

Tracers and Timescales: Tools for Distilling and Simplifying Complex Fluid Mechanical Problems

Lisa V. Lucas ^{1,*}  and Eric Deleersnijder ² 

¹ Integrated Modeling and Prediction Division, Water Mission Area, U.S. Geological Survey, 345 Middlefield Road, MS #496, Menlo Park, CA 94025, USA

² Institute of Mechanics, Materials and Civil Engineering (IMMC) & Earth and Life Institute (ELI), Université Catholique de Louvain, Bte L4.05.02, Avenue Georges Lemaître 4, 1348 Louvain-la-Neuve, Belgium; eric.deleersnijder@uclouvain.be

* Correspondence: llucas@usgs.gov; Tel.: +1-650-329-4588

1. Introduction

The last several decades have seen significant advances in fluid–mechanical, water–quality, and ecological observation systems, as well as in related scientific computing capabilities. These leaps forward have provided an increasingly detailed view of fluid flow and reactive transport in natural and engineered systems, thus enriching our process of understanding and improving (1) science-based resource management, (2) the design of anthropogenic structures, (3) the interpretation of field- and laboratory-scale phenomena, and (4) predictive capacity. The benefits of these advancements are easily apparent if one considers (as just a few examples):

- The ability to observe turbulent transport at scales of centimeters and seconds, enabling the more accurate characterization of oxygen, nutrient, carbon, contaminant, or other scalar fluxes through the water column;
- The capacity to model whole or multiple connected aquatic systems in multiple dimensions at a spatial resolution of tens to hundreds of meters and timesteps of seconds to minutes, helping us understand how riverine, oceanic, and atmospheric drivers influence constituent transport or habitat connectivity (e.g., [1–3]);
- The capability to remotely track hundreds of physical drifters across hundreds of kilometers and over timescales of days, revealing complex Lagrangian transport patterns not discernible from moored (Eulerian) sensor measurements ([4]).

Thus, the current technological capacity in environmental fluid mechanics and hydraulic engineering is, clearly, impressive. However, so is the massive amount of generated data requiring processing and analysis in order to transform it into useful information [5]. Furthermore, this intensive data-generating capacity enriches our awareness and understanding of individual processes operating over a broad range of spatial and temporal scales, but the net effect—the “upshot”—of those processes and their interactions may be challenging to identify. Techniques for distilling, simplifying, and extracting the essence from large, complex environmental datasets have arguably never been more necessary [5–7].

It is in this realm—the extraction of meaningful information—where tracers and timescales shine. Both are tools that can paint a simplified, digestible (yet quantitative; [6]) picture of a large number of reactive transport processes that co-exist and interact in aquatic environments. These techniques thereby help us understand and interpret those processes, identifying the most crucial ones and establishing causal relationships between them [6,7]. The contributions to this Special Issue relate to one or both of these commonly related tools, providing new methodologies, applications, or reviews of tracers or timescales in fluid mechanics.

So, what precisely are “timescales” and “tracers”, as discussed in this Special Issue? A timescale is a diagnostic parameter that communicates approximately how long a process



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takes [8]. A timescale can be defined for any process, be it physical, biological, chemical, or radiological but, because all timescales carry the same units (time), they serve as a common currency [9], allowing disparate processes to be directly compared and easily integrated. Timescales have several other virtues, including the ability to encapsulate spatial, temporal, and multi-process complexity into a single number (for example, the use of a “residence time” to capture the net effect of all transport processes operating on a transported substance (e.g., [8,10]). One might consider this timescale role as that of an integration tool. Depending on how they are estimated, though, timescales may also be devised to deconstruct a complex problem, separating key processes and assessing their relative overall contributions to observed or modeled outcomes. Importantly, timescales may also help in building simplified reactive transport models, which may be regarded as a form of model reduction (i.e., replacing a model containing many variables or parameters with a model containing far fewer variables/parameters that are deemed to be satisfactory indicators of the state of the system; [11]).

A tracer, on the other hand, is a distinguishable dye or chemical compound that is added to a fluid system [12] and is used to learn something about the physical, biological, or chemical functioning of that system. Tracers may be natural or anthropogenic, and can be introduced either intentionally, accidentally, or without any human intervention. They are used in field, laboratory, and numerical studies of aquatic habitats and, as such, may be real or virtual. As discussed in the tracer-related papers within this Issue, there are some scientific questions for which conservative (i.e., inert, non-reactive) tracers present the ideal tool, whereas in other situations, reactive (or both types of) tracers are needed.

