A PROCEDURE FOR SISO CONTROLLABILITY ANALYSIS
- with application to design of pH processes

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Abstract. A procedure for analyzing the input-output controllability of single-input single-output (SISO) systems is presented. This procedure is applied to a pH neutralization process which must be redesigned to get acceptable controllability. It is found that more or less heuristic design rules given in the literature follow directly. The key point in the example is to consider disturbances and scale the variables properly.

1 INTRODUCTION

In this paper the term “controllability” has the meaning of “achievable control performance” and provides a link between process control and process design. More precisely, we use the following definition:

Definition of (input-output) controllability: The ability to achieve acceptable control performance, that is, to keep the outputs (y) within specified bounds from their setpoints (r), in spite of unknown variations in the plant (e.g., disturbances (d) and model perturbations) using available inputs (u) and available measurements (e.g., y_m or d_m).

In summary, a plant is controllable if there exists a controller (connecting measurements and inputs) that yields acceptable performance for all expected plant variations. Thus, controllability is independent of the controller, and is a property of the plant (process) only. It can only be affected by changing the plant itself, that is, by design modifications. These may include:

1. Change the process itself, for example, by changing the size or type of equipment.
2. Move measurements and actuators.
3. Add new equipment to dampen disturbances, for example, buffer (mixing) tanks.
4. Add extra measurements (cascade control).
5. Add extra actuators (parallel control).
6. Change the control objectives.
7. Change the control structure of the lower levels.

(It may be discussed whether it is appropriate to label the last two items as design modifications, but at least they address issues which come before the actual controller design.)

Surprisingly, in spite of the fact that mathematical methods are used extensively for control system design, the methods available when it comes to controllability analysis are mostly qualitative. In most cases the “simulation approach” is used. However, this requires a specific controller design and specific values of disturbances and setpoint changes. In the end one never really knows if a result is a fundamental property of the plant or if it depends on these specific choices. In a companion paper (Skogstad, 1994) a procedure for controllability analysis of SISO systems is presented. The objective of the present paper is to apply this procedure, and in particular to consider the design of a pH neutralization process.

One shortcoming with the controllability analysis presented in this paper is that all the measures are linear. This may seem very restrictive, but in most cases it is not. In fact, one of the most important nonlinearities, namely input constraints, can be handled with the linear approach. To deal with slowly varying changes one may perform a controllability analysis at several selected operating points. As a last step one may perform some nonlinear simulations to confirm the linear controllability analysis. The experience from a large number of case studies is that the agreement generally is very good.

Remarks on the definition of controllability.

The above definition is in agreement with most persons intuitive feeling about the term, and was also how the term was used historically in the control literature. For example, Ziegler and Nichols (1943) define controllability as “the ability of the process to achieve and maintain the desired equilibrium value”. Unfortunately, in the 60’s the term “controllability” became synonymous with the rather narrow concept of “state controllability” introduced by Kalman, and the term is still used in this restrictive manner in the system theory community. “State controllability” is the ability to bring a system from a given initial state to any final state (but with no regard to the quality of the response between these two states). This concept is of interest for realizations and numerical calculations, but as long as we know that all the unstable modes are both controllable and observable, it has little practical significance. For example, Rosenbrock (1970, p. 177) notes that “most industrial plants are controlled quite satisfactorily though they are not [state] controllable”. To avoid confusion with Kalman’s state controllability, Morari (1983) introduced the term “dynamic resilience”. However, this term does not capture the fact that “controllability” it is related to control, and instead it is proposed to use the term “input-output controllability” if one explicitly want to make the distinction with “state controllability”. 
2 CONTROLLABILITY ANALYSIS

PROCEDURE

Notation. Consider a linear process model in terms of deviation variables

\[ y = gu + gd \quad (1) \]

Here \( y \) denotes the output, \( u \) the manipulated input and \( d \) the disturbance (including what is often referred to as "load changes"). \( g(s) \) and \( gd(s) \) are transfer function models for the effect on the output of the input and disturbance, and all controllability results in this paper are based on this information. The Laplace variable \( s \) is often deleted to simplify notation. The control error \( e \) is defined as

\[ e = y - r \quad (2) \]

where \( r \) denotes the reference value (setpoint) for the output. In the paper we mostly consider feedback control as illustrated in Figure 1 where

\[ u = c(s)(r - y) \quad (3) \]

and \( c(s) \) is the controller. Eliminating \( u \) from equations (1) and (3) yields the closed-loop response

\[ y = T \sigma + Sgd \quad (4) \]

where the sensitivity is \( S = (1 + gc)^{-1} \) and the complementary sensitivity is \( T = gc(1 + gc)^{-1} = 1 - S \). The transfer function around the feedback loop is denoted \( L \). In this case \( L = gc \).

