About Travel Times and related quantities

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Introduction and definitions

This is to look for a unification of concepts developed in theory. Our reference work is (hyd) however, this matter has been developed since the sixties in Chemical engineering. Notably, here, we want to bridge (Nauman, 1969) to recent work which milestone can be considered (Botter et al., 2011). Let's start with definitions:

- V is the control volume which we are analysing
- t is the clock time, or simply the time (as measured by a clock) which in (Nauman, 1969) is called θ
- Particles are injected into the the control volume at time t_{in}
- and exit the control volume at time t_{ex}, called the *exit time*
- Either t_{in} and t_{ex} can be random variables.
- Throughout the paper will be always assumed that $t_{in} \leq t \leq t_{ex}$
- $T := t_{ex} - t_{in}$ is called *travel time* of the particles
- If we take a snapshot of the control volume at time t particles in the volume will have a *residence time* $T_r := t - t_{in}$

Therefore, after these definitions, we have two distinct distribution to care of: the distribution of travel times and the distribution of residence times. Notably, if we collect outgoing particles at the boundary of the control volume, i.e. the discharge (or evapotranspiration that we neglect here for simplicity), and we have their injection time distribution, for them $t_{ex} = t$ and we are measuring their travel time.

The definition of residence times opens also to a new definition. Particles inside the control volume can have a

- *life expectancy:* $T_e := t_{ex} - t$, a random variable which will also have a distribution.
- Let D be the discharge.

Let's assume then that we can label each particle with its injection time and exit time (because eventually we found a way to forecast future). We can define then, relative to the control volume, the quantity:

- $v(t, t_{in}, t_{ex})$ being the volume of particles inside the control volume

We can normalize it over the total volume V to obtain:

- $p(t_{in}, t_{ex}|t) := v(t, t_{in}, t_{ex})/V(t)$ that, assumed that injection time and exit time are random variables is their joint probability conditional to the clock time

Based on the above probability, we can define the marginals:

- the probability of life expectancy:

$p(t_{ex}|t) \equiv p(t_{ex}-t|t) := \int_{-\infty}^{\infty} p(t_{in}, t_{ex}|t)dt_{in}$

- the probability of residence time:

$p(t_{in}|t) \equiv p(t-t_{in}|t) := \int_{-\infty}^{\infty} p(t_{in}, t_{ex}|t)dt_{ex}$

The two probabilities above are clearly different (also in form) and we do not use further subscripts to say that, since it is clear from the argument (two diverse variables)

- "the fraction of material entering the reactor (control volume) at time t which will remain in the reactor for a duration greater than t' " (citation from Neuman paper) can be then expressed as an integral over the first of the above probabilities:

$$R(t,t') = \int_{t+t'}^{\infty} p(t_{in}=t, t_{ex}|t)dt_{ex} \tag{1}$$

At the same time, "the fraction of material leaving the reactor at time t which remained in the reactor for a duration greater than t', i.e. the fraction of material leaving at time t which entered before $t-t'$" can be expressed as:

$$S(t,t') = \int_{-\infty}^{t-t'} p(t_{in}, t_{ex}=t|t)dt_{in} \tag{2}$$

R(t,t')

Further insight on R and S functions can be derived arguing again on their definition in (1) and (2). For what regards R,

we can observe that , by definition,

$$p(t_{in}=t, t_{ex}|t) = \frac{v(t, t_{in}=t, t_{ex})}{F(t=t_{in})} \tag{3}$$

Volume v, said in words is: the volume at time t that entered at time t and will exit at time t_{ex}. Once integrated over all t_{ex}, this is actually the the definition of the feeding $F\left(t=t_{in}\right)$ to the reactor, the input to the control volume. Therefore we can write:

$$p(t_{in}=t, t_{ex}|t_{in}) = \frac{v(t, t_{in}=t, t_{ex})}{F(t_{in})} = \frac{q(t=t_{in}, t_{ex})}{F(t_{in})} \tag{4}$$

where we denoted

- $q\left(t_{in}, t_{ex}\right)$ as the input to the system at time $t_{in}=t$ and will exit at time t_{ex}.

