



## Using travel times to simulate multi-dimensional bioreactive transport in time-periodic flows



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### ABSTRACT

In travel-time models, the spatially explicit description of reactive transport is replaced by associating reactive-species concentrations with the travel time or groundwater age at all locations. These models have been shown adequate for reactive transport in river-bank filtration under steady-state flow conditions. Dynamic hydrological conditions, however, can lead to fluctuations of infiltration velocities, putting the validity of travel-time models into question. In transient flow, the local travel-time distributions change with time. We show that a modified version of travel-time based reactive transport models is valid if only the magnitude of the velocity fluctuates, whereas its spatial orientation remains constant. We simulate nonlinear, one-dimensional, bioreactive transport involving oxygen, nitrate, dissolved organic carbon, aerobic and denitrifying bacteria, considering periodic fluctuations of velocity. These fluctuations make the bioreactive system pulsate: The aerobic zone decreases at times of low velocity and increases at those of high velocity. For the case of diurnal fluctuations, the biomass concentrations cannot follow the hydrological fluctuations and a transition zone containing both aerobic and obligatory denitrifying bacteria is established, whereas a clear separation of the two types of bacteria prevails in the case of seasonal velocity fluctuations. We map the 1-D results to a heterogeneous, two-dimensional domain by means of the mean groundwater age for steady-state flow in both domains. The mapped results are compared to simulation results of spatially explicit, two-dimensional, advective-dispersive-bioreactive transport subject to the same relative fluctuations of velocity as in the one-dimensional model. The agreement between the mapped 1-D and the explicit 2-D results is excellent. We conclude that travel-time models of nonlinear bioreactive transport are adequate in systems of time-periodic flow if the flow direction does not change.

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### 1. Introduction

Numerical simulation is indispensable for the quantitative understanding of compounds undergoing transport and chemical transformations in the subsurface (e.g., Barry et al., 2002; MacQuarrie and Mayer, 2005; Steefel et al., 2005). The most typical approach taken is to solve the coupled, multi-dimensional advection-dispersion-reaction equations of all reactants, either as a single system of nonlinear partial differential equations, or as decoupled equations in sequential or iterative

operator-split approaches. The resulting computational effort is high, and the spatially explicit description requires hydraulic and reactive parameters as spatial fields throughout the domain. In order to reduce the computational effort and avoid the spatially explicit description of the required multi-dimensional parameter fields, travel-time based reactive transport models (hereafter denoted simply as travel-time models) may be preferred over spatially explicit Eulerian methods (e.g., Cirpka and Kitanidis, 2000; Cvetkovic et al., 1996; Cvetkovic and Dagan, 1996; Dagan and Cvetkovic, 1996; Ginn et al., 1995; Janssen et al., 2006; Kaluarachchi et al., 2000; Malmström et al., 2004; Sanz-Prat et al., 2015; Simmons et al., 1995; Yabusaki et al., 1998). While in spatially explicit models the spatial

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coordinates (together with time) are considered as independent variables, travel-time models replace space by travel time. This leads to quasi one-dimensional transport under the assumption that reaction fronts coincide with groundwater isochrones (i.e., lines of equal travel time).

The travel time,  $\tau(\mathbf{x})[T]$ , is defined as the time that a water particle resides in the domain of interest, from the entry point at the domain inlet to the point of observation  $\mathbf{x}[L]$ . There are at least four reasons why the travel time is not a unique value: (1) Pore-scale dispersion leads to a local distribution of travel time,  $p(\tau(\mathbf{x}))[T^{-1}]$  at any point within the domain even for deterministic flow fields, (2) dynamic boundary conditions or time-varying fluid and aquifer properties cause velocity variations in time, making the local travel-time distributions dependent on time, (3) sampling over a larger control plane (or considering breakthrough curves in pumping wells) in a non-uniform flow field leads to a distribution of arrival times within the observation plane, and (4) considering the uncertainty of aquifer properties using stochastic methods leads to a statistical distribution of travel time over an ensemble of aquifer realizations (e.g., Cvetkovic et al., 1992; Dagan et al., 1992; Dagan and Nguyen, 1989; Shapiro and Cvetkovic, 1988, among others). In this study, we restrict ourselves to point observations in single aquifer realizations so that only the first two causes of non-unique travel times are considered.