In this paper bandwidth is defined as the frequency \( \omega_B \) where the loop gain is one in magnitude, i.e., \( |L(j\omega)| = 1 \) (or more precisely where the low-frequency asymptote of \( |L| \) first crosses 1 from above). This frequency is frequently called the "crossover frequency". At frequencies lower than the bandwidth \( \omega < \omega_B \) feedback is effective and will affect the frequency response. However, for sinusoidal signals (for example, a disturbance) with frequencies higher than \( \omega_B \) the response will not be much affected by the feedback.

A frequency domain analysis, and in particular of the frequency-region corresponding to the bandwidth, is very useful for systems under feedback control. This is the case even when the disturbances and setpoints entering the system are not sinusoids. The reason is that the effect of disturbances is usually largest around the bandwidth frequencies; slower disturbances are attenuated by the feedback control, and faster disturbances are usually attenuated by the process itself.

Scaling. The interpretation of most measures presented in this paper assumes that the transfer functions \( g \) and \( gd \) are in terms of scaled variables. The first step in a controllability analysis is therefore to scale (normalize) all variables (input, disturbance, output) to be less than 1 in magnitude (i.e., within the interval -1 to 1) by normalizing each variable by its maximum value.

Thus, in the following we assume that the signals are persistent sinusoids, and that \( g \) and \( gd \) have been scaled, such that at each frequency the allowed input \( |u(j\omega)| < 1 \), the expected disturbance \( |d(j\omega)| < 1 \), the allowed control error \( |e(j\omega)| < 1 \), and the expected reference signal \( |r(j\omega)| < R_{max} \). Note that \( e \) and \( r \) are measured in the same units so \( R_{max} \) is the magnitude of the expected setpoint change relative to the allowed control error.

Summary of controllability rules

Let \( \omega_B \) denote the closed-loop bandwidth of the system. The following approximate requirements apply for feedback control (Skogestad, 1994).

1. Speed of response to reject disturbances. Must require \( \omega_B > \omega_d \). Here \( \omega_d \) is the frequency at which \( |gd(j\omega_d)| \) crosses 1 from above. Below this frequency the error will be unacceptable \((|e| > 1)\) for a disturbance \( d = 1 \) unless control is used. Alternatively, the requirement can be formulated as

\[ |gd(j\omega_B)| \leq 1 \quad (5) \]

2. Speed of response to follow setpoints with minimum required response time \( \tau_r = 1/\omega_r \). Must require \( \omega_B > \omega_r \). The requirement comes in addition to the bandwidth requirement imposed by the disturbances.

3. Input constraints for disturbances, must require \( |g(j\omega)| > |gd(j\omega)| \), \( \forall \omega < \omega_d \). This is needed to avoid input constraints for perfect rejection of disturbance \( d(j\omega) = 1 \).

4. Input constraints for setpoints, must require \( |g(j\omega)| > R_{max}, \forall \omega < \omega_r \). This is needed to avoid input constraints \(|u(j\omega)| < 1\) for perfect tracking of \( |r(j\omega)| = R_{max} \). Here \( \omega_r \) is the frequency up to which setpoint tracking is desired, and \( R_{max} \) is the magnitude of the setpoint change relative to the allowed control error. Often \( R_{max} = 1 \).

In the frequency range up to the bandwidth \( \omega_B \) there should not be any time delays, RHP-zeros and high-order plant dynamics that need to be counteracted. We get

5. Time delay \( \theta \). Must require \( \omega_B < 1/\theta \).

6. Real RHP-zero at \( s = z \). Must require \( \omega_B < z/2 \).

7. Phase lag constraint. In most practical cases: \( \omega_B < \omega_{180} \).
Here $\omega_{g180}$ is the frequency at which the phase of $g(j\omega)$ is $-180^\circ$. This condition is not a fundamental limitation, but more of a practical limitation. In particular it applies if the phase drops rather quickly around the frequency $\omega_{g180}$.

