A new modeling approach for advective and dispersive pollutant transport in 3D discrete fracture network backbones of heterogeneous aquifers

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Key Points

- A well-to-well tracer test validated results of the new combined particle-tracking/channeling modeling approach showing its potentiality
- The proposed modeling approach depicted the preferential 3D spatial spreading of the tracer injected into a fractured aquifer
- The new modeling approach could predict the 3D pollutant transport in a DFN up to 100,000 fractures, owing to simulations in the backbones

Abstract

In the present study, we demonstrate comprehensive three-dimensional breakthrough pollutant advection-dispersion curve predictions throughout the 3D block of a highly heterogeneous fractured aquifer, using a combination of 3D particle-following tracking (P-FT) outputs and channeling theory results, without substantial computations. The P-FT method neglects slow tracer pathways in groundwater, owing to pollutant recirculation and dead-end pathways, when applied to backbones extracted from discrete fracture networks (DFNs), providing a non-exhaustive advection and dispersion solution in a 3D DFN characterized by preferential flow path formation. The combination of proposed models was positively verified at a local scale using a benchmark DFN in a fractured limestone aquifer in Bari (Italy) to evaluate its suitability for use in larger scale simulations with comprehensive DFNs (up to 100,000 fractures). The modeling results were validated using tracer (chlorophyll-A) concentrations obtained from a well-to-well monitoring/injection test. The P-FT simulations to the DFN-extracted backbones helped to instantly generate suitable histograms of the pollutant concentration as a function of time, providing input for the 3D channeling model solution of the tracer advection-dispersion in the rock aquifer. Unlike other Lagrangian or stochastic models, which accommodate the tail of the expected concentration curve, the solution of the proposed model does not require tail improvements because, in groundwater, the advection-dispersion theory helps to explain the complete trend of pollutant spreading, including macro-scale channeling effects. In addition to the dispersion coefficients and

Peclet number, the P-FT output provides information on actual 3D particle displacement, i.e., the 3D pollutant plume spreading through the studied aquifer.

Keywords: Discrete fractured aquifers; Backbones; Well-to-well tracer test; Particle tracking; 3D advective–dispersive pollutant transport.

Plain Language Summary

Analysis of recent articles dealing with three-dimensional water flow and pollutant transport in rock aquifers shows impressive progress of studies aimed at relating the complex 3D structure of interconnected fracture networks (DFNs) within rocky systems to specific fractures properties, measurable on the rock outcrops using field tracer tests. Anyway, the complex geometry of real aquifers makes challenging model computations, especially for a high number (>7,000) of interconnected fractures, owing to the huge computations required. Available models apply a "purely advective" computational method in transport models that may require amendments in the case of groundwater flows characterized by abrupt changes in fracture permeability. In these aquifers, the dispersion of pollutants cannot be neglected.

We developed a new modeling approach combining a new 3D "advective and dispersive" computational method, which accounts for the channelization of the pollutant pathway in a pipe network rather than in the whole DFN, and new theoretical achievements explaining the preferential transport in groundwater. The proposed method was validated into the Bari (Italy) fractured groundwater using results from a specific tracer test. The fine results obtained support the possible upscaling of the proposed method to large 3D DFNs up to 100,000 fractures, owing to fewer computational requirements.

Introduction

The development of new and effective modeling approaches is needed for predicting three-dimensional (3D) sorbing and non-sorbing pollutant transport in groundwater discrete fracture networks (DFNs). The study of pollutant transport in discrete fractured aquifers should address the preferential fluxes and specific physical characteristics of the fractures and rock matrix, owing to the heterogeneity of the dominant rock permeability in these aquifers. Moreover, the 3D pollutant flow and transport modeling of fractured aquifers with an impermeable matrix or those with low permeability—considered "equivalent continua"—using common advective–diffusive and dispersive methods, often results in inconsistent outputs. Particle tracking (PT) techniques can be utilized to evaluate the hydrodynamic control of pollutant migration in DFNs in fractured reservoirs. In such cases, deterministic or stochastic flow modeling and "purely advective" PT techniques can be used for effective pollutant flow and transport estimation in 3D stochastic DFNs, in which the geometry of the 3D fracture is predicted or assigned (Hyman et al., 2021; Makedonska et al., 2015) using specific codes, such as DFNTRANS in DFNWORKS (Hyman et al., 2015).

