ON THE USE OF CONTROLLER PARAMETRIZATION IN THE OPTIMAL DESIGN OF DYNAMICALLY OPERABLE PLANTS

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Abstract: This paper explores some issues pertaining to the use of Q–parametrization in the optimal design of dynamically operable plants. An optimization–based plant design formulation in which a discrete-time implementation of the controller parametrization is embedded, is described. Its application is demonstrated through a reactor case study in which the resulting design is compared against that obtained using PI control. Differences in results obtained are discussed and related to the design problem formulation. The impact of other assumptions, such as the disturbance dynamics, is also discussed.

Keywords: integrated design and control; PI control; Q–parametrization

1. INTRODUCTION

The impact that the design of a plant can have on its ability to be satisfactorily controlled has led to a significant research effort both in the development of techniques for dynamic operability assessment and in the incorporation of dynamic operability criteria directly within plant design calculations. Reviews of work in this area include those of Walsh and Perkins [1996], van Schijndel and Pistikopoulos [2000], and Pistikopoulos and Sakizlis [2002].

Optimization-based approaches are particularly effective both for the quantitative assessment of dynamic operability, and for the design of plants that are both economically optimal and dynamically operable. This framework enables the plant-inherent control performance limitations of non-minimum phase characteristics, input constraints and uncertainty [Morari, 1983] to be simultaneously accounted for, and offers considerable flexibility in the problem formulation. Inclusion of various controller types is possible, including no control [Bahri et al., 1996], perfect control, and controllers of specified type such as multi-loop PI control [Mohideen et al., 1996; Bansal et al., 2002]. Swartz [1996] utilized Q–parametrization within an optimization-based framework to provide a controller-independent measure of operability for alternative designs; its extension to plant design formulations is described in Swartz et al. [2000].

In this paper, we outline the general optimization-based approach to integrated plant and control system design, focusing in particular on the use of Q–parametrization and PI control as the regulatory control strategy. These strategies are implemented on a comprehensive reactor case study, and the results compared. We show that the control performance metric induced by the economic objective function coupled with path constraints explains much of the similarity in the results obtained. This issue, along with other features of the optimization-based formulation, are discussed.

2. PROBLEM FORMULATION

The optimal design formulation considered here is as follows:

Maximize: objective function

subject to:
- dynamic process model;
- operating constraints;
- and controller equations

for all disturbances within a specified set

To provide:
- an optimal design;
- an optimal operating point;
- and optimal controller tuning.

Each aspect of this formulation will now be briefly described.

2.1 Objective function

The objectives in process design vary widely, are multifaceted and are frequently conflicting. A strategy that is widely adopted is to use an economic–based objective function, as is typically followed in steady-state design. This single measure is not likely to completely and accurately encapsulate all features of interest, such as ease of operation. These remaining features are incorporated as constraints.

The objective function in the case study that follows is formulated in terms of a physical design variable and steady-state values of certain operating variables. The optimal steady-state must be such that the operation remains feasible over a specified time horizon for all disturbances within a specified set.

2.2 The dynamic process model equations

Continuous time processes with a differential and algebraic equation (DAE) model description are considered in this formulation. As a simultaneous solution strategy is employed in this work, the differential equation elements of the model are converted to algebraic equations by using orthogonal collocation on finite elements. The complete set of algebraic, equality equations is then incorporated into the problem as constraints.

Discrete time controllers are used in this study and it is important to align their sampling time with the finite element representation of the process model. Many finite elements per sampling period are used in the model discretization strategy to capture the range of process dynamics that may occur within one sampling interval.

2.3 Operating constraints

The process operating constraints define desirable and feasible process behaviour. Collectively they define the required dynamic operability and also aide in the the solution of the optimization problem by limiting the search space.

2.4 Disturbances

Step–like disturbances will be used in this paper, going from nominal to upper or lower bound values. Combinations of disturbances are handled by using a set of parallel process models – one for each disturbance combination. All these parallel models are constrained to use the same physical design, operating point and controller tuning, thereby increasing the problem's size, but maintaining the same degrees of freedom.

2.5 Controller equations

Two feedback controller types are considered here: PI control and Q–parametrization.

2.5.1. PI control The velocity form of the digital PI controller is given by

$$\Delta u_k = K_c \left[e_k - e_{k-1} + \frac{\Delta t}{\tau_I} e_k \right] \quad (1)$$

where: $\Delta u_k = u_k - u_{k-1}$

Two controller tuning variables, K_c and τ_I, are introduced for every PI loop added to the process.

