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Economically Optimal Controlled Variables for Parallel Units – Application to Chemical Reactors ⋆

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Abstract: Adding parallel process lines is a common way to increase the capacity of a chemical plant. Generally, the process units will be similar, but not identical. The optimal distribution of load between the lines will vary depending on the parameters and disturbances which affect the individual units, and controlling the distribution optimally can lead to significant savings in the operational costs. We derive a method for finding optimal controlled variables which involve only measurements from two lines at a time. Controlling these variables to equal values leads to the optimal load distribution, with no need to re-optimize online when disturbances occur. As an example, we consider a system of parallel continuous stirred tank reactors with the general reaction $aA + bB \rightarrow cC + dD$, which follows a polynomial reaction law.

Keywords: Parallel reactors, Optimal operation, Controlled variable selection, Real-time optimization, Optimizing control, Optimization

1. INTRODUCTION

During the lifetime of a process plant, its capacity is often increased due to a rising demand for products. Starting at some initial capacity, a common solution to cater for increased demand is to add one or more parallel process lines. The resulting parallel plants will often be similar, and in many cases share one common feed or product stream, which is distributed between the different lines.

In practice, it cannot be expected that the optimal value of the distribution remains constant. It is rather a function of changing disturbances and operating conditions in each line. To operate the process at maximum profitability, a strategy is required for distributing the flow optimally between the parallel lines.

In this work we consider the case where we have several continuous stirred tank reactors (CSTR), which are operated in parallel. This is often the case when reactors are required which have a high ratio of heat transfer area to volume [Luyben, 2007], or where deactivation of the catalyst requires regular catalyst changes or reactivation. In particular, we present a method for distributing the load between the reactors, when the operating conditions of the individual reactors differ from the nominal conditions. The resulting unconstrained optima are relatively flat, such that a suboptimal split will in general not immediately show a drastic profit reduction. However, as these processes are operated over a long time period, the accumulated savings which come with adjusting the split optimally become large in the long run.

The most common operational strategy in industrial practice is to determine a split between the lines, that gives good performance for some nominal conditions, and to keep the split constant at that value. This open loop strategy has the advantage that it is very simple, but it will give rise to economic losses when the operating conditions differ from the nominal conditions.

A second approach is "real-time optimization" (RTO) [Marlin and Hrymak, 1997]. It involves estimating and updating the parameters and the states of a mathematical process model for formulating an optimization problem. Using the newest parameter and state estimates, this optimization problem is solved on-line at given sample times. If a dynamic model is used in the optimization, this approach is referred to as dynamic RTO, [Diehl et al., 2002]. The success of this approach depends strongly on an adequate process model [Forbes et al., 1994], and the ability to estimate the states [Kolås et al., 2008] correctly. In addition, the resulting optimization problem needs to be solved in a sufficiently short time, so that the obtained solution can be used online. These factors generally make RTO a relative expensive technology.

A third approach, which is followed in this paper, is to determine a feedback control structure which keeps some variables at constant setpoints. This strategy is very common in practice, for example controlling the same output temperatures or the same compositions in all passes. However, the design of the control structure is often done based on engineering intuition and without systematically including economic considerations. The goal of this paper is therefore to systematically use results from optimization and to show how one can obtain steady state optimal controlled variables (CV) for parallel systems. Controlling these variables at a constant setpoint value leads to steady state optimal operation without the need to reoptimize when the operating conditions change. Such variables are

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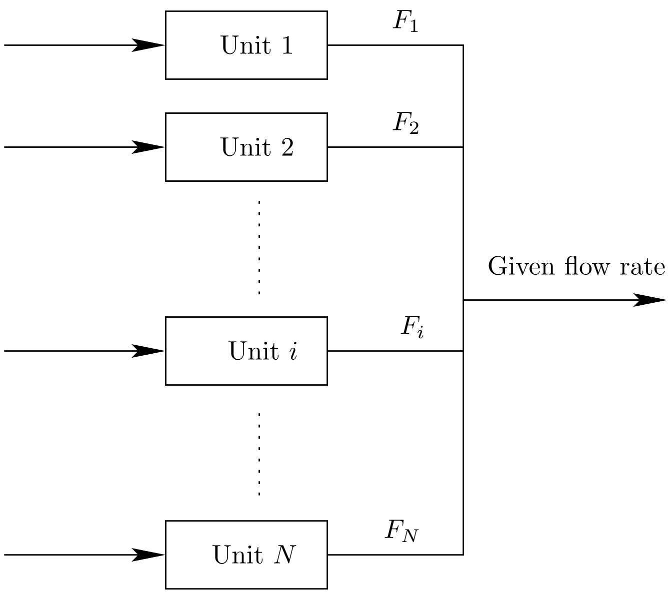