Please, notice the double role of such a function: integrated over t_{ex} it gives the input at t_{in}.

$$F(t_{in}) = \int_{t_{in}}^{\infty} q(t_{in}, t_{ex}) dt_{ex} \tag{5}$$

Rigon et al 2016, would suggest to define a probability density function as:

- $p\ _{ex}(t_{ex}|t_{in} = t) := \frac{q(t_{in}=t, t_{ex})}{F(t_{in}=t)}$ representing the probability that a quantity of water entered at time t_{in} will exit at time t_{ex}

and relabeling t_{ex}as t (and dropping, necessarily, $t = t_{in}$, letting t_{in}), it is easy to recognize that this is the so called forward in time distribution (or response time distribution) . Therefore

$$p(t_{in} = t, t_{ex}|t_{in}) = p(t_{ex}|t_{in} = t) \leftrightarrow p_{ex}(t|t_{in}) \tag{6}$$

where $\leftrightarrow$ means relabeling of the independent variable. By definition, see equation (4):

$$D(t) = \int_{-\infty}^{t} p_{ex}(t|t_{in}) F(t_{in}) dt_{in} \tag{7}$$

where the substitution $t_{ex} \to t$ has been made, as it is usual when talking about discharge. An expression for R, alternative to (1) is then:

$$R(t = t_{in}, t') = \int_{t+t'}^{\infty} p_{ex}(t_{ex}|t = t_{in}) dt_{ex} \tag{8}$$

which implies:

$$R(t, t') \equiv P[T_{ex} > t'|t] \tag{9}$$

i.e., R is the probability that life expectancy is larger than t' conditional to the clock time, t. Accordingly, the mean Nauman is estimating in his equation (6) is the mean life expectancy. In the new notation, it reads:

$$t_e(t = t_{in}) = \int_{t}^{\infty} (t_{ex} - t)\, p_{ex}(t_{ex}|t_{in}) dt_{ex} \tag{10}$$

Interestingly, life expectancy results as expressed by the forward probability distribution function, the one which, under simplifications was used since the 1930s of the las century to express, in hydrology, the instantaneous unit hydrograph (IUH). In this case, however, the IUH was usually taken as time-invariant, and (11) represents its generalisation. For those who miss it, R is know just if we make strong assumptions about the future. It is clear in fact, that we should know all the inputs still to come to get constructively the forward probability. Otherwise, the approach followed in the past was to assume a form of p_{ex} directly, as chosen from one of the known distribution function families, and verify a-posteriore its fitting to data.

S(t,t')

The function $q\left(t_{in}, t_{ex}\right)$, integrated over t_{in}, it gives all the discharge at t_{ex}:

$$D(t_{ex}) = \int_{-\infty}^{t_{ex}} q(t_{in}, t_{ex}) dt_{in} \tag{11}$$

For $S\left(t, t'\right)$ we will follow the same path used for $R\left(t, t'\right)$. Therefore, starting from definition:

$$p(t_{in}, t_{ex} = t|t) = \frac{v(t, t_{in}, t_{ex} = t)}{D(t = t_{ex})} \tag{12}$$

Volume v, in this case , is the volume injected inside the control volume at time t_{in} which at time t is exiting. It is arguably easy to understand that:

$$v(t, t_{in}, t_{ex} = t) \equiv q(t_{in}, t) \tag{13}$$

and it equals the part of discharge at time $t = t_{ex}$ which was injected in the system at time t_{in}.

As in the previous case of R, it is possible to define:

$$p_{in}(t_{in}|t) = p(t_{in}, t_{ex} = t|t) := \frac{v(t, t_{in}, t_{ex} = t)}{D(t = t_{ex})} = \frac{q(t_{in}, t)}{D(t = t_{ex})} \tag{14}$$

Therefore it is also:

$$S(t, t') \equiv P[T > t'|t] = \int_{-\infty}^{t-t'} p_{in}(t_{in}|t) dt_{in} \tag{15}$$

$S\left(t, t'\right)$ is then the probability that the travel time T is larger than t'.

