Optimal process analyzer selection and positioning for plant-wide monitoring
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2. Selection and Positioning: Deterministic Grounds

Selection of Optimal Sensor Position in a Tubular Reactor using Robust Degree of Observability Criteria

Abstract - Robust selection criteria for the optimal location for in-process concentration or temperature sensors along the length of a tubular reactor for the partial oxidation of benzene to maleic anhydride are developed. A model of the reactor is constructed by rewriting the Pde's describing the mass and heat balances into a set of Ode's through the method of lines on a grid defined over the reactor length. The linearized model is described as a continuous, time invariant state-space model where the state is formed by temperature and concentration profiles on the grid-points. The best sensor location for the reactor is found by specifying scalar measures on the observability Gramian integral from the linear least squares state estimation problem. New robust criteria for a degree of observability are specified. The scores on these criteria are determined by the amount of signal received by a sensor for a specific system configuration. These new selection criteria are compared with known measures for degree of observability for the optimal sensor location problem from the literature.
2.1 Introduction - The implementation and operation of in-process measurements - either compositional/analytical or physical in nature - can be quite expensive. The cost of purchasing and maintenance often form an obstacle for the number of sensors that can be implemented for monitoring and/or control purposes. These costs naturally lead to the following question: what is the best location to place the limited number of sensors available (typically one) in a process? Stated differently, what type of sensor on what position delivers the information best suited to monitor the system under observation?

In this chapter we investigate the optimal sensor position for the purpose of state estimation of a unit operation. As an example we will use a computer simulation model of a fixed bed tubular reactor for the catalytic partial oxidation of benzene to produce maleic anhydride. The state of this system is formed by the concentration and temperature profiles over the reactor tube, which has to be determined from measuring one of these variables. We will examine both the position of the sensor along the reactor tube, as well as compare four different types of measurements. The measurements used are two process analyzers (for reactant and product) and two temperature measurements (fluid and solid phase). The present study will be limited to the hypothetical case of continuous, error free and immediate response signal transducers. Selection of the best configuration of in-process sensors with the purpose of monitoring a process by estimating the state of the system is done by defining a degree of observability.

State observability is an established definition for systems represented in the well-known state-space notation. The state of a dynamic system at any time may be (loosely) defined as the collection of information which is both necessary and sufficient to determine the future behavior of the system, assuming that all future inputs are also known. The state-space consists of all those values, which the state may take on [9]. Observability defines whether the state can be observed given a certain output. In this work the outputs are the sensor responses acquired through measurements.

The systems theoretical definition of observability is binary in nature: a system is either state observable or state unobservable. A consequence of
this definition is that unobservability is a 'singular' condition, in the sense that if a system is unobservable, any small perturbation of the systems elements might cause it to become observable. As a consequence, most simulation models with physical constants are completely observable [9]. This makes the yes/no definition impracticable when comparing different system configurations. If we want to study e.g. different sensor locations in one unit operation we need a degree of observability for comparison.

Many authors have looked for possible expressions for a degree of state observability and its dual, the state controllability (see e.g. [10]-[15]). All these criteria are scalar functions of the observability Gramian integral (the unscaled Fisher information matrix), or the observability matrix in case of a discrete time system. The interpretation of these criteria for state controllability is straightforward. The energy required by the control action for disturbance reduction must be minimized, and the degree of controllability criterion should show a minimum for the configuration that optimizes this performance. For a degree of observability the explanation is less obvious. A possible interpretation is that the best sensor position is the one that gives maximum signal response on the sensor when changes due to input disturbances in the system - thus the state vector specifying the system - occur. The scalar degree of observability criteria must again indicate the best configuration by some minimum or maximum value.

The most frequently encountered criteria for a degree of observability are those introduced by Müller and Weber [11]. They define measures that are dominated by those elements in the state vector that show only minimal changes for disturbances and thus are difficult to estimate from the measurements. For the tubular reactor in our study this leads to impractical solutions for the optimal sensor location problem. By utilizing the idea of maximal measurement response or maximal 'energy' collected by a particular choice of sensor we will derive alternative measures for degree of observability. With these supplementary criteria we hope to come to so-called 'robust' selection procedures for sensor placement. The central idea for optimal sensor location with these new criteria is to monitor only major changes in the state variables for the system under observation. This concept resembles the theory previously developed by others for complete state versus input-output controllability [16], [17].
The chapter is organized as follows. The next section gives a short description of the tubular reactor simulation model. The third section explains the theoretical meaning of observability as defined in systems theory and introduces the different scalar measures for a degree of observability. In the fourth section we present the result for the optimal sensor location problem for the tubular reactor, and the last section is used to discuss these results.

