Optimal Measurement System Design for Chemical Processes

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A procedure for the optimal determination of measured variables in chemical processes is presented. This procedure is based on quantifying the trade-off between the process information that can be obtained and the total cost of the sensors making up the measurement system. The resulting trade-off is specified as a Pareto optimization problem. The optimal measurement systems that should be considered for installation are determined from the set of solutions to this Pareto optimization problem. The approach is demonstrated using a CSTR process example.

Introduction

Monitoring and control of chemical processes are based on the measured values available from the installed measurement system. The information that can be obtained from the process is dependent on the number of process sensors and the selection of the corresponding measured variables. Increasing the number of sensors will increase the information that can be obtained from the process, but also increase the measurement cost associated with the process measurement system. The result is a trade-off between the information that can be obtained and the total measurement cost. In this work, we quantify this trade-off as a Pareto optimization problem. The set of Pareto optimal solutions to this problem are then taken as possible optimal measurement system designs.

Previous work by Joseph and Brosilow (1978) and Morari and Stephanopoulos (1980) considered the selection of measured variables to reduce the reconstruction error in inferential controlled variables. Scalar measures of the quality or degree of observability, such as the trace, determinant, and maximal eigenvalue of the inverse characteristic observability matrix, are presented by Muller and Weber (1972). Waldraff et al. (1998) use similar observability metrics for sensor location in tubular reactors. The effect of sensor placement on the condition number of the observability matrix for a linearized, fixed-bed bioreactor model is discussed by Dochain et al. (1996). Ali and Narasimhan (1993) extend the observability metric for sensor selection by considering the reliability of measurement systems in the presence of sensor failure.

Other measures that consider the trace, determinate, or norm of the state prediction error covariance matrix are discussed by Mehra (1976) for linear dynamic systems, and Omatu et al. (1978) and Kumar and Seinfeld (1978a) for linear distributed-parameter systems. These measures are used to optimize the sensor location for tubular reactors in Colantuoni and Padmanabhan (1977), Kumar and Seinfeld (1978b), Harris et al. (1980), and Jorgensen et al. (1984). Morari and O'Dowd (1980) present an optimal projection approach for sensor location in linear distributed-parameter systems. Optimization of the determinate of the Fischer information matrix is presented by Qureshi et al. (1980) in the context of distributed-parameter system identification. Optimal sensor location based on the determinate of a sensor response matrix for distributed-parameter systems is discussed by Sadegh and Spall (1998). A similar measure is presented by Wouwer et al. (2000) and demonstrated using a tubular reactor.

Alvarez et al. (1981) discuss optimal selection within a variable measurement structure for the adaptive control of a tubular reactor. Romagnoli et al. (1981) also consider variable measurement structures for distillation and tubular reactor control. Control-based metrics for sensor selection in the context of distillation control are discussed by Yu and Luyben (1984). Narraway and Perkins (1993) consider the selection of the economically optimal controlled and manipulated

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variables for regulatory control of square, linear, time-invariant systems. The optimal sensor selection in square inferential control systems for distillation control is presented by Kookos and Perkins (1999).

None of these previous works explicitly consider measurement cost in the optimization of the various observability or controllability metrics. Measurement cost is considered by Athans (1972) in the context of optimal switching times between a series of sensors and by Mellefont and Sargent (1977) in the context of optimal measurement subset selection for linear stochastic systems. The selection of sensors based on the minimization of an objective that includes both the measurement cost and the covariance of the state prediction error is presented by Mellefont and Sargent (1978). The minimization of measurement cost subject to measurement-system performance constraints related to data reconciliation requirements is discussed by Madron and Veverka (1992), Bagajewicz (1997), and Chmielewski et al. (2002). The work of Chmielewski et al. (2002) also addresses dynamic systems.

The trade-off between measurement cost and process information in the optimal determination of measurement systems for chemical processes is directly considered in this work. In the following sections, we present the optimal measurement system design method. The process model used in the analysis is first discussed. We then define the process information and cost metrics, discuss other metrics proposed in the literature in relation to the present work, and present the optimal measurement-system selection procedure along with the computations required to implement the technique. Finally, we introduce a CSTR process example to illustrate the procedure.