Travel-time models of reactive transport conceptualize a multi-dimensional transport domain as an ensemble of independent 1-D systems, i.e., stream tubes, in which the longitudinal coordinate is the associated travel time along the stream tube (e.g., Luo, 2012). As the stream tubes along different groundwater flow paths are treated as independent systems, transverse dispersion and related mixing processes cannot explicitly be considered. In stochastic-convective transport, pore-scale dispersion is neglected altogether, and typically breakthrough curves averaged over an extended control plane or an ensemble of many aquifer realizations are considered (e.g., Dagan et al., 1992; Dagan and Nguyen, 1989; Shapiro and Cvetkovic, 1988; Simmons, 1982). Stochastic-convective transport models also have a long tradition in soil science, where they are used to describe solute transport in percolating soil water (see the reviews of Feyen et al., 1998; Köhne et al., 2009). First extensions towards advective-reactive transport included linear kinetic sorption and first-order decay (Cvetkovic and Dagan, 1994; Cvetkovic and Shapiro, 1990; Selroos and Cvetkovic, 1992; Severino et al., 2012).

The extension to nonlinear reactions (stochastic convective reactive transport – SCR), including reactions between mobile and immobile phases, is straightforward in steady-state flow fields (e.g., Cvetkovic et al., 1996; Cvetkovic and Dagan, 1996; Dagan and Cvetkovic, 1996; Simmons et al., 1995): The spatial coordinates of the standard advection-reaction equation are replaced by the advective travel time (or kinematic age),  $\tau_{adv}[T]$ , and the velocity becomes unity; nonlinear multi-component reactive transport is solved in these coordinates; and the reactive-species concentrations at a point  $\mathbf{x}$  within the domain are obtained by looking up the reactive-species concentrations in the travel-time domain at the specific kinematic age  $\tau_{adv}(\mathbf{x})$  of the observation point. While closed-form expressions can be derived for comparably simple reaction laws (e.g., Ginn et al., 1995), numerical simulation of 1-D reactive transport is computationally so inexpensive that the approach is feasible also

for more complex reaction systems (e.g., Kaluarachchi et al., 2000; Malmström et al., 2004; Yabusaki et al., 1998).

A major concern with convective-reactive models is their conceptual inadequacy in describing mixing-controlled reactions (Luo and Cirpka, 2008, 2011). In the stochastic-convective framework a distribution of travel times, observed over a larger control plane, is interpreted as the result of many non-interacting stream tubes being mixed upon the observation rather than within the domain. To predict reactive-species concentrations, the advection-reaction equation is solved in the travel-time domain, the resulting concentrations are weighted by the probability density of a certain kinematic age to occur within the control plane and integrated over all advective travel times. By construction, this approach cannot handle reactions that are controlled by dispersive solute mixing within the domain. In reactive-transport applications that don't require dispersive mixing, the SCR models perform much better than models in which "macrodispersive" spreading is introduced into macroscale advective-dispersive-reactive transport (Molz and Widdowson, 1988). In order to handle mixing-controlled reactions in travel-time models, Cirpka and Kitanidis (2000) developed the advective-dispersive stream-tube model (ADS), which parametrizes the effects of local transverse dispersion on macroscopic longitudinal mixing by an increasing within-stream-tube dispersion coefficient and handles the variability of the mean groundwater age within a control plane by a stochastic description. Intra-streamtube mixing was also accounted for in other stream-tube models (e.g., Ginn, 2001; Ginn et al., 2001).

In a preceding study, we analyzed which error is introduced by the mapping of reactive-species concentrations from the travel-time domain to the spatial domain using the mean groundwater age assuming advective-dispersive transport in a heterogeneous domain (Sanz-Prat et al., 2015). The application involved oxygen, nitrate, dissolved organic carbon as dissolved species as well as aerobic and denitrifying bacteria as immobile species. All dissolved compounds were introduced jointly into the domain; the concentration in the inflow were spatially uniform; reactive parameters did not vary within the domain; and flow was at steady state. We found that the spatial concentration distributions of all compounds organized themselves in zones that are essentially aligned with isochrones: A water parcel carrying a certain chemical signature kinetically interacts with the immobile phases, which in turn are modified by the reactions. We could predict local reactive-species concentrations quite accurately from the mean groundwater age at that location combined with one-dimensional simulations of the same reactive-transport problem by mapping the 1-D results to the 2-D domain according to the mean travel time. The mapping performed best with an advective-dispersive-reactive 1-D model in which the longitudinal mixing coefficient increased with distance, which was calibrated by the relationship between second-central and first temporal moments in the 2-D simulations. However, mapping by the kinematic age, which is conceptually much simpler, did not introduce a large error.

The assumption of steady-state flow, made in the preceding study, is crucial and not very realistic in many situations. An exemplary zone with intensive natural biogeochemical cycling is the surface-water/groundwater interface, where infiltrating river water gets in contact with microbial biomass in the river sediments. These transition zones are known to be dynamic with

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