2.2 Tubular Reactor Model - The theory developed in this chapter is illustrated in combination with a simulation model of a fixed bed tubular reactor for the production of maleic anhydride by partial oxidation of benzene. Most of the information used in this computer model can be found in the papers by Wohlfahrt and Emig [18] and Ramirez and Calderbank [19]. Some essential data not included in these two sources were assessed from general literature.

Three exothermic, irreversible gas phase reactions take place on a solid $V_2O_5$-$MoO_3$-$P_2O_5$ catalyst particles packed in a one-inch diameter tube

\[
\begin{align*}
C_6H_6 + 4 O_2 & \rightarrow C_4H_2O_3 + CO + CO_2 + 2 H_2O & (2.1) \\
C_6H_6 + 6 O_2 & \rightarrow 3 CO + 3 CO_2 + 3 H_2O & (2.2) \\
C_4H_2O_3 + 2 O_2 & \rightarrow 2 CO + 2 CO_2 + H_2O & (2.3)
\end{align*}
\]

Reaction (2.1) is the desired path for the formation of maleic anhydride - the product - from benzene. Reactions (2.2) and (2.3) represent the undesired oxidation (burning) of reactant and product, respectively. The feed stream to the reactor is air mixed with approximately 0.009 mol.s$^{-1}$ benzene. Because of the oxygen excess in the feed all reactions are assumed to be pseudo first order for the limiting reactant. The Arrhenius equation for the reaction rates in formula (2.1)-(2.3) is given by equation (2.4). The frequency factors, activation energies and the reaction heat used are shown in Table 2.1.

\[
k_i(t, z) = A_i e^{-\frac{E_i}{RT(t, z)}}
\]

(2.4)
The two mass balances used in the model are molar flow benzene $F_B$ (mol.s$^{-1}$) and molar flow maleic anhydride $F_{MA}$ (mol.s$^{-1}$) in the fluid phase stream. The partial differential equations are given by (2.5) and (2.6). The parameters for these two equations are shown in Table 2.2 ($t$ (s) denotes time; $z$ (m) indicates axial position in the reactor; total length is 3.2 m).

$$\frac{\partial F_B(t,z)}{\partial t} = -v \frac{\partial F_B(t,z)}{\partial z} + D_{eff} \frac{\partial^2 F_B(t,z)}{\partial z^2} - k_1(t,z)F_B(t,z) - k_2(t,z)F_B(t,z) \quad (2.5)$$

$$\frac{\partial F_{MA}(t,z)}{\partial t} = -v \frac{\partial F_{MA}(t,z)}{\partial z} + D_{eff} \frac{\partial^2 F_{MA}(t,z)}{\partial z^2} + k_1(t,z)F_B(t,z) - k_3(t,z)F_{MA}(t,z) \quad (2.6)$$

Two heat balances are included in the simulation, namely the temperature of the fluid phase $T_f$ (K) (the gas flow) and the temperature of the stagnant solid phase catalyst $T_s$ (K). The corresponding (partial) differential equations are shown in (2.7) and (2.8); the parameters are given in Table 2.2.

$$\frac{\partial T_f(t,z)}{\partial t} = -v \frac{\partial T_f(t,z)}{\partial z} + k_{eff} \frac{\partial^2 T_f(t,z)}{\partial z^2} - U_{f-w}(T_f(t,z) - T_w) - U_{s-f}(T_s(t,z) - T_f(t,z)) \quad (2.7)$$

$$\frac{dT_s(t,z)}{dt} = -U_{s-f}(T_s(t,z) - T_f(t,z)) + c_s \Delta H_1 k_1(t,z)F_B(t,z) + c_s \Delta H_2 k_2(t,z)F_B(t,z) + c_s \Delta H_3 k_3(t,z)F_{MA}(t,z) \quad (2.8)$$
<table>
<thead>
<tr>
<th>Parameter</th>
<th>value (unit)</th>
</tr>
</thead>
<tbody>
<tr>
<td>linear gas velocity v</td>
<td>2.48 (m.s⁻¹)</td>
</tr>
<tr>
<td>Effective mass diffusion coefficient D_{eff}</td>
<td>3.17x10⁻³ (m².s⁻¹)</td>
</tr>
<tr>
<td>Effective heat diffusion coefficient k_{eff}</td>
<td>3.17x10⁻² (m².s⁻¹)</td>
</tr>
<tr>
<td>Effective heat transfer coefficient fluid</td>
<td>10.6 (s⁻¹)</td>
</tr>
<tr>
<td>phase-wall temp. U_{f,w}</td>
<td></td>
</tr>
<tr>
<td>wall temperature T_w</td>
<td>733 (K)</td>
</tr>
<tr>
<td><em>effective heat transfer coefficient solid-fluid phase U</em>{s,f}</td>
<td>84.0 (s⁻¹)</td>
</tr>
<tr>
<td>solid phase heat balance constant c_s</td>
<td>0.729 (s.K.J⁻¹)</td>
</tr>
</tbody>
</table>

Table 2.2

We would like to emphasize that our aim was not to make a detailed study of the reactor setup used in the simulations. Many aspects (for example pressure drop, radial diffusion, etc.) are not included in the model. Their impact on the subject of our study – optimal sensor location – is assumed to be of less importance.