Measurement-System Design Procedure

We define an optimal measurement system as any sensor combination for which there is no other combination that provides increased process information at a lower measurement cost (Muske and Georgakis, 2002). The inverse norm of a weighted steady-state state prediction error covariance matrix is used as a scalar measure of the process information associated with a given measurement system. The measurement cost associated with this system is determined from the summation of the installed cost and the present value of the future expected operating cost for each sensor. The resulting optimal sensor combinations comprise a Pareto optimal set that represent the optimal trade-off between measurement cost and process information. We note that if a process sensor combination is not optimal, there is some other combination that provides increased process information at a reduced measurement cost. Therefore, only optimal process sensor combinations should be considered for installation.

The incorporation of measurement cost and process information into a single objective function (Mellefont and Sargent, 1978) or the minimization of measurement cost subject to minimum process information constraints (Bagajewicz, 1997) and (Chmielewski et al., 2002) provides a single sensor combination that does not consider other potentially attractive measurement systems. For example, it may be possible to accept a slight increase in measurement cost to attain a significant increase in process information or to accept a slight decrease in process information to attain a significant decrease in measurement-system cost. This information is not available from the solution of a single optimization problem.

Process model

We begin with a physical state-space model of the process. Because a physical process model is used, each of the states represents a physical quantity that can potentially be measured and selected as a measured variable. If the state-space process model is nonlinear, it is linearized about the nominal steady-state operating point of interest. If a number of nominal operating points exist for the process, the system model is linearized at each and a separate analysis is carried out. The states of the state-space process model are partitioned into dependent states and independent states. The independent states include the independent variables for the nominal operation such as the manipulated and disturbance variables. We include these independent variables in the state-space model because we are interested in quantifying the effect of disturbances that enter the system through these variables. The result is a partitioned stochastic linear system of the form

$$\begin{bmatrix} \dot{\boldsymbol{z}} \\ \dot{\boldsymbol{u}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{A}_z & \boldsymbol{A}_u \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{z} \\ \boldsymbol{u} \end{bmatrix} + \begin{bmatrix} \boldsymbol{G}_z \\ \boldsymbol{G}_u \end{bmatrix} \boldsymbol{w} \tag{1}$$

$$\boldsymbol{y} = \boldsymbol{C} \begin{bmatrix} \boldsymbol{z} \\ \boldsymbol{u} \end{bmatrix} + \boldsymbol{v} \tag{2}$$

where $\boldsymbol{z} \in \Re^{n_d}$ are the dependent states of the system, $\boldsymbol{u} \in \Re^{n_i}$ are the independent states of the system, $n_d + n_i = n$, $\boldsymbol{y} \in \Re^{l}$ are the measured variables, $\boldsymbol{w} \in \Re^{m}$ are the state disturbances, and $\boldsymbol{v} \in \Re^{l}$ is the sensor noise. We assume zero mean, normally distributed sensor noise and state disturbances in this work. In the sequel, we will denote the partitioned system in Eqs. 1 and 2 using the simplified notation in Eq. 3

$$\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{G}\boldsymbol{w}, \qquad \boldsymbol{y} = \boldsymbol{C}_{\boldsymbol{x}} + \boldsymbol{v}, \qquad \boldsymbol{x} = \begin{bmatrix} \boldsymbol{z} \\ \boldsymbol{u} \end{bmatrix} \tag{3}$$

Because each state represents a physical quantity in the state-space model, each row of the $\boldsymbol{C} \in \Re^{l \times n}$ matrix will take the form

$$[0, \ldots, 0, 1, 0, \ldots, 0]$$

in which the nonzero entry indicates the state corresponding to the measured physical variable. Sensors that measure some linear combination of the physical variables of the system, such as a total flowmeter, can be represented within this framework by including additional unit entries in the row vector.