Fig. 1. Parallel reactor units

called "self-optimizing" controlled variables. According to Skogestad [2000] self-optimizing control is achieved if:

> "we can achieve an acceptable loss with constant setpoint values for the controlled variables (without the need to reoptimize when disturbances occur)."

We present first some general concepts for finding nonlinear self-optimizing controlled variables for a class of parallel processes, and apply the ideas to a system of parallel continuous stirred tank reactors (CSTR). We combine the theory of "equal marginal utility" [Downs and Skogestad, 2011], with the ideas from Jäschke and Skogestad [2012], where (1) the optimality conditions are formulated using a simple model, (2) all unknown variables are eliminated from the optimality conditions, and (3), the obtained expressions are used as controlled variables. In this work we add an additional step, where we show that for the parallel CSTRs in consideration, the resulting expressions can be approximated by very simple measurements.

A big advantage of the nonlinear controlled variables is that it is not necessary to determine or adjust their optimal setpoint. As they are derived from the optimality conditions, the optimal setpoint results from the derivation.

In the next section we present the problem formulation, and in Section 3 we present some general results for parallel processes, which are applied to a system of CSTRs in Section 4. In Section 5 we illustrate our results with a numerical case study, and the paper is closed with a discussion and conclusions, Sections 6 and 7.

2. PROBLEM FORMULATION

We assume that we have N parallel process units, Fig. 1. Each unit has an associated operating cost, and the overall cost J is the sum of the N individual costs J_i,

$$J = \sum_{i=1}^{N} J_i(F_i). \tag{1}$$

Here F_i denotes the load allocated to the unit F_i. In the rest of this paper, we will use the terms "load" and "flow" interchangeably. It is assumed that the total load F is fixed, that is, the total load is the sum of the individual loads F_i through all lines:

$$F = \sum_{i}^{N} F_i. \tag{2}$$

Optimal operation can be formulated mathematically as

$$\min_{F_1,\ldots F_N} J(F_1 \ldots F_N), \tag{3}$$

where the flow rates F_i have to satisfy the constraint

$$\sum_{i=1}^{N} F_i - F = 0. \tag{4}$$

This results in $N-1$ degrees of freedom to optimize the total cost J, namely the distribution of the flow rates between the N units.

Under normal plant operation, the individual units are subject to varying disturbances which can have either positive or negative influence on the cost. To achieve optimal operation, it is necessary to adjust the distribution of the load (split) between the different units on-line. This adjustment will be dependent on the type and magnitude of the disturbance.

The aim of this work is to find variable combinations, which can be controlled using the $N-1$ degrees of freedom, and which, when controlled at a constant setpoint, automatically lead to the optimal adjustments in the load distribution between the individual units.

3. CONTROLLED VARIABLES FOR PARALLEL PROCESSES

3.1 Optimality conditions

The first order necessary optimality conditions [Nocedal and Wright, 2006] require that at the optimum

$$\frac{\mathrm{d}J}{\mathrm{d}F_i} = 0. \tag{5}$$

The flows F_i, however, are not completely independent, but have to satisfy the relation (4). This results in $N-1$ flows, which can be freely chosen, and one flow, which is determined once the other $N-1$ flows are fixed. In the sequel, the subscript j will denote the dependent load, while the subscript i will be used for loads which can be freely chosen, so we will always assume

$$i \neq j. \tag{6}$$

The total derivative of the cost (1) with respect to F_i can then be written as

$$\frac{\mathrm{d}J}{\mathrm{d}F_i} = \frac{\partial J}{\partial F_i} + \frac{\partial J}{\partial F_j}\frac{\partial F_j}{\partial F_i}. \tag{7}$$

