How are characteristic times (τ_{char}) and non-dimensional numbers related?

Systems Analysis and Mathematical Modeling in Urban Water Management (Fall 2015)
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This document provides some background on characteristic times, how they can be useful to differentiate between very fast/very slow processes, and how ratios of characteristic times can be used to calculate non-dimensional numbers such as the Reynolds number, the Turbulence Number, or the second Damköhler number.

An introduction to characteristic times with some examples is also provided in section "10.4 Discussion of Time Constants" in Gujer, 2008.

1 Characteristic times (τ_{char}) describes how fast a process is

The concept of characteristic times (sometimes referred to as time constants) is frequently used in textbooks and the scientific literature - but the background of the concept is seldom explained. The concept can be introduced using the following example. For a first order reaction rate the mass balance equation for the degradation of a substrate C_S in a batch process is:

$$\frac{dC_S}{dt} = -k_1 \cdot C_S \tag{1}$$

where C_S is the substrate concentration, $M\,L^{-3}$, k_1 is the first order reaction rate, T^{-1}, and t = time, T. Solving Eq. (1) with $C_S(t = 0) = C_{S,0}$ results in

$$\frac{C_S(t)}{C_{S,0}} = e^{-k_1 \cdot t} \tag{2}$$

Based on Eq. (2) one way to define the characteristic time for a first order reaction rate ($\tau_{reaction,1}$) is

$$\tau_{reaction,1} = \frac{1}{k_1} \tag{3}$$

Note that for a first order reaction rate this selection of the characteristic time results in $C_S(t=\tau)$ = exp(-1)·$C_{S,0}$ = 36.8 %·$C_{S,0}$. However, there is nothing special about the value of 36.8 % (there are others); it is simply mathematically convenient (Clark, 2009). For example the characteristic time for a zero order reaction rate $\tau_{reaction,0}$ corresponds to $C_S(t=\tau)$ = 0 in a batch reaction. A characteristic time is simply a measure of how fast a process will proceed, e.g., will the specific process approach equilibrium within seconds, hours, days, or weeks. In Table 1 characteristic times for reaction rates and mixing processes are summarized and some examples using these definitions are shown in Figure 1.
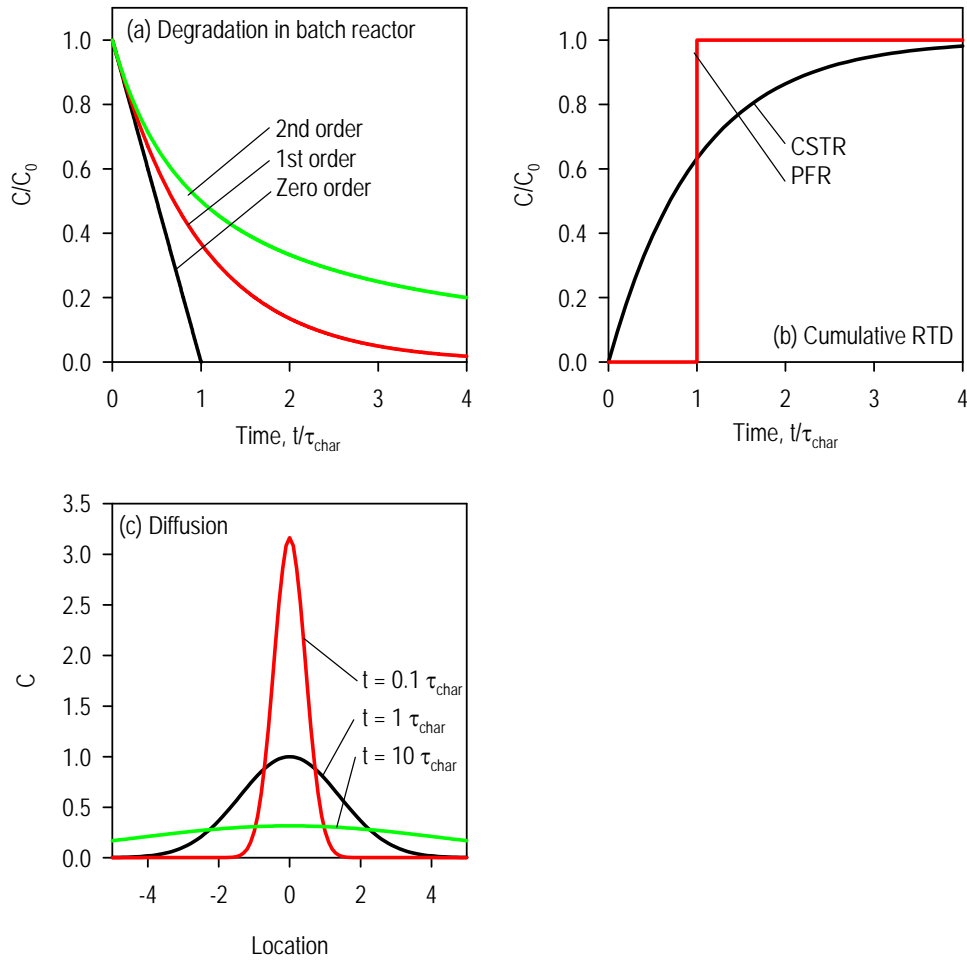
Figure 1. Characteristic times (τ_{char}) provide an order of magnitude approximation of how fast a reaction is occurring: (a) Degradation with zero, first, and second order kinetics, (From **Table 1** τ_{char} = C_0/k_0, $1/k_1$, $1/(C_0 \cdot k_2)$) (b) cumulative residence time distributions for CSTR and PFR, and (c) diffusion of a dirac pulse added at time zero over space and time ($\tau_{char} = L^2/D$).