Process information metric

We define a scalar measure for the process information associated with a particular sensor combination based on the steady-state state prediction-error covariance matrix. Because it is the state estimates that will be used for control and monitoring of the process, the prediction error covariance matrix provides a good process information metric for sensor selection. We do not use observability-based metrics,

since they do not provide direct information about the information content of the estimated states. We also wish to avoid the potential numerical difficulties associated with computing the observability matrix as pointed out in Paige (1981) and Laub (1985). We note that other scalar metrics that quantify the information provided by a measurement system, such as those discussed in Qureshi et al. (1980), Sadegh and Spall (1998), and Wouwer et al. (2000), are equally appropriate.

The state prediction error covariance matrix for the linearized system can be computed using the algebraic Riccati equation (Jazwinski, 1970)

$$\boldsymbol{AP} + \boldsymbol{PA}^T - \boldsymbol{PC}^T\boldsymbol{R}^{-1}\boldsymbol{CP} + \boldsymbol{GQG}^T = \boldsymbol{0} \tag{4}$$

in which $\boldsymbol{P}$ is the state error covariance matrix, $\boldsymbol{R}$ is the covariance matrix associated with the sensor noise, and $\boldsymbol{Q}$ is the covariance matrix associated with the state disturbances entering the system. We note that the solution of Eq. 4 will only represent the true linearized estimated error covariance if the disturbances to the system are accurately modeled. Of particular concern is the determination of $\boldsymbol{G}_u$ and $\boldsymbol{Q}_u$ for the independent variables. Unless one has prior knowledge of these disturbances or is able to perform time-series analysis experiments, both of which may not be practical in the context of sensor placement, the selection of this disturbance model may be considered as a choice of tuning parameters for the algorithm. The information obtained from the inclusion of the independent variables with some reasonable noise model, however, can provide a representative information metric value for measurement system design.

A scalar process information metric based on the state error covariance matrix can be determined from the following inverse matrix p-norm

$$a = \left\| \frac{1}{w}\boldsymbol{WSPS} \right\|_p^{-1}, \qquad p \in \{2, \infty\} \tag{5}$$

in which $\boldsymbol{P}$ is determined from the solution of Eq. 4, $\boldsymbol{W}$ is a diagonal weighting matrix that specifies the relative importance of each state, $\boldsymbol{S}$ is a diagonal scaling matrix used to normalize the covariance terms, w is a normalization term, and a is a scalar metric of the information content provided by the measurement system.

In this work, we consider only the two-norm, which includes a contribution from every state with a nonzero weight, and the ∞-norm, which includes only the state with the largest weighted and scaled covariance. The weighting matrix, $\boldsymbol{W}$, is used to specify the relative contribution to the process information metric from each state. In most process systems, there are a number of critical states that are key indicators of product quality and process safety. There are other states that are less critical for the process operation. This relative importance can be incorporated into the measurement-system design procedure through the entries on the diagonal of the weighting matrix. A convenient scaling matrix $\boldsymbol{S}$ can be constructed by taking the inverse standard deviations of the state reconstruction error in the case of all possible measured outputs as the diagonal. This choice of scaling provides an unweighted, process information metric in the range of zero to one. The normalization term, w, is used to retain this range for the particular choice of $\boldsymbol{W}$.

Only those sensor combinations that result in observability of the states with nonzero weights in the weighting matrix $\boldsymbol{W}$ are considered as potentially optimal measurement systems. This restriction guarantees that each process variable with a nonzero weight can be completely reconstructed from the process measurements. Therefore, all sensor combinations for which the nonzero weighted states are measured, in addition to all combinations that result in $(\boldsymbol{C}, \boldsymbol{A})$ observable, are considered. For those sensor combinations that do not result in $(\boldsymbol{C}, \boldsymbol{A})$ observable when all weighted states are measured, a solution to the algebraic Riccati equation in Eq. 4 can be obtained by including high variance fictitious sensors to achieve system observability, as suggested by Chmielewski et al. (2002). In the present work, the effect of these sensors on the process information metric can be essentially eliminated through the selection of the scaling matrix entries corresponding to the states with fictitious sensors.