8. Real open-loop unstable pole at $s = p$. We need fast control to stabilize the system and must approximately require $\omega_B > p$.

3 SIMPLE EXAMPLES

3.1 First-order with delay process

Consider disturbance rejection for the following process

$$g(s) = \frac{e^{-qs}}{1 + \tau s}; \quad g_d(s) = \frac{e^{-q_d s}}{1 + \tau_d s}$$

(6)

In addition there is a measurement delay $\theta_m$ for the output and $\theta_{md}$ for the disturbance. All parameters have been appropriately scaled such that at each frequency $|u| < 1$, $|d| < 1$ and we want $|y| < 1$. One interesting question is: For each of the eight parameters $k, \tau, \theta, k_d, \tau_d, \theta_d, \theta_m, \theta_{md}$ what value is preferred to have good controllability (large, small, no effect)?

<table>
<thead>
<tr>
<th>Feedback control</th>
<th>Feedforward control</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$</td>
<td>Large</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Small</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Small</td>
</tr>
<tr>
<td>$k_d$</td>
<td>Small</td>
</tr>
<tr>
<td>$\tau_d$</td>
<td>Large</td>
</tr>
<tr>
<td>$\theta_d$</td>
<td>No effect</td>
</tr>
<tr>
<td>$\theta_m$</td>
<td>Small</td>
</tr>
<tr>
<td>$\theta_{md}$</td>
<td>No effect</td>
</tr>
</tbody>
</table>

Table 1: Desired value of parameters to have good controllability.

Qualitative results are given in Table 1. Essentially, the effect of the input should be as large and quick as possible, whereas the opposite is true for the disturbance. The main difference between feedback and feedforward control is that a delay for the disturbance has no effect for feedback control, while it is an advantage for feedforward control as it leaves more time to take the appropriate control action.

We now want to quantify the statements in Table 1. Assume $k_d > 1$ such that control is needed to have acceptable performance ($|y| < 1$). From Rule 1 control is needed up to the frequency

$$\omega_d \approx \frac{k_d}{\tau_d}$$

(7)

Thus, from Rule 5 we must require for feedback control that $\omega_d < 1/\theta_{tot}$, where $\theta_{tot}$ is the total delay around the loop. That is, to have $|y| < 1$ for feedback control we require

$$\theta + \theta_m < \frac{\tau_d}{k_d}$$

(8)

Fig. 2: Response for step disturbance, $g_d = \frac{k_d e^{-q_d s}}{(1 + s \tau_d)}$.

For feedforward control any delay for the disturbance itself yields a smaller "net delay", and to have $|y| < 1$ we require

$$\theta + \theta_{md} < \frac{\tau_d}{k_d + \theta_d}$$

(9)

From Rule 4 to avoid input saturation we must require $|g(j\omega)| > |g_d(j\omega)|$ for frequencies $\omega < \omega_d$. Specifically, for both feedback and feedforward control

$$k > k_d; \quad k/\tau > k_d/\tau_d$$

(10)

3.2 Step response controllability analysis

The controllability analysis presented in this paper is based on the frequency domain. However, most engineers feel much more comfortable with the time domain and step responses. Consider a unit step disturbance, $d = 1$, to the first-order with delay disturbance model in Eq.(6). Without control the output response is

$$y(t - \tau_d) = k_d(1 - e^{-t/\tau_d})$$

(11)

The response is shown graphically in Fig. 2. Since $k_d > 1$ the output $y(t)$ will exceed 1 after some time. Disregarding for a moment the delay, the time where $y(t) = 1$ is at $t = -\tau_d \ln(1 - \frac{1}{k_d}) \approx \tau_d/k_d$ (the approximation holds for $k_d >> 1$ and corresponds to the point where the initial tangent of the time response crosses 1, see Fig. 2). Assuming that we measure the disturbance, the "minimum reaction time" to achieve $|y| < 1$ is then (see Fig. 2) $\tau_d/k_d + \theta_d$. This is then an upper bound on the allowed delay in the process. This is the same value as was obtained in Eq.9 using the frequency domain in the case of feedforward control.