However, when using purely advective PT, many authors (Hyman et al., 2016; Painter et al., 2002) have proposed accommodations be made for the tail of the model outputs, following power-law stochastic distributions, to account for the heterogeneity of the fracture permeability, a factor that leads to non-Fickian (i.e., asymmetric) behavior in the pollutant concentration breakthrough curve (BTC) (Fig. 1). Similarly, Kang et al. (2015) suggested that accommodations be made for the spatial spreading curves of classical random walk solutions in 2D DFNs via truncated power-law velocity distribution and three other suitable parameters that still captured the main properties of the velocity field relevant to tracer transport, based on different mixing rules at every intersection node of the particle pathways.

Figure 1. Literature (Hyman et al., 2016; Painter et al., 2002) and proposed (blue text) computational methods for modeling the breakthrough curve (BTC), based on a tracer pulse injection into a 3D discrete fracture network (DFN) of a fractured aquifer. PT, particle tracking; P-FT, particle-following tracking.

When using PT in channel networks, the particle-following tracking (P-FT) method can help to determine the apparent spatial dispersion of pollutants, i.e., their preferential pathways in a 3D DFN in a rock mass, as opposed to the more general, purely advective PT models that are used to simulate single-particle trajectories, independently. Purely advective PT models are mainly applied to estimate the BTCs of the pollutant arrival times at the outlets of DFNs; they cannot be used to determine the 3D spatial spreading of pollutant concentrations owing to particle displacement. However, especially in heterogeneous aquifers, P-FT pollutant transport simulations in the backbones extracted from 3D DFNs can also provide information on the non-exhaustive tails of BTCs because pollutant flux is characterized by preferential flow path formation, neglecting the slow tracer pathways in groundwater owing to pollutant recirculation and dead-end channels,

In this study, we present a new modeling approach that does not require improvements to the BTC of the solution which was validated experimentally via a specific tracer field test. Precisely (see Fig. 1), the new modeling approach consists of a combination of the outputs of a 3D P-FT backbone simulation and a 3D channel model (Tsang et al., 2015; Tsang and Neretnieks, 1998; Shahkarami et al., 2019) analytical solution to obtain information on the accurate BTC of passive pollutant (or tracer) advection-dispersion in discrete fractured aquifers. Tsang et al. (1996) presented the channeling theory and proposed the P-FT numerical solution for pollutant transport in regular (2- or 3D) fracture network (lattice) models. Moreno et al. (1988) and Moreno and Neretnieks (1993) used the same P-FT method in both 2D and 3D lattices. Masciopinto et al. (2008; 2010) applied an in-house 2D P-FT code to pollutant advective–dispersive transport in a layered variable-aperture fractured aquifer and assessed the results using field investigations. In this study, P-FT simulations were performed using a recently developed open-source code (Particle3D; http://alghalandis.net) that is suitable for simulating particle advection and the macro-scale dispersion of tracers in the 3D backbones of DFNs. The Bari limestone aquifer was selected as a benchmark case for the proposed modeling approach. Here, results derived from a field tracer (chlorophyll-A) well-to-well test were considered to validate the proposed flow and transport solution. The injection/monitoring well-to-well test was conducted in the well field at the *Istituto di Ricerca Sulle Acque*, Bari, Italy, during a specific investigation on the permeability and porosity of the fractured limestone aquifer.