Figure 2.1 shows the steady-state concentration and temperature profiles over the reactor tube for three different benzene feeds. The boundary conditions used in the calculations are $F_{b}(t,0) = \text{[feed]} \ mol.s^{-1}$, $F_{MA}(t,0) = 0 \ mol.s^{-1}$ and $T_{i}(t,0) = 733 \ K$. Diffusion effects at the entrance and exit are neglected.
Figure 2.1 a) molar flow benzene b) molar flow maleic anhydride c) fluid phase temperature d) solid phase temperature; benzene feed 0.00900 (-), 0.00873 (..) and 0.00927 mol.s⁻¹ (--)  

The systems theoretical definitions for observability that are used in the remainder of this chapter require a linear, finite dimensional state-space reactor model. The first step is to divide the reactor length into $m$ equidistant segments indicated by $z_i$ (where $z_0$ is the reactor entrance which is not included in the dynamic simulation model). The distance between two successive grid points is $\Delta z$ meters. For every grid-point $z_i$, we define four (partial) differential equations from formula (2.5)-(2.8). In the next step the first and second order differential terms in partial the differential equations on every grid-point $z_i$ are approximated by second order upwind and central difference terms according (2.9) and (2.10), respectively (where $f$ is $F_B$, $F_{MA}$ or $T_f$).

$$\frac{\partial f(t,z_i)}{\partial z_i} = \frac{3f(t,z_i) - 4f(t,z_i) + f(t,z_i)}{2\Delta z} + O(\Delta z^2) \quad (2.9)$$
After these modifications the original reactor model is transformed into a set of $n = 4 \times m$ ordinary differential equations, two mass and two heat balances on all $m$ grid-point over the reactor length ('Method Of Lines' approximation).

The last step is to linearize all non-linear terms in the reactor model (more precisely, the cross products of the Arrhenius equation and molar fractions in equations (2.5), (2.6) and (2.8)). This is done by a first order Taylor-series approximation.

After these two modifications we have transformed the original reactor model (2.5)-(2.8) into $n$ linear time invariant ordinary differential equations. They can then be reorganized into state-space notation as shown in the next equation (see e.g. [9])

$$
\frac{d\mathbf{x}(t)}{dt} = A\mathbf{x}(t) + B\mathbf{u}(t) \tag{2.11a}
$$

In this formula state vector $\mathbf{x}$ ($n \times 1$) contains four variables for all $m$ grid points. The state vector is organized in an alternating fashion $\mathbf{x} = [F_B(t,z_1), F_{MA}(t,z_1), T_1(t,z_1), T_s(t,z_1), F_B(t,z_2), \ldots, T_s(t_m,z_m)]'$. The other components of (2.11a) are the band diagonal system or dynamic coefficients matrix $A$ ($n \times n$) with appropriate constants connecting the $n$ linear differential equations for successive grid points, the input coupling coefficients or control matrix $B$ ($n \times p$) and the input vector $\mathbf{u}$ ($p \times 1$). In our reactor model $p$ is one because benzene concentration in the feed stream is the only variable to manipulate. Because we use derivative variables the boundary conditions for equation (2.11a) simplify to $\mathbf{x}(t_0) = \mathbf{0}$.

In Figure 2.2 the (complex) eigenvalues of the system matrix $A$ are plotted for a grid size of $m = 32$ ($\Delta z = 0.1$ m). These eigenvalues are the poles of the system and the reciprocal values of their real parts are time constants of the natural frequencies of the process. In the plot we see
that all eigenvalues have negative real parts. This means that the system is asymptotically stable.

**Figure 2.2** eigenvalues system matrix A for grid-size $m = 32$ ($n = 128$)

The second conclusion we draw from Figure 2.2 is that four clusters of eigenvalues can be distinguished, corresponding with the four differential equations (2.5)-(2.8) of the original reactor model. Although there is a strong connection between these four equations and the four clusters there is no simple one-on-one relation because of the coupling between the equations. The cluster with the fastest dynamic response (left side of the plot) is closely connected to the solid phase temperature balance. The 'slower system poles' (real part near zero) could suggest neglecting the former. However, all balances are fully connected and fixing one of the balances on a steady-state value would influence the overall dynamic behavior of the simulation model. For complete state estimation we keep all sources of dynamics in the model.

