# Optimally Invariant Variable Combinations for Nonlinear Systems

**Johannes E. P. Jäschke Sigurd Skogestad**

*Norwegian University of Science and Technology (NTNU), Trondheim, Norway (e-mail: skoge@chemeng.ntnu.no).*

**Abstract:** Optimal operation of chemical processes becomes increasingly important in order to be able to compete in the international markets and to minimize environmental impact. A well established tool to achieve this goal is real-time optimization (RTO), where the optimal set-points are computed on-line based on measurements taken at given sample times. This involves setting up and maintaining an real-time computation system, which can be very expensive and time consuming. In this article we present a different approach for achieving optimal operation, by performing all calculations off-line and by determining optimally invariant variable combinations, which when kept constant, yield optimal operation. Once these variable combinations have been identified and the control structure is set up, there is no need for on-line optimization.
The procedure presented here is applicable to nonlinear steady state optimization problems and consists of four steps. First, regions of constant active constraints are defined. Second, optimally invariant nonlinear variable combinations are determined for each of the regions. Third, the unknown internal variables and disturbances are eliminated from the invariants to obtain variable combinations containing only known variable (measurements). Finally a strategy to detect changes in the active set is found in order to be able to operate the process over a large disturbance range. The method is tested on a model of a four component isothermal CSTR taken from Srinivasan and Bonvin (2008).

*Keywords:* Optimizing control, Nonlinear control systems, Real-time optimization, Self-optmizing control, Optimally invariant measurement combinations

## 1. INTRODUCTION

Strong competition, high commodity prices and environment protection issues have raised the importance of operating chemical plants as close to optimality as possible while satisfying the several constraints as equipment limits or environmental regulations.

In order to operate a chemical process optimally in presence of changing disturbances, two main approaches are currently found in industry and literature. The first approach is Real-Time Optimization (RTO). This strategy involves using a nonlinear process model to calculate the optimal set-points for the system on-line at certain sample times based on the last available measurements. Setting up and solving the optimization problem online can be very complex, as the usually large optimization problem has to be solved within a certain time interval.

The second approach is to minimize or avoid all complex on-line computations, and to find optimally invariant variable combinations (self-optimizing variable combinations). Controlling these variable combinations to their setpoints guarantees to operate the process optimal or close to optimal, with a certain acceptable loss (Skogestad (2000)). After these invariant variables have been identified, a simple, control structure based on PI controllers can be set up to control them to their setpoints yielding optimal process operation. The conventional Real-Time Optimization problem can either be replaced completely or partially by controlling the invariants.

In practice many processes are operated by the second approach, although not always deliberately. Often the optimization problem is not formulated explicitly and the control variables are chosen from experience and engineering intuition.

To the authors knowledge, optimally invariant variable combinations have been considered systematically only for linear plants with quadratic performance index (Alstad et al. (2008)). This contribution extends the idea of self-optimizing control from unconstrained, linear models to constrained nonlinear models. This extension to nonlinear constrained optimization problems makes this systematic method relevant for Real-Time Optimization applications, where nonlinear models are optimized for large disturbance variations and where the optimum generally is unconstrained.

The paper is structured as follows. First the concept of using invariant variable combinations for obtaining optimal operation in regions defined by active constraints is described. Then we show how optimally invariant variable combinations can be found for a well-posed system. If it is possible to eliminate the unknown disturbances and internal variables from the invariant variable combinations, the obtained measurement combinations can be used for control. Finally we present and example of how these results are applied to a nonlinear model of an isothermal CSTR from Srinivasan and Bonvin (2008).

## 2. PROCEDURE FOR FINDING INVARIANT MEASUREMENT COMBINATIONS

We consider a plant at steady state and assume the plant performance can be modelled as an optimization problem with a performance index $J$ together with equality and inequality constraints, $g(\mathbf{u},\mathbf{x},\mathbf{d})$ and $h(\mathbf{u},\mathbf{x},\mathbf{d})$:

$$\begin{aligned} \min f \\ \text{s.t} \\ g(\mathbf{u},\mathbf{x},\mathbf{d}) = 0 \\ h(\mathbf{u},\mathbf{x},\mathbf{d}) \leq 0 \end{aligned} \tag{1}$$

The variables $\mathbf{u}$, $\mathbf{x}$, $\mathbf{d}$ denote the manipulated input variables, the internal states, and the disturbance variables, respectively. In addition there we assume that there are measurements $\mathbf{y} = p(\mathbf{x},\mathbf{u},\mathbf{d})$ which provide information about the internal states and the disturbance of the process.