Solving (4) for F_j gives

$$F_j = F - \sum_{i=1}^{j-1} F_i - \sum_{i=j+1}^{N} F_i, \tag{8}$$

and differentiating with respect to an arbitrary F_i yields

$$\frac{\partial F_j}{\partial F_i} = -1. \tag{9}$$

Inserting (9) into (7), the optimality condition can be stated as:

$$\frac{\mathrm{d}J}{\mathrm{d}F_i} = \frac{\partial J}{\partial F_i} - \frac{\partial J}{\partial F_j} = 0 \quad \text{for } i \neq j. \tag{10}$$

Under the assumption that the cost is the sum of the costs for each unit, see (1), we have that

$$\frac{\partial J}{\partial F_i} = \frac{\partial J_i}{\partial F_i}, \tag{11}$$

and inserting into (11) into (10), we rewrite the optimality condition as

$$\frac{\partial J_i}{\partial F_i} = \frac{\partial J_j}{\partial F_j} \quad \text{for } i \neq j. \tag{12}$$

The interpretation of this equation is that at the optimum, the gain (utility) resulting from an incremental increase of flow rate F_i must result in an equal loss caused by the decrease of flow rate F_j. The partial derivatives $\frac{\partial J_i}{\partial F_i}$ are also called "marginal costs" or "marginal utilities" [Lipsey and Harbury, 1992], and at the optimum it is required to have equal marginal utilities for all units.

Remark 1. This result on equal marginal costs (or utilities) is not new, it has been suggested for process control applications among others by Urbanczyk and Wattenbarger [1994], and Downs and Skogestad [2011]. However, in most cases the marginal costs will not be directly measurable, and have to be estimated. Urbanczyk and Wattenbarger [1994] use simulations and finite difference to estimate the marginal costs, which goes into the direction of NCO tracking [Srinivasan et al., 2008, Jäschke and Skogestad, 2011] and extremum seeking control [Krstic and Wang, 2000]. We however, following the approach of Jäschke and Skogestad [2012], use a plant model to express (or approximate) the marginal costs in terms of variables, which can be easily measured online and used for feedback control.

Eq. (12) has been derived for a given j, but since j can be chosen arbitrarily, this has to hold for all pairs i and j. Thus, the $N-1$ splits between the process units should be used to control

$$c_{i,j} = \frac{\partial J_i}{\partial F_i} - \frac{\partial J_j}{\partial F_j} \quad \text{for all pairs } i \neq j \tag{13}$$

to zero,

$$c_{i,j} = 0. \tag{14}$$

Remark 2. The form of Eq. (13) has significant influence on the implementation of optimal operation. It shows that we can optimize the process by controlling differences in the marginal costs pair-wise, that is we can restrict our considerations on (or optimize) two parallel units at a time.

Before we can use $c_{i,j}$ for control, we must express the marginal costs in terms of known variables (measurements only). This is done using simple models. Finding simple expressions for the marginal costs $\frac{\partial J_i}{\partial F_i}$ is not always easy, and depends heavily on the model structure and complexity. However, in many cases it is possible to use simplified models to find controlled variables which result in performance with acceptable loss.

The expressions for the marginal costs $\frac{\partial J_i}{\partial F_i}$ which are obtained after eliminating the unmeasured disturbances will be denoted as γ_i. Once we have obtained expressions for γ_i, the optimal controlled variables based on (13) become

$$c_{ij} = \gamma_i - \gamma_j. \tag{15}$$

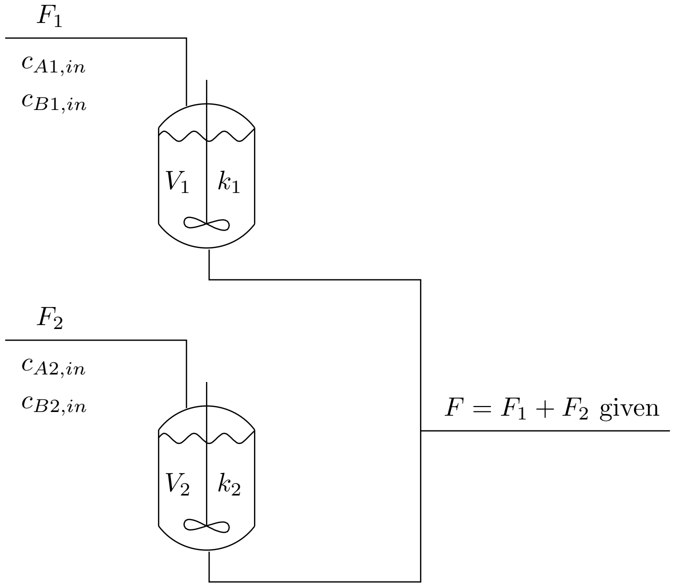

Fig. 2. 2 CSTR operated in parallel

4. APPLICATION TO A GENERAL CSTR

In this section, we will show how to determine a good variable combination which can be used for controlling the split optimally for a system of reactors. Without loss of generality we can consider a system of two CSTRs, Fig. 2. In each of the reactors, we have the general reaction