The eigenvalues in Figure 2.2 also warn us that state estimation will be a difficult task. This situation is comparable with the one encountered in many control applications: some small disturbances of the system might be very hard to control. From a systems theoretical point of view a particular configuration might even be state uncontrollable, but by focusing the control action on the dominant effects in the system the overall controller performance can be very efficient [16]. Comparable
reasoning holds for the optimal sensor position problem for the reactor state determination in this study: focusing the selection criteria on the dominating effects instead of the minor phenomena that are hardest to observe leads to different results.

To simulate measurements on the reactor the system in (2.11a) is expanded with a measurement equation

\[ y(t) = Cx(t) \]  

(2.11b)

The output or measurement sensitivity matrix \( C (q \times n) \) selects the elements of the state vectors that can be observed, and \( y (q \times 1) \) contains the measurement results. Simulating for instance a fluid phase temperature sensor on the \( k \)th grid point along the reactor length can be done by placing an element one on the proper place (in this case position \( 4 \times (k-1) + 3 \)) in a all-zero row vector \( C \). Other measurements can be introduced by adding new rows to \( C \).

The sensor response \( y(t_1) \) for time \( t_1 \) can by found from the solution of the system in equation (2.11)

\[ y(t_1) = Ce^{A(t_1-t_0)}x(t_0) + \int_{t_0}^{t_1}Ce^{A(t-t_0)}Bu(t)dt \]  

(2.12)

In this equation \( x(t_0) \) is the known state at time \( t_0 \) and \( u(t) \) is the known input signal on the time trajectory \( t_0 \leq t \leq t_1 \). On the right hand side of (2.12) we recognize the first term as the natural response of the system and the second term as the input part or forced response.

2.3 Theory - Observability concerns the extent to which the state of a linear system influences the outputs [9]. In this chapter the state vector \( x(t) \) contains the concentration and temperature profiles on the grid-points over the reactor tube, and the output is the signal received from measurements as formulated in equation (2.11). To determine whether a system is state observable on the time trajectory \( t_0 \) to \( t_1 \) (for any \( t_1 > t_0 \))
we define the positive (semi) definite observability Gramian $W_0(t_1,t_0)$ $(n \times n)$ in equation (2.13). The role of the observability Gramian matrix in state determination is explained in Appendix 2.A.

$$W_0(t_1,t_0) = \int_{t_0}^{t_1} e^{A(t-t_0)}C'Ce^{A(t-t_0)}dt$$

(2.13)

A state $x(t_0)$ is unobservable if it belongs to the null space of this symmetric observability Gramian. Consequently, (2.11) is completely observable if and only if $W_0(t_1,t_0)$ is of full rank $n$ (nonsingular). This rank determination is the mathematical solution to the question of (binary) observability: a system is either observable ($\text{rank}(W_0(t_1,t_0)) = n$) or unobservable ($\text{rank}(W_0(t_1,t_0)) < n$).

Closely related to state observability — determine $x(t_0)$ from measurements $y(t)$, $t_0 \leq t \leq t_1$; estimating a state in the past — is state construction (also known as state reconstruction or determinability) which is the ability to estimate the state vector $x(t_1)$ based on measurements $y(t)$, $t_0 \leq t \leq t_1$ (estimating the present state from past measurements). It can be shown that for linear, continuous time invariant systems state observation and construction are equivalent [16], [20].

An analytical solution for the Gramian matrix in equation (2.13) can be found by solving the corresponding Lyapunov equation (2.14) for the special case of a stable system on the time trajectory $t_0 = 0$ and $t_1 = \infty$ (see e.g. Ogata [21]). Since the definition of observability for continuous systems is valid for any $t_1 > t_0$, we will use equation (2.14) to compute the observability Gramian's in the remainder this study.

$$A'W_0(\infty,0) + W_0(\infty,0)A + C'C = A'W_0 + W_0A + C'C = 0$$

(2.14)

From the state observability test by establishing the rank of $W_0$, as formulated above, there can be no comparison between different configurations, meaning for our study different sensors on different positions. The only distinction possible by the original definition is between systems that are completely state observable and systems that are
unobservable. It is not possible to determine a ranking in the set of observable systems. What is needed is a degree or quality of observability, preferably some scalar function of the observability Gramian.