In order to obtain optimal operation we do not optimize the model on-line at given sample times. Instead, we use the structure of the problem in order to find optimally invariant variable combinations. Using PI or any other kind of controller to keep these variable combinations at their setpoints will result in optimal operation without re-optimizing when disturbances occur.

Since the available number of degrees of freedom changes when an inequality constraint becomes active, we have to find a new set of invariant measurement combinations for each set of constraints that becomes active during operation of the plant. This makes it necessary to define separate control structures for each region. Therefore, the first step is to partition the operating space into regions defined by the set of active constraints, i.e. the system is optimized for all possible disturbances and the active constraints in each region are identified.

In the second step, we determine (nonlinear) variable combinations which yield optimal operation when kept at their constant setpoint. The variables resulting from this first step cannot yet be used for control, because they contain unknown disturbance variables and internal states which are not directly known.

To be able to use the invariant measurement variables for control we eliminate the unknown variables using the equations from the active set and the measurements. After all unknown variables are eliminated from these expressions, the *measurement* invariants can be used for control in feedback loops.

The last step in this procedure is do define rules to detect and to switch region when the active constraints change. In many cases this can be done by monitoring the controlled variables of the neighbouring region and switching when the controlled variable of the neighbouring region reaches its optimal value. However, this assumes that it is not possible to skip regions and that the controlled variables are monotone rising or falling in the current region, which not always is the case. However for the CSTR example studied here, this method is applicable and gives good results.

### *2.1 Invariants for quadratic objective with linear constraints and measurements*

To illustrate the idea of finding invariant variable combinations we will first consider a problem with a quadratic objective and linear constraints. Later we will extend the result to nonlinear problems. After having defined $n_r$ regions we can define an equality constrained optimization problem for each region, by only considering the active constraints. In the following we will consider a problem with a quadratic objective and linear constraints. Later we will extend the result to nonlinear problems. For each of the $n_r$ regions of active constraints we have:

*Theorem 1.* (Linear invariants). Let $\mathbf{u} \in \mathbb{R}^{n_u \times 1}, \mathbf{x} \in \mathbb{R}^{n_x \times 1}, \mathbf{d} \in \mathbb{R}^{n_d \times 1}$, and let $\mathbf{A} \in \mathbb{R}^{(n_c \times n_u + n_x)}$ have full rank and let $n_c < n_u + n_x$. Furthermore let $\mathbf{A}_d \in \mathbb{R}^{n_c \times n_d}$, $\mathbf{b} \in \mathbb{R}^{n_c \times 1}$, and let $\mathbf{Q} \in \mathbb{R}^{(n_u+n_x+n_d)\times(n_u+n_x+n_d)}$ be a positive definite matrix made up of submatrices $\mathbf{DJ}, \mathbf{J_{ud}}, \mathbf{J_{xd}}$ and $\mathbf{J_{dd}}$ of suitable dimensions.

Consider the optimization problem:

$$\min\,[\mathbf{u}^{\mathrm{T}}\mathbf{x}^{\mathrm{T}}\mathbf{d}^{\mathrm{T}}] \underbrace{\begin{bmatrix} \mathbf{DJ} \\ \mathbf{J_{ud}}^{\mathrm{T}} \ \mathbf{J_{xd}}^{\mathrm{T}} \ \mathbf{J_{dd}} \end{bmatrix}}_{\mathbf{Q}} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \\ \mathbf{d} \end{bmatrix}$$

$$\text{s.t.} \quad [\mathbf{A}\,,\mathbf{A}_d] \begin{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \end{bmatrix} \\ \mathbf{d} \end{bmatrix} = \mathbf{b}$$

with measurements $\mathbf{y} = \tilde{\mathbf{G}}^y \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \\ \mathbf{d} \end{bmatrix}$.

