### 4.3 PT1: First order lag (single capacity)

This is a so-called single capacity element because a single capacity process behaves this way; see the examples in this section.
Note: Non-linearly behaving capacity elements are also modeled with PT1. In those cases linearization is applied around a working point, as is demonstrated in the examples of liquid level with free outflow and general order chemical reactor.

### 4.3.1 General properties

Its equation:

$$
\mathrm{T} \frac{\mathrm{dy}(\mathrm{t})}{\mathrm{dt}}+\mathrm{y}(\mathrm{t})=\mathrm{A} \cdot \mathrm{x}(\mathrm{t})
$$

Its two parameters are the gain A and the time constant or delay T . As it is derived in section 2.5.1, its transfer function is

$$
G(s)=\frac{A}{T \cdot s+1}
$$

### 4.3.1.1 Response functions of PT1

Its impulse response can be derived by first computing the Laplacian answer:

$$
\mathrm{Y}(\mathrm{~s})=\mathrm{G}(\mathrm{~s}) \cdot \mathrm{X}(\mathrm{~s})=\frac{\mathrm{A}}{\mathrm{~T} \cdot \mathrm{~s}+1} \cdot \mathrm{a}=\frac{\mathrm{A} \cdot \mathrm{a}}{\mathrm{~T} \cdot \mathrm{~s}+1}
$$

Its inverse Laplacian is: $\hat{y}(t)=\frac{A \cdot a}{T} \cdot e^{-\frac{t}{T}}$, thus $y(t)=y_{0}+\frac{A \cdot a}{T} \cdot e^{-\frac{t}{T}}$.
Its step response for step a is derived in section 2.4. Using the transfer function as starting point and input function $x(t)=a$ :

$$
\mathrm{Y}(\mathrm{~s})=\mathrm{G}(\mathrm{~s}) \cdot \mathrm{X}(\mathrm{~s})=\frac{\mathrm{A}}{\mathrm{~T} \cdot \mathrm{~s}+1} \cdot \frac{\mathrm{a}}{\mathrm{~s}}=\frac{\mathrm{A} \cdot \mathrm{a}}{(\mathrm{~T} \cdot \mathrm{~s}+1) \cdot \mathrm{s}}
$$

Its inverse Laplacian is: $\hat{y}(t)=A \cdot a \cdot\left(1-e^{-\frac{t}{T}}\right)$, thus $y(t)=y_{0}+A \cdot a \cdot\left(1-e^{-\frac{t}{T}}\right)$
In the same way, for a rump input with slope a, i.e. $x(t)=a \cdot t$ :

$$
Y(s)=G(s) \cdot X(s)=\frac{A}{T \cdot s+1} \cdot \frac{a}{s^{2}}=\frac{A \cdot a}{(T \cdot s+1) \cdot s^{2}}
$$

Its inverse Laplacian is: $\hat{\mathrm{y}}(\mathrm{t})=\mathrm{A} \cdot \mathrm{a} \cdot\left(\mathrm{t}-\mathrm{T} \cdot\left(1-\mathrm{e}^{-\frac{\mathrm{t}}{\mathrm{T}}}\right)\right)$
At high t values this answer fits asymptotically to $\mathrm{y}(\mathrm{t}) \approx \mathrm{A} \cdot \mathrm{a} \cdot(\mathrm{t}-\mathrm{T})$, this is why the time parameter T is also called time delay.

The response functions are shown below.




Response functions of PT1

### 4.3.1.2 Frequency function of PT1

$$
\begin{aligned}
\mathrm{g}(\omega)= & \frac{\mathrm{A}}{\mathrm{~T} \cdot(\mathrm{i} \cdot \omega)+1}=\frac{\mathrm{A} \cdot(1-\mathrm{T} \cdot \mathrm{i} \cdot \omega)}{(1+\mathrm{T} \cdot \mathrm{i} \cdot \omega) \cdot(1-\mathrm{T} \cdot \mathrm{i} \cdot \omega)}=\frac{\mathrm{A} \cdot(1-\mathrm{T} \cdot \mathrm{i} \cdot \omega)}{1+\mathrm{T}^{2} \cdot \omega^{2}} \\
& =\mathrm{A} \cdot\left(\frac{1}{1+\mathrm{T}^{2} \cdot \omega^{2}}-\mathfrak{i} \cdot \frac{\mathrm{T} \cdot \omega}{1+\mathrm{T}^{2} \cdot \omega^{2}}\right) \\
|\mathrm{g}(\omega)| & =|\mathrm{A}| \cdot \frac{1}{1+\mathrm{T}^{2} \cdot \omega^{2}} \cdot \sqrt{1+\mathrm{T}^{2} \cdot \omega^{2}}=\frac{|\mathrm{A}|}{\sqrt{1+\mathrm{T}^{2} \cdot \omega^{2}}} \\
\varphi(\omega) & =\arctan \left(\frac{-\frac{\mathrm{T} \cdot \omega}{1+\mathrm{T}^{2} \cdot \omega^{2}}}{\frac{1}{1+\mathrm{T}^{2} \cdot \omega^{2}}}\right)=\arctan (-\mathrm{T} \cdot \omega)=-\arctan (\mathrm{T} \cdot \omega)
\end{aligned}
$$