$$aA + bB \rightarrow cC + dD, \tag{16}$$

where the reaction rate of component l is calculated as [Fogler, 2006]:

$$r_l = \frac{1}{\nu_l} k c_A^{\alpha} c_B^{\beta}, \tag{17}$$

where r_l is the rate of reaction of species l, ν_l is the stoichiometric coefficient, which is negative for the reactants and positive for the products, k is the temperature dependent reaction constant, and c_A and c_B are the concentrations of the reactants A and B, respectively.

The operational goal is to produce a given stream $F = F_1 + F_2$ with a maximum concentration of component C. That is, the cost function to minimize is

$$J = \Phi_1 + \Phi_2 \tag{18}$$

with

$$\Phi_i = -p_C F_i c_{Ci}, \tag{19}$$

where p_C denotes the revenue from selling product C, and the variables F_i and c_{Ci} denote the flow rate, and the concentration of valuable product in reactor i, respectively. This kind of problem occurs often in industry when the capacity of the subsequent separation is the bottleneck of the process. Since the profit cannot be improved by increasing F further (e.g. because of flooding in the distillation column), we want to maximize the total production of component C.

As disturbances which affect the reactors in our plant, we consider the product of reaction constant and reactor volume k_iV_i and the feed compositions $c_{Ai,in}$ and $c_{Bi,in}$ for each line:

$$d_i = \begin{bmatrix} k_iV_i \\ c_{Ai,in} \\ c_{Bi,in} \end{bmatrix} \qquad i = 1, 2. \tag{20}$$

To obtain an optimal controlled variable which is based on the general optimality conditions for the parallel reactors (12), we define a model which is used for setting up the optimality conditions and eliminating the unknowns. Our goal is to find an expression for the marginal costs $\partial J_i/\partial F_i$ in terms of measurements and known parameters only, that is, we want to eliminate disturbances d_i from the optimality conditions. Controlling the resulting expressions γ_i to equal values leads to optimal operation in spite of varying feed composition $(c_{Ai,in}, c_{Bi,in})$, catalyst decay or reactor levels (k_iV_i).

As all variables of reactor i appear only in the marginal cost $\frac{\partial J_i}{\partial F_i}$ of reactor i, and all variables of the reactor j appear only in $\frac{\partial J_j}{\partial F_j}$, we consider one reactor at a time.

For CSTR i, the mass balances for unit i yield

$$g_1 = F_ic_{Ai,in} - F_ic_{Ai} - ac_{Ai}^{\alpha}c_{Bi}^{\beta}k_iV_i = 0 \tag{21a}$$
$$g_2 = F_ic_{Bi,in} - F_ic_{Bi} - bc_{Ai}^{\alpha}c_{Bi}^{\beta}k_iV_i = 0 \tag{21b}$$
$$g_3 = -F_ic_{Ci} + cc_{Ai}^{\alpha}c_{Bi}^{\beta}k_iV_i = 0 \tag{21c}$$
$$g_3 = -F_ic_{Di} + dc_{Ai}^{\alpha}c_{Bi}^{\beta}k_iV_i = 0. \tag{21d}$$

Introducing $x_i = [c_{Ai}, c_{Bi}, c_{Ci}, c_{Di}]^{\boldsymbol{T}}$, we write the model in compact form as

$$g_i(x_i, F_i) = 0. \tag{22}$$

The cost associated to this reactor is

$$\Phi_i(x_i, F_i) = -px_iF_ip_C, \tag{23}$$

where $p = [0\ 0\ 1\ 0]$. Using the compact notation, the expression for the marginal cost becomes

$$\begin{aligned} \frac{\partial J_i}{\partial F_i} &= \frac{\mathrm{d}\Phi_i}{\mathrm{d}F_i} \\ &= \frac{\partial \Phi_i}{\partial F_i} - \frac{\partial g_i}{\partial F_i}\left(\frac{\partial g_i}{\partial x_i}\right)^{-1}\frac{\partial \Phi_i}{\partial x_i}. \end{aligned} \tag{24}$$

where we have used the inverse function theorem to incorporate the relationships given by the model.