If the problem is feasible, $\mathbf{Q} > 0$, and $\tilde{\mathbf{G}}^y$ invertible, we can find $\mathbf{c} = \mathbf{Hy}$ such that controlling $\mathbf{c}$ to zero yields optimal operation.

**Proof.** To obtain an optimally invariant variable combination we first write down the Karush-Kuhn-Tucker conditions:

$$\begin{aligned} 0 &= [\mathbf{A}\,,\mathbf{A}_d] \begin{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \end{bmatrix} \\ \mathbf{d} \end{bmatrix} - \mathbf{b} \\ \nabla L &= \mathbf{DJ} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \\ \mathbf{d} \end{bmatrix} + \mathbf{A^T}\lambda = 0 \end{aligned} \tag{2}$$

We can write the second equation as

$$\mathbf{A^T}\lambda = \underbrace{\mathbf{DJ} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \\ \mathbf{d} \end{bmatrix}}_{\mathbf{B}} = \mathbf{B} \tag{3}$$

Note that (3) is linear and overdetermined in $\lambda$, since $\lambda \in \mathbb{R}^{n_c \times 1}$ and $\mathbf{A^T} \in \mathbb{R}^{n_u + n_x \times n_c}$. Hence, depending on the right hand side of (3), there is either none or one unique solution for $\lambda$. From linear algebra it is known that the system is solvable if and only if $y^{\mathbf{T}}\mathbf{B} = 0$ whenever $y^{\mathbf{T}}\mathbf{A^T} = 0$. The feasible right hand side is therefore obtained by setting

$$\underbrace{\mathbf{N^T A^T}}_{=0}\lambda + \underbrace{\mathbf{N^T B}}_{:=\mathbf{c}^v} = 0. \tag{4}$$

Where $\mathbf{N}$ is a basis for the null space of $\mathbf{A}$. At the same time this is the desired optimally invariant variable combination since keeping it constant yields unique $\lambda$ which satisfy the KKT conditions. As a consequence it is found that $\mathbf{c} = \mathbf{N^T B} \in \mathbb{R}^{n_u+n_x-n_c\times 1}$, making the system

$$\mathbf{c}^v = \mathbf{N^T B} = 0$$
$$[\mathbf{A},\ \mathbf{A}_d] \begin{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \end{bmatrix} \\ \mathbf{d} \end{bmatrix} = \mathbf{b} \tag{5}$$

fully specified.

The unknown variables can now be eliminated from $\mathbf{B}$ using the measurements to yield the measurement invariant $\mathbf{c}_s^v$:

$$\mathbf{c}_s^v = \mathbf{N^T B} = \mathbf{N^T D J} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \\ \mathbf{d} \end{bmatrix} = \mathbf{N^T D J} [\tilde{\mathbf{G}}^y]^{-1} \mathbf{y} \tag{6}$$

□

*2.2 Invariants for nonlinear systems*

An analog approach may be taken for obtaining invariant variable combinations for more general systems described by nonlinear equations. Initially all regions defined by constant sets of active constraints are determined. For each region we then have:

*Theorem 2.* (Nonlinear invariants). Given $\mathbf{u}, \mathbf{x}, \mathbf{d}$ as in theorem 1, consider the nonlinear optimization problem

$$\begin{gathered} \min J(\mathbf{u}, \mathbf{x}, \mathbf{d}) \\ \text{s.t} \\ p_{c,i}(\mathbf{u}, \mathbf{x}, \mathbf{d}) = 0, \quad i = 1 \dots n_c \end{gathered} \tag{7}$$

and $n_j$ implicit measurement relations $p_{y,j}(\mathbf{y}, \mathbf{u}, \mathbf{x}, \mathbf{d}) = 0$. If the transposed of the Jacobian $\mathbf{A^T} = [\nabla p_{c,i}]$ has constant rank $n_c$ there are $n_{DOF} = n_u + n_x - n_c$ independent invariant variable combinations $c_s^v$.

If it is possible to eliminate the unknown variables and disturbances using measurements, these measurements can be used for controlling the system optimally.