The phase angle at $\omega=0$ starts at 0 and monotonically decreases with increasing $\omega$, but never goes below $-90 .{ }^{\circ}$ The Nyquist plot is a curve starting from $[A, 0]$ and going toward $[0,0]$ in the first negative quadrant:


Nyquist plot of PT1

For drawing the Bode plot, take into account that

$$
\lg |g(\omega)|=\lg |\mathrm{A}|-\frac{1}{2} \lg \left(1+\mathrm{T}^{2} \cdot \omega^{2}\right)
$$

At low $\omega$ frequencies the term $\mathrm{T}^{2} \cdot \omega^{2}$ is negligible in the bracket, whereas at high $\omega$ frequencies the unity is negligible in the bracket. Therefore

$$
\begin{aligned}
& \text { at low frequencies } \lg |g(\omega)| \approx \lg |\mathrm{A}| \text {, and } \\
& \text { at high frequencies } \lg |\mathbf{g}(\omega)|=\lg |\mathrm{A}|-\lg T-\lg \omega
\end{aligned}
$$

Hence at low frequencies the curve asymptotically fits to a horizontal line whereas at high frequencies it asymptotically fits to a straight line with slope -1 . The two asymptotic straight lines intersect at a frequency $\omega=\frac{1}{\mathrm{~T}}$. (This is called: corner frequency.) Note that the frequency $\omega$ is measured in [radian/time unit] in these formulas.
The normalized Bode plot is shown below. Normalization means: $\mathrm{A}=1$ and $\omega \cdot \mathrm{T}$ is used in the horizontal axis:


Normalized Bode plot of PT1

### 4.3.2 Identifying PT1 from empirical data

Given the step response of a PT1 element, its gain A can be determined from the estimated response step at infinite time, and the time constant T can be computed from any point's co-ordinates or the slope of a tangent line to a point, according to the analytically known answer function.
However, we cannot be sure that the actual physical element really behaves as (i.e. can be well approximated by) a PT1 element. This can be checked by plotting $\ln \frac{y_{\infty}-y(t)}{y_{\infty}}$
against $t$, because $y_{\infty}=A \cdot a$ so that $\frac{y_{\infty}-y(t)}{y_{\infty}}=e^{-\frac{t}{T}}$ and thus $\ln \frac{y_{\infty}-y(t)}{y_{\infty}}=-\frac{t}{T}$, a straight line in t with slope $-\frac{1}{\mathrm{~T}}$.

The unit behaves as a PT1 element if the plot is approximately a straight line, and the time constant can be determined by fitting a straight line to the plot and reading its slope:


Identification of PT1

### 4.3.3 Example: Stirred tank

The stirred tank in the example serves as a concentration buffer. Liquid solution flows through a tank so that the liquid level in the tank is somehow kept constant and thus the volume V of the liquid momentarily contained in the vessel is also constant. As a result, the momentary flow rate w leaving the vessel is always equal to the flow rate entering the vessel. The liquid consists of a solvent and a solute. The concentration $\mathrm{c}_{\mathrm{in}}$ of the solute in the incoming flow is subject to change in time, and thus the average concentration of the solute in the vessel at any moment is also subject to change. The vessel is perfectly mixed so that the concentration in any point of the vessel is the same, and equal to the average, and the concentration $\mathrm{c}_{\text {out }}$ in the effluent stream in any moment is the same as in the vessel.

Suppose, for the sake of simplicity, that the flow rate w is constant. Suppose, as well, that there is an initial steady state characterized by some $\mathrm{c}_{\text {in }}=\mathrm{c}_{0}=\mathrm{c}_{\text {out }}$ concentration. How does the outlet concentration $\mathrm{c}_{\text {out }}$ change in time if the inlet concentration $\mathrm{c}_{\text {in }}$ changes? The
inlet concentration can change according to any arbitrary (but non-negative and finite) function of time.


In order to find a proper answer, consider a dynamic balance of the solute around the vessel:

$$
\mathrm{w} \cdot \mathrm{c}_{\text {in }}(\mathrm{t})=\mathrm{w} \cdot \mathrm{c}_{\text {out }}(\mathrm{t})+\mathrm{v} \cdot \frac{\mathrm{dc}}{\text { out }}(\mathrm{t})
$$

The balance says: What comes into the vessel (left hand side) is equal to a sum of two parts: that part which flows out from the vessel, and another part which increments the amount accumulated in the vessel. (This second part can be zero or negative, as well.)
By rearranging of the equation, we obtain the general form of a first order lag:

$$
\frac{\mathrm{V}}{\mathrm{w}} \cdot \frac{\mathrm{~d} \mathrm{c}_{\text {out }}(\mathrm{t})}{\mathrm{dt}}+\mathrm{c}_{\text {out }}(\mathrm{t})=\mathrm{c}_{\text {in }}(\mathrm{t})
$$