Inserting the model (21a-21d) and the cost (23) into (24), we obtain with help of maple

$$\frac{\partial J_i}{\partial F_i} = p_Ccc_{Ai}^{\alpha}c_{Bi}^{\beta}k_iV_i\frac{c_{Ai}c_{Bi}(\alpha+\beta) - \alpha c_{Ai,in}c_{Bi} - \beta c_{Ai}c_{Bi,in}}{c_{Ai}c_{Bi}F_i + \alpha ac_{Bi}c_{Ai}^{\alpha}c_{Bi}^{\beta}k_iV_i + \beta bc_{Ai}c_{Ai}^{\alpha}c_{Bi}^{\beta}k_iV_i} \tag{25}$$

This expression cannot be controlled directly via feedback, because it contains the unmeasured disturbances $c_{Ai,in}, c_{Bi,in}, k_i$ and V_i. Using the model equations (21a-21c) to eliminate these unknowns and simplifying, yields

$$\gamma_i = -p_Cc_{Ci}^2\frac{\alpha ac_{Bi} + \beta bc_{Ai}}{cc_{Ai}c_{Bi} + c_{Ci}(\alpha ac_{Bi} + \beta bc_{Ai})}, \tag{26}$$

which can be reformulated as

$$\gamma_i = c_{Ci}\frac{-p_C}{1 + \left(\frac{cc_{Ai}c_{Bi}}{c_{Ci}(\alpha ac_{Bi}+\beta bc_{Ai})}\right)}. \tag{27}$$

This variable combination contains only known (measured) variables, and can be evaluated online for each reactor. Adjusting the feed flow rates for Reactor 1 and Reactor 2 such that

$$c = \gamma_1 - \gamma_2 = 0 \tag{28}$$

will result in optimal operation in spite of varying disturbances.

Inspecting (27) further, we find an even simpler near-optimal controlled variable. When the term in parenthesis is small, (which will be the case in many practical cases when c_{Ai} and/or c_{Bi} is small) its contribution becomes negligible, and since p_C is equal for Reactor 1 and Reactor 2, a very simple strategy is to keep the outlet concentrations of the valuable product in both reactors equal:

$$c = \gamma_1 - \gamma_2 \approx (c_{C1} - c_{C2})p_C \tag{29}$$

This results in an extremely simple controlled variable, which is very suitable for practical implementation. The interpretation of this is that the main contribution to disturbance rejection comes from controlling $c_{C1} - c_{C2}$ to zero. The factor

$$\frac{1}{1 + \left(\frac{cc_{Ai}c_{Bi}}{c_{Ci}(\alpha ac_{Bi}+\beta bc_{Ai})}\right)} \tag{30}$$

in (27) may be considered as "correction" factor, which fine-tunes the performance.

5. NUMERICAL EXAMPLE

We consider two reactors in parallel with the reactions

$$A + 2B \rightarrow 2C + D. \tag{31}$$

The same reaction takes place in both reactors, however, due to imperfect temperature control or catalyst decay, the reaction rate may differ between the two reactors, and the feed composition is assumed to differ between the different reactors, too.

As above, the goal is to produce a given amount of product stream F, which contains a maximum amount of the desired product C. We introduce the variable $z \in (0, 1)$, which is the defined as the fraction of the total flow F, which is produced in the first reactor, thus the load of Reactor 1 is

$$F_1 = zF \tag{32}$$

and the load of Reactor 2 is

$$F_2 = (1 - z)F. \tag{33}$$

It is assumed that the total product stream F is fixed at 500 l/h due to capacity constraints in the subsequent separation process. Nominally, the reactors are designed identically with a nominal reaction constant of $k_1 = k_2 = 8$ l/(mol h)$^{-1}$, and the resulting split should be $z = 0.5$, that is the total load should be split equally between the two lines. All parameter values are given in Table 1.