Many authors have formulated measures to establish the degree of observability based on the matrix $W_0$. The approach most frequently used is the one formulated by Müller and Weber. They define a series of imbedded means on the symmetric Gramian ($s \leq 0$)

$$m_i = (\Lambda(W_0)) = \left(\sum_{i=1}^{n} \frac{1}{n} \lambda_i^s\right)^{\frac{1}{s}}$$

(2.15)

In this equation $\Lambda(W_0)$ is a $n$-dimensional diagonal matrix with the eigenvalues of the observability Gramian as its elements. Higher scores for the criteria formulated in equation (2.15) correspond with better degree of observability for the system under investigation. Three cases of the series in (2.15) are of special interest

$$\mu_1 = \lim_{s \to \infty} m_s(W_0) = \lambda_{\min}(W_0)$$

(2.16)

$$\mu_2 = m_{-1}(W_0) = n \frac{1}{\text{trace}(W_0^{-1})}$$

(2.17)

$$\mu_3 = \lim_{s \to 0} m_s(W_0) = \sqrt[n]{\det(W_0)}$$

(2.18)

As stated previously, the series (2.15) are imbedded - meaning $\mu_1 \leq \mu_2 \leq \mu_3$ - for one particular system (one particular sensor position). The interpretation when comparing degrees of observability for different configurations is less obvious. In terms of the observability Gramian the comparison of the costs can be formulated as $W_{0A} > W_{0B}$ when system $A$ is better observable than system $B$. This matrix inequality is equivalent to $n$ scalar conditions of which (2.16)-(2.18) are possible candidates. There is however no guarantee that all $n$ criteria will select the same optimal sensor position, a situation encountered in e.g. [14]. An example in
Appendix 2.B illustrates the situation where the criteria (2.16)-(2.18) led to contradictory conclusions for the optimal sensor location problem. Another criterion for degree of observability is proposed by Dochain et. al. [15]. They use the condition number of the observability Gramian to select the best observable system.

$$\gamma(W_0) = \frac{\sigma_{\text{max}}(W_0)}{\sigma_{\text{min}}(W_0)}$$ (2.19)

where the $\sigma$'s are the singular values of a matrix. Smaller condition numbers indicate better observable systems leading to improved state estimations.

All the preceding criteria for degree of observability place strong emphasis on smallest eigenvalues (or singular values) of the Gramian $W_0$. The reason for selecting these measures is that if a system is near singular, inversion of the Gramian (see Appendix 2.A) or errors introduced by this inversion are dominated by the smallest eigenvalues. This effect is illustrated by the example in Appendix 2.B, where it is shown that using the definitions (2.16)-(2.19) the selection for optimal sensor location is dominated by the smallest eigenvalue of the original system. This corresponds with dynamic phenomena related to those state vector elements that are the most difficult to determine. When monitoring a process we are primarily interested in detecting principal changes in the system (observed by changes in the state vector elements). For the reactor under study this means that we are interested in the significant changes taking place in the hot-spot region $z = 0.4-0.7$ m (see Figure 2.1) and not in trivial alterations in the last part of the reactor tube. For this purpose we would like to introduce two 'robust' selection criteria for optimal sensor location. They are based on the idea of maximizing the signal received by a sensor for a system disrupted from steady state. We also formulate an alternative interpretation of criterion (2.16) and use this for comparison with the new robust selection criteria.
The first measure is the spectral 'norm' defined as (since Gramian's are by definition symmetric positive (semi) definite, eigenvalues and singular values are equivalent)

\[ \rho(W_0) = \sigma_{\text{max}}(W_0) \]  \hspace{1cm} (2.20)

The set of eigenvalues of \( W_0 \) are called the spectrum of the matrix, and the largest one the spectral radius. It is not a norm for general matrices because the triangular inequality does not generally hold. However, for the special case of symmetric positive definite matrices the spectral radius is a matrix norm (the induced 2-norm; see e.g. [17]). It can be interpreted as an indicator of the geometric size of a matrix. Taking into consideration the position of the observability Gramian in state determination, as explained in Appendix 2.A, this means that larger values for spectral norm (2.20) correspond with a better ('larger') \( W_0 \).

The second criterion we propose is the trace of the observability Gramian

\[ \text{trace}(W_0) = \sum_{i=1}^{n} \sigma_i(W_0) \]  \hspace{1cm} (2.21)

Trace can be interpreted as a (weighted) size criterion of the singular values for the matrix under investigation. A larger value for (2.21) means that a certain configuration of the state-space model (2.11) is better equipped for state estimation. Maximization of equation (2.21) bears close resemblance to the A-optimality criterion in experimental design theory [22].

The third criterion - near singularity (2.22) - is an alternative interpretation of equation (2.16). It is used to illustrate the difference between the robust sensor selection measures presented above and the criteria proposed in literature.

\[ NS(W_0) = \sigma_{\text{min}}(W_0) \]  \hspace{1cm} (2.22)
Equation (2.A3) in Appendix 2.A tells us that if the observability matrix $W_0$ is singular the system under investigation is unobservable. However, as mentioned in the introduction most physical systems are always observable. Let us assume that the Gramian $W_0$ is nonsingular and the sum $W_0 + E$ is singular. One particular choice of $E$ that satisfies this assumption is $E = -u_{min} \sigma_{min}(W_0) u'_{min}$, where $W_0 = U \Sigma U'$ is the singular value decomposition of $W_0$. Thus, the smallest singular value tells us how near a matrix is to being rank deficient [17]. The configuration with the highest value for this near singularity criterion is furthest from being unobservable. The near singularity measure (2.22), as well as the criteria (2.16)-(2.18), are closely related to D- and E-optimal experimental design methods [22].