2.5.2. Q–parametrization is an established part of control theory and provides a convenient mechanism for representing and parameterizing all stable closed-loop maps from a set of exogenous inputs to regulated outputs in a linear feedback system [Francis, 1987; Green and Limebeer, 1995]. The IMC controller [Garcia and Morari, 1982; Morari and Zafiriou, 1989] shown in Figure 1 yields a parametrization of this type for stable plants. The feedback system is stable if Q is stable.

The significance of this representation in the present operable design application is that by including a finite dimensional approximation of Q in the decision space, a design is obtained that represents an optimum for linear control independent of controller type or tuning.

A finite impulse representation is used for Q, which for SISO systems takes the form,

$$Q(z^{-1}) = \sum_{i=0}^{L} q_i z^{-i} \qquad L = (t_f - t_0)/\Delta t \quad (2)$$

The controller decision variables are the coefficients q_i, $i = 0, 1, \ldots, L$.

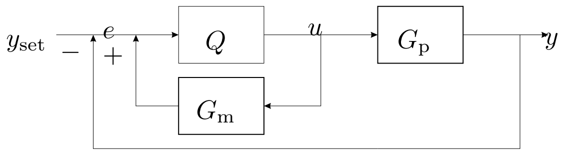


Fig. 1. The Q–parametrization structure used

Asymptotic tracking may be achieved by requiring

$$\left(\sum_{i=0}^{L} q_i\right)\overline{G}_{\mathrm{m}} = 1$$

where $\overline{G}_{\mathrm{m}}$ is the model gain. In addition, this condition yields an initial guess strategy for $q(z^{-1})$ by setting $q_0 = 1/\overline{G}_{\mathrm{m}}$ and $q_i = 0$ for the remaining coefficients.

In the case study that follows, the optimization is carried out on the *nonlinear* dynamic model. The linear model required for the Q–parametrization is obtained by linearizing the nonlinear model around the current iterate of the steady-state operating variables. Upon convergence of the optimization, the Q–parametrization is consistent with the optimal steady-state operating point.

2.6 Solution Strategy

Cervantes and Biegler [2001] review solution methods for dynamic optimization problems and divide them into two major classes, Direct and Indirect methods. The Direct methods are widely used and are again divided into two categories: the *sequential* and *simultaneous* methods. In this paper a simultaneous solution strategy is used and since no integer variables are present, it results in a nonlinear programming (NLP) problem.

3. CASE STUDY

The case study presented here considers the integrated design and control of a stirred tank reactor in which an irreversible, exothermic reaction takes place. The study is based, in part, on the work of Loeblein and Perkins [1998].

The objectives of this study are to:

- find a design that is dynamically operable with respect to the given process constraints;
- determine the difference between designs using PI control and designs using a controller described by Q–parametrization;
- analyze the design by investigating the assumptions and constraints.

3.1 Process description

The process model is given by the equations in (3) with parameter values in Table 1. Values in the lower half of this table represent the values of the variables at the steady–state economic optimum, with the objective function given by Equation (3f) and constraints in Equation (4).

The disturbances are taken to be step changes from the nominal value, in parentheses, of the following two variables to their upper and lower bounds:

- $18 \leqslant C_{\mathrm{in}}(t) \leqslant 22$ kmol/m^3 (20 kmol/m^3)
- $290 \leqslant T_{\mathrm{in}}(t) \leqslant 310$ K (300 K)

$$\frac{dC}{dt} = \frac{F_{\mathrm{in}}}{V}\left(C_{\mathrm{in}} - C\right) - k_0 e^{-\frac{E}{RT}} C \tag{3a}$$

$$\frac{dT}{dt} = \frac{F_{\mathrm{in}}}{V}\left(T_{\mathrm{in}} - T\right) + \left(-\frac{\Delta H_{\mathrm{R}}}{\rho C_p}\right) k_0 e^{-\frac{E}{RT}} C - \frac{Q_{\mathrm{cool}}}{V} \tag{3b}$$

$$Q_{\mathrm{cool}} = U_{\mathrm{A}}(T - T_{\mathrm{mean}}) \tag{3c}$$

$$Q_{\mathrm{cool}} = F_{\mathrm{c}}(T_{\mathrm{cool}} - T_{\mathrm{cool,in}}) \tag{3d}$$