Here $c_{\text {in }}(t)$ is the input signal, and $c_{\text {out }}(t)$ is the output signal of the element. The time constant is $\mathrm{T}=\frac{\mathrm{V}}{\mathrm{W}}$, the average residence time of the fluid particles (you can check its dimension is time), and the gain is $\mathrm{A}=1$ concentration/concentration, i.e. dimensionless).
In order to apply this model properly, we have to use deviation variables $\hat{c}_{\text {in }}(\mathrm{t})=\mathrm{c}_{\text {in }}(\mathrm{t})-\mathrm{c}_{0}$ and $\hat{\mathrm{c}}_{\text {out }}(\mathrm{t})=\mathrm{c}_{\text {out }}(\mathrm{t})-\mathrm{c}_{0}$. By introducing them to the equation, we get

$$
\frac{\mathrm{V}}{\mathrm{w}} \cdot \frac{\mathrm{~d}\left(\mathrm{c}_{0}+\hat{\mathrm{c}}_{\text {out }}(\mathrm{t})\right)}{\mathrm{dt}}+\left(\mathrm{c}_{0}+\hat{\mathrm{c}}_{\text {out }}(\mathrm{t})\right)=\left(\mathrm{c}_{0}+\hat{\mathrm{c}}_{\text {in }}(\mathrm{t})\right)
$$

i.e. $\quad \frac{V}{W} \cdot \frac{d \hat{c}_{\text {out }}(t)}{d t}+\hat{c}_{\text {out }}(t)=\hat{c}_{\text {in }}(t)$

The equation for the deviation variables is the same as that for the original ones. This is generally true for linear forms.
After Laplace transformation we get $\frac{\mathrm{V}}{\mathrm{W}} \cdot \mathrm{C}_{\text {out }}(\mathrm{s}) \cdot \mathrm{s}+\mathrm{C}_{\text {out }}(\mathrm{s})=\mathrm{C}_{\text {in }}(\mathrm{s})$ where capitals are used for the Laplacians. Thus the transfer function from $\mathrm{c}_{\text {in }}$ to $\mathrm{c}_{\text {out }}$ is

$$
\mathrm{G}(\mathrm{~s})=\frac{1}{\left(\frac{\mathrm{~V}}{\mathrm{~W}}\right) \cdot \mathrm{s}+1}=\frac{1}{\tau \cdot \mathrm{~s}+1}
$$

where $\tau$ is the residence time of the liquid in the vessel.
For example, if $\mathrm{c}_{\text {in }}$ changes by a sudden step from $\mathrm{c}_{0}$ up to $\mathrm{c}_{1}$, then the response function is

$$
\hat{c}_{\text {out }}(t)=1 \cdot\left(c_{1}-c_{0}\right) \cdot\left(1-e^{-\frac{t}{V / w}}\right)
$$

and the measured output concentration changes according to the following function:

$$
c_{\text {out }}(t)=c_{0}+\left(c_{1}-c_{0}\right) \cdot\left(1-e^{-\frac{t}{V / w}}\right)
$$

### 4.3.4 Example: Thermometer

Consider a mercury thermometer submerging in a fluid of temperature $\mathrm{T}_{\mathrm{F}}$. Denote the temperature of (and shown by) the thermometer by $\mathrm{T}_{\mathrm{th}}$. Suppose that the heat transfer coefficient between the fluid and the thermometer is U , and the heat transfer area (of the mercury jacket) is B. Let the heat capacity C of the thermometer is as small as to be negligible comparing it to the heat capacity of the fluid.
Suppose that initially the system was in steady state at some equilibrium temperature $\mathrm{T}_{\mathrm{F}}=\mathrm{T}_{0}=\mathrm{T}_{\mathrm{th}}$, and then $\mathrm{T}_{\mathrm{F}}$ is changed. How will $\mathrm{T}_{\mathrm{th}}$ change? We are looking for the answer with any arbitrary change of $\mathrm{T}_{\mathrm{F}}$.
The dynamic heat balance of the thermometer can be written as

$$
\mathrm{U} \cdot \mathrm{~B} \cdot\left(\mathrm{~T}_{\mathrm{F}}(\mathrm{t})-\mathrm{T}_{\mathrm{th}}(\mathrm{t})\right)=\mathrm{C} \cdot \frac{\mathrm{~d} \mathrm{~T}_{\mathrm{th}}(\mathrm{t})}{\mathrm{dt}}
$$

Here the left hand side tells how much heat is taken up by the thermometer in a unit time, whereas the right hand side counts the increase of $\mathrm{T}_{\mathrm{th}}$ as a result of taking up that heat.
Now the input signal is $\mathrm{T}_{\mathrm{F}}$, and the output signal is $\mathrm{T}_{\mathrm{th}}$. The equation is rearranged:

$$
\frac{\mathrm{C}}{\mathrm{U} \cdot \mathrm{~B}} \cdot \frac{\mathrm{dT} \mathrm{~T}_{\mathrm{th}}(\mathrm{t})}{\mathrm{dt}}+\mathrm{T}_{\mathrm{th}}(\mathrm{t})=\mathrm{T}_{\mathrm{F}}(\mathrm{t})
$$

This is the equation of a first order lag with gain $\mathrm{A}=1$ (temperature/temperature, i.e. dimensionless) and time constant $T=\frac{C}{U \cdot B}$.
We have to consider deviation variables, but the form of the equation does not change.

$$
\mathrm{G}(\mathrm{~s})=\frac{1}{\left(\frac{\mathrm{C}}{\mathrm{U} \cdot \mathrm{~B}}\right) \cdot \mathrm{s}+1}
$$

If the temperature of the fluid changes with a constant slope K degree/time_unit (a ramp function), for example, then the measured temperature will be

$$
T_{t h}(t)=T_{0}+1 \cdot K \cdot\left(t-\frac{C}{U \cdot B} \cdot\left(1-e^{-\frac{U B}{C} \cdot t}\right)\right)
$$

That is, the measured temperature will be delayed by $T=\frac{C}{U \cdot B}$ at high $t$.

