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A METHODOLOGY FOR CONTROL STRUCTURE SELECTION BASED ON RIGOROUS PROCESS MODELS

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Abstract: In this contribution, a systematic procedure for control structure selection based on rigorous models is presented. The basic idea is that a feedback controller that regulates certain measurable quantities to their set-points should steer the process towards its economic optimum in the presence of disturbances and model uncertainties. This part of the analysis is performed for the stationary behaviour of the regulated process, dynamic aspects are considered in a second step where the dynamic controllability of the economically superior structures is assessed. The stationary analysis is performed for rigorous nonlinear plant models. The methodology is applied to a reactive distillation process.

Keywords: Control Structure Selection, Integrated Processes, Reactive Distillation

1. INTRODUCTION

Control structure selection deals with the choice of measured and manipulated variables that are used for feedback control. This selection is of particular importance in chemical process control, where a considerable number of degrees of freedom and of measurements is available and the choice of the controlled and of the manipulated variables and of the controller structure is by no means trivial. Most of the available literature in this area focuses on the dynamic controllability analysis based upon linear process models. The state of the art is well described in the recent book (Seferlis and Georgiadis, 2004). Several authors have also investigated the issue of control structure selection from the point of view of the performance and operability of the controlled plant rather than focussing on the ability of the control structure to regulate the chosen variables well. Several important aspects of the control of chemical processes were discussed in the early contribution by (Morari *et al.*, 1980). Shinnar and co-authors developed the concept of partial control in a series of papers, evolving around the example of the operation of catalytic crackers (Arbel *et al.*, 1995*b*), (Arbel *et al.*, 1995*a*), (Arbel *et al.*, 1996), (Arbel *et al.*, 1997), (Shinnar *et al.*, 2000). In their approach, the final choices were strongly influenced by their knowledge about how the operators would run the type of plants under consideration what allowed them, for example, to justify a control structure that was not recommended by the RGA analysis.

In many contributions, engineering insight and simulations are used to arrive at a suitable control structure for a given plant. A recent representative is (Al-Arfaj and Luyben, 2002).

Skogestad (Skogestad, 2000) advocated to choose the regulated variables such that a profit function is maximized in the presence of disturbances by keeping the controlled variables close to their set-points. This approach was applied to the Tennesee Eastmann Process (Larsson *et al.*, 2001), as well as to others (Larsson *et al.*, 2003).

A different approach is taken in (Schenk *et al.*, 2002). Here the choice of the control structure as well as the computation of the controller parameters is included in the optimization of the plant design, leading to

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a large mixed-integer dynamic optimization problem. The structure of the individual controllers is fixed a priori, e.g. as PI controllers. Despite the admirable progress in the solution of large mixed-integer optimization problems in recent years, convergence problems are usually encountered and a suitable initialization is crucial for the success of this approach.

We therefore propose a stepwise approach, were first promising control structures are found from a stationary analysis, followed by dynamic controllability analysis (without assuming a fixed control structure), and finally the computation and testing of fixed-structure controllers. In this paper, the focus is on the stationary analysis. We proceed along the same line of thinking as (Skogestad, 2000) but refine the approach in several respects. In general, we aim at the replacement of informed judgements by objective criteria and optimization wherever possible.

The paper is structured as follows: First the general idea is presented. Then the realization of the approach by the solution of a sequence of optimization problems is described in detail. The method is then applied to a reactive distillation process and conclusions for further research are drawn.

2. CONTROL STRUCTURE SELECTION FOR OPTIMAL PLANT PERFORMANCE

From a process engineering point of view, the purpose of automatic feedback control (as well as that of manual control) is not to keep some variables at their set-points as well as possible or to nicely track set-point changes but to establish a close-to-optimal operation of the plant under the presence of disturbances and while the model used for plant design does not represent the real process exactly so that an operating regime that was optimized for the plant model will not lead to an optimal operation of the real plant. While an online optimization of the available degrees of freedom based upon a full nonlinear model in order to maximize the profit over a finite horizon is nowadays possible for slow processes see e. g. (Engell and Toumi, 2004), in industrial practice usually feedback (or manual) control of selected variables is preferred to counteract the effect of disturbances and plant-model mismatch because of the simplicity and reliability even of multivariable controllers compared to online optimization.