2. Materials and Methods

Representative DFN generation in fractured aquifers

The DFN can be considered an equivalent fracture network (Huang et al., 2017) to the study aquifer, developed using interconnected "smoothed" fractures of different apertures, although recent investigations (Hyman et al., 2021; Hyman, 2020) focused on important 3D flow (and transport) "channeling effects" (scale-bridging) when, at a micro-scale, the variable apertures in each fracture plane are considered. The fracture network connectivity in the DFN and the fracture properties, such as apertures, density, length, direction, and dip are deemed key factors for characterizing the flow and transport in fractured aquifers. However, only a small fraction of the fracture intersections and properties of an entire geological rock formation can generally be directly observed and analyzed during field investigations. Therefore, deterministic DFN generation from actual aquifers is usually not possible (Chilés, 2008). This leads to stochastic and geostatistical methods frequently being applied in DFN flow and transport models, because minimal field data input is required compared to the input requirements for deterministic or hybrid methods. Moreover, with the use of experimental variograms, geostatistic-based DFNs can be used to indirectly incorporate observed fractured rock properties and interconnections, via field hydraulic conductivity estimations (Berkowitz, 2002). This indicates that, in geostatistic DFNs, field investigation results could be a link between the actual velocity of the flow field and the DFN flow model output.

Otherwise, explicitly stochastic DFN generation can be considered when field measurements are insufficient. Probability distributions (Darcel et al., 2009) are applied to the fracture properties; specifically, the truncated power-law distribution is used to determine fracture sizes, the Poisson (or uniform) distribution is used for fracture spatial positions, and the Fisher distribution is used for orientations. In certain cases, stochastic DFN realizations and flow simulations are necessary for DFN flow model simulations based on ensemble averages of DFN properties (Berkowitz, 2002). Monte Carlo simulations (Dessirier et al., 2018) are then used to fit the available experimental values, i.e., fracture permeabilities, at specific sites.

Backbone extraction from 3D DFNs

A DFN realization should be based on field measurements of fracture parameters, including fracture number, orientation, dip angles and lengths, and aperture sizes. Hence, the DFN can help to provide an accurate flow simulation of the underlying interconnected fracture network and, consequently, of pollutant transport. Reliant meshing methods may prove to be inadequate in practical DFN modeling, as a considerable number of fractures and nodes (e.g., 16 million), even at a field scale (<200 m) (Hyman et al., 2018), is necessary to determine the flow solution using meshing methods incorporating every DFN fracture. Alternatively, the finite-volume method can be used for each interconnected fracture (meshed volume) within "equivalent fracture sub-networks," i.e., backbones (Karra et al., 2018) or pipe networks (Fadakar-Alghalandis, 2014), to reduce the computational load of pollutant flow and transport simulations in DFNs composed of many thousands of fractures. The "backbones" in previously reported DFN flow and transport simulations were defined as connected "subsets" of fractures forming flow paths in the fracture network, thus, facilitating "a significant amount" of DFN water flow and pollutant transport. According to the percolation theory, the backbone through a percolation channel network is defined as the "conductive" fragment of the percolation clusters, i.e., the links in the percolation fractures exhibiting non-zero flowrates (Hendrick and Renard, 2016). The backbones are thus deemed "subsets" of the DFN that do not include fluid flow recirculation or dead-end fractures. The percolation skeleton (or "effective backbone") of the DFN can be extracted utilizing the direct electrifying method (Li and Chou, 2009).

The pipe network flow solution was executed by extracting the backbone (Fadakar-Alghalandis, 2014) of the DFN, establishing a graph structure, and subsequently solving a substantial system of linear flow equations. The prior conversion of the DFN models into pipe networks was performed based on intersection analysis (Fadakar-Alghalandis et al., 2011), following which all fracture interconnections (i.e., pipes) in the DFN were identified. The backbone was then extracted by removing the isolated pipes, in addition to those with free ends. This method enabled the immediate identification of fluid flow solutions for comprehensive DFN models (<100,000 fractures), while aiding the use of sparse matrices for adequately manageable memory requirements. The solution of the subset model helped to define the representative subset of the DFN that formed flow paths with a significant amount of fluid flow and pollutant transport.