The mean travel time is then obtained from:

$$t_l = t - \int_{-\infty}^{t} t_{in} p_{in}(t_{in}|t) dt_{in} \tag{16}$$

Please observe that $p_{in}(t_{in}|t)$ is a so called backward probability, since it does not depend upon any future time. It can be constructed by available information about inputs and discharges only assuming to know everything necessary since $t = -\infty$. This is obviously wishful thinking, because we have usually knowledge of the past up to some initial time t_0 and not before.

Niemi's identity

Niemi's relation follows equating results from equation (4) and (14)

$$p_{ex}(t_{ex}|t_{in}) F(t_{in}) = q(t_{in}, t_{ex}) = p_{in}(t_{in}|t_{ex}) D(t_{ex}) \tag{17}$$

though in literature t_{ex} is usually labeled as t.

Summary of probabilities

In our analysis we encountered several different probabilities of which we try a list here:

- $p(t_{in}, t_{ex}|t) := v(t, t_{in}, t_{ex})/V(t)$: the joint residence time and life expectancy probability of particles in reactor conditional to clock time, t
- $p(t_{ex}|t) \equiv p(t_{ex} - t|t)$: the probability of life expectancy of particle inside the reactor (a snapshot of expected particle lives) conditional to clock time.
- $p(t_{in}|t) \equiv p(t - t_{in}|t)$: the probability of residence time of particle inside the reactor (a snapshot of particles ages) conditional to clock time.
- $p_{ex}(t|t_{in})$: the probability of response times (i.e. probability of exit times), i.e. a certain restriction of the joint residence times probability, conditional to injection time.
- $p_{in}(t_{in}|t)$: the travel time probability, also a restriction on the travel time probabilities (p_Q in Rigon et al., 2016), conditional to clock time (which, in this case, is equal to exit times).

It is evident that all of these probabilities derive from the joint one, but under different operations. Niemi's identity relates p_{ex} and p_{in} .

One interesting goal is to find also a relation, for instance, between $p_{ex}\,(t|t_{in})$ and $p(t_{ex}|t_{in})$ (and correspondingly between $p_{in}(t_{in}|t)$ and $p(t_{in}|t)$). In Botter et al., 2011, this relation is set to be a function $\omega(t, t_{in})$ for which:

$$p(t_{in}|t) = \omega(t, t_{in}) p_{in}(t_{in}|t) \tag{18}$$

this function was named StorAge Selection function (SAS).

In many physical cases, t_{in} and/or t_{ex} are not random variables and therefore, it could be improper to talk about probabilities. However, using this nomenclature is still efficient and bringing immediate understanding of the properties of the functions. So we will maintain it also in those cases, instead of talking about fractions.

Determination of $R\,(t, t')$

Understood the relation between R and S functions and probabilities, Rigon at al., 2016 can be used to find the one to one correspondence they have with the mass budget. According to Nauman's notation, the global continuity equation is expressed as:

$$\frac{dV(t)}{dt} = F(t) - D(t) \tag{19}$$

From this the mass budget is obtained by multiplying all the terms by the particle density, $\rho \equiv M(t)/V(t)$ which is assumed constant. Then:

$$\frac{dM(t)}{dt} = M_{t_{in}} \delta(t - t_{in}) - M(t)D(t)/V(t) \tag{20}$$

where, it was further assumed that the input mass was an impulse at t_{in} . This equation can be formally solved in:

$$M(t) = M_{t_{in}} e^{-\int_{t_{in}}^{t} D(x)/V(x)dx} \tag{21}$$

which was written as in Neuman, 1969. Now two observations can be made:

- Eq (13) notation is not fully explicative, since it does not explicitly explain that it refers to an unitary impulse at time t_{in}. It should be better written as:

$$\frac{dM(t,t_{in})}{dt} = M_{t_{in}}\delta(t-t_{in}) - M(t,t_{in})q(t_{in},t)/v(t,t_{in}) \tag{22}$$