From this example we see that a step response controllability analysis yields results similar to the frequency domain, at least for a first-order process and feedforward control. For feedback control a step response controllability analysis is generally less suitable. For example, one cannot simply measure the time it takes from the disturbance enters to the output exceeds its maximum value (which is 1 in terms of the scaled variables used in this paper). As shown by Fig. 2 this time depends on the delay in the disturbance model, whereas we know that this delay should not matter for rejecting disturbances with feedback control. In conclusion, the frequency domain should generally be used for controllability analysis, and the purpose of this example was not to suggest using step responses, but to provide another justification for the usefulness of the frequency domain.
4 NEUTRALIZATION PROCESS

One tank. Consider the process in Figure 3 where a strong acid (pH=−1) is neutralized by a strong base (pH=15) in one mixing tank with volume \( V = 10 \, \text{m}^3 \) to make \( q = 0.01 \, \text{m}^3/\text{s} \) of "salt water". The pH in the product stream is adjusted to be in the range \( 7 \pm 1 \) ("salt water") by manipulating the amount of base, \( q_B \). The delay for the measurement of pH is \( \theta = 10 \) s. Details about the dynamic model are given in Appendix. Introduce the excess of acid \( c \) [mol/l] defined as

\[
c = c_H - c_{OH} \tag{12}
\]

Somewhat surprisingly, we find that in terms of \( c \) the dynamic model, which is usually believed to be strongly nonlinear, is given by that of a simple mixing process

\[
\frac{dc}{dt} = q_A c_A + q_B c_B - q c \tag{13}
\]

Introduce the following scaled variables

\[
y = \frac{c}{10^{-6}}; \quad u = \frac{q_B}{q}; \quad d = \frac{q_A}{0.5q^2} \tag{14}
\]

where superscript * denotes the steady-state value. The appropriately scaled linear model then becomes (see Appendix)

\[
y = \frac{k_d}{1+\frac{1}{\tau_s}}(-2u + d); \quad k_d = 2.5 \cdot 10^6 \tag{15}
\]

where \( \tau = V/q = 1000 \) s. The output is extremely sensitive to both \( u \) and \( d \) and the large gain is easily explained: A change \( d = 1 \) corresponds to a 50% increase in the amount of acid which has a concentration of 10 mol/l of \( H^+ \) (pH=−1). This increases the amount of \( H^+ \) in the product from 0 to 2.5 mol/l, while the largest allowed amount of \( H^+ \) in the product is \( 10^{-6} \) mol/l (pH=6), thus the gain in terms of scaled variables is \( k_d = 2.5 \cdot 10^6 \).

Input constraints do not pose a problem since \( |g| = 2 |g_d| \) at all frequencies. The main control problem is the high disturbance sensitivity, and from (7) we find the frequency up to which feedback is needed

\[
\omega_d \approx k_d / \tau = 5000 \, \text{rad/s} \tag{16}
\]

This requires a response time of \( 1/5000 = 0.2 \) millisecond which is clearly impossible.

Design change: Multiple tanks. The only way to improve the controllability is by design changes. The most useful change in this case is to do the neutralization in several steps. With \( n \) equal mixing tanks in series the transfer function for the effect of the disturbance becomes

\[
g_d(s) = k_d b_n(s); \quad h_n(s) = \frac{1}{(2n \theta s + 1)^n} \tag{17}
\]

where \( k_d = 2.5 \cdot 10^6 \) is the gain for the mixing process, \( h_n(s) \) is the transfer function of the mixing tanks and \( \tau_n = \theta = V_{tot}/q \). The magnitude of \( h_n(s) \) as a function of frequency is shown in Figure 5 for one to four equal tanks in series.