Some studies have suggested specific algorithms based on flow topology graphs (Aldrich et al., 2016; Hyman et al., 2016; Hyman et al., 2018) to isolate the effective backbone of a DFN. To elaborate, a prescribed constant unidirectional water flux was initially imposed on the DFN to maintain water flow in the percolation subset cluster of fractures from the upstream surface to the downstream boundary of the DFN. The flow velocities in the fracture network clusters were numerically estimated by imposing mass flow continuity (Kirchhoff's equation) at every fracture intersection node and by applying the Hagen–Poiseuille equation (i.e., the cubic law) for flow resistance estimations (see section 3.3) in each individual pathway. The results of the flow calculations were collated in a flow topology "graph" (FTG), a dual representation of the investigated fracture subnetwork topology, suitable for identifying the various subsets of fractures comprising the backbone from a network of interconnected edges (i.e., pipes) and nodes (i.e., fractures). Furthermore, several FTGs can be generated from a DFN; the purely advective PT analytical solution can be determined for every possible FTG by preserving both the particle count and the travel time at each node and edge. Thus, a successive optimization algorithm was applied to the FTGs to isolate the effective backbone. The backbone was expected to collate the highest particle count via the fastest and shortest pathways that exhibited minimal fractures, while excluding the slowest flowing and recirculating pathways (Hyman et al., 2018). However, based on its definition, the topology of a backbone extracted from the DFN of a heterogeneous aquifer is not exhaustive of all the pathways followed by pollutants, owing to the slow non-preferential flow paths in actual limestone aquifers, which demonstrate prevalent secondary permeability and a quasi-impermeable rock matrix.

3D P-FT computational methods

PT techniques rely on a Lagrangian-based transport observation framework as opposed to an Eulerian framework. In Lagrangian flow fields, the observer moves in tandem with a single particle along its pathway. This enables the description of the governing flow and transport equations in a simple mathematical form, with a straightforward post-time integration solution. Thus, Lagrangian frameworks require an established flow field, i.e., the water velocities in the DFN or extracted backbones. PT analytical solutions aid in the identification of the elapsed time during the transport of injected pollutant particles from the inlet to the outlet positions in a 3D DFN. In the DFN, particles follow specific pathways with low flow resistance, i.e., highly conductive channels. Cvetkovic and Frampton (2012) applied PT to examine the purely advective transport of pollutants, i.e., without macro-scale dispersion, using generic boundary conditions applied to a DFN.

The P-FT method applied in the present study involved the utilization of a numerical method to generate a histogram of particles collected in the observation section (i.e., outlet or well), as a function of the assigned time intervals, as opposed to the analytical PT output of the purely advective PT solution (Hayman et al., 2016; Cvetkovic, and Frampton, 2012). The P-FT transport simulation for a generic, saturated 3D DFN (Figure 2a) involves the release of particles at the inlets (e.g., left boundary nodes) and their collection at the outlets (e.g., right boundary nodes). According to the Lagrangian approach, particles entering the intersection (node) of a pipe (or channel) are dispersed into the outlet channels, obeying the probability function $f(\mathbf{x})$ values, where $\mathbf{x}(\mathrm{t})$ is the spatial particle position vector. Hence, the numerical P-FT method helps determine pollutant pathways, i.e., the spatial distribution of the pollutant particles as a consequence of advection and dispersion phenomena. Specifically, the mixing of pollutant fluxes in all subsequent intersection nodes along the preferential flow pathways originates the macro-scale dispersion affected by the channeling effect. This study assumed the complete and instantaneous mixing of the pollutant at every channel intersection node during the simulation. In contrast, previous studies have reported alternative pollutant mixing possibilities and $f(\mathrm{x})$ probability distributions at each channel intersection, associated with the fluid velocity or Peclet number (Berkowitz et al., 1994). In the applied Particle3D code, $f(\mathrm{x})$ denotes the probability distribution function of the pathway direction followed by the particles at every channel intersection. A uniform random distribution was selected to achieve the objectives of this study. Kang et al. (2015) observed that the high heterogeneity ($^{2}{}_{\mathrm{lnK}} > 5$) caused by changes in the single fracture hydraulic conductivity, K (Lt^{-1}), and a limited (or discrete) number of fractures in the network, resulted in negligible spatial spreading effects when using the "routing" mixing option, i.e., when all pollutant particles followed the pathway adjacent to the outflow of each node. The outlet section receives particles at different arrival times (Fig. 2b,c), and this is attributed to differences in the pathway characteristics, such as the conductivity, or fracture apertures, and length. The final simulation result, represented by the frequency distribution of the particles (Fig. 2d), depicts the possible BTC of a passive pollutant. Calculations performed to investigate the effect of the number of particles on the BTCs can utilize 500 or more released particles. Moreno et al. (1988) recommended a total of 1000 particles to aid the generation of reliable model outputs.

