Advances in Water Resources 52 (2013) 7–18

Contents lists available at SciVerse ScienceDirect

Advances in Water Resources

journal homepage: www.elsevier.com/locate/advwatres

A particle-tracking scheme for simulating pathlines in coupled surface-subsurface flows

Rob de Rooij [a,*], Wendy Graham [a], Reed M. Maxwell [b]

[a] Water Institute, University of Florida, 570 Weil Hall, P.O. Box 116601, Gainesville, FL 32611-6601, USA
[b] Department of Geology and Geological Engineering, Colorado School of Mines, 1500 Illinois Street, Golden, CO 8040, USA

ARTICLE INFO

Article history:
Received 21 February 2012
Received in revised form 16 July 2012
Accepted 22 July 2012
Available online 1 August 2012

Keywords:
Particle-tracking
Surface/subsurface flow coupling
Particle transfer probability
Transit time

ABSTRACT

A Lagrangian particle tracking scheme has been extended to simulate advective transport through coupled surface and subsurface flows. This extended scheme assumes a two-dimensional flow field for the overland domain and a three-dimensional flow field for the subsurface domain. Moreover it is assumed that the flow fields are simulated by a cell centered finite difference method. Pathlines in both the subsurface and the overland domain are simulated by classical particle tracking methods. Exchange of particles between the two domains is simulated by newly-developed algorithms presented in this study. Different algorithms are used depending on the direction of the exchange across the interface between the two domains. In the subsurface domain knowledge about a particle's pathline is enough to detect a transfer to the surface domain and the solution is straightforward. However, in the two-dimensional overland domain pathlines are parallel to the land surface. Therefore the velocity field in the overland domain alone cannot be used to detect a transfer to the subsurface. We propose a relatively simple algorithm to estimate the probability of transfer to the subsurface domain. It is shown that this algorithm can also be used to handle the transfer from the overland domain to the atmosphere domain. The algorithm to estimate the transfer probabilities is based on the mass balance of water on a streamtube aligned with the particle's pathline. This newly developed technique ensures that transit time distributions can be simulated accurately. These new relationships are implemented in an existing particle tracking code and are verified using analytical solutions for transit times.

1. Introduction

It has been widely recognized that a variety of hydrogeological problems require an integrated analysis of surface/subsurface flows. This has been the main motivation for the development of physically-based, distributed parameter models for coupling surface and subsurface flows. Well-known process-based models for coupling surface-subsurface flows include InHM [1], HydroGeoSphere [2], CATHY [3], WASH123D [4], ParFlow [5], OpenGeoSys [6] and PAWS [7]. The attractive feature of process-based models is that they account for the underlying physical processes and the spatial distribution of physical parameters. As such these models not only have the potential to obtain good simulation results while accounting for the physical processes, but they are also considered as useful tools for gaining insights into physical processes that are not yet fully understood. For example these type of models have been used for gaining insights in residence time distributions [8,9], runoff generation [10,11] and contaminant transport [12]. Except for PAWS and ParFlow, these models can also simulate contaminant transport using an Eulerian approach.

The Lagrangian particle tracking scheme presented in this study intends to fill a gap in simulating transport in coupled surface-subsurface flows. With respect to Eulerian schemes, Lagrangian particle tracking schemes have the advantage that they do not suffer from numerical dispersion or spurious oscillations [13,14]. Moreover, it is relatively straightforward to extend particle tracking schemes to simulate transit time distributions. Whereas the extension of Eulerian transport schemes to simulate the average transit time is relatively straightforward [15], Eulerian transport schemes to simulate transit time distributions are generally more complicated [16–18].

Our Lagrangian particle tracking scheme is tailored for flow fields generated with ParFlow and has been developed by implementing additional routines in the code Slim-Fast [19]. The scheme assumes a regular cell-centered finite difference grid on which the flow field has been calculated. On such grids the semi-analytical technique of Pollock [20] is a very efficient method to simulate the advection of particles. In our scheme Pollock's method is used for generating pathlines in the subsurface domain as well as in the overland domain. The current scheme does not account dispersion.

* Corresponding author. Tel.: +1-352-392-5893; fax: +1-352-392-6855.
E-mail addresses: r.derooij@ufl.edu (R. de Rooij), wgraham@ufl.edu (W. Graham), rmaxwell@mines.edu (R.M. Maxwell).

0309-1708/$ - see front matter © 2012 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.advwatres.2012.07.022

Although the scheme is tailored for usage in conjunction with ParFlow, it is emphasized that our scheme can also be applied on flow fields generated by other codes as long as the flow fields are being generated with a cell-centered finite difference model.

Coupled surface–subsurface flow models typically simulate a two-dimensional flow field for the overland domain and a three-dimensional flow field for the subsurface domain.

Since the flow fields do not have the same dimension standard particle tracking methods such as the semi-analytical technique of Pollock do not permit the simulation of particle transfer across the surface-subsurface interface. The primary challenge is to develop an accurate computational scheme to simulate particle transfer from the overland domain to the subsurface domain. Since the trajectory of a particle in the overland domain is parallel to the surface-subsurface interface, the trajectory itself cannot be used to detect a transfer to the subsurface domain. This is different when a particle moves from the subsurface domain to the overland domain. Advective transfer from the subsurface to surface domain is simply detected when a particle's trajectory ends on the surface-subsurface interface.