What do tracers and diagnostic timescales have to do with each other, and why does this Special Issue incorporate papers from both realms? First, tracers and timescales are both useful diagnostic tools that can help us understand, visualize, and quantify the net effect of one or multiple interacting processes. Both tools can therefore aid us in answering practical questions, such as:

1. To where will a particle travel if it is released at Point A and Time t in a fluid body?
2. How much time will be required for a particle to travel from Point A to Point B?
3. Will the travel time between Points A and B be sufficient to allow for any particle reactions to run to completion?
4. How long will a particle or collection of particles remain within a defined fluid environment?

Second, tracers are often implemented to mark a water “mass” or “type”, such as that originating in a specific region or released into the domain from a point or boundary source. As such, tracers frequently form a basis for the estimation of characteristic timescales, whether experimentally (e.g., [13]) or numerically [14]. For example, a number of the papers in this Special Issue describe studies in which transport timescales such as age, residence time, and exposure time are computed from the solution of partial differential problems (“PDPs”, which include partial differential equations plus initial and boundary conditions). These PDPs describe the evolution of numerical tracers and tracer-like quantities, including tagged water types or masses, which are treated as passive tracers (e.g., [2,15–17]).

This Special Issue includes papers relevant to a variety of fluid–mechanical domains: idealized model environments, seas, gulfs, estuaries, human-made impoundments, lakes, deltas, river networks, reservoirs, marinas, and other hydrogeologic environments. Below, we provide an integrative summary of the contributions in this Special Issue, following the imperfect delineation between papers focused on tracers and those focused on timescales, acknowledging that there is overlap for the reasons mentioned above. We also attempt to identify key remaining gaps in general understanding or capability and areas ripe for future work.

2. Tracer-Focused Contributions

Two papers in this volume provide useful reviews of different classes of tracers implemented in physical experiments. Cao et al. [12] delineate tracer types at the highest

level based on the degree of interaction with the aquatic system to which they are added, with: (1) “conservative” tracers displaying virtually no interaction with materials within the system, thus behaving as inert substances under the conditions characteristic of that system and flowing passively with the fluid, and (2) “reactive” tracers defined as “compounds that undergo a chemical reaction or physicochemical interaction processes in a predictable way.” Those authors explain that conservative tracers are typically used to assess physical transport processes or hydromechanical properties such as porosity, whereas reactive tracers—which are used in tandem with conservative tracers—can provide information on physicochemical properties such as sorption capacity, redox condition, or microbial activity [12]. While conservative tracer compounds have been the subject of other reviews, Cao et al. [12] note that there had not previously been a systematic review of reactive tracers—a need which they fill herein, with an emphasis on subsurface and hyporheic processes. Those authors then discuss in detail the properties, behaviors, and potential applications of three major subgroups of reactive tracers: (A) partitioning tracers (whose breakthrough curves display a retardation—or time shift—relative to conservative tracers), (B) kinetic tracers (which experience degradation but no retardation), and (C) hybrid tracers (which experience both retardation and degradation). Cao et al. [12] emphasize that the selection of an optimal tracer compound for a given purpose is a complex “art” and describe a general approach for designing and creating tracers tailored for specific applications.

Bailly du Bois et al. [1] review a different class of tracers: dissolved anthropogenic radionuclides (or “artificial radiotracers”), which may be inadvertently or intentionally discharged into ocean waters and emanate from atmospheric nuclear tests, nuclear fuel reprocessing plants, or nuclear power plants (e.g., Chernobyl, Fukushima Daiichi). Regardless of how such tracers are introduced into the aquatic environment, these authors demonstrate the valuable role that dissolved radionuclides can play as oceanographic tools. Bailly du Bois et al. [1] present an extensive, updated dataset of in situ radionuclide (e.g., ^3H , ^{137}Cs , ^{134}Cs , ^{125}Sb) measurements collected between 1982 and 2016 aboard 80 oceanographic campaigns across the English Channel, Bay of Biscay, Celtic Sea, Irish Sea, and the North Sea. With a focus on the measured tracers behaving most conservatively in seawater (^3H and ^{125}Sb), the authors describe useful applications of radiotracer data for illuminating physical transport processes and pathways and for validating hydrodynamic models. Additionally, they describe how measured tracers could be used to deduce percentages of water masses originating in different regions, construct radionuclide inventories, ascertain transport timescales, or assess seawater–sediment or seawater–organism exchange. The many applications demonstrated in this paper could be relevant to other parts of the globe receiving inputs of radionuclides, such as the Gulf of Mexico and the Mediterranean, Arctic, China, and Arabian Seas, all of which are within reach of nuclear power plants [1].