### 4.3.5 Example: Steam heater

Let a stream to be heated up at a constant flow rate w through a perfectly mixed tank of volume V that serves as a heat exchanger with heat transfer area B . The material properties of the fluid are its density $\rho$ and specific heat $\mathrm{c}_{\mathrm{p}}$. Let the fluid heated up by steam of a given pressure, involving its condensation temperature $\mathrm{T}_{\mathrm{S}}$, and let the overall heat transfer coefficient be $U$. Denote the inlet temperature by $T_{i n}$, the outlet temperature by $\mathrm{T}_{\text {out }}$.


Suppose that there is initially a steady state with data $\mathrm{T}_{\mathrm{in}, 0}, \mathrm{~T}_{\mathrm{S}, 0}$, and $\mathrm{T}_{\text {out }, 0}$, and then some change happens either in $\mathrm{T}_{\text {in }}$ or in $\mathrm{T}_{\mathrm{S}}$, or both. How will $\mathrm{T}_{\text {out }}$ react?
The steady state heat balance can be written as

$$
\mathrm{w} \cdot \rho \cdot \mathrm{C}_{\mathrm{p}} \cdot \mathrm{~T}_{\text {in }}(\mathrm{t})+\mathrm{U} \cdot \mathrm{~B} \cdot\left(\mathrm{~T}_{\mathrm{s}}(\mathrm{t})-\mathrm{T}_{\text {out }}(\mathrm{t})\right)=\mathrm{w} \cdot \rho \cdot \mathrm{c}_{\mathrm{p}} \cdot \mathrm{~T}_{\text {out }}(\mathrm{t})
$$

Note that, because of perfect mixing, temperature of the effluent stream equals the temperature inside the vessel. The left hand size is a sum of the heat content carried in by the inlet stream and the heat transported through the wall separating the two media. This sum must be equal to the heat content of the effluent stream (right hand side) in steady state.

If there is no steady state, i.e. in the general case (dynamic balance), the accumulation of heat in the vessel is also taken into account by an additional member:

$$
\mathrm{w} \cdot \rho \cdot \mathrm{c}_{\mathrm{p}} \cdot \mathrm{~T}_{\text {in }}(\mathrm{t})+\mathrm{U} \cdot \mathrm{~B} \cdot\left(\mathrm{~T}_{\mathrm{s}}(\mathrm{t})-\mathrm{T}_{\text {out }}(\mathrm{t})\right)=\mathrm{w} \cdot \rho \cdot \mathrm{c}_{\mathrm{p}} \cdot \mathrm{~T}_{\text {out }}(\mathrm{t})+\mathrm{V} \cdot \rho \cdot \mathrm{c}_{\mathrm{p}} \cdot \frac{\mathrm{~d} \mathrm{~T}_{\text {out }}(\mathrm{t})}{\mathrm{dt}}
$$

We may apply deviation variables and the equation can be rearranged as

$$
\frac{V \cdot \rho \cdot c_{p}}{U \cdot B+W \cdot \rho \cdot c_{p}} \cdot \frac{d \hat{T}_{\text {out }}(t)}{d t}+\hat{T}_{\text {out }}(t)=\frac{W \cdot \rho \cdot C_{p}}{U \cdot B+W \cdot \rho \cdot C_{p}} \cdot \hat{T}_{\text {in }}(t)+\frac{U \cdot B}{U \cdot B+W \cdot \rho \cdot c_{p}} \cdot \hat{T}_{s}(t)
$$

Here there are two input signals, and the output signal responses as first order lag to both of them.

The Laplacian form is

$$
T_{\text {out }}(s)=\frac{A_{T_{\text {in }}}}{T \cdot s_{1}+1} \cdot T_{\text {in }}(s)+\frac{A_{T_{s}}}{T \cdot s+1} \cdot T_{s}(s)
$$

where time constant is common

$$
T=\frac{V \cdot \rho \cdot c_{p}}{U \cdot B+W \cdot \rho \cdot c_{p}}
$$

but the gains are different:

$$
\begin{aligned}
& \mathrm{A}_{\mathrm{T}_{\text {in }}}=\frac{\mathrm{W} \cdot \rho \cdot \mathrm{C}_{\mathrm{p}}}{\mathrm{U} \cdot \mathrm{~B}+\mathrm{W} \cdot \rho \cdot \mathrm{C}_{\mathrm{p}}} \\
& \mathrm{~A}_{\mathrm{T}_{\mathrm{s}}}=\frac{\mathrm{U} \cdot \mathrm{~B}}{\mathrm{U} \cdot \mathrm{~B}+\mathrm{W} \cdot \rho \cdot \mathrm{C}_{\mathrm{p}}}
\end{aligned}
$$

### 4.3.6 Example: Liquid level in tank with free outflow

Fluid flows in with flow rate $\mathrm{w}_{\text {in }}$ to a vessel with vertical walls and constant horizontal cross section area $B$, and flows out from it with $w_{\text {out }}$ through an open hole into a pipe. The liquid level in the vessel is denoted by H .


The driving force of the outflow is the weight of the liquid over the hole, i.e. the pressure of the liquid column over the level of the hole.
(Note that this is a self-controlling process because the higher level causes faster outflow, and if the tank is high enough then there is a level where the outflow equals the inflow.)