**Proof.** Calculate the Jacobian

$$\mathbf{A} = \begin{bmatrix} \nabla p_{c,1}(\mathbf{u}, \mathbf{x}, \mathbf{d}) \\ \vdots \\ \nabla p_{c,n_c}(\mathbf{u}, \mathbf{x}, \mathbf{d}) \end{bmatrix} \tag{8}$$

and calculate its null space $\mathbf{N}$. Since the rows of $\mathbf{A}$ are independent, the null space has constant dimension. Apart from that $\mathbf{A}$ and $\mathbf{N}$ now are functions, the proof is analog to the proof of theorem 1. Set up the KKT conditions and use the fact that the KKT conditions are linear in $\lambda$. The KKT conditions and the conditions for existence and uniqueness for $\lambda$ are:

$$\begin{gathered} \nabla J(\mathbf{u}, \mathbf{x}, \mathbf{d}) + \mathbf{A^T} \lambda = 0 \\ \mathbf{N^T} \nabla J = \mathbf{N^T A^T} \lambda = 0 \end{gathered} \tag{9}$$

The invariant variable combination is then given by:

$$\mathbf{c}^v = \mathbf{N^T} \nabla J(\mathbf{x}, \mathbf{u}, \mathbf{d}) \tag{10}$$

If the unknown variables $(\mathbf{x}, \mathbf{d})$ can be eliminated from (10) we have obtained the desired measurement invariants which when controlled at their setpoints yield optimal operation. □

*Remark 1.* When calculating the matrix $\mathbf{N} = \mathcal{N}(\mathbf{A})$ it is important that the rank remains constant (i.e. that the rows of $\mathbf{A}$ remain linear independent for every realization of $\mathbf{A}$ in the operating region). If this is not the case at some point, the $\mathbf{N}$ will change dimension implying that the number of degrees of freedom for the problem changes (increases). Such phenomena are not covered by this method.

*Remark 2.* If for every $c_s^v$ there exist some $h_{c,i}, g_{y,j}$ such it can be written in the form $c_s^v = \sum_{i,j} (h_{c,i} p_{c,i} + g_{y,j} p_{y,j}) + r(\mathbf{y})$, the term $r(\mathbf{y})$ is the desired measurement invariant $c_s^y$. This follows from the implicit relations $p_{c,i} = 0$ and $p_{y,j} = 0$. This is in particular useful for polynomial systems, where $c_s^v$ can be obtained by polynomial reduction.

## 3. EXAMPLE

As an application example, we consider the model of an isothermal CSTR with two parallel reactions, Fig. 1 (Srinivasan and Bonvin (2008)). Two feed streams $F_A$ and $F_B$ with the concentrations $c_A$ and $c_B$ react in a tank to the desired product $C$ and the undesired side product $D$. The tank is equipped with one outflow in which all components are present. In order to enable isothermal reaction conditions a temperature loop is closed such that the correct amount of heat is removed from the system. The temperature control is assumed to be perfect.

In the CSTR, the reaction products $C$ and $D$ are formed according to following reaction equations:

$$\begin{aligned} \text{A} + \text{B} &\xrightarrow{k_1} \text{C} \\ 2\,\text{B} &\xrightarrow{k_2} \text{D} \end{aligned} \tag{11}$$

As optimization objective we wish to maximize the desired product $(F_A + F_B)c_C$ weighted by the yield factor $(F_A + F_B)c_C/(F_A c_{A,in})$. Due to the installed equipment the amount of heat to remove and the maximum flow rate are limited to some upper bound. The corresponding optimization problem of the system is formulated as follows:

$$\max_{F_A, F_B} \frac{(F_A + F_B)c_C}{F_A c_{A_{in}}} (F_A + F_B) c_C \tag{12}$$

subject to

$$\begin{aligned} F_A c_{A_{in}} - (F_A + F_B)c_A - k_1 c_A c_B V &= 0 \\ F_B c_{B_{in}} - (F_A + F_B)c_B - k_1 c_A c_B V - 2k_2 c_B^2 V &= 0 \\ -(F_A + F_B)c_C + k_1 c_A c_B V &= 0 \\ F_A + F_B - F &= 0 \\ k_1 c_A c_B V(-\Delta H_1) + 2k_2 c_B V(-\Delta H_2) - q &= 0 \\ q - q_{max} &\le 0 \\ F - F_{max} &\le 0 \end{aligned} \tag{13}$$

The variables $k_1$ and $k_2$ are the isothermal rate constants for the two reactions, $(-\Delta H_1)$ and $(-\Delta H_2)$ are the corresponding reaction enthalpies, $q$ the heat produced by the reactions, $V$ the reactor volume. The measured variables ($\mathbf{y}$), the manipulated variables (MV) and the disturbance variable ($\mathbf{d}$) are listed in table 1, and the parameter values of the system are listed in table 2.