Other tracer-focused papers in this issue assess or advance methodologies for measuring or modeling tracers or tracer-like quantities. For example, Staneva et al. [18] investigate processes influencing particle transport by comparing different ocean-modeling approaches to observed paths of physical drifters in the North Sea. Specifically, those authors compare particle tracks computed with a stand-alone ocean circulation model to those computed with the same ocean circulation model coupled with a wave model, examining the fidelity of each model set-up to observed drifter trajectories, as well as high-frequency radar-based observations of current velocity. It is shown that wave-induced drift significantly influences particle transport in the upper layers of the ocean. This work demonstrates that the coupling of circulation models to wave models may greatly improve simulations of the transport of marine litter, oil, larvae, or other biological materials.

So et al. [19] tackle the ongoing challenge of improving measurements of turbulent tracer transport. They note that (1) “most fluid motions in nature and engineering are turbulent”, and (2) estimates of tracer transport under turbulent conditions in shallow waters can be contaminated by wave action. As So et al. [19] explain, observations of turbulence properties may be confounded by velocity fluctuations that include orbital

velocities generated by waves, potentially leading to tracer transport overestimates by one or more orders of magnitude. Therein lies their motivation to improve available methods for eliminating the wave-induced contamination of ADCP (Acoustic Doppler Current Profiler) measurements. The authors propose a new method—the Harmonic Analysis or “HA” method—and demonstrate that it performs better than a previously introduced approach under conditions with energetic surface gravity waves, potentially leading to more accurate estimates of tracer flux in shallow coastal waters.

The intersection of tracer measurements and modeling is explored by Tomkovic et al. [3], who employ both approaches while pursuing a deeper understanding of source water provenance in a branching tidal river system. Their field-based approach focuses on the utilization of stable isotope compositions of oxygen and hydrogen in water samples to build a mixing model. Their numerical approach involves the implementation of a two-dimensional (vertically averaged) model of the study domain and its adjacent environments, allowing for the computational depiction of tracer transport through the domain. Results from the two approaches are compared and are shown to agree well with each other, with each approach providing validation of the other and providing the authors with an opportunity to evaluate the strengths and shortcomings of each. Although Tomkovic et al. [3] implement this dual-track study with the aim of supporting ecosystem restoration efforts in the Sacramento–San Joaquin Delta (California, USA), their approaches and findings can be applied in other systems as well.

3. Timescale-Focused Contributions

The review by Lucas and Deleersnijder [8] describes diagnostic timescale uses and methods of estimation, primarily in the coastal zone. Citing numerous examples from the literature, they demonstrate how timescales can improve the understanding of aquatic systems by helping us distill large datasets, compare systems across space or time, compare relative speeds of disparate processes, and build simple and tractable models. The authors reiterate what numerous others have before them: the one point of consistency in diagnostic timescale use across the aquatic sciences is the inconsistency in how (or whether) terms are defined and calculated. Different definitions and calculation methods can lead to substantially different values and represent different phenomena, so it is most constructive for all employing diagnostic timescales to choose, define, calculate, and present them with care and clarity.

Several papers in this volume provide examples of computationally derived transport timescales (e.g., water age, residence time, exposure time, and flushing time) for the purposes of supporting engineering design, guiding resource management, or strengthening the understanding of physical processes in aquatic systems. This selection of papers provides a window into a variety of approaches for implementing state-of-the-art numerical models for computing transport timescales.

For example, in their investigation of water renewal in La Rochelle Marina (France), Hugué et al. [17] implement a hydrodynamic and transport model with conservative numerical tracer and particle tracking capabilities to compute spatially variable residence, exposure, and *e*-folding flushing times, as well as return flow parameters. Timescales for several scenarios are compared in a sensitivity analysis assessing the effects of wind and spring–neap tidal phase. A particularly novel aspect of this study is the incorporation of floating structures (docks and moorings) into the modeling and assessment of the sensitivity of water renewal in the marina to the presence of those structures.