Suppose an initial steady state is characterized by $\mathrm{W}_{\text {in }}=\mathrm{W}_{0}=\mathrm{W}_{\text {out }}$ and $\mathrm{H}=\mathrm{H}_{0}$, and then the inlet flow rate changes arbitrarily. How will liquid level H change in time?

The dynamic material balance is

$$
W_{\text {in }}(t)=W_{\text {out }}(t)+B \cdot \frac{d H(t)}{d t}
$$

We know from physics or unit operations that the outlet flow rate depends on the actual level by a square root formula

$$
W_{\text {out }}=K \cdot \sqrt{H}
$$

where K is constant factor. Substitute this formula to the balance:

$$
\mathrm{W}_{\mathrm{in}}(\mathrm{t})=\mathrm{K} \cdot \sqrt{\mathrm{H}(\mathrm{t})}+\mathrm{B} \cdot \frac{\mathrm{dH}(\mathrm{t})}{\mathrm{dt}}
$$

then this is not a linear equation. Thus, the free outflow level process is not a linear unit. In such cases, however, the process can be linearized around a working point, which is taken as the initial steady state. For example, if y depends on x in a non-linear manner then the linearization, according to the figure below, is


$$
y-y_{0}=\left.\frac{d y}{d x}\right|_{x_{0}} \cdot\left(x-x_{0}\right), \quad \text { i.e. } \quad \hat{y}=\left.\frac{d y}{d x}\right|_{x_{0}} \cdot \hat{x}
$$

In our particular case we have

$$
\hat{W}_{\text {out }}=\frac{d \hat{W}_{\text {out }}}{d H} \cdot \hat{H}
$$

and the linearized balance equation is

$$
\hat{W}_{\text {in }}(\mathrm{t})=\left.\frac{\mathrm{d} \hat{W}_{\text {out }}}{\mathrm{dH}}\right|_{0} \cdot \hat{H}(\mathrm{t})+\mathrm{B} \cdot \frac{\mathrm{~d} \hat{H}(\mathrm{t})}{\mathrm{dt}}
$$

By differentiation we get

$$
\begin{aligned}
& \frac{d W_{\text {out }}}{d H}=\frac{K}{2 \cdot \sqrt{H}}=\frac{K \cdot \sqrt{H}}{2 \cdot H}=\frac{W_{\text {out }}}{2 \cdot H} \\
& \left.\frac{d \hat{W}_{\text {out }}}{d H}\right|_{0}=\frac{W_{\text {out }, 0}}{2 \cdot H_{0}}
\end{aligned}
$$

thus the linearized balance is

$$
\hat{W}_{\text {in }}(\mathrm{t})=\frac{\mathrm{W}_{\text {out }, 0}}{2 \cdot H_{0}} \cdot \hat{H}(\mathrm{t})+\mathrm{B} \cdot \frac{\mathrm{~d} \hat{H}(\mathrm{t})}{\mathrm{dt}}
$$

By rearrangement:

$$
\frac{2 \cdot \mathrm{H}_{0} \cdot \mathrm{~B}}{\mathrm{~W}_{\text {out }, 0}} \cdot \frac{\mathrm{~d} \hat{\mathrm{H}}(\mathrm{t})}{\mathrm{dt}}+\hat{\mathrm{H}}(\mathrm{t})=\frac{2 \cdot \mathrm{H}_{0}}{\mathrm{~W}_{\text {out }, 0}} \cdot \hat{\mathrm{~W}}_{\text {in }}(\mathrm{t})
$$

This is a PT1 element with gain

$$
\mathrm{A}=\frac{2 \cdot \mathrm{H}_{0}}{\mathrm{w}_{\text {out }, 0}}
$$

and time constant

$$
\mathrm{T}=\frac{2 \cdot \mathrm{H}_{0} \cdot \mathrm{~B}}{\mathrm{w}_{\mathrm{out}, \mathrm{O}}}
$$

Note that $\mathrm{H} \cdot \mathrm{B}=\mathrm{V}$, the volume of the liquid in the vessel, and then $\frac{\mathrm{H}_{0} \cdot \mathrm{~B}}{\mathrm{~W}_{0}}=\tau$, the residence time of the liquid in the vessel in steady state. Thus

$$
\mathrm{T}=2 \cdot \tau_{0}
$$

and the transfer function is

$$
\mathrm{G}(\mathrm{~s})=\frac{\left(\frac{2 \cdot \mathrm{H}_{0}}{\mathrm{~W}_{\text {out }, 0}}\right)}{\left(2 \cdot \tau_{0}\right) \cdot \mathrm{s}+1}
$$

### 4.3.7 Example: Stirred chemical tank reactor

Consider a perfectly stirred chemical tank reactor (CSTR) with constant liquid volume V and flow rate w.
Let the chemical reaction be of order n so that the reaction rate [ $\mathrm{mol} /$ (volume-time) $]$ is $r=k \cdot c^{n}$. (A given component whose concentration is $c$ reacts off from the solution. The concentration of the reaction product is not part of the model.) Because of perfect mixing, c inside the vessel is $\mathrm{c}=\mathrm{c}_{\text {out }}$.