Alternate information metrics

Other measurement-system performance metrics that are related to data reconciliation such as availability, gross error detectability, and resilience can also be considered. Previous work by Bagajewicz (1997) and Chmielewski et al. (2002) minimized measured cost subject to minimum constraints on these metrics. Within the present framework, these metrics can either replace the process information metric in Eq. 5 or they can be treated as constraints on the Pareto optimization of the present information metric that an optimal measurement system must satisfy. We refer the reader to Bagajewicz (1997) and Chmielewski et al. (2002) for the details concerning the implementation of these metrics.

Reliability of the measurement system can be included in this analysis by considering the failure rate of the sensors comprising the measurement system. Previous work by Ali and Narasimhan (1993) defined the reliability of a measured variable as the probability of estimating its value for a given measurement system and sensor failure probabilities. The minimum reliability among all variables was then maximized in the optimization procedure presented in Ali and Narasimhan (1993), and the measurement cost was minimized subject to a reliability constraint in Chmielewski et al. (2002). This metric can either be optimized or treated as a constraint on the Pareto optimization of the information metric.

A third possibility is the incorporation of reliability into the process-information metric by considering the expected value of the metric in Eq. 5. The expectation is computed as

$$\xi(a) = \sum_i Pr(\Omega_i)\,\Theta(\Omega_i)\,\| \boldsymbol{WSP}(\Omega_i)\boldsymbol{S} \|_p^{-1}, \qquad p \in \{2,\infty\} \tag{6}$$

where the set Ω_i represents the ith possible subset of sensors for a given measurement system, $Pr(\Omega_i)$ is probability of the occurrence of this subset due to sensor failure, and $\Theta(\Omega_i) = 1$ if the subset results in an observable system or $\Theta(\Omega_i) = 0$ otherwise. Assuming that sensor failures are independent events, the probability of the occurrence of any subset of sensors in a measurement system can be computed by taking the product of the on-line probabilities or reliabilities

for each working sensor and the off-line probabilities for each failed sensor in the subset.

Cost metric

We define a scalar metric for the measurement cost as

$$c = \| \boldsymbol{Ce} \|_1 \tag{7}$$

in which $\boldsymbol{e} = [e_1, e_2, \ldots, e_n]^T$ is a vector containing the sensor expense for each physical property represented by the system states, $x_1 - x_n$. The sensor expense comprises the installed cost and present value of the future expected operating cost on either a relative or absolute basis. The incremental expense of the sensor is typically a more appropriate value to compare for most common process measurements. However, the proper value may depend on the specified measurement system. Composition measurements, for example, may not scale linearly with the number of measurements, because the infrastructure necessary to support each measurement may not have to be replicated. In this case, a more representative cost metric is

$$c = \sum_{i=1}^{l} \sum_{j=1}^{l} t_{i,j}, \qquad \boldsymbol{T} = \boldsymbol{CEC}^T \tag{8}$$

in which $t_{i,j}$ are the elements of the matrix $\boldsymbol{T}$. The matrix $\boldsymbol{E}$ contains the vector $\boldsymbol{e}$ on the diagonal, with off-diagonal terms representing any additional costs or savings associated with particular sensor combinations in a similar manner to the metric presented in Mellefont and Sargent (1978). We note that when $\boldsymbol{E}$ is a diagonal matrix, Eq. 8 produces the same value as Eq. 7.

Numerical computation

Generation of the Pareto optimal measurement system set requires the determination of the process information and cost metrics for observable measured variable combinations. An efficient search procedure to determine the combinations that comprise the Pareto optimal set can be based on the observation that if a given $\boldsymbol{C}$ matrix does not result in an observable system, removing rows from that matrix (eliminating measured variables) also will not result in an observable system. Therefore, a significant number of combinations can be eliminated. However, the resulting search is combinatorial in nature and can be prohibitive for large-scale systems (Korte and Vygen, 2000).