2.4 Results - In this paragraph the three criteria (2.20)-(2.22) for optimal sensor location are computed for the tubular reactor model described earlier. A state-space model of the form (2.11a) is constructed with a maze size of $m = 32$ equidistant grid points ($\Delta z = 0.1$ m). This results in an intrinsically stable system since all eigenvalues of the A-matrix have negative real parts (see Figure 2.2). In this model one sensor on one grid point is selected through equation (2.11b). For this system $W_0$ from equation (2.14) is computed [23]. From this matrix the different norms (2.20)-(2.22) for optimal sensor location are calculated. This procedure is repeated for every element in the state vector ($n$ times), selecting the corresponding measurements (benzene, maleic anhydride, fluid phase and solid phase temperature) through equation (2.11b). The results are shown in Figure 2.3.
Interpreting the results for spectral radius (2.20) (Figures 2.3a-b) we see that the best sensor position for maleic anhydride concentration (the product of interest), fluid or solid phase temperature is on the hot-spot in the reactor tube (see Figures 2.1c-d). For benzene (the reactant) the optimal sensor position is after the hot-spot. This observation agrees with the 'negative feed-back' as observed in Figure 2.1 and the reaction rate parameters in Table 2.1. The increase (or decrease) of benzene concentration in the feed stream has little or no effect on the benzene concentration profile over the reactor range $z = 0.4-0.7$ m. These findings are also in good agreement with the results presented by other authors studying the subject of optimal sensor location in tubular reactors [2], [24], [26].

The results also indicate that for the case of continuous error free measurements temperature sensors are preferred over concentration sensors for state estimation. Looking at Figure 2.1 these results also
corresponds with engineering intuition. Small variations in the benzene feed show noticeable effects in the temperature curves in the region \( z = 0.4-0.9 \) m.

Using equation (2.21) – the trace of the observability Gramian (Figure 2.3c-d) – as selection criterion the best sensor position for concentration measurements is found down stream at the reactor outlet. For temperature the optimal position is still at the hot-spot of the reactor tube. From the results in Figure 2.3 and the definition for trace in (2.21) we concluded that the spectrum of the Gramian for temperature measurements is dominated by the spectral radius. For concentration measurements trace as optimal sensor position selection criterion forms an intermediate between spectral (2.20) norm and near singularity (2.22) (see below).

For the near singularity criterion (2.22) the results indicate two things (Figure 2.3e-f; notice the logarithmic y-scale; equations (2.17)-(2.19) for degree of observability give similar results). First of all, the size of the smallest singular values tells us that all the observability Gramian’s are very close to being singular. The algorithms used in these calculations have great difficulty computing these small numbers. This causes the noisy appearance of the curves, but the overall trend is clear. The second conclusion from these last results is that for measurements placed at the beginning of the reactor the observability Gramian is much closer to being singular than for sensors at the end of the reactor. To interpret this result we have to go back to the original reactor model. Looking at the differential equations (2.5)-(2.8) and the parameters of the simulation model in Table 2.2 we see that the fluid phase travels down stream (from reactor entrance to exit) with a velocity \( v = 2.48 \) m.s\(^{-1}\). The only possible method of transporting information upstream (from exit to entrance) is by the small mass and thermal diffusion coefficients opposing the down stream flow. If we look again at Figure 2.1c-d, we observe that the last part of the temperature profiles (beyond \( z = 2 \) m) hardly change when manipulating the benzene feed. If complete state observability is required from for instance a maleic anhydride measurement on the first grid point
it is very hard to detect minuscule changes in the reactor temperature down stream, and very hard in this context means a near singular observability matrix. This confirms that calculating the degree of observability by near singularity (2.22) - aimed at complete state observability - is dominated by those state vector elements that are the most difficult to estimate, which clearly leads to undesirable solutions for the optimal sensor location problem for our reactor model. The same conclusion holds for the degree of observability criteria (2.16)-(2.19) retrieved from literature.

2.5 Conclusions - In this chapter we introduce new and robust selection criteria for optimal sensor location for state estimation of a tubular reactor model. The two criteria we propose are scalar measures calculated from the observability Gramian for the system configuration under investigation. The spectral norm (2.20) focuses on maximizing the energy received by the sensor. The trace (2.21) is an average measure of the estimation performance. For comparison we use the near singularity criterion (2.22), a measure indicating how far a system is from being unobservable. This criterion focuses on complete state observability. For the tubular reactor simulation used as an example in this chapter the last criterion was of little use. Its outcome for the optimal sensor location problem is dominated by the minuscule changes in components and temperature profiles in the last part of the reactor tube for disturbances in the benzene feed. The same conclusion holds for measures for degree of observability (2.17)-(2.19) proposed in literature.