From a process optimization point of view, the purpose of feedback control is to set the process inputs if disturbances or plant-model mismatch are encountered such that a (fictitious) online optimizing controller is approximated. In other words, the goal is to establish a relation between the manipulated variables $\underline{u}$ and the disturbances $\underline{d}$ such that the function $\underline{u}_{con} = f(\underline{y}_{set}, \underline{d}_i)$ which is (implicitly) realized by regulating the chosen variables to their set-points is an approximation of the optimal input $\underline{u}_{opt}(\underline{d}_i)$. The effect of feedback control on the profit function J under the presence of disturbances can be expressed as

$$\begin{aligned}\Delta J = & J(\underline{u}_{nom}, \underline{d} = \underline{0}) - J(\underline{u}_{nom} \underline{d}_i) \\ & + J(\underline{u}_{nom}, \underline{d}_i - J(\underline{u}_{opt}, \underline{d}_i) \\ & + J(\underline{u}_{opt}, \underline{d}_i) - J(\underline{u}_{con}, \underline{d}_i).\end{aligned} \quad (1)$$

The first term is the loss that is encountered if the manipulated variables are fixed at their nominal values, the second term represents the effect of an optimal adaptation of the manipulated variables to the disturbance $\underline{d}_i$, and the third term is the difference of the optimal compensation of the disturbance and the compensation which is achieved by the chosen feedback control structure. If the first term in (1) is much larger than the second one, or if all terms are comparatively small, then a variation of the manipulated variables offers no advantage, and neither optimization nor feedback control are required for this disturbance. If the third term is not small compared to the attainable profit for optimized inputs for all possible regulating structures, then online optimization or an adaptation of the set-points should be performed rather than just regulation of the chosen variables to fixed set-points.

Equation (1) represents the loss (which may also be negative, i.e. a gain) of profit for one particular disturbance d_i and a fixed control structure. To evaluate the performance of a control structure, the expected value of (1) should be used:

$$\begin{aligned}\Delta J = \int_{-d_{1,max}}^{d_{1,max}} \ldots \int_{-d_{n,max}}^{d_{n,max}} & w(\underline{d}) \, (J(\underline{u}_{nom}, \underline{d}) \\ & - J(\underline{u}_{con}, \underline{d})) \, dd_1 \ldots dd_n\end{aligned} \quad (2)$$

where $w(\underline{d})$ is the probability of the occurrence of the disturbance $\underline{d}$. In practice, $w(\underline{d})$ is usually not known, we therefore approximate (2) by a weighted sum over a set of disturbance scenarios.

In regulating control, errors of the measurements of the controlled variables must be taken into account. E.g. quality parameters often cannot be determined very accurately online in process control. A variable may be very suitable for regulatory control in the sense that the resulting inputs are a good approximation of the optimal inputs in the nominal case, but due to a large measurement error and/or a small sensitivity to changes in the inputs, the resulting values $\underline{u}_{con}$ may differ considerably from the desired values. We take this into account by considering the worst case control performance for regulation to values in a range around the nominal set-point $\underline{y}_{set}$ that is defined by the measurement errors. So for each disturbance scenario $\underline{d}_i$, the performance measure of a control structure (i.e. a selection of measured and manipulated variables) is:

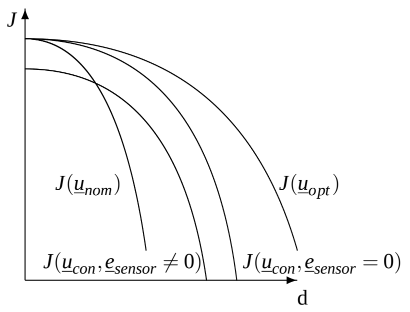


Fig. 1. Schematic representation of the influence of a disturbance on the profit for different control approaches and measurement errors

$$\min_{\underline{u}} J(\underline{u}, \underline{d}_i, \underline{x}) \tag{3}$$
$$s.t.: \quad \dot{\underline{x}} = \underline{f}(\underline{u}, \underline{d}_i, \underline{x}) = \underline{0}$$
$$\underline{y} = \underline{m}(\underline{x}) = \underline{M}(\underline{u}, \underline{d}_i)$$
$$\underline{y}_{set} - \underline{e}_{sensor} \leq \underline{y} \leq \underline{y}_{set} + \underline{e}_{sensor},$$

where $\underline{f}$ represents the plant dynamics. A control structure that yields a comparatively small value of the minimal profit is not able to avoid a poor performance of the process under the presence of measurement errors and hence is not suitable.

Note that this formulation also represents the realistic situation where closed-loop control leads to a worse result than keeping the manipulated variables constant at their nominal value. This may happen for small disturbances, as illustrated by figure 1. It is therefore important to include scenarios with small disturbances and not only those with very large ones into the set of disturbances considered in the analysis. In the next section, we describe how the general idea presented in this section is realized by a step-by-step procedure which provides a number of potential control structures which are suitable from the point of view of profitable operation of the controlled process. Whether these structures are also suitable from the point of view of the dynamics of the closed-loop system is then checked using tools from linear control theory.