The numerical computations required for each sensor combination in this procedure involve the determination of the rank of the observability matrix and the solution of the steady-state algebraic Riccati equation. The Schur method described in Laub (1979) is used to determine the steady-state state prediction error covariance matrix. Determination of observability is based on the Lanczos Arnoldi algorithm in Boley and Golub (1984). The numerical procedure is described in Golub and Van Loan (1989) with the exception of the complete reorthogonalization used to obtain an orthogonal basis for the Krylov subspace at each Arnoldi iteration, which is outlined in Saad (1996). The rank of the observability matrix is then determined from the number orthogonal-

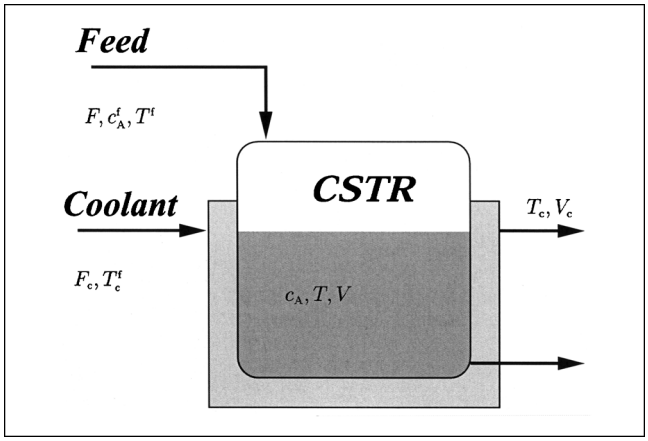

Figure 1. CSTR reactor diagram.

F is the feed flow rate, c_A^f is the feed composition, T^f is the feed temperature, F_c is the coolant flow rate, T_c^f is the coolant inlet temperature, T_c is the coolant temperature, V_c is the cooling jacket volume, c_A is the reactor composition, T is the reactor temperature, and V is the reactor liquid volume.

basis vectors for the observable subspace. We note that computational difficulties can arise in determining the rank of the observability matrix; however, this value is not used in the calculation of the information metric. If desired, measurement systems that are numerically unobservable can still be considered within this framework by the addition of high variance fictitious sensors, as discussed previously.

Example

We illustrate the design approach using the CSTR reaction system shown in Figure 1. In this example, component A undergoes a first-order, exothermic reaction to form a product component B

$$A \rightarrow B, \quad \Re_A = k \exp(-E/RT) c_A \tag{9}$$

The heat of reaction is removed by a cooling jacket surrounding the reactor, through which a coolant flow is maintained. The CSTR system can be described by the following nine ODEs. The first three are obtained from a mole balance over component A and an energy balance over the reactor fluid and the coolant in the cooling jacket, assuming perfect mixing and constant physical properties. The six independent variables are included in the state space model in order to take into account disturbances entering the system

$$\dot{c}_A = \frac{F}{V}(c_A^f - c_A) - \Re_A \tag{10}$$

$$\dot{T} = \frac{F}{V}(T^f - T) + \frac{\Delta H}{\rho C_p} \Re_A - \frac{hA}{\rho C_p V}(T - T_c) \tag{11}$$

$$\dot{T}_c = \frac{F_c}{V_c}(T_c^f - T_c) + \frac{hA}{\rho_c C_{p_c} V_c} \tag{12}$$

$$\dot{V} = 0 \tag{13}$$

Table 1. Nominal Operating Values

Parameter	Variable	Value
Feed flow	F	0.1 m^3/h
Feed temperature	T^f	20°C
Feed composition	c_A^f	2,500 mol/m^3
Reactor volume	V	0.2 m^3
Heat transfer area	A	4.5 m^2
Fluid density	ρ	1,025 kg/m^3
Fluid heat capacity	C_p	1.55 kJ/kg·C
Heat of reaction	ΔH	160 kJ/mol
Activation energy	E/R	255 K
Preexponential factor	k	2.5 h^{-1}
Coolant flow rate	F_c	0.15 m^3/h
Coolant inlet temp.	T_c	10°C
Cooling jacket volume	V_c	0.055 m^3
Coolant density	ρ_c	1,000 kg/m^3
Coolant heat capacity	C_{p_c}	1.2 kJ/kg·C

$$\dot{F} = 0 \tag{14}$$

$$\dot{c}_A^f = 0 \tag{15}$$

$$\dot{T}^f = 0 \tag{16}$$

$$\dot{F}_c = 0 \tag{17}$$

$$\dot{T}_c^f = 0 \tag{18}$$

The reactor model used for the analysis comprises the system of equations in Eqs. 9–18, linearized around the stable nominal steady-state operating point outlined in Table 1.