Additionally, using a 3D hydrodynamic and transport model, Liu et al. [16] employ a straightforward method utilizing pairs of conservative and decayable numerical tracers (each pair associated with a group of tributaries) to assess spatially variable water age in Taihu Lake (China). This environment is widely known for its large size, economic and ecological importance, and for its challenges with eutrophication and harmful cyanobacteria blooms. Liu et al. [16] conduct their study of water age to quantitatively investigate nutrient loads from different source regions to Taihu Lake and to understand the influence

of wind and river discharge on transport times. It is seen that age is a useful water-quality related diagnostic parameter, which may be of use for decision making at the basin scale.

Some articles in this Issue contribute to the development and use of the Constituent-oriented Age and Residence time Theory (CART, www.climate.be/cart, accessed on 25 September 2021). This conceptual toolbox provides a consistent set of partial differential equations, along with relevant initial and boundary conditions, aimed at estimating various diagnostic timescales at every time and position, chiefly the age and the residence or exposure time. These timescales may be derived for every constituent of fresh or salty water (or any other liquid mixture) or aggregates of them (i.e., groups of constituents), including the water itself.

Deleersnijder et al. [7] investigate the boundary conditions for age calculations. In CART, the mean age is computed as the ratio of the “age concentration” to the concentration of a numerical tracer. These variables are not independent, for the former is the first-order moment of the age distribution function, whilst the latter is the zeroth order moment. Therefore, the boundary conditions cannot be prescribed independently; rather, they must be consistent with each other. This paper shows how to do this and also illustrates the impact of inconsistent boundary conditions. Based on these considerations, a strategy to design meaningful age diagnoses is outlined.

Using consistent boundary conditions, Pham Van et al. [15] apply the water renewal assessment strategy of de Brye et al. [20] to the delta of the Mahakam River (Indonesia). Water renewal timescales (i.e., age, residence, and exposure times) are quite short (i.e., a few days to a couple of weeks) and crucially depend on the river discharge in spite of the large influence of tides on the hydrodynamics. The return coefficient (a measure of the propensity of water particles to re-enter the domain after leaving it for the first time) is of the order of 0.3 far away from the boundaries, suggesting that re-entering due to tides is important almost everywhere. Overall, this study illustrates how forward- and backward-looking diagnostic timescales (residence/exposure time and age, respectively) may be combined to gain insight into the water renewal processes of a river delta whose hydrodynamics are driven mostly by tides and river discharge.

In the northern San Francisco Estuary (USA), Gross et al. [14] compare water age estimated from field data (isotopic water composition) and numerical estimates derived from a thoroughly validated hydrodynamic and tracer transport model. The discrepancies, which are relatively small, are investigated in detail, suggesting avenues of improvement for both approaches. Interestingly, a new concept is introduced—namely, the mean property experienced by a tracer—which may be seen as a generalization of CART’s philosophy. This concept may be applied to non-positive-definite variables, which would have been impossible using the diagnoses based on partial differential equations developed up to now. This novelty deserves to be investigated further and, above all, put to use.

For rectangular, flat-bottomed reservoirs commonly used in urban hydraulics or river engineering, Dewals et al. [21] compute the depth-integrated, steady-state, position-dependent water age distribution function (i.e., the histogram of the water age in every water parcel). No other article in the present issue evaluates such a distribution function. It is shown that (A) simple indicators such as the ratio of domain volume to volumetric flow rate or (B) a more sophisticated diagnosis, namely the position-dependent mean water age (i.e., the mean time elapsed since entering the domain), provide insufficient information regarding the pathways of water particles in the domain. This is because particles follow both slow and fast routes from the inlet to the outlet, causing, in many instances, the age histogram to exhibit several maxima. This rather complex behavior could not have been anticipated from a simple inspection of the flow field, underscoring the need for suitably designed diagnostic timescales.

Cheng et al. [22] compute the three-dimensional, time-dependent residence time in a typical tributary bay of the reservoir of Three Gorges Dam (China). They adopt the adjoint approach of Delhez et al. [23] and perform a detailed sensitivity analysis aimed at identifying the processes that have the largest impact on the exchanges of the domain

of interest with its environment. It is shown that water-level regulation of the dam and density currents crucially influence the residence time, whereas surface wind force and river discharge are much less significant. A strengthened understanding of these issues is important because of the poor water quality in the bay under study, as in many such bays. This investigation is one of those that suggests that diagnostic timescales can provide useful pieces of information for water quality management.