3. CONTROL STRUCTURE SELECTION PROCEDURE

3.1 *Definition of the optimization problem*

The investigation starts with an analysis of the degrees of freedom of the process which are available during plant operation. These degrees of freedom are the same for online optimization and for regulatory control. The profit function J has to be defined and constraints of the process must be formulated mathematically.

3.2 *Selection of disturbances*

The second step is to define the disturbance scenarios. In contrast to (Skogestad, 2000) we distinguish between disturbances (including plant-model mismatch) and measurement errors. The size of the measurement errors usually can be estimated, e.g. from the manufacturers' data-sheets. Worst case disturbances are computed by performing a minimization of the profit that is obtained by optimal adaptation of the manipulated variables:

$$\underline{d}_{max} = \text{argmin}(\max_{\underline{u}} J(\underline{u}, \underline{d})). \tag{4}$$

As mentioned before, smaller disturbances are also considered, as the worst case is not typical for the day-to-day operation of the process and the performance of a control structure can be qualitatively different for large and for small disturbances due to the effect of measurement errors. Each disturbance scenario $\underline{d}_i$ is investigated individually in an optimization (eq. 3). The results of different control structures are compared using a weighted sum of the values of the objective function for the chosen scenarios.

3.3 *Pre-selection of controlled variables*

In this approach, the resulting worst case profit is computed for each control structure and each disturbances scenario. As the number of structures increases rapidly with an increasing number of measurements and manipulated variables, as given by

$$C_n^k = \begin{pmatrix} n \\ k \end{pmatrix} = \frac{n!}{(n-k)! \;\; k!} \tag{5}$$
$$\text{with } n = dim(\underline{y}) \text{ and } k = dim(\underline{u}),$$

an a priori exclusion of unsuitable variables is very useful or even necessary for larger problems. Usually the key problem is the selection of the controlled variables because the number of available measurements is larger than the number of manipulated variables. A set of measured variables is unsuitable for control if the resulting inputs under closed-loop control are too sensitive to the sensor errors. The sensor errors usually are small compared to the absolute values, so a linear analysis is justified here. Let

$$\underline{u}_{con} = \underline{h}(\underline{y}_{set}, \underline{d}) \tag{6}$$

denote the dependency of the manipulated variables on the measurements ($\underline{h}$ is the inverse of the measurement mapping $\underline{y} = \underline{M}(\underline{u}, \underline{d})$. Then the sensitivity of $\underline{u}$ for small measurement errors is given by the Jacobian of $\underline{h}$, and the normalized matrix

$$\underline{S} = \text{diag}(\Delta\underline{u})^{-1} \frac{\partial \underline{h}}{\partial \underline{y}} \text{diag}(\underline{e}_{sensor}) \tag{7}$$

where

$$\Delta\underline{u} = \max_{\underline{d}}(\text{argmax} J(\underline{u}, \underline{d})) \tag{8}$$
$$- \min_{\underline{d}}(\text{argmax} J(\underline{u}, \underline{d}))$$

represents the normalized propagation of the sensor errors to the manipulated variables. Small singular values of $\underline{S}$ indicate a small influence of the sensor errors. Therefore structures with a large maximal singular value of S are excluded, because for these structures either some measurement error is comparatively large or the sensitivity of some measurements to the inputs is small or the measurements are not independently influenced by the inputs such that the mapping $\underline{M}$ is ill-conditioned.

3.4 *Selection of the set-points for regulatory control*

A simple choice of the set-points of the regulated variables would be to choose them as the values which result for optimal operation under nominal conditions (i.e. no plant-model mismatch, no disturbances). This however underestimates the potential of feedback control. We therefore determine the set-points $\underline{y}_{set}$ by optimization over the set of disturbance scenarios.
The optimal set-point results from solving

$$\max_{\underline{y}_{set}} \sum_{i=1}^{n} J(\underline{u}_{i,con}, \underline{d}_i) \quad (9)$$

$$\begin{aligned} &\text{s.t.: } \forall \underline{d}_i : \\ &\quad \dot{\underline{x}} = \underline{f}(\underline{u}_{i,con}, \underline{x}, \underline{d}_i) = 0 \\ &\quad \underline{y}_{set} = \underline{m}(\underline{x}) = \underline{M}(\underline{u}_{i,con}, \underline{d}_i) \\ &\quad \underline{u}_{min} \leq \underline{u}_{i,con} \leq \underline{u}_{max} \\ &\quad \underline{x}_{min} \leq \underline{x} \leq \underline{x}_{max}. \end{aligned}$$

Note that the constraints on the inputs and on the state variables in (9) may be infeasible, indicating that this control structure is unsuitable for regulatory control to a fixed set-point because there exists no set-point that can be attained for all disturbances considered for the given constraints on the process inputs and process states.