*3.1 Identifying operational regions*

The first step of the procedure, optimizing the system offline for all possible values shows that the system operation

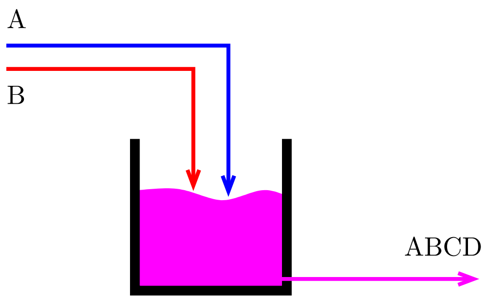


Fig. 1. CSTR with two reactions

space can be divided into three regions defined by the set of active constraints. In region 1, for values of $k_1$ below about 0.65 only the flow constraint is active (Fig. 2). In region 2 for values between 0.65 and 0.8 both constraints are active, and in region 3 above 0.8 only the heat constraint is active.

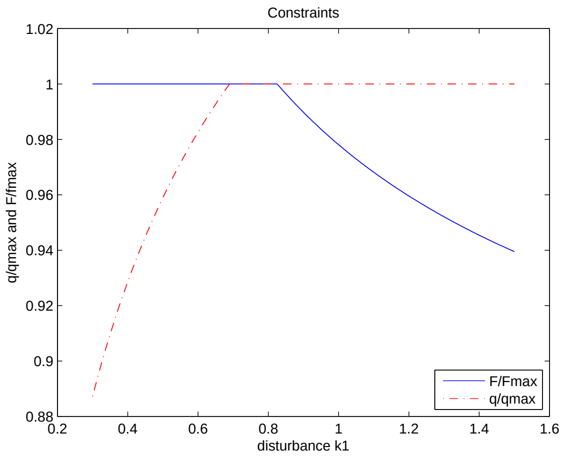


Fig. 2. Optimal values of the constrained variables

After satisfying the active constraints in the regions we are left with $N_{\text{DOF},1} = 1$ for region 1, $N_{\text{DOF},2} = 0$ for region 2, and $N_{\text{DOF},1} = 1$ for region 3.

In region 1, one of the MVs (flow rates) is used to control the active constraint (maximum flow) and the other MV is used to control the invariant measurement combination of the region. In region 2 we simply control the active constraints, keeping $q$ at $q_{\max}$ and $F$ at $F_{\max}$. In region 3, again one of the MVs is used to control the active constraint (maximum heat removal) and the other MV is used to control the invariant measurement combination of region 3.

Table 1. Variables relevant for control

| | |
|---|---|
| Measurements $\mathbf{y}$ | $F_A, F_B, c_A, c_b, q$ |
| Manipulated variables $\mathbf{u}$ | $F_A, F_B$ |
| Unknown disturbance $\mathbf{d}$ | Rate constant $k_1$ |

Table 2. Parameters

| | | |
|---|---|---|
| $k_1$ | l/(mol h) | 0.3-1.5 |
| $k_2$ | l/(mol h) | 0.0014 |
| $(-\Delta H_1)$ | j/mol | $7 \times 10^4$ |
| $(-\Delta H_2)$ | j/mol | $5 \times 10^4$ |
| $c_{A,in}$ | mol/l | 2 |
| $c_{B,in}$ | mol/l | 1.5 |
| $V$ | l | 500 |
| $F_{\max}$ | l | 22 |
| $q_{max}$ | kJ/h | 1000 |

In regions 1 and 3, where the system has one degree of freedom, finding invariant variable combinations is non-trivial, while in region 2 the invariants are simply the active constraints, $q = q_{\max}$ and $F = F_{\max}$.