Hong et al. [2] divide the upstream boundary of the Pearl River Estuary (China) into several parts. Then, the three-dimensional, time-dependent age of passive tracers emanating from those sub-regions is evaluated, and a thorough sensitivity analysis is carried out. A strong correlation between river discharge and transport time is found. The ultimate objective of this study is to contribute to an understanding of the dynamics of pollution caused by terrestrial substances. The approach of Hong et al. (2020) is based on the hypothesis that the age of passive tracers is a diagnostic tool capable of providing information relevant to the fate of numerous terrestrial substances entering the domain of interest. Similar hypotheses have guided other investigations to implement conservative tracers to gain insights into the dynamics of non-conservative substances. Validation of this hypothesis (for the Pearl River Estuary and other deltas or estuaries as well) is yet to be achieved in full and is likely to require a vast amount of dedicated research. Hong et al. (2020) thus provide novel and valuable results and, by doing so, highlight important areas for future work.

4. Conclusions

The articles of this Special Issue deal with topics related to a wide variety of domains of interest that are investigated with a wide range of approaches. Clearly, tracer and timescale methods are alive and well, with the need for such tools only expanding over time and the related methods and technologies continually advancing.

A range of timescale quantification approaches exists, with many such methods relying on tracers or tracer-like substances (e.g., particles, drifters) to characterize and track fluid movement. Similarly, a range of diagnostic timescales themselves exist, with some integrating across space and/or time (e.g., the volume/flow advective flushing time) and others defined and calculated as varying fields across one to four dimensions, such as with the CART methods [23,24].

Another classification approach distinguishes timescales by the degree of “holism” or “process richness” incorporated into them [8]. At the low end of the holism spectrum, “atomistic” timescales depict the time associated with a single process (e.g., advection, diffusion, or a reaction). Atomistic timescales can be relatively easy to estimate, often relying on simple algebraic relationships (e.g., distance/velocity), and have been used for many decades (e.g., [25–28]). These, which we might think of as “Grandma and Grandpa’s” timescales, can help assess the relative importance of individual terms of the governing equations and also form the basis for simple, process-based mathematical models [8,29]. However, more often than not, they cannot paint a satisfactory picture of the overall impact of transport and reaction processes taking place in a fluid environment. More holistic approaches are often needed.

“Holistic” timescales each represent the time associated with a collection of processes (e.g., multiple transport and/or reaction processes), producing a parameter conveying the net effect of those processes and their interplay with each other [8]. Over the past several decades, the ability to compute holistic timescales with numerical models, or quantify them in the field using drifters or tracers, has exploded—at least with respect to transport timescales. Additionally, the last ~20 years have brought increasingly sophisticated methods for doing so. The articles in this Special Issue collectively describe a smorgasbord of these new and powerful approaches, presenting new applications, innovative directions for validation, and novel extensions of what is now the established state of the art (these are not your grandparents’ timescales.) Similarly, observational approaches for characterizing and quantifying the net effect of multiple interacting

transport processes and hydraulic connectivity have experienced significant advancements and are well represented in this Issue.

Notwithstanding the exciting capabilities and continual methodological improvements demonstrated, some key questions remain:

1. Is it always necessary to use the most advanced methods? For example, is it always needed to solve PDPs to obtain tracer fields and/or timescales at every location within a fluid domain? Indeed, the most sophisticated methods are not always the best option. Such detailed information is not always necessary and, sometimes, simpler timescales are precisely what is needed, for example, to compare relative speeds of processes.
2. Are the most sophisticated methods clearly “better”? Possibly, if detailed spatial and/or temporal variations in timescales or scalar fields are needed. However, although powerful numerical approaches hold enormous potential, they also present some important limitations and critical open questions, such as:
 - Significant data requirements for driving, calibrating, and validating a complex numerical model (not to mention research-and-development resources).
 - The challenge of directly validating the new (e.g., CART- and PDP-based) methods. Diagnostic timescales cannot be directly measured in situ like salinity or temperature. Rather, in the field or laboratory, they must be deduced from other measured quantities, which will carry increased errors.
 - Remaining challenges in incorporating particle dynamics or biogeochemical reactions and transformations into models, thus limiting models from achieving 100% holism for transported reactive constituents.

How to select the most suitable holistic diagnostic approach, be it based on tracers alone, timescales closely related to tracers, or more simplistic atomistic timescales, is clearly still an open question. Additionally, in our view, the need for the full spectrum of diagnostic approaches—from the very simple to the mathematically complex and cutting edge—remains.

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