3.5 *Quantitative evaluation of the benefits of the control structures*

For all scenarios $\underline{d}_i$, the optimization problems (3) are solved and the weighted sum of the values is determined. This yields the expected worst-case profit for each structure. In addition, maximization instead of minimization in (3) over the possible sensor errors may be performed. If the results of the two computations are close to each other, the selected variables constrain the process efficiently, whereas a large difference indicates that constraining this set of variables does not constrain the inputs very strongly. Some of the variables then are not efficient to control the process.

3.6 *Dynamic analysis*

Steps 3.1-3.5 yield an ordered set of control structures which are attractive with respect to the expected profit for stationary or slowly varying disturbances. It is however possible (if not likely) that some of these structures are not suitable for dynamic operation. Dynamic controllability is therefore assessed in the next step using linear techniques. The approach used is described in detail in (Engell *et al.*, 2004). The key idea is that after using performance indices to exclude e.g. structures with small right half plane zeros, the attainable dynamic performance is computed over all stabilizing linear time-invariant controllers. The corresponding controllers are of high order. For a detailed analysis of the resulting dynamic performance, these controllers are approximated by low-order controllers with prescribed structure by the method described in (Müller *et al.*, 1995) and then tested in simulations with the rigorous dynamic model.

4. EXAMPLE: REACTIVE DISTILLATION

The methodology described above is applied to the reactive distillation column for the production of methyl acetate shown in figure 2. The column with an inner

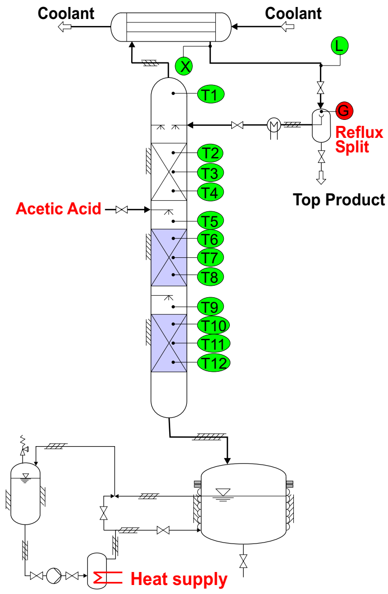


Fig. 2. Reacitve Distillation Column

diameter of 100mm is operated at our university as a pilot plant. Its height is about six meters. The column has three packings of one meter height each. The upper packing is used for separation, while the two lower packings include an ion exchange resin to catalyze the chemical reaction of methanol (MeOH) and acetic acid (HAc) to methyl acetate (MeAc) and water:

$$MeOH + HAc \rightleftharpoons MeAc + H_2O.$$

The reaction is an equilibrium reaction and the resulting mixture is difficult to separate. By integrating reaction and distillation, pure methyl acetate can be obtained at the top (Agreda *et al.*, 1990) and (Huss *et al.*, 2003). In our case, the re-boiler is filled with methanol at the beginning of the batch and the by-product water accumulates in the re-boiler. We assume that the trajectory of the acetic acid flow over the batch run is given as the result of an optimization as described in (Engell and Fernholz, 2003) while the reflux ratio and the heat supply are operating degrees of freedom. Measurable variables are four temperatures in each packing, the distillate flow, and the molar fractions in the distillate stream. For a conventional square control structure, there are

$$\begin{pmatrix} \dim(\underline{y}) \\ \dim(\underline{u}) \end{pmatrix} = \begin{pmatrix} 17 \\ 2 \end{pmatrix} = \frac{17!}{(17-2)!2!} = 136$$

possibilities to control two measured variables by the two available manipulated variables.

The objective function for this process describes the earnings from the main product minus the costs of methanol and heating:

$$J = c_{MeAc}\dot{n}_{MeAc} - c_{MeOH}\dot{n}_{MeOH} - c_{heat}q_{heat}. \quad (10)$$

As the acetic acid stream is not manipulated, its cost is not included here. To guarantee the required quality of the main product, the molar fraction of MeAc in the top product is constrained to values not less than 0.8.