Table 1. Characteristic times for transport and conversion processes (cited from Morgenroth, 2008, based on Clark, 2009; Esener et al., 1983; Gujer and Wanner, 1990; Ingham et al., 2007; Kissel et al., 1984; Picioreanu et al., 2000)

Process	Characteristic time	Eq.
Advection	$\tau_{convection} = \dfrac{L}{u}$	(4)
Retention in CSTR	$\tau_{CSTR} = \dfrac{V}{Q} = \dfrac{1}{\text{dilution rate}}$	(5)
Diffusion (mass)	$\tau_{diffusion,mass} = \dfrac{L^2}{D}$	(6)
Diffusion (viscous)	$\tau_{diffusion,viscous} = \dfrac{L^2}{\nu}$	(7)
Growth	$\tau_{growth} = \dfrac{1}{\mu_{max}}$	(8)
	$\tau_{growth}^{\;*} = \dfrac{C_S}{\mu_{max} \cdot X_H}$	(9)
Decay	$\tau_{decay} = \dfrac{1}{b_{decay}}$	(10)
Reaction	$\tau_{reaction,0} = \dfrac{C_S}{k_0}$ (zero order)	(11)
	$\tau_{reaction,1} = \dfrac{1}{k_1}$ (first order)	(12)
	$\tau_{reaction,Monod} = \dfrac{Y}{\mu_{max}} \cdot \dfrac{(K_S + C_S)}{X_H}$ (Monod)	(13)

L = characteristic distance (L), u = velocity ($L\,T^{-1}$), D = diffusion coefficient ($L^2\,T^{-1}$), dilution rate (D^1) = Q/V, ν = viscosity ($L^2\,T^{-1}$), k_0, k_1 = zero and first order volumetric reaction rates ($M\,L^{-3}\,T^{-1}$ and T^{-1}, respectively), b_{decay} = decay coefficient (T^{-1}), μ, μ_{max} = growth rate, maximum growth rate (T^{-1}), Y = yield coefficient ($M\,M^{-1}$), C_S, X_H = substrate, biomass concentration ($M\,L^{-3}$), K_S = Monod half saturation constant, ($M\,L^{-3}$)

2 How fast is a process relative to the time scale of interest (τ_0)?

When evaluating a dynamic system, one has to define a time scale of interest (τ_0). All processes with much smaller time scales (i.e., faster processes) than τ_0 can be assumed to be at a pseudo steady state. Processes with much larger time scales (i.e., slower processes) can be described as if they were "frozen" in time (Benjamin and Lawler, 2013; Esener et al., 1983; Picioreanu et al., 2000; Wanner et al., 2006).