The corresponding P-FT solution following the step injection of the pollutant into a target section of groundwater can be obtained using the following equation:

$C_T\left[\mathbf{x}(t)\right] = C_m \frac{m_k}{M_0} f\left(\mathbf{x}_k\right);\ for\ k = 1, \dots, nc$ (1),

where m_k $f(\mathbf{x}_k)$ represents the expected mass-fraction of the total injected pollutant mass, M_0, which is transported by every parent cluster of particles with a travel time of $\mathrm{t_k}$ provided by the P-FT output; *nc* denotes the number of particle clusters with different travel times at the outlet position; and C_m (ML^{-3}) indicates the maximum expected concentration in the groundwater that can reach vector position $\boldsymbol{x}(t)$, considering possible reductions in the initial concentration, C_0, owing to sorption, mass transfer, and pollutant decay during transport through the fractures. For conservative pollutants or tracers, $C_m = C_0$.

Figure 2. **a**) Discrete fracture network (DFN) representation of a fractured aquifer and backbone; particle-following tracking (P-FT) outputs at two subsequent simulation times**:** **b**) 2979 s (49.7 min) and **c**) 4086 s (68.1 min). **d)** Typical histogram of the arrival times of the particle clusters at the outlets.

Furthermore, the spatial spread of the pollutant through the fractured aquifer was depicted by the pollutant particles' pathways in the 3D backbone network. The Particle3D code helps independently facilitate the simultaneous tracking of multiple particles and each individual particle over time. In the example shown in Fig. 2a, the particles were released simultaneously at several inlet nodes. Each particle may have followed a different pathway from the others, as f(x) is random (Fig. 2b,c). The simulation ended when all particles arrived at the outlets (larger colored solid circles in Fig. 2b,c). The cumulative, i.e., per cluster, arrival times of the particles at the outlet nodes are represented by a projected histogram (Fig. 2d), depicting the one-directional transport of the pollutant through the DFN backbone.

Proposed modeling approach

As mentioned above (see the Introduction), the output of the 3D P-FT applied to the backbones may not exhaust all the pollutant pathways in the DFN, as non-preferential flow paths, including flow recirculation in fractures or dead-end pathways, are not considered in the backbone simulations. Thus, in 3D simulations, where backbone extraction is necessary owing to the substantial computations caused by the high number of fractures (>7,000; Aldrich et al., 2016) and their intersections, BTC tail improvements are required, especially for highly heterogeneous media, i.e., those with high variance ($_{\mathrm{b}}{}^{2}$) in the fracture aperture ("b") or a low Peclet number.

In this study, instead of using stochastic power-law distribution trends for the BTC tails, as suggested in the literature, we determined the appropriate complete trend of the pollutant concentrations via the application of the 3D analytical solution of the channeling model. Specifically, we preserved information derived from the significant component of the histogram predicted by performing the 3D P-FT simulation, which yielded the preferential mean (or most frequent in DFN) particle velocity U (Lt^{-1}) throughout the DFN and the hydrodynamic dispersion coefficient D ($\mathrm{L}^2\mathrm{t}^{-1}$) of the transported pollutant throughout the DFN, defined as follows (Neretnieks, 1983; Yeo, 2001):