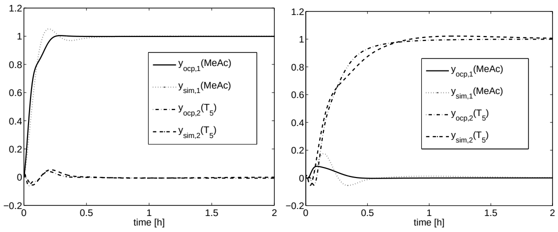
For the control structure selection, we consider the batch process as quasi-stationary. This corresponds to an infinitely large re-boiler and a constant composition of the vapour entering the column. The vapour composition used in the analysis corresponds to the batch run at three hours after the start of the regular operation. The variation over the batch is taken into account as a disturbance in the control structure selection process. For the final validation of the control performance, a rigorous dynamic simulation of the batch process is performed.

To reduce the number of 136 structures, the influence of the sensor errors was investigated first. The result was that 66 structures can be discarded because $\sigma_{max}(\underline{S})$ is more than 10 times larger than in the best case. The excluded structures use measurements with large relative sensor errors, e. g. the molar fraction of acetic acid in the top product, or measured variables in the lower part of the column, which are only weakly affected by the disturbances. The disturbance scenarios were chosen by a worst case analysis. We consider an additional heat loss in the heat-supply system of 500W, a reduction of the reaction rate by 10% and subcooling of the condensate by 40K. An additional scenario describes the change in the vapour composition during the batch run. The methanol fraction changes from 93% at 3h to 70% at 12h of the optimal trajectory of the batch.

The nominal operating point is defined by a heating power of 3250W, a reflux ratio of 0.63 and a feed of acetic acid of $0.0387\frac{mol}{s}$, the profit at this point is set to 100 percent.

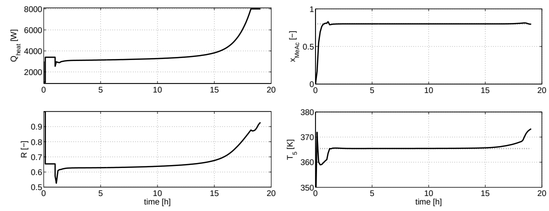
As result of the optimization referring to (9) five structures are excluded from the further investigation, because no common set-point could be found.

During the minimizations (3) the hard constraints on the product quality are omitted and the control structure is required to keep meet this constraint. Seven structures can not guarantee a required quality of 77% MeAc. Only 77% are specified as a sensor error of 3 mol% is assumed for the concentration measurement.



(a) step in x_{MeAc} (b) step in T_5

Fig. 3. Response of the controlled variables on a step in the set-points



(a) manipulates variables (b) controlled variables

Fig. 4. Performance in non-linear simulations

The errors of the temperature sensors is assumed to be 0.3K and the flow can be measured with an accuracy of 1%.

17 additional structures are excluded because the average profit decreases to approx. 75%. For the remaining 41 structures the dynamic behaviour is evaluated similar to (Dadhe *et al.*, 2002).

First the zeros of the transfer function of each structure are calculated. Small zeros in the right half plane denote a large rise time. Here rhp zeros with absolute values smaller than 0.01 are not acceptable. Eleven of the 41 structures are rejected by this criterium. Another five structures are discarded by the investigation of the condition number. A condition number smaller than ten in the area of the crossover frequency $(10^{-2}\ldots10^{-3})$ is requested for suitable structures. The next step is to calculate the optimal control performance (Völker and Engell, 2004) and to design a controller for the most promising structure, which uses the measurements x_{MeAc} and T_5. The responses of the ideal and the real controller for a linearized model on a set-point-step is shown in the figure 3. The temperature and x_{MeAc} are scaled such that 5K and 5% are mapped to one, respectively. The figure shows that the real controller achieves nearly the same performance as the ideal one and there are only small couplings between the controlled variables. Also the settling time of two hours is very good for this system. Figure 4 shows the control performance during a final test in a non-linear simulation of the batch run. The first hour is used for the start-up of the plant. Then closed-loop control is applied and the controlled variables are adjusted to their setpoints. These setpoints can be kept for more than 10 hours, until the controlled temperature drifts away. At this moment the fraction of methanol in the reboiler is less then 10%, what usually denotes the end of the batch. The manipulated variables also reflect this situation, as they reach their upper bounds. Over the complete batch the profit grows continuously.

For the worst case disturbance of a 20% decrease in the reaction rate the profit for closed-loop control drops to 95%. This is clearly more than the 80%, which are achieved by applying the nominal open-loop input values in this case. Even if disturbances are considered, that are larger than supposed during the optimizations, the controller is able to maintain the controlled variables at their set-points.

5. CONCLUSIONS AND FUTURE WORK

A methodology for control structure selection was presented that takes the steady state economy into account as well as the dynamic behaviour. The method was successfully applied to the example of a reactive distillation column.

6. ACKNOWLEDGEMENTS

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