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[1] Note: We use the symbol "D" for the diffusion coefficient and also for the dilution rate (= Q/V). In most cases, the meaning of the symbol can be derived from the specific context (e.g., dimensions).
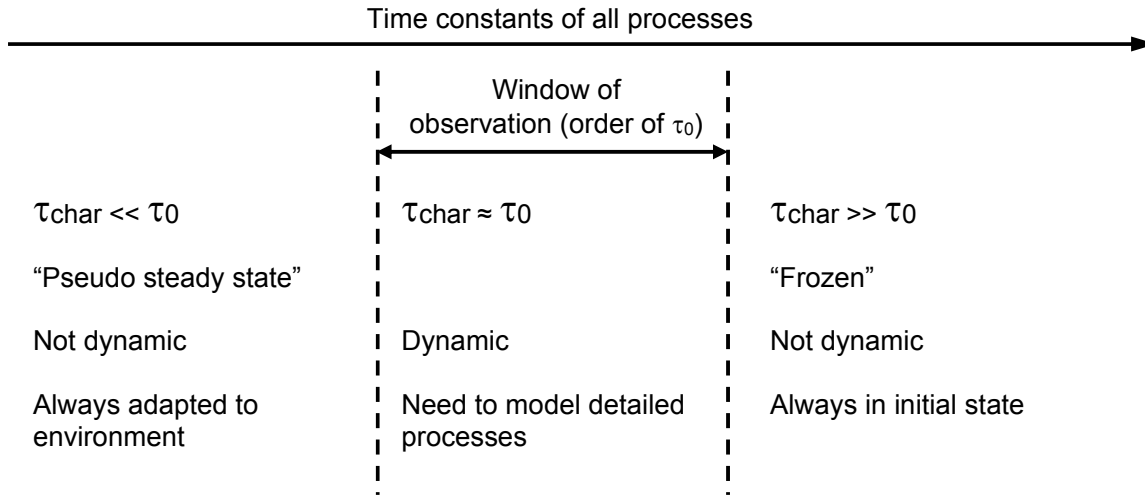
Time constants of all processes

$\tau_{char} \ll \tau_0$	$\tau_{char} \approx \tau_0$	$\tau_{char} \gg \tau_0$
"Pseudo steady state"		"Frozen"
Not dynamic	Dynamic	Not dynamic
Always adapted to environment	Need to model detailed processes	Always in initial state

Window of observation (order of τ_0)

Figure 2. Comparing time constants for very fast ($\tau_{char} \ll \tau_0$) and very slow ($\tau_{char} \gg \tau_0$) processes with relevant system dynamics (τ_0) (based on Esener et al., 1983; Roels, 1982).

When comparing the rates of different processes (i.e., their characteristic times) one has to differentiate whether processes occur in sequence (e.g., oxidation of ammonia to nitrite followed by oxidation of nitrite to nitrate) or in parallel (e.g., utilization of oxygen for heterotrophic or autotrophic growth) (Figure 3). If reactions occur in sequence then the overall process rate is determined by the slowest process (i.e., the process with the highest characteristic time). If reactions occur in parallel then the slower processes are of minor importance and the overall process rate is determined by the fastest process (i.e., the process with the smallest characteristic time) (Table 2).
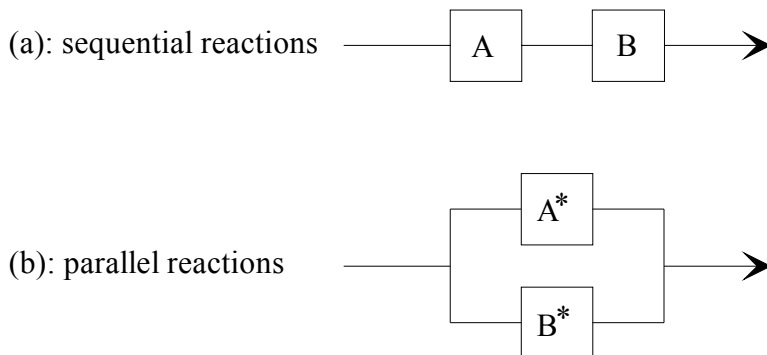
(a): sequential reactions

(b): parallel reactions

Figure 3. In sequencing reactions (a) the system is dominated by the slowest process while in parallel reactions (b) the slower process is not relevant and the fastest process dominates.

Table 2. Time constants determine which process dominates system performance where system response depends on whether processes are sequential or in parallel (Figure 3).

Type of process combination	General case	For $\tau_A \ll \tau_B$	For $\tau_A \gg \tau_B$
Processes A and B in sequence	Slowest process limits process combination	Process B dominates	Process A dominates
Processes A and B in parallel	Fastest process dominates and the slowest process can be neglected	Process A dominates	Process B dominates

3 Non dimensional numbers as ratios of two characteristic times

In many cases we are more interested in the ratios of characteristic times for two processes than in the characteristic times themselves. Ratios of characteristic times provides information on which of the two processes is dominating.