$$T_{\mathrm{mean}} = 0.5(T_{\mathrm{cool}} + T_{\mathrm{cool,in}}) \tag{3e}$$

$$\phi_{\mathrm{econ}} = 10\overline{F}_{\mathrm{in}}\left(C_{\mathrm{in}} - \overline{C}\right) - 0.01\overline{Q}_{\mathrm{cool}} - 0.1\overline{F}_{\mathrm{in}} - 0.075V^{0.7} \tag{3f}$$

$$T(t) \leqslant 350 \text{ K} \tag{4a}$$

$$0.05 \leqslant F_{\mathrm{in}}(t) \leqslant 0.8 \text{ m}^3/\text{s} \tag{4b}$$

$$T_{\mathrm{cool}}(t) \leqslant 330 \text{ K} \tag{4c}$$

$$T_{\mathrm{cool}}(t) < T(t) \tag{4d}$$

$$C(t) \leqslant 0.1 \text{ kmol/m}^3 \tag{4e}$$

$$V \leqslant 10 \text{ m}^3. \tag{4f}$$

Table 1. Nomenclature and value for the process model

Variable Name	**Nominal Values**	**Units**	**Lagrange Multiplier**
C_{in}	20	kmol/m^3	–
T_{in}	300	K	–
$T_{\mathrm{cool,in}}$	300	K	–
F_{c}	0.7	m^3/s	–
k_0	2.7×10^8	s^{-1}	–
E/R	6000	K	–
U_{A}	0.35	m^3/s	–
$\frac{-\Delta H_{\mathrm{R}}}{(\rho C_p)}$	5	m^3.K/kmol	–
C	0.1	kmol/m^3	4.6437
T	350	K	2.2603
F_{in}	0.2828	m^3/s	0
V	5.808	m^3	0
T_{cool}	320	K	0
T_{mean}	310	K	0
Q_{cool}	14	m^3.K/s	0
ϕ_{econ}	55.86	\$/hr	–

3.2 Integrated design and control

The steady–state economic optimum presented in Table 1 is not dynamically operable, even with feedback control, since a disturbance could cause

Table 2. Steady–state values for open–loop operation

Name	Value	Name	Value
$\overline{C}$	0.07146 kmol/m^3	$\overline{Q}_{\text{cool}}$	11.65 m^3.K/s
$\overline{T}$	341.6 K	$\overline{T}_{\text{mean}}$	308.3 K
$\overline{F}_{\text{in}}$	0.2007 m^3/s	$\overline{T}_{\text{cool}}$	316.6 K
V	8.803 m^3	ϕ_{econ}	39.52 \$/hr

C and/or T to violate their respective active constraints. The process operating point must be changed to achieve dynamic operability. An analysis of the design degrees of freedom shows that two independent variables may be selected in order to fix the remaining variables. Of the seven variables in the lower half of Table 1, one is a design variable, V, while the remaining are constrained operating variables, such as C, T, F_{in} and T_{cool}.

3.2.1. No feedback control: An operating point can be found for this particular example which does not require feedback control. This operating point is within the permanent feasible region, so that no constraint violation occurs when the given disturbances impact on the process either separately or together. This operating point is found by using the formulation described above without controllers where the search variables are then the tank volume and the steady state inlet flowrate, $\overline{F}_{\text{in}}$.

The design summary is given in Table 2 which shows that a sacrifice in the profit has to be made in order to operate at this point – the price to be paid to remain operable without feedback control. This design has all variability appearing in the process outputs, with the process inputs remaining constant.

3.2.2. With feedback control: The sacrifice in process profit can be reduced by implementing feedback control, but the aim of this study is to investigate how much improvement is to be had by using either PI control or Q–parametrization.

The tank temperature with a 10 second measurement delay is selected as the controlled variable; the inlet flowrate is chosen to be the manipulated variable in this study, as was done in the work of Loeblein and Perkins [1998]. The search space now consists of the process design and operating variables from the lower half of Table 1 as well as the controller tuning variables of the two controller types.