It may be noted that the particular problem of simulating a particle transfer from a flow domain of a lower dimension to a flow domain of a higher dimension can also occur in other coupled flow problems. Fractures may be represented as a two-dimensional flow domain embedded in a three-dimensional porous matrix [2,21]. One-dimensional flow domains may be used to represent rivers, conduits or tile-drains within a three-dimensional porous medium [2,22]. Pathlines in one-dimensional and two-dimensional flow domains are parallel to the interface with the surrounding three-dimensional porous matrix and cannot be used to detect to transfer to the matrix.

In the literature only a few particle tracking techniques have been described that deal specifically with simulating particle transfer between coupled flow domains. Liu et al. [23] and Pan and Bodvarsson. [24] presented a random walk particle method for particle transfer in fractured porous media. However, this scheme is based on a dual continuum concept in which the matrix and the fractures are represented by two overlapping flow domains of the same dimension. Nevertheless, since the interface between the fractures and the porous medium is not represented explicitly, the problem of detecting a transfer is similar to coupled overland flow in that the particle trajectories alone cannot be used to detect a transfer between the two flow domains. Instead the transfer is based on so-called particle transfer probabilities between the fractures and the matrix. These transfer probabilities are estimated using the Eulerian concept of an average concentration within the grid cell. As such the transfer of particles is based on the assumption of completely mixed conditions within the grid cell. To apply the transfer probability to individual particles Liu et al. [23] and Pan and Bodvarsson [24] express the transfer probability as a function of the time step associated with a particle tracking step. In other words the particle transfer probability is a function of the Lagrangian travel time of a particle. However, as we show in this work, if the transfer probability is derived by assuming complete mixing then it may only be expressed as a function of the Eulerian residence time of a particle. Therefore this methodology can produce inaccurate transit time distributions.

Another example of a problem where the fate of a particle cannot be deduced from its trajectory is when the standard scheme of Pollock is applied to a cell-centered finite difference model containing a so-called weak sink. A weak sink is a sink that does not capture all the water entering a cell. With the standard scheme of Pollock the pathlines in a cell containing a weak sink do not converge towards the position of the sink and without any modification to this scheme all the particles pass the cell without being captured by the weak sink. One solution to this problem is to extend the standard scheme of Pollock with a specific semi-analytical solution that accounts for the radial flow pattern around the sink [25]. A second probability-based solution is found in the adapted MODPATH code called SplitPath [26]. This solution assumes that the cell containing a weak sink can be regarded as a completely mixed reservoir. The probability that a particle is being discharged by the sink then equals the volume of water being discharged by the weak sink as a fraction of the total volume of water being discharged by the cell.

In this work we have extended the classical advective particle tracking method of Pollock [20] such that particles can be tracked across the surface–subsurface interface. The new particle-tracking scheme is built upon the code Slim-Fast [19]. Slim-Fast is based on Pollock's method and the original code permits to track particles through variably saturated subsurface flows. The new scheme detects a transfer from the subsurface to surface domain if a particle's trajectory ends on the land surface. To simulate the transfer from the overland domain to the subsurface domain we have developed an algorithm that that estimates the transfer probability of leaving the overland domain. This algorithm is based on a mass balance of water on a streamtube aligned with the simulated pathline. Using this technique we are able to define specific transfer probabilities along the individual pathlines. These probabilities are not based on the assumption of complete mixing of particles within the cell. As we show, the advantage of using pathline specific transfer probabilities is that the accuracy of simulated transit time distributions is improved.

Our particle-tracking scheme also accounts for particle transfer on the interface with the atmosphere. Particles may enter or leave the computational domain along this interface. Simulating a transfer from the subsurface to the atmosphere is relatively straightforward and is analogous to simulating a transfer from the subsurface to the surface. The algorithm for simulating a transfer from the overland domain to the atmosphere is similar to the algorithm dealing with a transfer from the overland to the subsurface.

To verify our particle tracking scheme we compare simulated transit times in a simple idealized synthetic watershed with analytical solutions. The scheme based on pathline specific transfer probabilities is compared with schemes based on complete mixing.

2. The flow model

2.1. Overland flow

Two-dimensional overland flow is governed by the following mass-balance:

$$\frac{\partial d}{dt} + \nabla \cdot (\mathbf{v}d) + q_{\mathrm{ov}\to\mathrm{sub}} - q_{\mathrm{atm}\to\mathrm{ov}} = 0 \tag{1}$$

where d is the water depth [L], t the time [T], $\mathbf{v}$ the velocity vector [LT^{-1}], $q_{\mathrm{atm}\to\mathrm{ov}}$ the effective rainfall per unit area on the overland domain [LT^{-1}] and $q_{\mathrm{ov}\to\mathrm{sub}}$ the flux per unit area into the subsurface coming from the overland domain [LT^{-1}]. In this study other source terms are not considered.

Manning's equation gives the scalar components of the velocity vector as a function of depth:

$$v_{\mathrm{i}} = \frac{d^{2/3} S_{\mathrm{fi}}}{n\sqrt{|S_{\mathrm{f}}|}} \tag{2}$$

where n is the Manning's coefficient [$TL^{-1/3}$], S_{fi} the friction slope [–] in the direction of v_{i} and S_{f} the friction slope [–] in the direction of $\mathbf{v}$. Eq. (2) assumes isotropy in Manning's coefficient.

The kinematic wave equation is obtained by combining Eqs. (1) and (2) and by making the assumption that the momentum