From controllability rule 5 we get that the best achievable closed-loop bandwidth is \( \omega_B = 1/\theta = \omega_d \). To be able to reject disturbances, we must then from Eq. 5 require

\[
|g_d(\omega_d)| \leq 1 \tag{18}
\]

Thus, the purpose of the mixing tanks is to reduce the effect of the disturbance by a factor \( k_d = 2.5 \cdot 10^6 \) at the frequency \( \omega_d = 1/\theta = 0.1 \) [rad/s]. Combining (17) and (18) yields the following condition for the minimum total residence time for \( n \) equal tanks in series

\[
\tau_n = \theta n \sqrt{(k_d)^{2/n} - 1} \tag{19}
\]

The corresponding total volume is \( V_{tot} = \tau_n q \) where \( q = 0.01 \, \text{m}^3/\text{s} \). With \( \theta = 10 \) s we find that the following designs have the same controllability with respect
to disturbance rejection:

<table>
<thead>
<tr>
<th>No. of tanks $n$</th>
<th>Total volume $V_{tot}$ [m$^3$]</th>
<th>Volume each tank $V$ [m$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>250000</td>
<td>250000</td>
</tr>
<tr>
<td>2</td>
<td>316</td>
<td>158</td>
</tr>
<tr>
<td>3</td>
<td>40.7</td>
<td>13.6</td>
</tr>
<tr>
<td>4</td>
<td>15.9</td>
<td>3.98</td>
</tr>
<tr>
<td>5</td>
<td>9.51</td>
<td>1.90</td>
</tr>
<tr>
<td>6</td>
<td>6.96</td>
<td>1.16</td>
</tr>
<tr>
<td>7</td>
<td>5.70</td>
<td>0.81</td>
</tr>
</tbody>
</table>

With one tank we need a volume corresponding to that of the world's largest ship to get acceptable controllability. The minimum total volume is obtained with 18 tanks of about 2031 each - giving a total volume of 3.662 m$^3$. However, taking into account the additional cost for extra equipment such as piping, mixing and level control, we would probably select a design with about 4 neutralization tanks for this example.

**Remarks.**

1. Walsh (1993, p. 31) uses the following data for the capital cost of large mixing tanks (in 1000 British pounds): $c$ [kGBP] = 20 + 2V$^{0.7}$ where $V$ is the tank volume in m$^3$. With these data 3 tanks is best for the above example (capital cost is 97 kGBP versus 101 kGBP for 4 tanks). We have here not taken into account the cost the pH control systems which according to Walsh is about 40 KGBP in capital and 40 KGBP/year in maintenance.

2. Another reason for preferring fewer steps is the delay in the transfer function $g(s)$ caused by piping and incomplete mixing. Clearly, if there are say five tanks the effective delay due to these effects will most probably be much larger than the measurement delay. To avoid this problem one may consider adding base gradually in each tank. This is commonly done in practice, and it is usually recommended to have a pH-controller for each tank (McMillan, 1984). This clearly increases the cost and may not be necessary. One simple solution which may be worth considering, is shown in Fig.6. Here a small base flow, $q_B$, is used to get quick response for the fine tuning in the last tank, while the main base flow into the first tank, $q_B$ is adjusted by resetting the small flow in a cascade manner.

3. The results given above compare well with results by other authors. A simple shortcut method given by McMillan (1984) is to use about one mixing tank for each 2 units change in pH. For example, with a pH change of 8, as in our example (from pH 15 to 7), four tanks is recommended.

4. McMillan (1984) also gives more rigorous method based on estimating the peak error when using PID control with Ziegler-Nichols tunings. This peak error is compared with the allowed error and the number of tanks is increased until acceptable control is possible. A closer inspection of his method reveals that it yields the same results as obtained with our frequency domain analysis, and is in fact identical to the controllability condition (18):

$$k_d \cdot |h_n(j\omega_p)| \leq 1$$

(20)

Here $g_d(e) = k_d$ is the open-loop error and $h_n(j\omega_p)$ is the attenuation of the peak error. The product of these yield the peak error which in terms of scaled variables should be less than one.

5. Traditionally, a “feedforward” approach has been taken when considering controllability of such processes, and one key argument has been that control is difficult because on needs to adjust the amount of base extremely accurately to counteract the disturbance in the acid. This is a valid argument for feedforward control, but not for feedback control as the feedback control action will be able to adjust the input accurately. As demonstrated above the key problem for feedback control is that the output is extremely sensitive to disturbances ($k_d$ and $\omega_d$ are large), which requires an extremely high bandwidth.