- This form, changed the notation and once divided by the particle density, is one of the set of age-ranked functions, formally equivalent to equation (9)in Rigon et al 2016. Therefore, the above (14) can be written in term of age-ranked functions as:

$$M(t,t_{in}) = M_{t_{in}} e^{-\int_{t_{in}}^{t} q(t_{in},x)/v(x,t_{in})dx} \tag{23}$$

Notationally, in Rigon et al 2016, all these functions were written with lowercase quantities. It can be argued that also the following equality holds:

$$P[T_{ex} > t' = t - t_{in}|t] = R(t, \underbrace{t-t_{in}}_{t'}) = \frac{M(t,t_{in})}{M_{t_{in}}} = e^{-\int_{t_{in}}^{t} q(t_{in},x)/v(x,t_{in})dx} \tag{24}$$

because it is just the (mass) "fraction of the molecules entering at time t_{in} which remain in the system at time $t_{in} \leq t \leq t_{ex}$" (cit. Nauman with appropriate notations modifications) and, therefore, by definition, the particles having life expectancy greater than t':

$$f(t,t') = p(t',t|t) = p_{ex}(t|t_{in}) = -\frac{dR(t,t')}{dt} = -\frac{dP[T_{ex} > t'|t]}{dt} = \frac{q(t,t_{in})}{v(t,t_{in})} e^{-\int_{t_{in}}^{t} q(x,t_{in})/v(x,t_{in})dx} \tag{25}$$

Observing the definition of $p_{in}(t_{in}|t)$, (24) can be written as:

$$p_{ex}(t|t_{in}) = \frac{q(t,t_{in})}{v(t,t_{in})} e^{-\int_{t_{in}}^{t} q(x,t_{in})/v(x,t_{in})dx} = p_{in}(t_{in}|t)\left[\frac{D(t)}{v(t,t_{in})} e^{-\int_{t_{in}}^{t} q(t_{in},x)/v(x,t_{in})dx}\right] \tag{26}$$

Comparing (26) with Niemi's identity, it follows:

$$F(t_{in}) = v(t,t_{in}) e^{\int_{t_{in}}^{t} q(t_{in},x)/v(x,t_{in})dx} \tag{27}$$

Which is a form of (24) expressed as a function of volumetric quantities.

Determination of $S(t, t')$

To be revised

Paraphrasing Neuman 1969. Suppose that a tracer stream is injected at the reactor inlet starting at time t_{in}. For $t > t_{in}$, let the concentration at the inlet be C_0. The concentration within the reactor is given by:

$$\frac{dV(t)C(t)}{dt} = F(t)C_0(t) - D(t)C(t) \tag{28}$$

with $C(t_{in}) = 0$ and $C_0(t) := \frac{F_s(t)}{F(t)}$being the volumetric concentration of the solute in input, if F_s(t) is the input of solute. The same arguments apply to $C(t) := \frac{V_s(t)}{V(t)}$being the concentration of solute in output. After using the continuity equation for the solvent represented by equation (12), (23) results in:

$$\frac{dC(t)}{dt} = \frac{F(t)}{V(t)}[C_0(t) - C(t)] \tag{29}$$

NOTE: In the following there is some ambiguity upon which I have to reflect a little. We are going to do the hypothesis of an instantaneous release of solute, this in order to obtain back Newman results. This does not automatically implies that the solvent is released just instantaneously which would require, $F(t) \rightarrow F(t, t_{in}) = M_0\delta(t - t_{in})$. I have certainly to compare the result below with what obtained in Rigon et al., 2016 (section 10) and (Duffy, 2010) to clarify all the issues. Please note that in Rigon et al., 2016, we did not fully exploited the concentration equation simplification (as Duffy 2010 does and we are required to do also here below) using the continuity equation (we did consciously for not adding further equation to the 104 ones already present) .

