As discussed in Section 2.1., those controlled variables associated with feasibility and consistency of control structure are decided in advance (explained below). In addition, the design space is limited to the controlled variables with reasonable measurement characteristics. These concerns can be employed to manage the size of the problem.

Degree of freedom analysis: if the feed is assumed as disturbance, then, in a total reflux column, there are five degrees of freedom including boil-up, cooling duty, reflux, and the flowrates of the overhead and bottom products. However, controlling the overhead and bottom level of liquid inventories, and column pressure of vapor inventory consume three degrees of freedom, and two degrees of freedom remain. In a column with side product stream, there is an extra degree of freedom.

Inferential control: having liquid level and pressure control loops closed, the distillation column is still unstable due to composition drift, (Skogestad 2007). However, direct measurement of the composition with an analyzer is expensive and involves delays. Therefore, temperatures should be measured for inferential composition control, (Luyben, 2005; Luyben 2006).

Flow control: If a degree of freedom remains from the last decisions, a flow or flow-ratio variable (D, B, R, D/F, R/F, B/F) will be selected.

4. Results of the case study
Table 2. presents the result of the simulation-optimization program. These include the controlled variables, which are selected by the optimizer for each distillation column. Table 3. shows that a very good trade-off between different competing objective functions is established. The implication is that while the manipulated variables are preserved from excessive movement in different disturbance scenarios, operational costs are minimized; the products specifications are met and minor changes in average
temperature profiles indicates short trajectories between different process steady states. For the case of distillation columns, process insights can be employed to partition the manipulated and control variables. For more complex processes (e.g. heat integration or recycle streams) RGA or RHP zeros analysis can be applied (Pham 2009). Assuming a decentralized control structure, Figure 3 shows the final control structure including the selected controlled variables for optimization and liquid/vapor inventories.

5. Conclusion

In this research, an optimization-simulation framework is presented for optimal selection of controlled variables. The criteria for selection of controlled variables are explained and a steady state simulation is employed for modelling, in order to avoid unnecessarily increasing the size of the problem. In addition, it is explained why nonlinear model is needed for ensuring operability of the closed loop process. The proposed methodology is benchmarked on an industrial case study of a distillation train. Engineering insights are applied to reduce the size of problem. The results show a very good trade-off between different objective functions is established which ensure controllability and profitability of the control structure. In addition, the methodology is not limited to the linearized space and is scalable and practicable to industrial problems.

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