Two scenarios are studied. In the first scenario, the reaction constant k_2 of reactor 2 is decreasing. This may be due to catalyst decay, but may also be caused by poor temperature control. In the second scenario, we consider a change in the feed composition of reactor 2.

5.1 Scenario 1: Varying reaction constant k_2

Due to impurities in the feed, the catalytic activity of reactor 2 is assumed to drop 50% ($k_2 = 0.5k_1$). In this case,

Table 1. Parameter values for CSTR example

Symbol	Description	Value
F_{total}	Total flow rate	500 l/h
k_1	Reaction constant	4-8 l (mol h)$^{-1}$
V	Reactor volume	500 l
z	Split ratio	0-1
$c_{A,in}$	Feed concentration of A	2 mol/l
$c_{B,in}$	Feed concentration of B	4 mol/l
p_C	Price for pure component C	1\$/mol

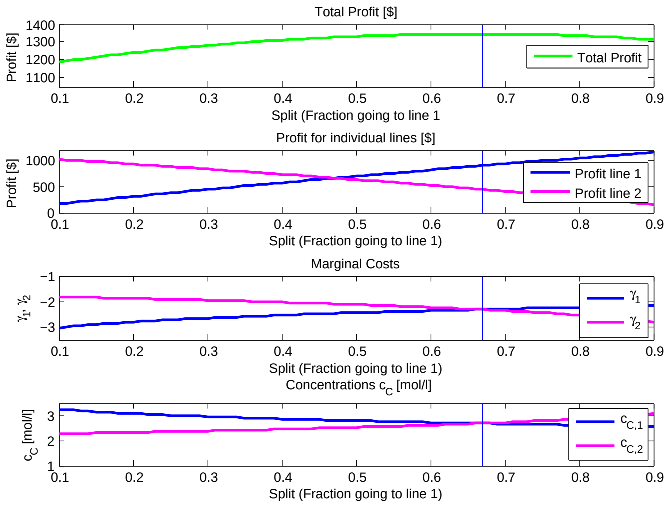

Fig. 3. Disturbance in k_2: Profit, γ_1, γ_2, and concentration of component C for different z

the new optimal split becomes 0.66, that is we produce two thirds of the required product in reactor 1 and the remaining third in reactor 2. If the rate constants k_i could be measured, it would be easy to adapt the split optimally to the new optimal value. However in practice, the reaction constant is generally not measurable. Since also the feed conditions can vary, we use the controlled variable

$$c = \gamma_1 - \gamma_2, \tag{34}$$

which is a function of measurements only, and which results in the optimal split when controlled to zero.

Fig. 3 shows how the total profit, the profits of the individual reactors, the invariants, and the concentrations of component C change with the split z. At the optimum (indicated by the vertical line), we see that $\gamma_1 = \gamma_2$. More importantly, also the simple approximation, $\gamma \approx c_C$, is equal at (or very close to) the optimum. So controlling

$$c = c_{C,1} - c_{C,2} \tag{35}$$

to zero leads to a load ratio which is very close to the optimum. The figure shows that the profit maximum is relatively flat. This is good for control purposes, because a small deviation from the optimal split does not affect the cost very strongly. However, for processes which process large amounts of material the savings resulting from optimally adjusting the split can become large. Using a product price of $p_C = 1\$/\text{mol}$, we obtain savings of 119892 per year (8760h). This corresponds to an increase of 1% in annual profit.

5.2 Scenario 2: Varying feed composition

In this scenario we consider the case when the concentration of component B in the second reactor is increased by

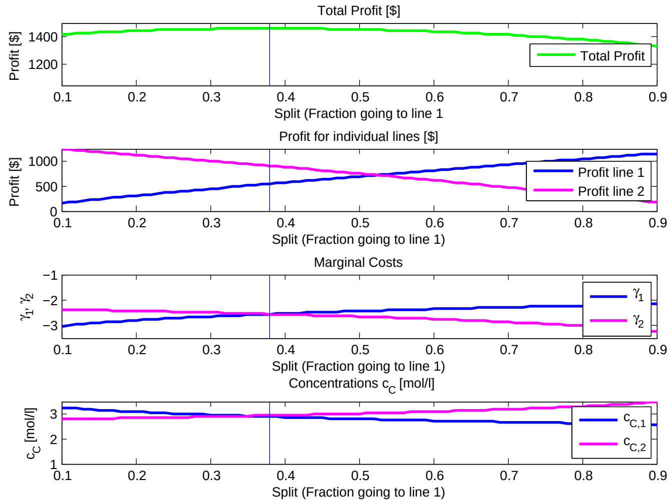

Fig. 4. Disturbance in feed composition: Profit, γ_1, γ_2, and concentration of component C for different z

10%. The reaction constants k_i and all other variables are the same for both reactors.