$D = \left\{\exp\left[4\left(\ln 10\cdot\ \ _b\right)^2\right] - 1\right\} \bullet \frac{1}{2}U \bullet L \bullet \lambda$ (2),

where D is a function of the mean flow velocity represented by the majority of the particles and of the coefficients of the exponential variogram model of log_{10} fracture apertures obtained in the study area, such as the standard deviation $_{\mathrm{b}}$ (L) of the fracture log-apertures, which is related to the scale (sill and nugget) and correlation length (-) of the variogram; L (m) represents the domain length. Equation (2) was derived from the analytical solution of flow and transport resulting from a pulse injection of a tracer at the inlet of a bundle of independent channels, with apertures following a log-normal distribution with variance $_{\mathrm{b}}{}^{2}$. Specifically, the estimation of the second order moment of the tracer concentration at the channel outlets could be expressed as follows:

$\frac{\sigma_t^2}{\bar{t}^2} = exp\left[4\left(\ln 10 \bullet \sigma_b\right)^2\right] - 1$ (2a).

The dispersion coefficient (2) can, thus, be provided using a well-known relationship (Fiori and Jankovic, 2005; Dagan, 1990):

$D = \frac{\mathrm{UL}}{2}\frac{\sigma_t^2}{\bar{t}^2}$ (2b),

where $\frac{\mathrm{UL}}{D}$ denotes the Peclet number, and $\bar{t}$ is the mean (or most frequent) residence time. Thus, we used the one-directional advective–dispersive transport equation in a spatially oriented 3D bundle of equivalent channels to determine the complete trend of the BTC at the outlets that was attributable to the tracer injection at the inlet. Essentially, we endeavored to satisfy the projected concentration trend using a 3D channeling analytical solution at the cross-section x = x_0 (van Genucthen and Alves, 1982; p. 11-12), for one-directional flow and pollutant transport in a 3D bundle of channels, using a conservative pollutant (or tracer) with a step injection at x = 0. This solution can be approximated (Fried, 1975, p. 63; Runkel, 1996, p. 831) as follows:

$C\left(x_0, t\right) = C_b + \frac{1}{2}\left(C_0 - C_b\right)\left[\mathrm{erf}\frac{x_0 - U\bullet(t-t_0)}{2\sqrt{D(t-t_0)}} - erf\frac{x_0 - U\bullet t}{2\sqrt{\mathrm{Dt}}}\right],\ for\ t > t_0,$ (3),

when the following initial and boundary conditions are considered:

$C(x,t) = C_b,\ for\ t \leq 0,$ (3a);

$C(0,t) = C_0,\ for\ t \leq t_0,$ (3b);

$C(0,t) = C_b,\ for\ t > t_0,$ (3c); and

$C(x,t) = C_b, for\ x \rightarrow \infty,$ (3d),

where t = t_0 is the completion time of tracer injection into the well, C_0 (ML^{-3}) represents the corresponding aqueous phase tracer concentration in the injection well (x = 0 m), and C_b (ML^{-3}) indicates the initial background (natural) tracer concentration in the groundwater. In Equation (3), the complementary error function *erfc* (x) was replaced by *1 – erf(x)*, via the error function (Abramovitz and Stegun, 1972, p. 297)

$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-z^2}\mathrm{dz}.$ (4).

The solution to Equation (3) can be used to define a comprehensive predictive concentration curve for a conservative pollutant (or tracer), based on inputs obtained via the simulation results obtained using the P-FT code, as well as for a high $_b^2$ value or a low Peclet number (Tsang et al., 1988; p. 2054) in highly heterogeneous aquifers.

1.