6. Of course, feedforward control based on measuring $q_A$ and $c_A$ can be used in addition to feedback to improve performance. According to McMillan (1984) one can typically save one mixing tank using a well designed feedforward controller.

7. In terms of minimizing the total volume it is almost always optimal to have mixing tanks of equal size. The only exception is for low-frequency disturbances (frequencies lower than about $1/\tau_h$, see Figure 5) where it is slightly better to use fewer tanks. Still, there are some suggestions in the literature regarding using tanks with of different sizes. One argument is that the tanks should be of different sizes such that with independent control of each tank it is less likely that the resonance peaks of the individual tanks are at the same frequency (McMillan, 1984, p. 208). This may have some merit, although one would expect that retuning the controllers would be better. There are also recommendations about having the small tank towards the end (McMillan, 1984, p. 208), but at least from a linear point of view the order makes no difference.

8. This example was motivated by the interesting thesis by Walsh (1993), who studied controllability of waste water systems using an open-loop step response analysis. He compared numerically (p. 150) estimates from an open-loop step response analysis, with the response of a step disturbance under closed loop with PI control of each tank. The discrepancy was quite large, especially for large $n$. However, the results
compare very well with the values obtained from our frequency-domain analysis.

9. It is instructive to study in more detail the difference between a step response and frequency domain controllability analysis for the case with \( n \) tanks in series. Let us follow Walsh (1993) and use the "disturbance attenuation" as a basis of comparison. Let \( d \) denote the concentration disturbance entering the first tank (after mixing), and \( y \) denote the concentration in the last tank. Then the disturbance attenuation is defined as

\[
\delta_d = \left| \frac{y\left(\omega_\beta\right)}{|d|} \right|_{\text{max}} \quad (21)
\]

where \( |d| \) is the magnitude of the concentration disturbance and \( |y\left(\omega_\beta\right)|_{\text{max}} \) is the largest effect this disturbance has on the product concentration.

Let us first consider a frequency domain analysis where we assume \( d(t) = \sin(w_\beta t) \). The disturbance attenuation depends on the frequency \( \omega \), and we want to find the "worst" disturbance attenuation. For \( n \) tanks with feedback control the attenuation is given by \( S(s)h_n(s) \) where \( S(s) \) is the sensitivity function and \( h_n(s) \) is given in (17). It is possible to make the sensitivity function small at low frequencies and thus achieve good disturbance attenuation here. However, with a delay \( \theta \) in the feedback loop we will have \( \left| S(j\omega\theta) \right| \approx 1 \). Thus, the disturbance attenuation at frequency \( \omega = \omega_\beta \) is approximately \( |h(j\omega_\beta)| \), and taking this as the worst value we get

\[
\delta_d \approx \left| h_n(j\omega_\beta) \right| \approx \left( \frac{\theta}{\tau_h/n} \right)^n \quad (22)
\]

where the approximation applies for \( \tau_h \gg \theta \), that is, for \( \delta_d \) small.

Let us now consider an open-loop step response analysis. For \( n \) identical tanks in series the time response to a step disturbance \( d(t) = 1 \) is given by (e.g., Walsh (1993) p. 94)

\[
y(t) = 1 - e^{-t/\tau_h} \sum_{i=0}^{n-1} \left( \frac{t}{\tau_h/n} \right)^i \quad (23)
\]

In the ideal case with a perfect (and probably unrealizable) controller which immediately detects the disturbance and takes the proper action, \( y(t) \) will reach its maximum value at time \( t = \theta \) (at the delay), thus \( 1/y(\theta) \) yields the ideal disturbance attenuation, and we have

\[
\delta_\Delta = 1/y(\theta) \approx \left( \frac{\theta}{\tau_h/n} \right)^n \quad (24)
\]

Recall that the expression for \( \delta_\Delta \) in (22) obtained from a frequency domain analysis, which compared very well with the numerical closed-loop step responses (Walsh, 1993). Thus, by comparing \( \delta_\Delta \) in (22) and (24) we see that the open-loop step response analysis is optimistic by a factor \( n! \). For \( n = 1 \) the results of the open-loop step response analysis and the frequency domain analysis are the same, but the difference is very large number for large \( n \). The reason for the discrepancy is that a real feedback control system will have a resonance frequency around \( \omega_\beta \), and a frequency analysis based on considering the behavior at this frequency will yield good predictions of the closed-loop step response.