### 3.2 *Determining the invariant variable combinations*

Using the information from the previous section, we can start finding invariant variable combinations for region 1 and 3. In the next step we calculate the null space of Jacobian of the active set $\mathbf{N^T}$ and multiply it with the gradient of the objective function as in (10) to obtain the invariant variable combination. Generally this will become a fractional expression, but since we are controlling it to zero, it is sufficient to consider only the numerator in all further calculation.

Evaluating the numerator of $\mathbf{N^T}\nabla J$ yields the invariant variable combination for region 1:

$$\begin{aligned}
\mathbf{c}_1^v = &-(F_A + F_B)^2 c_C \big[-3c_C F_B^2 F_A - 3c_C F_A^2 F_B \\
&- 4c_C c_B F_A^2 k_2 V - 4c_C k_2 V^2 k_1 c_B^2 F_A - c_C F_A^3 \\
&- c_C F_B^3 - 4c_C k_2 V^2 k_1 c_B^2 F_B - c_C c_B F_A^2 k_1 V \\
&- 4c_C c_B F_B^2 k_2 V - c_C c_B F_B^2 k_1 V - c_C F_A^2 c_A k_1 V \\
&- c_C F_B^2 c_A k_1 V - 8c_C F_A c_B F_B k_2 V \\
&- 2c_C F_A c_B F_B k_1 V - 2c_C F_A F_B c_A k_1 V \\
&+ 8F_A k_1 V^2 c_{A,in} k_2 c_B^2 + 2F_A^2 k_1 V c_B c_{A,in} \\
&+ 2F_A k_1 V F_B c_B c_{A,in} - 2F_A^2 k_1 V c_{B,in} c_A \\
&-2F_A k_1 V F_B c_{B,in} c_A\big]
\end{aligned} \tag{14}$$

This invariant may be simplified even more knowing that $(F_A + F_C)c_C \neq 0$, so it is sufficient to control the second term in (14) to zero.

As mentioned above, region 2 does not have any unconstrained degree of freedom, so satisfying all active constraints yields optimal operation. In other words, the optimally invariant variable combinations are the equations of the inequality constraints in (13).

In region 3 the procedure is exactly the same, yielding a similar expression for $\mathbf{c}_3^v$.

### 3.3 *Eliminating unknown variables*

The invariant variable combinations still contain the unknown and internal variables $k_1$ and $c_C$, so they cannot be used for feed back control directly. In the next step the unknown variables have to be replaced by expressions in the measured variables, so that this invariant can be used for control. Depending on the type of the system equations, different methods may be applied in this step. The general idea is that we use the measurements together with the equations that are satisfied in the active set to express the invariant. As all equations in this case study are polynomial (rational expressions equal to zero can transformed to polynomials by multiplication with the denominator), we attempt to reduce the invariants modulo the active set with a variable ordering that eliminates the unknowns.

It is found that by only reducing the invariant modulo the active constraints and with an appropriate term order, $k_1$ was not eliminated. In order to be eliminated, the leading term of the polynomial of $c^v$ has to be a multiple of a leading term of the set of polynomials that describe the active constraints or the measurements.

However, this could be resolved by solving the third equality constraint for $k_1$

$$k_1 = (F_A + F_B)c_C/(c_A c_B V) \tag{15}$$

and inserting it into (14). Having eliminated $k_1$ in this way, the other unknown variable was eliminated using polynomial reduction and the resulting *measurement* invariant becomes:

$$\begin{aligned}
c_{s,1} = &-c_B c_A^2 F_B c_{A,in} F_{max}^4 - 2c_B c_A F_B^2 c_{A,in}^2 F_{max}^3 \\
&- c_B F_B^3 c_{A,in}^3 F_{max}^2 + c_B c_A^2 c_{A,in} F_{max}^5 \\
&+ 4c_B c_A F_B c_{A,in}^2 F_{max}^4 + 3c_B F_B^2 c_{A,in}^3 F_{max}^3 \\
&- 2c_B c_A c_{A,in}^2 F_{max}^5 - 3c_B F_B c_{A,in}^3 F_{max}^4 \\
&+ c_B c_{A,in}^3 F_{max}^5 - c_A^4 F_{max}^5 - c_A^3 F_B c_{A,in} F_{max}^4 \\
&- 2c_A^3 F_B c_{B,in} F_{max}^4 + 3c_A^2 F_B^2 c_{A,in}^2 F_{max}^3 \\
&- 2c_A^2 F_B^2 c_{A,in} c_{B,in} F_{max}^3 + 5c_A F_B^3 c_{A,in}^3 F_{max}^2 \\
&+ 2c_A F_B^3 c_{A,in}^2 c_{B,in} F_{max}^2 + 2F_B^4 c_{A,in}^4 F_{max} \\
&+ 2F_B^4 c_{A,in}^3 c_{B,in} F_{max} + c_A^3 c_{A,in} F_{max}^5 + 2c_A^3 c_{B,in} F_{max}^5 \\
&- 6c_A^2 F_B c_{A,in}^2 F_{max}^4 + 6c_A^2 F_B c_{A,in} c_{B,in} F_{max}^4 \\
&- 15c_A F_B^2 c_{A,in}^3 F_{max}^3 - 2c_A F_B^2 c_{A,in}^2 c_{B,in} F_{max}^3 \\
&- 8F_B^3 c_{A,in}^4 F_{max}^2 - 6F_B^3 c_{A,in}^3 c_{B,in} F_{max}^2 \\
&+ 3c_A^2 c_{A,in}^2 F_{max}^5 - 4c_A^2 c_{A,in} c_{B,in} F_{max}^5 \\
&+ 15c_A F_B c_{A,in}^3 F_{max}^4 - 2c_A F_B c_{A,in}^2 c_{B,in} F_{max}^4 \\
&+ 12F_B^2 c_{A,in}^4 F_{max}^3 + 6F_B^2 c_{A,in}^3 c_{B,in} F_{max}^3 \\
&- 5c_A c_{A,in}^3 F_{max}^5 + 2c_A c_{A,in}^2 c_{B,in} F_{max}^5 \\
&- 8F_B c_{A,in}^4 F_{max}^4 - 2F_B c_{A,in}^3 c_{B,in} F_{max}^4 + 2c_{A,in}^4 F_{max}^5
\end{aligned} \tag{16}$$

Although this expression seems rather complicated, it contains only known variables and therefore it can be easily evaluated and controlled to its setpoint using a PI controller.

The measurement invariant for region 3 is found in the same way as the previous one:

$$\begin{aligned}
c_{s,3} = &\, 2Fc_A^2 q_{max} - 2F^2 c_{A,in}^2 \Delta H_2 c_B \\
&+ 2F^2 c_{A,in}^2 \Delta H_2 c_{B,in} - 2F^2 c_{A,in} \Delta H_2 c_B^2 \\
&+ 3F^2 c_A^2 \Delta H_2 c_{B,in} - 2F c_A q_{max} c_{A,in} \\
&- F c_A c_{B,in} q_{max} - 2F_B^2 c_{A,in}^2 \Delta H_2 c_B \\
&+ 2F_B^2 c_{A,in}^2 \Delta H_2 c_{B,in} + 2F_B^2 c_{A,in} \Delta H_2 c_{B,in}^2 \\
&- 2F_B^2 c_A \Delta H_2 c_{B,in}^2 + 2F_B c_A q_{max} c_{A,in} \\
&- 2F_B^2 c_{A,in} c_B \Delta H_2 c_{B,in} - 2F_B^2 c_{A,in} c_A \Delta H_2 c_{B,in} \\
&- 4F_B F c_{A,in}^2 \Delta H_2 c_{B,in} + 4F_B F c_{A,in}^2 \Delta H_2 c_B \\
&+ 2F_B F c_{A,in} \Delta H_2 c_B^2 - 2F_B F c_{A,in} \Delta H_2 c_{B,in}^2 \\
&+ 7F_B F c_{A,in} c_A \Delta H_2 c_{B,in} + 2F^2 c_{A,in} c_B c_A \Delta H_2 \\
&- 5F^2 c_{A,in} c_A \Delta H_2 c_{B,in} + 2F^2 c_{A,in} c_B \Delta H_2 c_{B,in} \\
&- 3F^2 c_B c_A \Delta H_2 c_{B,in} - 2F_B F c_{A,in} c_B c_A \Delta H_2 \\
&- 2F_B F c_A^2 \Delta H_2 c_{B,in} + 2F_B F c_B c_A \Delta H_2 c_{B,in} \\
&+ 3F_B F c_A \Delta H_2 c_{B,in}^2 + 2F_B c_A c_{B,in} q_{max}
\end{aligned} \tag{17}$$