Solving the design problem with PI control results in the operating point given in Table 3. An improvement of \$ 6.62 per hour is achieved compared to the profit with open–loop operation. The integral square error (ISE) values are computed from Equation 5 with $\psi = 0$, the weighted ISE (wISE) values have $\psi = 30\ 000$ for all possible disturbance combinations, J, over a time horizon with $t_f = 500$ s.

$$w\text{ISE} = \sum_{j=1}^{J} \sum_{k=0}^{L-1} \left[\left(\overline{T} - T_{k,j}\right)^2 + \psi \left(\Delta F_{\text{in},k,j}\right)^2 \right] \Delta t \tag{5}$$

$$L = (t_f - t_0)/\Delta t \qquad J = 8 \tag{6}$$

Table 3. Design with PI control

Name	Value	Name	Value
$\overline{C}$	0.06054 kmol/m^3	$\overline{Q}_{\text{cool}}$	12.71 m^3.K/s
$\overline{T}$	345.4 K	$\overline{T}_{\text{mean}}$	309.1 K
$\overline{F}_{\text{in}}$	0.2341 m^3/s	$\overline{T}_{\text{cool}}$	318.2 K
V	10.00 m^3	ϕ_{econ}	46.14 \$/hr
K_c	0.01511	τ_I	28.50
ISE	1586	wISE	1885

Solving the same design problem using Q–parametrization yields an improvement of \$ 7.26 per hour when using 2 or more coefficients for $q(z^{-1})$. Table 4 shows the values at the nominal operating point, which do not change after two coefficients for $Q(z^{-1})$. Only the integral squared error metrics are reduced by adding further coefficients, as seen in Table 5.

Table 4. Design with Q–parametrization

Name	Value	Name	Value
$\overline{C}$	0.06034 kmol/m^3	$\overline{Q}_{\text{cool}}$	12.80 m^3.K/s
$\overline{T}$	345.7 K	$\overline{T}_{\text{mean}}$	309.1 K
$\overline{F}_{\text{in}}$	0.2372 m^3/s	$\overline{T}_{\text{cool}}$	318.3 K
V	10.00 m^3	ϕ_{econ}	46.78 \$/hr
ISE	877	wISE	1571

Table 5. Varying the number of FIR coefficients in $Q(z^{-1})$

$Q(z^{-1})$	ϕ_{econ} (\$/hr)	ISE	wISE
0.009336	45.51	3236	3306
$0.07148 - 0.06191z^{-1}$	46.78	1400	2184
$q_0 + \ldots + q_4 z^{-1}$	46.78	878	1620
$q_0 + \ldots + q_9 z^{-1}$	46.78	904	1584
$q_0 + \ldots + q_{19} z^{-1}$	46.78	877	1571

Figures 2 and 3 show trajectories for the design under PI control and for design with Q–parametrization. These trajectories represent the closed–loop response and manipulated variable inputs respectively for the case when both disturbances are stepped to their upper limits simultaneously at $t = 20$. These figures also serve to illustrate the difference between using 2 and 20 coefficients for $Q(z^{-1})$ and contrast to PI control.

3.3 Design Analysis

The above results indicate that there is not much difference, in this case study, between using PI control or the more advanced Q–parametrization strategy to maintain dynamically operable process behaviour while still remaining economically

Fig. 2. Controlled variable trajectories

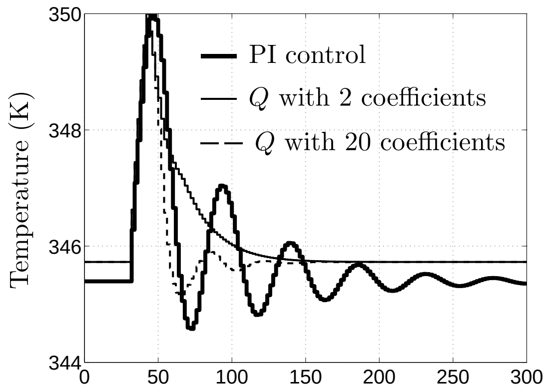
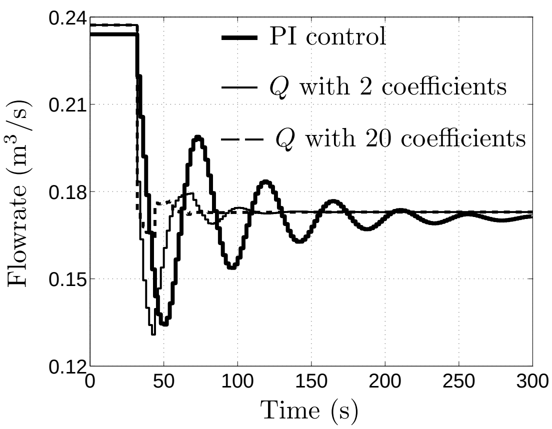


Fig. 3. Manipulated variable trajectories



optimal. This occurs because the distance from the constraints for both controller types is approximately the same. The integral squared error is however less for the more advanced controller and unless this has a significant economic benefit the standard PI controller would be economically acceptable.

