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A class of compartmental models for long-distance tracer transport in plants

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HIGHLIGHTS

- Systematic comparison of models regarding quality of fit to tracer transport data.
- Model class allows construction of numerous models with adjustable complexity.
- A designated model filter removes irrelevant and redundant models.
- Different optimal models were found for exemplary data sets.

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ABSTRACT

Studies of long-distance tracer transport in plants result in spatio-temporal data sets. Compartmental tracer transport models can be used to quantitatively characterize or compare such data sets derived from different experiments. Depending on the specific experimental situation it might be necessary to apply different models. Here, we present a general class of compartmental tracer transport models which allows a systematic comparison of different models regarding the quality of fitting to the experimental data. This model class is defined by a system of partial differential equations (PDEs) for an arbitrary number of parallel compartments with individual transport velocities and numerous lateral exchange connections. A large number of model instances with adjustable complexity can be derived from this model class by permitting only certain model parameters such as flux velocities or exchange rates between compartments to be non-zero. Since some of these models are either inconsistent or redundant we designed a model filter using combinatory rules in order to keep only valid and unique models. A numerical solver for the PDEs was implemented using finite volumes and a weighted essentially non-oscillatory (WENO) scheme. Several candidate models were fitted to experimental data using a Monte Carlo multi-start strategy to approximate the global optimum within a certain parameter space. Analysis of exemplary tracer transport experiments on sugar beet, radish and maize root resulted in different best models depending on the respective data and the required fit quality.

1. Introduction

In a recent publication we presented a mechanistic model for long distance tracer transport in plants including an analytic solution of the respective partial differential equations (PDEs) (Bühler et al., 2011). Fitting such a model to data sets from tracer studies (measured e.g. with positron emission tomography, PET, or magnetic resonance imaging, MRI) results in model parameter estimates which characterize the dynamical behavior of the tracer and can be used for quantitative comparison of different data sets, e.g. from plant phenotyping studies (Fiorani and Schurr, 2013). For a recent application of this method, see De Schepper et al. (2013). The model used in Bühler et al. (2011) was chosen on the basis of physiological considerations and consisted of three neighboring compartments roughly representing the main functions of vascular transport pathways (e.g. phloem or xylem) and the adjacent tissues. These functions include: (1) axial transport of tracer, simulated by a plug flow in the first compartment, (2) reversible lateral exchange of tracer between the first and second compartment, (3) storage of tracer in the third compartment, and (4) diffusion in axial direction within the first two compartments, see Fig. 1 in Bühler et al. (2011). The capability of the model to represent experimental data acquired by PET was demonstrated. However, it is not clear whether this model is the 'best' model according to the principle of parsimony: the most

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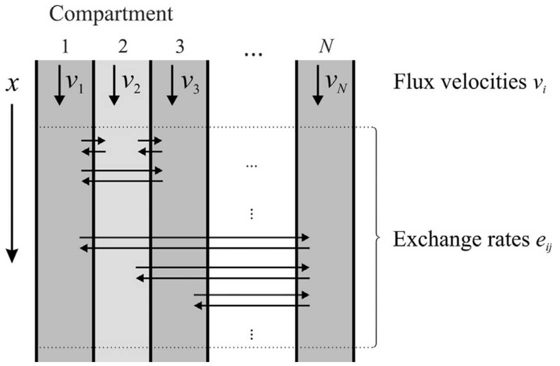

Fig. 1. Sketch of general mechanistic tracer transport model class. The model class consists of N one-dimensional compartments arranged in parallel along a spatial coordinate x. Within the ith compartment, tracer movement is controlled by flux velocities v_i. Lateral exchange of tracer between each of the compartments is controlled by individual exchange rates e_{ij}. From this model class, single model instances can be defined by allowing a specific set of model parameters to be non-zero. Tracer enters the system by arbitrary initial and boundary conditions.

exact and at the same time most simple data representation possible (Burnham and Anderson, 2002). For example, considering that the model appeared to be over-parameterized when fitted to some of the studied experimental data sets, it is a legitimate question whether or not a simpler model (e.g. with only two compartments) could fit the same data equally well. On the other hand, only slightly more complex models with several independent transport conduits (representing e.g. a bundle of parallel phloem sieve tubes) instead of just a single transporting compartment may fit the data better in other cases. The 'best' model choice will generally depend on the investigated plant species or the analyzed plant organ, e.g. stem, root system, or storage organ.