When one is interested in monitoring major changes in the state variables through state estimation (e.g. alterations in the temperature profile near the hot-spot to avoid possible damage) the robust spectral norm is a more suitable selection criterion than near singularity (or the criteria proposed in literature) for optimal sensor positioning. This distinction between complete state versus important disturbances for degree observability criteria resembles the differentiation made by e.g. Rosenbrock [16] and Skogestad and Postlethwaite [17] between (complete) state and input/output controllability.
In this study we assumed the hypothetical case of continuous, error free and immediate sensor responses, while disregarding uncertainty in the process model. Although these are deviations from real in-process measurements, the methods developed in this chapter can serve as early screening tools for the possibilities of in-process measurements implementation, avoiding the necessity of specifying the performance characteristics of real sensors. This aspect distinguishes our approach from other solutions to the optimal sensor location popular in literature [24]-[32]. In these publications the error covariance matrix from a state estimation Kalman filter is minimized by varying the sensor position. Implementing a Kalman filter however, requires knowledge (or at least assumptions) about the measurement dynamics and process uncertainty, which again directly influence the sensor location problem. Research on including sensor performance in the optimal location selection criteria is presented in later chapters of this thesis.

2.A Appendix - In this appendix we illustrate the role of the observability Gramian – also known as the unscaled Fisher information matrix – in state vector determination. In the formal statistical definition the information matrix represents the information obtained from a sample of values from a known probability distribution. It is a scaled version of the Gramian matrix when the measurement errors in \( y(t) \) have a joint Gaussian distribution. The information matrix is a quantitative statistical characterization of the 'information' that is in the data \( y(t) \) used for estimating \( x(t) \). The Gramian primarily serves as a qualitative algebraic characterization of the uniqueness of a solution [32], [33].

Consider the following problem: we want to determine a state vector \( x(t_0) \) from the observations \( y(t), t_0 \leq t \leq t_1 \), through equation (2.1)

\[
y(t) = Ce^{A(t-t_0)}x(t_0)
\]  

(2.1)
In (2.A1) we recognize the natural response of a system as given by equation (2.12). If we wish to determine $x(t_0)$, the solution can be found through the normal equations for (2.A1)

$$e^{A(t-t_0)}C'y(t) = e^{A(t-t_0)}C'e^{A(t-t_0)}x(t_0)$$  \hspace{1cm} (2.A2)

Integrating over the entire measured time trajectory $y(t)$ we find the following solution for $x(t_0)$

$$x(t_0) = \left( \int_{t_0}^{t_f} e^{A(t-t_0)}C'e^{A(t-t_0)}dt \right)^{-1} \int_{t_0}^{t_f} e^{A(t-t_0)}C'y(t)dt = W_0^{-1}(t_1,t_0) -1 \int_{t_0}^{t_f} e^{A(t-t_0)}C'y(t)dt$$  \hspace{1cm} (2.A3)

We recognize the term in brackets as the observability Gramian of the system, equation (2.13). From equation (2.A3) we notice that the solution is only possible if the inverse of $W_0(t_1,t_0)$ exists. This is the same as stating that the Gramian has to be full rank, which immediately leads to the original (binary) definition of observability.

For classical parameter estimation the inverse of the scaled information matrix (scaled by a function of the known distribution of the errors assumed to be present in the sensor responses $y(t)$) is equal to the estimation covariance matrix of $x(t_0)$. This covariance or 'estimation error' matrix obviously should be minimized to optimize the estimation procedure. This corresponds to maximizing a scaled observability Gramian. For classical estimation, using a proper experimental design will guarantee an optimal information matrix in the corresponding regression models [22].

The objective of this study is optimal sensor location. The only parameter to investigate is the sensor type and position as specified by the output or measurement matrix $C$. From (2.A3) we concluded that the 'size' or 'norm' of the observability Gramian $W_0(t_1,t_0)$ be can used to judge the performance of experiments for different configurations.

From a theoretically point of view, by assuming continuous, error free and immediate response measurement we have to assume finite arithmetic
precision. If we would assume infinite precise computations all systems in (2.A3) would give equal outcomes.