Suppose an initial steady state with $\mathrm{c}_{\mathrm{in}, 0}$ and $\mathrm{c}_{\mathrm{out}, 0}$, and then some change in $\mathrm{c}_{\mathrm{in}}$. How will $\mathrm{c}_{\text {out }}$ change in time?

Before answering the question, note that $\mathrm{c}_{\mathrm{out}, 0}$ is not independent of $\mathrm{c}_{\mathrm{in}, 0}$ since according to the steady state balance

$$
\begin{aligned}
& \mathrm{W} \cdot \mathrm{c}_{\mathrm{in}, 0}=\mathrm{V} \cdot \mathrm{r}_{0}+\mathrm{W} \cdot \mathrm{C}_{\mathrm{out}, 0} \\
& \mathrm{~W} \cdot \mathrm{c}_{\mathrm{in}, 0}=\mathrm{V} \cdot \mathrm{k} \cdot \mathrm{c}_{\mathrm{out}, 0}^{\mathrm{n}}+\mathrm{W} \cdot \mathrm{c}_{\mathrm{out}, 0} \\
& \mathrm{c}_{\mathrm{in}, 0}=\tau \cdot \mathrm{k} \cdot \mathrm{c}_{\mathrm{out}, 0}^{\mathrm{n}}+\mathrm{c}_{\mathrm{out}, 0}
\end{aligned}
$$

where $\tau$ is the residence time.
The dynamic balance is

$$
\mathrm{w} \cdot \mathrm{c}_{\text {in }}(\mathrm{t})=\mathrm{V} \cdot \mathrm{k} \cdot \mathrm{c}_{\text {out }}^{\mathrm{n}}(\mathrm{t})+\mathrm{w} \cdot \mathrm{c}_{\text {out }}(\mathrm{t})+\mathrm{V} \cdot \frac{\mathrm{dc}_{\text {out }}(\mathrm{t})}{\mathrm{dt}}
$$

which, in general, is a non-linear equation.

### 4.3.7.1 First order reaction

In this case the equation is linear.

$$
\mathrm{w} \cdot \mathrm{c}_{\text {in }}(\mathrm{t})=(\mathrm{V} \cdot \mathrm{k}+\mathrm{w}) \cdot \mathrm{c}_{\text {out }}(\mathrm{t})+\mathrm{V} \cdot \frac{\mathrm{dc}_{\text {out }}(\mathrm{t})}{\mathrm{dt}}
$$

After introducing the deviation variables and rearrangement:

$$
\frac{V}{V \cdot k+w} \cdot \frac{d \hat{c}_{\text {out }}(t)}{d t}+\hat{c}_{\text {out }}(t)=\frac{w}{V \cdot k+w} \cdot \hat{c}_{\text {in }}(t)
$$

or

$$
\frac{\tau}{\tau \cdot \mathrm{k}+1} \cdot \frac{\mathrm{~d} \hat{\mathrm{c}}_{\mathrm{out}}(\mathrm{t})}{\mathrm{dt}}+\hat{\mathrm{c}}_{\mathrm{out}}(\mathrm{t})=\frac{1}{\tau \cdot \mathrm{k}+1} \cdot \hat{\mathrm{c}}_{\mathrm{in}}(\mathrm{t})
$$

where $\tau$ is the residence time.
Thus, this is a PT1 element with gain and time delay as

$$
\begin{aligned}
& \mathrm{A}=\frac{\mathrm{W}}{\mathrm{~V} \cdot \mathrm{k}+\mathrm{w}}=\frac{1}{\tau \cdot \mathrm{k}+1} \\
& \mathrm{~T}=\frac{\mathrm{V}}{\mathrm{~V} \cdot \mathrm{k}+\mathrm{w}}=\frac{\tau}{\tau \cdot \mathrm{k}+1}
\end{aligned}
$$

### 4.3.7.2 General case

In the general case the reaction rate is linearized around the point of $\left[\mathrm{c}_{\mathrm{out}, 0,}, \mathrm{r}_{0}\right]$. (Note that $\mathrm{r}_{0}=\mathrm{k} \cdot \mathrm{c}_{\text {out }, 0}^{\mathrm{n}}$ )

$$
\left.\frac{\mathrm{dr}}{\mathrm{dc} \mathrm{c}_{\text {out }}}\right|_{0}=\mathrm{n} \cdot \mathrm{k} \cdot \mathrm{c}_{\text {out }, 0}^{\mathrm{n}-1}
$$

Substituting this to the balance equation, applying deviation variables and rearrangement:

$$
\frac{V}{V \cdot\left(\frac{d r}{d c_{\text {out }}}\right)_{0}+w} \cdot \frac{d \hat{c}_{\text {out }}(t)}{d t}+\hat{c}_{\text {out }}(\mathrm{t})=\frac{\mathrm{w}}{\mathrm{~V} \cdot\left(\frac{\mathrm{dr}}{d \mathrm{c}_{\text {out }}}\right)_{0}+\mathrm{w}} \cdot \hat{c}_{\text {in }}(\mathrm{t})
$$

or

$$
\frac{\tau}{\tau \cdot\left(\frac{\mathrm{dr}}{\mathrm{dc}_{\text {out }}}\right)_{0}+1} \cdot \frac{\mathrm{~d} \hat{\mathrm{c}}_{\text {out }}(\mathrm{t})}{\mathrm{dt}}+\hat{\mathrm{c}}_{\text {out }}(\mathrm{t})=\frac{1}{\tau \cdot\left(\frac{\mathrm{dr}}{\mathrm{dc}}\right)_{\text {out }}+1} \cdot \hat{c}_{\text {in }}(\mathrm{t})
$$