In order to systematically compare different models we set up a generalized class of mechanistic transport models, with an arbitrary number of compartments and flux along one or more compartments as well as lateral material exchange between all compartments. While generalizing the model structure, we still restricted ourselves to pure tracer models with parameters constant in time and space. In addition, the same model restrictions hold as described in Bühler et al. (2011), i.e., geometrical and anatomical details are disregarded, transport is allowed only in positive axial direction, and axial transport and lateral exchange in our models average the specific and complex mechanisms of processes in the plant (Patrick, 2013) such as passive or active axial transport and lateral exchange of labeled molecules. In contrast to Bühler et al. (2011), we excluded diffusion in axial direction for simplicity.

Each model instance (hereafter just called model) is defined by a specific system of PDEs characterized by a certain set of non-zero parameters. Consequentially, the model of Bühler et al. (2011) now becomes just one member of the much more general set of possible models defined by the model class. We applied finite volumes and a robust and fast WENO scheme (Shu, 1998) for the numerical solution (forward simulation) of the resulting PDEs, since no analytical solution is available for most models. The framework of model fitting and error analysis (bootstrapping) is similar to Bühler et al. (2011). A Monte Carlo multi-start approach was applied to avoid local optima.

The introduced set of possible models is very large even for a small number of compartments N. Therefore, a model filter was designed to eliminate redundant and obviously invalid models. We applied a 'bottom-up' approach for evaluating models with an increasing number of model parameters k until the quality of the achieved fits ceased to improve significantly. We ranked the resulting models according to their fitting quality, number of model parameters and parameter certainty.

2. A general mechanistic tracer transport model class

2.1. Model class definition

The basic composition of the model class is sketched in Fig. 1. Tracer is present in N parallel compartments. Each compartment can have individual transport velocities in axial direction (spatial coordinate x). Tracer is allowed to transfer between all compartments, determined by respective exchange rates.

This model class is defined by a system of partial differential equations

$$\frac{\partial \vec{\rho}(x,t)}{\partial t} = \left(\mathbf{A}^T - \mathbf{V}\frac{\partial}{\partial x} \right) \vec{\rho}(x,t) \tag{1}$$

The vector $\vec{\rho} = (\rho_1 \cdots \rho_N)^T$ denotes the tracer density distribution (arbitrary units) within each compartment at all spatial positions x and time points t. Here and in the following, we omit space and time dependence in our notation, i.e. $\vec{\rho} = \vec{\rho}(x,t)$ and $\rho_i = \rho_i(x,t)$. The coupling matrix $\mathbf{A}$ describes tracer entering compartment j coming from compartment i by an exchange rate e_{ij} (first term of Eq. (2)) in units of s^{-1}. The second term of Eq. (2) ensures mass conservation by removing exchanged tracer from the respective compartment. The third term of Eq. (2) describes decay of a radioactive tracer by a material specific rate λ, e.g. $\lambda \approx 5.67 \times 10^{-4}\ \mathrm{s}^{-1}$ for the isotope ^{11}C frequently used in PET measurements on plants.

$$\mathbf{A} = \begin{pmatrix} 0 & e_{12} & \cdots & e_{1N} \\ e_{21} & \ddots & & \vdots \\ \vdots & & \ddots & e_{(N-1)N} \\ e_{N1} & \cdots & e_{N(N-1)} & 0 \end{pmatrix} - \begin{pmatrix} \sum\limits_{k=1}^{N} e_{1k} & & 0 \\ & \ddots & \\ 0 & & \sum\limits_{k=1}^{N} e_{Nk} \end{pmatrix} - \lambda I \tag{2}$$

All diagonal elements e_{ii} are zero ($e_{ii}=0$ for $i=1 \ldots N$) since there is no tracer exchange of one compartment with itself. The matrix $\mathbf{V}$

$$\mathbf{V} = \begin{pmatrix} v_1 & & 0 \\ & \ddots & \\ 0 & & v_N \end{pmatrix} \tag{3}$$

contains the flux velocities for each compartment. The exchange rates e_{ij} and the elements of $\mathbf{V}$ are the parameters influencing the spatial and temporal tracer distribution and are therefore referred to as the model parameters. The complexity of the system of PDEs in Eq. (1) depends on how many of the model parameters are non-zero. Each set of non-zero parameters characterizes a specific model instance (model) of the model class.

Current tracer imaging methods typically do not allow a separation of tracer in different tissues. Thus, the compartments cannot be individually observed. For that reason, we compare the measured signal to the sum ρ_{tr} of the simulated tracer distribution over all compartments

$$\rho_{tr} = \sum_{i=1}^{N} \rho_i \tag{4}$$

Tracer entering the system is described either by a spatial initial condition at time $t = t_{\mathrm{ini}}$

$$\vec{\rho}_0(x) = \vec{\rho}(x, t = t_{\mathrm{ini}}) \tag{5}$$

or by a time dependent boundary condition at position $x = x_b$

$$\vec{\rho}_b(t) = \vec{\rho}(x = x_b, t) \tag{6}$$