In this example, we assume thermocouples for temperature measurement, differential pressure transmitters for volume and flow measurement, and optical spectrometry for composition measurement. We assume that the sensor noise and state disturbances are independent, white-noise sequences, and construct diagonal covariance matrices from the individual sensor noise and process disturbance variances

$$\boldsymbol{R} = \text{diag}\left(\sigma^2(v_1), \ldots, \sigma^2(v_l)\right) \tag{19}$$

$$\boldsymbol{Q} = \text{diag}\left(\sigma^2(w_1), \ldots, \sigma^2(w_m)\right) \tag{20}$$

in which $\sigma^2(v_i)$ is the sensor noise variance for sensor i, and $\sigma^2(w_i)$ is the state disturbance variance for state i. Although the independence assumption is generally valid for sensor noise, correlation between the state disturbances, reactor vol-

Table 2. Sensor Measurement Noise Variance

Sensor	Variance	Error
Reactor composition	25	±0.01 M
Reactor temperature	0.25	±1°C
Coolant temperature	0.25	±1°C
Reactor volume	1×10^{-5}	±0.5%
Feed flow rate	6.25×10^{-6}	±5%
Feed composition	25	±0.01 M
Feed temperature	0.25	±1°C
Coolant flow rate	1.4×10^{-5}	±5%
Coolant inlet temp.	0.25	±1°C

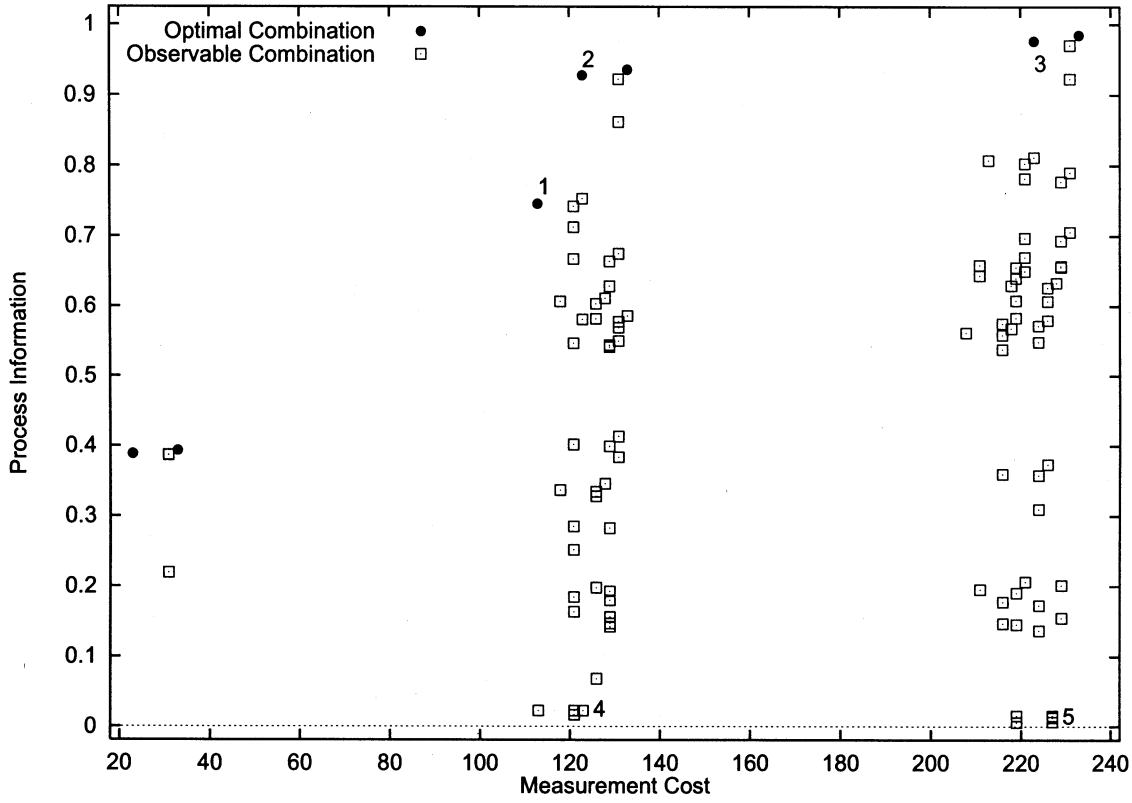

Figure 2. Process information vs. cost for observable sensor combinations.