Two aspects of the study require some further analysis and discussion for completion. The first aspect is the volume constraint that is active in all of the above designs and the second is the assumption of disturbance type and its dynamics.

3.3.1. The volume constraint: Table 6 shows the result of using the formulation to relax the volume constraint in Equation 4. It is understandable that a larger tank volume would attenuate the initial deviation for the controlled variable when the disturbance impacts the process. This allows for $\overline{T}$ to be closer to the constraints of 350 K, resulting in increased profit in ϕ_{econ}.

Note that if the volume constraint is completely removed, the economically optimal tank volume is calculated as 114 m^3. Increasing the volume to such a large value may be considered as downgrading the process equipment, but it is necessary to maintain an operable system at the calculated

Table 6. Effect of the volume constraint on the process design and operation

Variable	PI Control			
	$V \leqslant 10$	$V \leqslant 20$	$V \leqslant 80$	$V \leqslant \infty$
$\overline{T}$ (K)	345.4	347.0	349.0	349.3
V (m^3)	**10.00**	**20.00**	**80.00**	**114.0**
ϕ_{econ} ($/hr)	46.14	48.93	52.07	52.19
wISE	1885	1255	686	600

set point. A point to also note is that assumptions of perfect mixing may not be valid at such high tank residence times and the model may need to be adjusted.

3.3.2. The disturbance dynamics: The PI controller design of Table 3 was used, but the step disturbance input was replaced with the following disturbance model:

$$C_{\text{in}}(t) = 2\sin(0.01t) + 20 \qquad t \in [t_0; t_{\text{f}}]$$
$$T_{\text{in}}(t) = 10\sin(0.01t + \varphi) + 300 \quad \varphi \in [0; 2\pi]$$

Figure 4 shows the output of the two constrained state variables at 10 equally spaced points in the range of φ. This ball of process operation can be seen to lie well within the constrained region, indicating that the nominal operating point of the current design could well be moved closer to the upper temperature and concentration constraints of 350 K and 0.1 kmol/m^3 respectively.

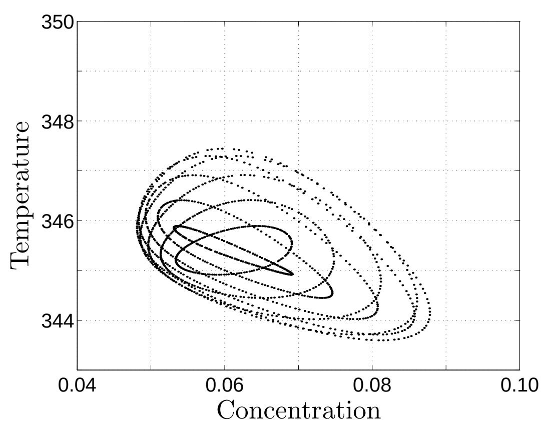


Fig. 4. The effect of sinusoidal disturbances on process variability with PI control

In summary, the effect of varying the process constraints can be understood and quantified using this formulation. It allows for more informed economic and operability trade–off when process parameters are to be investigated. Furthermore, the assumption of step–like disturbance dynamics was shown to lead to a conservative design and improved profit could be had if the disturbance dynamics were known more accurately.

4. CONCLUSIONS

An implementation of an integrated plant and control system design formulation is described, focusing in particular on the use of PI control and a parametrization of all linear stabilizing controllers. The integrated design strategy is illustrated through an application to a reactor case study. Various scenarios are considered – steady-state optimal design; dynamic optimization without control; the inclusion of PI control; controller parametrization; relaxation of the maximum volume constraint and the effect of disturbance dynamics.

The difference between PI control and the result using controller parametrization was found to be slight. One reason for this is that the control performance metric induced by the objective function and path constraints is the distance of the steady-state operating point to active constraints, and PI control appears to be essentially as good as the best linear controller in minimizing the peak output variation in the direction of the active constraints. While the difference between the closed-loop performance as measured by the integral square error is significant, this measure is incorporated neither into the objective function nor constraints. This illustrates the importance of accurately capturing the desired design and operational objectives.

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