2.B Appendix - The system in (2.B1) serves as an example to study the different criteria for degree of observability

\[
\dot{x}(t) = A x(t) = \begin{bmatrix} -1 & 1 & 1.5 \\ 1 & -2 & 1 \\ 0 & 1 & -3 \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \end{bmatrix}
\] (2.B1a)

The eigenvalues \(A\) are \(\lambda_1 = -0.06, \lambda_2 = -2.56\) and \(\lambda_3 = -3.38\), thus (2.B1) is stable. Three different models are formed from three different measurement vectors

\[y_i(t) = c_i x(t)\] (2.B1b)
\[
c_1 = [1 \ 0 \ 0] \quad c_2 = [0 \ 1 \ 0] \quad c_3 = [0 \ 0 \ 1]
\] (2.B1c)

The squared responses calculated from equation (2.12) for a unit impulse disturbance at \(t = 0\) for these three systems are shown in Figure 2.B1. The maximum signal response ('energy') for these three observable configurations is clearly number one, measuring the first element in the state vector.

---

**Figure 2.B1** squared impulse response for system (2.B1): \(y_1\) (---), \(y_2\) (--) and \(y_3\) (---)
The Gramian's from equation (2.14) plus the corresponding eigenvalues for these three systems are

\[
\begin{align*}
W_{o1} &= \begin{bmatrix} 3.03 & 2.53 & 2.28 \\ 2.53 & 2.28 & 2.03 \\ 2.28 & 2.03 & 1.82 \end{bmatrix} & \lambda_{W_{o1}} &= \begin{bmatrix} 7.00 \\ 0.12 \\ 8.10^{-4} \end{bmatrix} \\
W_{o2} &= \begin{bmatrix} 1.02 & 1.02 & 0.85 \\ 1.02 & 1.19 & 0.86 \\ 0.85 & 0.86 & 0.71 \end{bmatrix} & \lambda_{W_{o2}} &= \begin{bmatrix} 2.82 \\ 0.10 \\ 1.10^{-4} \end{bmatrix} \\
W_{o3} &= \begin{bmatrix} 0.11 & 0.11 & 0.10 \\ 0.11 & 0.12 & 0.13 \\ 0.10 & 0.13 & 0.26 \end{bmatrix} & \lambda_{W_{o3}} &= \begin{bmatrix} 0.41 \\ 0.08 \\ 26.10^{-4} \end{bmatrix}
\end{align*}
\]

(2.B2a)  

(2.B2b)  

(2.B2c)

The matrices (2.B2) all have positive distinct eigenvalues, thus the observability Gramian's are positive definite. None of the differences between the Gramian's in (2.B2) are however positive definite, e.g. the difference between the first and the third system is

\[
W_{o1} - W_{o3} = \begin{bmatrix} 2.92 & 2.42 & 2.17 \\ 2.42 & 2.16 & 1.90 \\ 2.17 & 1.90 & 1.55 \end{bmatrix} & \lambda_{W_{o1}-W_{o3}} &= \begin{bmatrix} 6.63 \\ 0.10 \\ -0.09 \end{bmatrix}
\]

(2.B3)

The criteria for degree of observability for the three configurations of (2.B1) from equations (2.16)-(2.22) of the theoretical section are shown in Table 2.B1. From these results we observe that for this (synthetic) example there is no clear overall winner. Even for the criteria \(\mu_1-\mu_3\) proposed by Müller and Weber there is no agreement (despite the imbedding for every individual system). The two robust selection criteria – \(\rho\) and trace – indicate measuring state one as the optimal position for state determination.
<table>
<thead>
<tr>
<th>criterion(^*)</th>
<th>Equation</th>
<th>(W_{01})</th>
<th>(W_{02})</th>
<th>(W_{03})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\mu_1)</td>
<td>(16)</td>
<td>0.0008</td>
<td>0.0001</td>
<td><strong>0.0026</strong></td>
</tr>
<tr>
<td>(\mu_2)</td>
<td>(17)</td>
<td>0.0024</td>
<td>0.0002</td>
<td><strong>0.0076</strong></td>
</tr>
<tr>
<td>(\mu_3)</td>
<td>(18)</td>
<td><strong>0.0871</strong></td>
<td>0.0280</td>
<td><strong>0.0444</strong></td>
</tr>
<tr>
<td>(\gamma)</td>
<td>(19)</td>
<td>8851</td>
<td>36510</td>
<td>157</td>
</tr>
<tr>
<td>(\rho)</td>
<td>(20)</td>
<td>7.00</td>
<td>2.82</td>
<td>0.41</td>
</tr>
<tr>
<td>Trace</td>
<td>(21)</td>
<td>7.12</td>
<td>2.92</td>
<td>0.50</td>
</tr>
<tr>
<td>NS (= (\mu_1))</td>
<td>(22)</td>
<td>0.0008</td>
<td>0.0001</td>
<td><strong>0.0026</strong></td>
</tr>
</tbody>
</table>

\(\text{Table 2.B1}\)

\(^*\) Underlined result is the 'winning' configuration for this particular criterion based on the explanation from the theoretical section.