**Conclusion.** The controllability results presented in Section 2 have been applied to a pH neutralization process, and it is found that more or less heuristic design rules given in the literature follow directly. The key point is to consider disturbances and scale the variables properly.

5 REFERENCES


APPENDIX. Neutralization model

Derivation of model: Consider Fig.3. Let \( C_H \) [mol/l] and \( C_{OH} \) [mol/l] denote the concentration of \( H^+ \) and \( OH^- \) ions, respectively. Material balances for these two species yields

\[
\frac{dc}{dt}(C_H) = q_{A\rightarrow H} + q_{B\rightarrow H} - q_{H^+} + rV
\]

\[
\frac{dc}{dt}(C_{OH}) = q_{A\rightarrow OH} + q_{B\rightarrow OH} - q_{OH^-} + rV
\]

where \( r \) [mol/m^2s] is the rate for the reaction \( H_2O = H^+ + OH^- \) which for completely dissociated ("strong") acids and bases is the only reaction in which \( H^+ \) and \( OH^- \) participate. We may eliminate \( r \) from the equations by taking the difference to get a differential equation in terms of the excess of acid, \( c = C_{H} - C_{OH} \):

\[
\frac{dc}{dt} = q_{A\rightarrow C} + q_{B\rightarrow c} - q_{c}
\]

Note: 1. This is the material balance for a mixing tank without reaction. The reason is that the quantity \( c = C_{H} - C_{OH} \) is not affected (invariant) by the reaction. 2. \( c \) is the excess of acid and will take on negative values when \( pH \) is above 7.

Assume the feed concentrations \( c_A \) and \( c_B \) are constant. Linearization and Laplace transform yields

\[
c(s) = \frac{1}{1 + \tau s} \left( c_A^* - c_B^* \right) + \frac{q_{A\rightarrow c}^* - c_{c}^*}{q_s^*} q_{A}^* + \frac{rV}{q_s^*} q_{B}\left(s\right)
\]

where \( r = V/q_s^* \) is the residence time and \( s \) is used to denote steady-state values. To derive this we have made use of the total material balance \( dV/dt = q_A + q_B = g \) (alternatively one may assume \( V \) is constant but this is not strictly necessary) and the corresponding steady-state balance \( c_A^* + c_B^* = q_s^* \). We now introduce the following scaled variables

\[
y(s) = \frac{c(s)}{c_{\text{max}}}; \quad d(s) = \frac{q_A(s)}{q_{\text{max}}}; \quad u(s) = \frac{q_B(s)}{q_{\text{max}}}\frac{1}{q_{B\text{max}}}
\]

We use the following numbers: \( V = 10 \text{ m}^3, c_A^* = 0.005 \text{ m}^3/\text{s}, c_B^* = 10 \text{ m}^3/\text{s}, c_{A\rightarrow H} = 10 \text{ mol/l} \) (corresponding to \( pH = 1 \) and \( c_{A\rightarrow OH} = 10 \text{ mol/l} \) (corresponding to \( pH = 15 \)), \( c_{B\rightarrow H} = 10^{-15} = 10 \text{ mol/l} \), \( c_{B\rightarrow OH} = 10^{-15} = 10 \text{ mol/l} \) (corresponding to \( pH = 15 \)). The following inputs \( q_{A\rightarrow c} = 0.005 \text{ m}^3/\text{s}, q_{B\rightarrow c} = 0.005 \text{ m}^3/\text{s}, q_{A\rightarrow c} = 0.005 \text{ m}^3/\text{s}, q_{B\rightarrow c} = 0.005 \text{ m}^3/\text{s}, q_{A\rightarrow c} = 0.005 \text{ m}^3/\text{s} \). Note from this that the largest disturbance is \( \pm 50\% \) of \( q_{A\rightarrow c} \), while the largest input is \( \pm 100\% \) of \( q_{B\rightarrow c} \).