where $\tau$ is the residence time.
Thus, this is a PT1 element with gain and time delay as

$$
\begin{aligned}
& \mathrm{A}=\frac{\mathrm{w}}{\mathrm{~V} \cdot\left(\frac{\mathrm{dr}}{\mathrm{dc}_{\text {out }}}\right)_{0}+\mathrm{w}}=\frac{1}{\tau \cdot\left(\frac{\mathrm{dr}}{\mathrm{dc}} \mathrm{cc}_{\text {out }}\right)_{0}+1} \\
& \mathrm{~T}=\frac{\mathrm{V}}{\mathrm{~V} \cdot\left(\frac{\mathrm{dr}}{\mathrm{dc}_{\text {out }}}\right)_{0}+\mathrm{w}}=\frac{\tau}{\tau \cdot\left(\frac{\mathrm{dr}}{\mathrm{dc}_{\text {out }}}\right)_{0}+1}
\end{aligned}
$$

This is an approximation around the working point.
This general case incorporates the particular case of the first order reaction, and even the case of no reaction, i.e. the mixed vessel. The first order case is not an approximation but is exact because then the derivative does not depend on the actual concentration.

### 4.4 PT2: Second order lag (double capacity)

Such a double capacity element is formed if two first order lags are connected in a series, but there are inherently second order lags that cannot be decomposed into two single capacities.

### 4.4.1 General properties

Its equation by definition:

$$
T_{2}^{2} \frac{d^{2} y(t)}{d t^{2}}+T_{1} \frac{d y(t)}{d t}+y(t)=A \cdot x(t)
$$

This element has three parameters: the gain $A$, the first order time constant $T_{1}$ and the second order time constant $T_{2}$. Its transfer function is

$$
G(s)=\frac{A}{T_{2}^{2} \cdot s^{2}+T_{1} \cdot s+1}
$$

but can be rewritten in the following form:

$$
\mathrm{G}(\mathrm{~s})=\frac{\mathrm{A}}{\mathrm{~T}^{2} \cdot \mathrm{~s}^{2}+2 \cdot \xi \cdot \mathrm{~T} \cdot \mathrm{~s}+1}
$$

where
$\mathrm{T}=\mathrm{T}_{2}$, the time constant of the element,

$$
\xi=\frac{T_{1}}{2 \cdot T_{2}} \text {, the damping factor of the element. }
$$

If two first order lags are connected in series then also a second order lag is formed:

$$
G(s)=\frac{A_{1}}{T_{1} \cdot s+1} \cdot \frac{A_{2}}{T_{2} \cdot s+1}=\frac{A_{1} \cdot A_{2}}{T_{1} \cdot T_{2} \cdot s^{2}+\left(T_{1}+T_{2}\right) \cdot s+1}
$$

so that in this case

$$
\begin{aligned}
& \mathrm{T}=\sqrt{\mathrm{T}_{1} \cdot \mathrm{~T}_{2}} \\
& \xi=\frac{\mathrm{T}_{1}+\mathrm{T}_{2}}{2 \cdot \sqrt{\mathrm{~T}_{1} \cdot \mathrm{~T}_{2}}}
\end{aligned}
$$

The second order lags can be classified into three cases according to the value of $\xi$. In all the three cases we show the impulse response and the step response for impulse value $a$ and step value $a$ :
a. $0<\xi<1$

This is the so-called oscillating case. Such a case cannot be formed by connecting two first order lags.
We use the following derived parameters:

$$
\begin{array}{ll}
\alpha=\frac{\xi}{\mathrm{T}} & \text { damping exponent } \\
\omega=\frac{\sqrt{1-\xi^{2}}}{\mathrm{~T}} & \text { oscillation frequency }
\end{array}
$$

The impulse response:

$$
\hat{\mathrm{y}}(\mathrm{t})=\mathrm{A} \cdot \mathrm{a} \cdot \frac{1}{\omega \cdot \mathrm{~T}^{2}} \cdot \mathrm{e}^{-\alpha \cdot \mathrm{t}} \cdot \sin (\omega \cdot \mathrm{t})
$$

The step response:

$$
\hat{\mathrm{y}}(\mathrm{t})=\mathrm{A} \cdot \mathrm{a} \cdot\left(1-\mathrm{e}^{-\alpha \cdot \mathrm{t}} \cdot\left[\cos (\omega \cdot \mathrm{t})+\frac{\alpha}{\omega} \cdot \sin (\omega \cdot \mathrm{t})\right]\right)
$$

b. $\xi=1$

This is the case when two first order lags with identical time constants T are connected in series.