Table 3. Process Disturbance Variance

Disturbance	Variance	Magnitude
Reactor volume	1×10^{-4}	$\pm10\%$
Feed flow rate	2.5×10^{-5}	$\pm10\%$
Feed composition	156.25	$\pm1\%$
Feed temperature	6.25	±5°C
Coolant flow rate	2.25×10^{-4}	$\pm20\%$
Coolant inlet temp.	25	±10°C

ume, and feed flow rate, for example, would be expected. However, we ignore state disturbance correlation in this example. The sensor noise variance and the corresponding repeatability used in this example are presented in Table 2. The state disturbance variances and the corresponding magnitude representing two standard deviations are presented in Table 3. Representative relative sensor costs based on installation, operation, and maintenance are shown in Table 4. Representative sensor reliabilities, or fractional on-line operating times, are also included in Table 4. The process-information metric presented in Eq. 6, the expected value of the inverse weighted steady-state state reconstruction error, with $p = 2$, and the following scaling and weighting matrices are used in this example

$$\boldsymbol{S} = \text{diag}\,(0.136, 1.86, 1.26, 188, 318, 0.127, 0.896, 145, 0.635)$$

$$\boldsymbol{W} = \text{diag}\,(1, 1, 0.5, 0.5, 0.5, 0, 0, 0, 0)$$

The scaling matrix is composed of the inverse state reconstruction error standard deviations in the case of full state measurement, and the weighting matrix considers only the reactor composition, temperature, volume, coolant temperature, and feed flow rate.

For the nine-state system presented in this example, there are 109 observable sensor combinations. Only seven of the possible 109 combinations result in an optimal selection, as shown in Figure 2. Due to the large relative composition sensor cost, there are three distinct groupings shown in Figure 2 that represent measurement of both reactor and feed compositions, measurement of a single composition, and no composition measurement. We note that a significant increase in the process information that can be attained is possible when measuring the reactor composition. The addition of the reactor feed composition measurement provides little additional benefit, as shown by points 2 and 3 on the figure. We also note that a significant increase in the process information metric is obtained by measuring the feed flow rate, as shown by points 1 and 2. Finally, we point out that it is possible to select very poor sensor combinations to determine the states of interest as shown by the grouping of points around 4 and 5. Although most of these combinations are easily discounted by heuristics for the example process, it may not be so obvious for more complicated processes. The sensors comprising points 1 through 5 in Figure 2 are summarized in Table 5.

Table 4. Relative Sensor Cost and Reliability

Sensor	Cost	Reliability
Reactor composition	100	0.9750
Reactor temperature	2	0.9975
Coolant temperature	2	0.9975
Reactor volume	5	0.9950
Feed flow rate	10	0.9925
Feed composition	100	0.9750
Feed temperature	2	0.9975
Coolant flow rate	10	0.9925
Coolant inlet temp.	2	0.9975

Table 5. Labeled Sensor Combinations

Point	Cost	Metric	Unmeasured States
1	113	0.746	Feed composition; feed flow; coolant flow
2	123	0.928	Feed composition; coolant flow
3	223	0.977	Coolant flow
4	123	0.015	Reactor composition; feed flow
5	227	0.022	Reactor, feed, and coolant inlet temperature

Conclusions

We have presented an optimal measurement-system design procedure that directly considers the trade-off between process-information and measurement-system cost. The advantage of this procedure is the identification of all possible optimal measurement systems. The resulting set of Pareto optimal measurement systems provides the measurement system design engineer with the ability to optimally choose between cost and process information. The disadvantage to this approach is the computational requirement for large-scale systems. We note, however, that many large-scale chemical process systems can be decomposed into a series of individual unit operations that can be analyzed individually. Analysis procedures for large-scale systems is an area for further study.

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