3.1 Examples of non-dimensional numbers

3.1.1 Reynolds number (Re)

Fluid flow is influenced by inertial and viscous forces. The Reynolds number compares the relevance of these two forces.

$$\text{Re} = \frac{\text{relevance of inertial forces}}{\text{relevance of viscous forces}} \tag{14}$$

can be expressed as a ratio of two characteristic times. Inertial and viscous processes can be viewed as "parallel processes" where the faster process or the process with the smaller time constant dominates.

$$\text{Re} = \frac{\left(\tau_{\text{advection}}\right)^{-1}}{\left(\tau_{\text{diffusion,viscous}}\right)^{-1}}$$

$$= \frac{\left(\dfrac{u}{L}\right)}{\left(\dfrac{\nu}{L^2}\right)} = \frac{u \cdot L}{\nu} \tag{15}$$

3.1.2 Turbulence number (N_T)

The turbulence number evaluates the relative importance of turbulence and advection

$$N_T = \frac{\text{relevance of turbulence}}{\text{relevance of advection}} \tag{16}$$

can be expressed as a ratio of two characteristic times. Mass transport due to turbulence and advection can be viewed as "parallel processes" where the faster process or the process with the smaller time constant dominates.

$$N_T = \frac{\left(\tau_{turbulence}\right)^{-1}}{\left(\tau_{advection}\right)^{-1}}$$

$$= \frac{\left(\dfrac{L^2}{D}\right)^{-1}}{\left(\dfrac{u}{L}\right)^{-1}} = \frac{D}{u \cdot L} \tag{17}$$

3.1.3 Second Damköhler number (Da^{II})

Substrate degradation in biofilms is a heterogeneous process where substrate has to diffuse into the biofilm and is subsequently degraded inside the biofilm. The second Damköhler number evaluated the relative importance of diffusion and reaction

$$Da^{II} = \frac{\text{relevance of reaction}}{\text{relevance of diffusion}} \tag{18}$$

Diffusion and reaction can be viewed as "sequential" processes as reactions inside the biofilm can take place only after the substrate has diffused into the biofilm so that the slower process with the larger characteristic time will limit the overall performance (Morgenroth, 2008).

$$Da^{II} = \frac{\tau_{reaction,0}}{\tau_{diffusion,mass}}$$

$$= \frac{\left(\dfrac{C_{S,0}}{k_0}\right)}{\left(\dfrac{L_F^{\,2}}{D}\right)} = \frac{C_{S,0}D}{k_0 L_F^{\,2}} \tag{19}$$

Note that for Da^{II} the slower process will dominate. Therefore, the non-dimensional number is calculated from the ratio of characteristic times (Eq. (19)) and not the ratio of the inverse of characteristic times as was the case previously (Eq. (15) and (17)). If the mass transport of substrate is slower than the reaction then the biofilm will be only partially penetrated (Da^{II} << 1) and the system will be transport limited. If Da^{II} >> 1 then transport is much faster than reaction and the biofilm is fully penetrated by the substrate.