The impulse response:

$$
\hat{\mathrm{y}}(\mathrm{t})=\mathrm{A} \cdot \mathrm{a} \cdot \frac{\mathrm{t}}{\mathrm{~T}^{2}} \cdot \mathrm{e}^{-\frac{\mathrm{t}}{\mathrm{~T}}}
$$

The step response:

$$
\hat{\mathrm{y}}(\mathrm{t})=\mathrm{A} \cdot \mathrm{a} \cdot\left(1-\mathrm{e}^{-\alpha \mathrm{t}} \cdot\left[1+\frac{1}{\mathrm{~T}}\right]\right)
$$

No oscillation is here. This is the limit case between oscillation and non-periodic damping.
c. $1<\xi$

This is the case when two first order lags with different time constants $T_{1}$ and $T_{2}$ are connected in series. $1<\xi$ because $\frac{T_{1}+T_{2}}{2} \geq \sqrt{T_{1} \cdot T_{2}}$ always holds.
The impulse response:

$$
\hat{y}(t)=A \cdot a \cdot \frac{1}{T_{1}-T_{2}} \cdot\left(e^{-\frac{t}{T_{1}}}-e^{-\frac{t}{T_{2}}}\right)
$$

The step response:

$$
\hat{\mathrm{y}}(\mathrm{t})=\mathrm{A} \cdot \mathrm{a} \cdot\left[1-\frac{1}{\mathrm{~T}_{1}-\mathrm{T}_{2}} \cdot\left(\mathrm{~T}_{1} \cdot \mathrm{e}^{-\frac{t}{T_{1}}}-\mathrm{T}_{2} \cdot \mathrm{e}^{-\frac{t}{T_{2}}}\right)\right]
$$

No oscillation is here. The larger $\xi$, the stronger approaching the final value.

The impulse responses for different damping factors are shown in the next figure:


The step responses for different damping factors are shown in the next figure:


Using the same technique of algebra as in the case of the first order lag (section 4.3.1.2), the frequency function can be derived:

$$
\begin{aligned}
& |\mathrm{g}(\omega)|=\frac{|\mathrm{A}|}{\sqrt{\left(1-\mathrm{T}^{2} \cdot \omega^{2}\right)^{2}+(2 \cdot \xi \cdot \mathrm{~T} \cdot \omega)^{2}}} \\
& \varphi(\omega)=\arctan \left(\frac{2 \cdot \xi \cdot \mathrm{~T} \cdot \omega}{1-\mathrm{T}^{2} \cdot \omega^{2}}\right)
\end{aligned}
$$

The phase angle at $\omega=0$ starts at 0 and monotonically decreases with increasing $\omega$, but never goes below $-180 .{ }^{\circ}$. The Nyquist plot of several second order lags with different damping factors is shown below here:


For drawing the Bode plot, note that

$$
\text { at low frequencies }|g(\omega)| \approx|\mathrm{A}|,
$$

at high frequencies $|g(\omega)| \approx \frac{|\mathrm{A}|}{\mathrm{T}^{2} \cdot \omega^{2}}$, i.e. $\lg |g(\omega)| \approx \lg |\mathrm{A}|-2 \lg T-2 \lg \omega$
Hence at low frequencies the curve asymptotically fits to a horizontal line whereas at high frequencies it asymptotically fits to a straight line with slope -2 . The Bode plot of several second order lags with different damping factors are shown below:


### 4.4.2 Example: U-tube manometer

Consider a U-tube manometer measuring the pressure difference between its two open ends:


The differential equation describing the behavior of the manometer is the following:

$$
\mathrm{F} \cdot \Delta \mathrm{p}-\mathrm{h} \cdot \mathrm{~F} \cdot \rho \cdot \mathrm{~g}-\mathrm{R} \cdot \mathrm{~F} \cdot \frac{\mathrm{dh}}{\mathrm{dt}}=\mathrm{L} \cdot \mathrm{~F} \cdot \rho \cdot \frac{\mathrm{~d}^{2} \mathrm{~h}}{\mathrm{dt}^{2}}
$$

where
F: the tube's cross section area
$\Delta \mathrm{p}$ : the pressure difference
$\mathrm{h}: \quad$ the level difference in the two arms of the manometer
$\rho$ : density of the liquid in the tube
g: gravitation acceleration constant
L : total length of the liquid column in the tube
R : friction resistance (a lumped factor)
( $R$ is a shorthand for
$\mathrm{R}=\frac{32 \cdot \mathrm{~L} \cdot \eta}{\mathrm{D}^{2}}$ where $\quad \eta$ : $\quad$ dynamic viscosity
D: internal diameter of the tube)

The leftmost member expresses the driving force that would push the liquid column to or back in the tube. The next member counts for the gravity difference that pushes back. The third member counts for the resistance against moving due to friction: this is proportional to the velocity of the liquid in the tube. The right hand side is a product of total liquid mass with the acceleration of the liquid in the tube, so that the whole equation stands for Newton's low of movement.
After rearranging the equation we get

$$
\frac{\mathrm{L}}{\mathrm{~g}} \cdot \frac{\mathrm{~d}^{2} \mathrm{~h}}{\mathrm{dt}^{2}}+\frac{\mathrm{R}}{\rho \cdot \mathrm{~g}} \cdot \frac{\mathrm{dh}}{\mathrm{dt}}+\mathrm{h}=\frac{1}{\rho \cdot \mathrm{~g}} \cdot \Delta \mathrm{p}
$$

This is the equation of a second order lag with input signal $\Delta \mathrm{p}$ and output signal h , gain $\mathrm{A}=\frac{1}{\rho \cdot \mathrm{~g}}$, and time constants $\mathrm{T}_{1}=\frac{\mathrm{R}}{\rho \cdot \mathrm{g}}, \mathrm{T}_{2}=\sqrt{\frac{\mathrm{L}}{\mathrm{g}}}$.