Assuming that we have an instantaneous input of both solvent and solute, i.e. $C_0(t) = C_0\delta(t - t_{in})$, then the

equation can be written:

$$\frac{dC(t, t_{in})}{dt} = \frac{F(t, t_{in})}{V(t, t_{in})}[C_0\delta(t - t_{in}) - C(t, t_{in})] \tag{30}$$

and solution is:

$$C(t, t_{in}) = C_0\left(1 - e^{-\int_{t_{in}}^{t} F(x,t_{in})/V(x,t_{in})dx}\right) \tag{31}$$

Accordingly, it can be seen that,

$$S(t, t') = 1 - C(t, t_{in})/C_0 = e^{-\int_{t_{in}}^{t} F(x,t_{in})/V(x,t_{in})dx} \tag{32}$$

because the second member is the fraction of the material in the exit stream at time t which has remained in the reactor for a duration greater than $t' = t - t_{in}$. Besides:

$$p(t', t|t) = g(t, t') = \frac{F(t, t_{in})}{V(t, t_{in})}e^{-\int_{t_{in}}^{t} \frac{F(x,t_{in})}{V(x,t_{in})}dx} \tag{33}$$

Some general properties (i.e. relations between $S\left(t,t'\right)$ *and* $R\left(t,t'\right)$)

NOTE: at present, I am just rewriting what Neman did with a minimum of change in notation to keep more easily track of the various times involved.

As Nauman says, "Expressions relating the function R and S can be easily obtained" from the continuity equation (12). We get in fact from (12):

$$D(t)dt - F(t)dt = dV \tag{34}$$

For which, after dividing for $V\left(t\right)$ and subsequent integration between $[t_{in},t]$ gives:

$$-\int_{t_{in}}^{t} \frac{D(t)}{V(t)} = -\int_{t_{in}}^{t} \frac{F(t)}{V(t)}dt + \int_{t_{in}}^{t} \frac{dV(t)}{dt}dt = \log\frac{V(t)}{V(t_{in})} - \int_{t_{in}}^{t} \frac{F(t)}{V(t)}dt \tag{35}$$

Taking the exponential of the leftmost member and rightmost member, we have, after equations (17) and (27):

$$R(t,\underbrace{t-t_{in}}_{t'}) = \frac{V(t)}{V(t_{in})}S(t,\underbrace{t-t_{in}}_{t'}) \tag{36}$$

or:

$$R(t,\underbrace{t-t_{in}}_{t'})V(t_{in}) = V(t)S(t,\underbrace{t-t_{in}}_{t'}) \tag{37}$$

which is consistent with equation (9) if V(tin)=F(tin) and V(t)=D(t)

Not sure to have done thing carefully here above. Because, I've kind of lost the different meaning of the t' which, in one case in the life expectancy, in the other, the travel time. I have to re-check above.

References

HESS - Abstract - Age-ranked hydrological budgets and a travel time description of catchment hydrology. https://www.hydrol-earth-syst-sci.net/20/4929/2016/. URL https://www.hydrol-earth-syst-sci.net/20/4929/2016/. Accessed on Thu, April 26, 2018.

Gianluca Botter, Enrico Bertuzzo, and Andrea Rinaldo. Catchment residence and travel time distributions: The master equation. *Geophysical Research Letters*, 38(11):n/a–n/a, jun 2011. doi: 10.1029/2011gl047666. URL https://doi.org/10.1029%2F2011gl047666.

Christopher J. Duffy. Dynamical modelling of concentration-age-discharge in watersheds. *Hydrological Processes*, 24(12):1711–1718, may 2010. doi: 10.1002/hyp.7691. URL https://doi.org/10.1002%2Fhyp.7691.

E.B. Nauman. Residence time distribution theory for unsteady stirred tank reactors. *Chemical Engineering Science*, 24(9):1461–1470, sep 1969. doi: 10.1016/0009-2509(69)85074-8. URL https://doi.org/10.1016%2F0009-2509%2869%2985074-8.