4 Examples of characteristic times

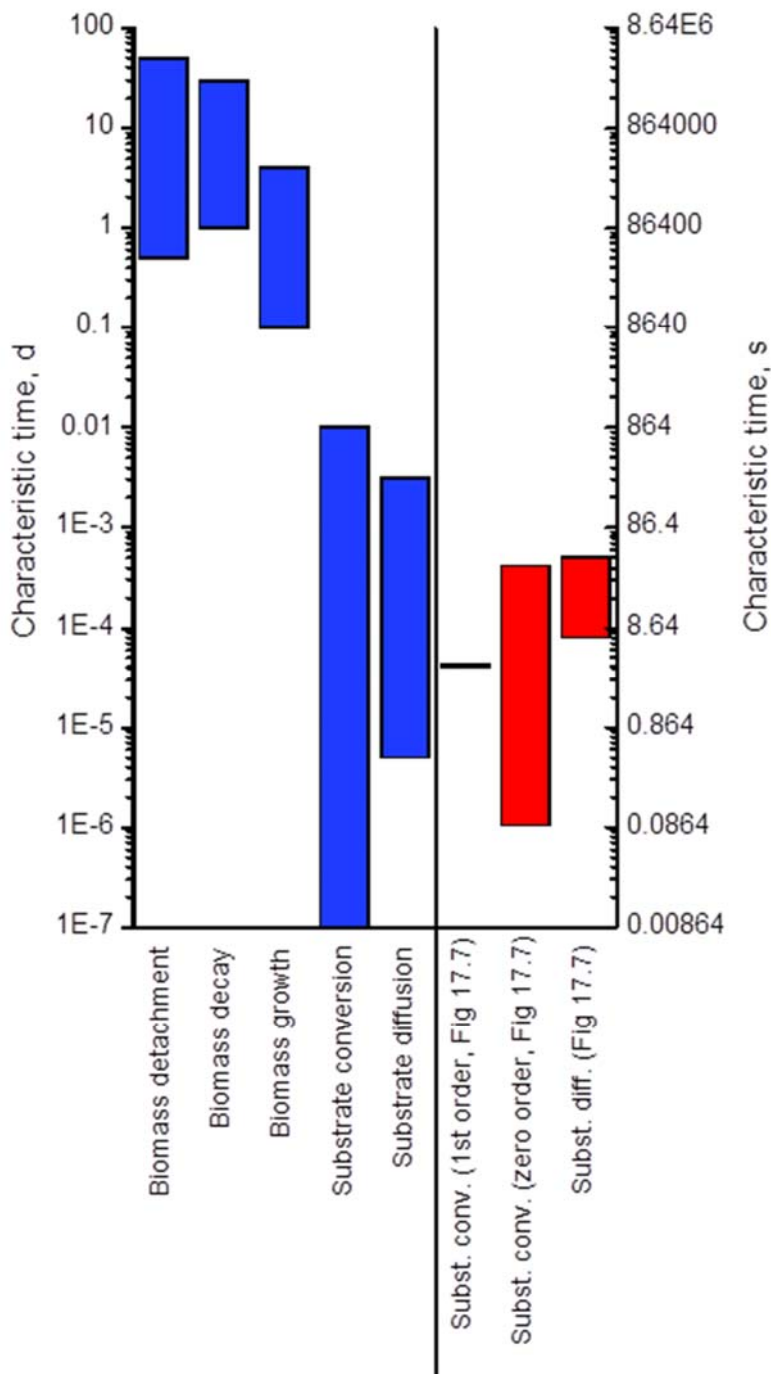Examples of characteristic times for biofilm processes are provided in Figure 4.

Figure 4. Characteristic times for biofilm processes (for details and underlying parameter values see Morgenroth, 2008).

5 References

Benjamin, M.M., Lawler, D.F., 2013. Water Quality Engineering: Physical-Chemical Treatment Processes. Wiley (available online at http://lib.myilibrary.com/Open.aspx?id=511704).

Clark, M.M., 2009. Transport modeling for environmental engineers and scientists, 2nd ed. Wiley, Hoboken.

Esener, A.A., Roels, J.A., Kossen, N.W.F., 1983. Theory and Applications of Unstructured Growth-Models - Kinetic and Energetic Aspects. Biotechnology and Bioengineering 25, (12) 2803-2841.

Gujer, W., 2008. Systems analysis for water technology. Springer-Verlag (available online at DOI:10.1007/978-3-540-77278-1 or http://link.springer.com/book/10.1007%2F978-3-540-77278-1), Berlin.

Gujer, W., Wanner, O., 1990. Modeling mixed population biofilms, in: Marshall, K.C. (Ed.), Biofilms. Wiley, New York, pp. 397-443.

Ingham, J., Dunn, I.J., Heinzle, E., Prenosil, J.E., Snape, J.B., 2007. Chemical engineering dynamics an introduction to modelling and computer simulation, 3rd compl. rev. ed. Wiley-VCH, Weinheim.

Kissel, J.C., McCarty, P.L., Street, R.L., 1984. Numerical simulation of mixed-culture biofilm. Journal of Environmental Engineering-ASCE 110, (2) 393-411.

Morgenroth, E., 2008. Modelling Biofilms, in: Henze, M., van Loosdrecht, M.C.M., Ekama, G., Brdjanovic, D. (Eds.), Biological Wastewater Treatment - Principles, Modelling, and Design. IWA Publishing, London.

Picioreanu, C., van Loosdrecht, M.C.M., Heijnen, J.J., 2000. Effect of diffusive and convective substrate transport on biofilm structure formation: A two-dimensional modeling study. Biotechnology and Bioengineering 69, (5) 504-515.

Roels, J.A., 1982. Mathematical-Models and the Design of Biochemical Reactors. Journal Of Chemical Technology And Biotechnology 32, (1) 59-72.

Wanner, O., Eberl, H.J., Morgenroth, E., Noguera, D.R., Picioreanu, C., Rittmann, B.E., van Loosdrecht, M.C.M., 2006. Mathematical Modeling of Biofilms. IWA Publishing, London, UK.