Fig. 4 shows the behaviour of the system. In contrast to Scenario 1, where controlling $c_{C,1} - c_{C,2}$ to zero gave the same performance as controlling $\gamma_1 - \gamma_2$, in Scenario 2 the concentration lines cross at a z-value which is slightly lower than the optimum, but the difference is still very small.

6. DISCUSSION

One advantage with optimizing the split in parallel processes is that it can be done "pair-wise". That means, the optimality conditions can be expressed pair wise. This facilitates the derivation of controlled variables. Moreover, since the only variable which couples the process lines is the common feed or product stream, each unit can be considered separately for formulating the marginal costs and eliminating unknown disturbances. Thus, the overall elimination problem is decomposed into smaller, easier elimination problems.

When using controlled variables based on the marginal costs, the optimal setpoint for the controlled variables is always zero. This is a clear advantage over other methods for selecting controlled variables, where a.) a set of controlled variables, and b.) the corresponding optimal setpoint has to be determined.

Parallel systems have among others also been studied by Woodward et al. [2009]. However, the scope of their multiple unit (MU) approach is quite different from ours. Their starting point is to have two identical units, and to apply a slightly different input to each. Using finite differences, the gradient is calculated and the inputs are updated to force the gradient to zero. As the units generally are not identical, the system is additionally excited with perturbations to obtain a usable gradient estimate.

In this work, however, the optimization variables are the splits between the parallel units. We assume that the units may be completely different, and that other degrees of freedom as e.g. heating or cooling are treated separately. To use the MU approach for a case with n degrees of freedom, we need $n + 1$ parallel systems. In the case study presented above, this would mean two systems, each containing two reactors in parallel, and where the same set of disturbances disturbance acts on two reactors simultaneously.

Although we used the same models for both lines in the case study, the models need not be the same, because the marginal costs $\partial J_i/\partial F_i$ are computed individually for each line. However, in most cases the parallel units will be quite similar, and we may use the same models for both lines.

Whether the analytical elimination of the disturbances is possible depends very much on the model structure and complexity. In many cases, however, simple models may be used to obtain expressions which give satisfactory performance. As the processes and the models become more complicated, it is reasonable to expect, that the optimal invariants also become more involved. Therefore, it is advised to try and find simple models, which describe the plant behavior well enough. And even if complicated expressions are obtained, they may be approximated by simpler controlled variables, as we have shown for the CSTRs. Since at the optimum an increase of load in one unit leads to an equal decrease of load in another unit, it may happen that the effects of model error cancel out, and that the error in one line compensates the model error in another line.

In the case that there are cross-overs between the lines, the presented approach will not work as easily, because the marginal costs are coupled. Then it will not be possible to consider one unit at a time to eliminate the unknowns. A direction for future work may be to investigate if results from graph-theory can be applied to this problem to give simple invariants

In case of more than two parallel reactors, there are several possibilities for the pairings of inputs (splits) and outputs (c_{ij}) which may result in different dynamic performance. A detailed treatment of implementation issues is outside the scope of this paper; however, a starting point could be to make all γ_i equal to $\gamma_{largest}$, where $\gamma_{largest}$ is the approximation of the marginal cost corresponding to the nominally largest stream. Alternatively one may apply a multivariable controller.

Compared to keeping the nominal split constant in open-loop, it is possible to achieve significant savings over time by just controlling a simple variable combination. It may be argued that an online real-time optimizer might perform equally or better. This is indeed true, however, it is much more expensive to set up and maintain a real-time optimizer than it is to simply control a simple function of measurements using PI controllers.

7. CONCLUSION

We presented a systematic approach to finding controlled variables for a class of industrially important problems. The idea is to use the split to control a combination of process variables at a constant setpoint. Controlling these variables gives optimal operation in spite of unmeasured disturbances. The resulting controlled variables are very easy and cheap to implement in the real process.

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