The values of these polynomial equations can vary over several order of magnitudes, so it is useful to scale the invariants in order to avoid numerical problems. Therefore the invariant of region 1 was scaled by the factor $10^5$ and the invariant of region 3 was scaled by $10^6$.

### 3.4 Using measurement invariants for control and region identification

For the system to be operated optimally we not only need to know which variables we want to keep constant during operation, but we need to know which region we currently operate in and when to change region. Assuming the initial region is known and it is not possible to skip regions, we can easily detect when to change region for this system by monitoring the controlled variables of the neighbouring regions.

Starting in region 1 optimal operation is achieved by using the two inputs $F_A$ and $F_B$ to control $c_{s,1} = 0$ and $F_A + F_B = F_{max}$. If $k_1$ increases, The amount of heat to be removed (the controlled variable of region 2) increases until it reaches the maximum possible value, $q_{max}$ (Fig 3). When this value is reached, the control structure has to changed to region 2. Now the inputs are used to control $q$ to $q_{max}$ and $F_A + F_B$ to $F_{max}$. While operating in region 2 the controlled variables of the neighbouring regions,$\mathbf{c}_{s,1}$ and $\mathbf{c}_{s,2}$ are monitored. If $k_1$ increases further, the $c_{s,3}$ approaches its optimal setpoint for region 3 and we switch region when the optimal value is reached. Switching back from the different regions is done in an analog manner.

## 4. CONCLUSION

In this paper we have presented an approach to obtain optimal steady state operation which does not require online calculations. After identifying the regions of constant active constraints, it is shown that there exist some optimally invariant variable combination for each region. If the unknown variables can be eliminated by measurements and system equations, the invariant combinations can be used for control.

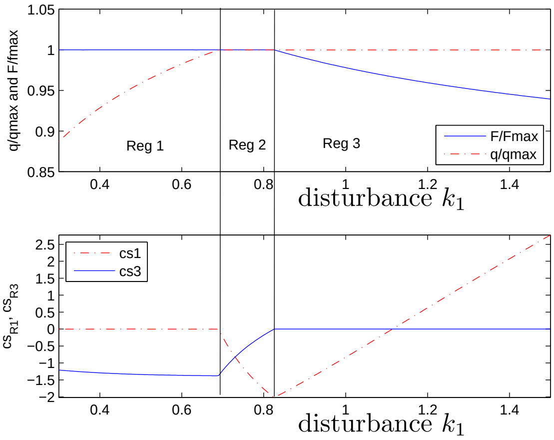


Fig. 3. Optimal values of controlled variables

In the example presented, the measurement invariants can be used for detecting changes in the active set and for finding the right region to switch to. This, however is not generally possible as an invariant may not be monotone increasing or decreasing within a regions. However as all these considerations are performed off-line, it can be determined in advance whether it is possible to track the regions by monitoring neighbouring control variables or if alternative approaches such as binary search trees have to be used. **citation?**

Although designing a self-optimizing control structure may require more work in advance, its implementation and maintenance is easy in practice. After the control structure is in place, optimal operation can achieved by simple PI controllers and there is no need to invest in expensive real-time equipment to operate the process optimally.


## ACKNOWLEDGEMENTS

**Funding ??**


## REFERENCES


Alstad, V., Skogestad, S., and Hori, E. (2008). Optimal measurement combinations as controlled variables. *Journal of Process Control*.

Skogestad, S. (2000). Plantwide control: The search for the self-optimizing control structure. *Journal of Process Control*, 10, 487–507.

Srinivasan, B. Biegler, L. and Bonvin, D. (2008). Tracking the necessary conditions of optimality with changing set of active constraints using a barrier-penalty function. *Computers and Chemical Engineering*, 32, 572–279.