Benchmark case for combined P-FT/channeling solution

(a)

Description of the field tracer test

Tracer concentration measurements derived from the dataset repository Masciopinto (2021) were used to validate the Particle3D code simulations in the 3D DFN representation of the actual fractured limestone aquifer in Bari. At the field-test site, pumped groundwater was mixed with 500 g of chlorophyll-A powder in a 1 m^3 tank using a mechanical agitator. Chlorophyll-A is a natural non-toxic compound that can be easily detected even at low concentrations in groundwater (Jones, 2019; Masciopinto et al., 1997). The traced water solution was injected with a mean flow rate of 1.1 L/s into a well (150 mm ID) upstream of the main groundwater flow using gravity and a three-inch pipeline. The traced water outflowed at a pre-assigned water depth of 3 m with an injection time of approximately 15 min. The injection pipeline was then removed, and the groundwater sampled at regular intervals at a monitoring well located 20 m downstream of the injection well. Sampling was performed using a pump with a flow rate of 5–6 L/min (Grundfos BTI/MP1, Downers Grove, IL, USA), placed at an assigned depth of 3 m in the monitoring well (150 mm ID). This sampling pump enabled the continuous monitoring of the chlorophyll-A content of the groundwater flow (Fig. 3).

Figure 3. (Left) Map of the Bari aquifer contour head (m) (above sea level), showing flow velocity vectors (Masciopinto et al., 2010) and the area (yellow polygon) of the tracer test wells; and (right) fluorometer set-up used for chlorophyll-A concentration measurements (FU) into the groundwater flows.

Additionally, to facilitate the convergence of the traced groundwater flow into the monitoring borehole, a second pump, operating constantly at the low rate of 0.88 L/s, was installed in the monitoring well, forcing the natural groundwater flow gradient ($\emptyset/L$) from 0.1% to 0.35% (calculated using 0.07 m/20 m). The maximum chlorophyll concentration in the groundwater was 115 mg/L (approximately 112,000 FU) in the injection well and 2.5 mg/L (6400 FU) in the monitoring well at a water depth of 3 m. The groundwater was sampled until the background chlorophyll value of 290 FU (0.08 mg/L) was reached. A model 10-005 fluorometer (Serial 5584 R, 230 V 50/400 Hz, Turner Design, Inc. Mt. View, CA, USA) (Fig. 3) was used for this purpose.

Fracture data description: input data

Data derived from local rock fracture reliefs (Healy et al., 2017; Panza et al., 2016) were depicted using ADFNE1.5, an open-source code (Fadakar-Alghalandis, 2017) for the DFN of the Bari aquifer. This software was preferred over other open-source codes, such as DFNWORKS or similar codes, because it can be operated in the MATLAB (v. 2014 or later) environment, which enables the immediate visualization of the 3D DFNs after slight changes to the source code. Geological surveys were used to supplement the representation of the DFN aquifer and included the following: 150 horizontal fractures, with a dip angle of 90° and direction of –45°; 70 vertical fractures, with a dip of 45° and direction of 45°; and 130 vertical fractures, with a dip and direction of 10° and

–15°, respectively. The maximum fracture length ranged from 50–80% of the 3D rock block border size (20 m) and the mean aperture of the DFN fractures (b) was 0.86 mm (Fig. 4a). This was obtained using a geostatistical 3D fracture aperture model (Masciopinto, 2005) based on the experimental variogram of the fracture apertures (Gelhar, 1993; Journel and Huijbregts, 1978) (Fig. 4b) estimated from the results of 30 pumping well tests conducted in the aquifer under investigation (Masciopinto et al., 2010).

Figure 4. **a)** Three-dimensional (3D) model of the fractures and backbone obtained using MATLAB R2019b, and **b)** fitted exponential model of the experimental variogram (indicated using a dashed line) of the fractured limestone aquifer in Bari, Southern Italy.

A sequence (i.e., matrix) of aperture values, derived from the variogram data using in-house software (Masciopinto, 1999), was used as the input to the GRAPH function in ADFNE1.5 to obtain actual flow resistances for the 497 backbone pipes of the representative DFN of the Bari aquifer, instead of using internally estimated apertures based on an assigned distribution (i.e., the power-law or similar). The rock block matrix of the DFN was considered impermeable owing to the known low permeability ($<10^{-12}$ cm^2; or $K < 10^{-7}$ cm/s) of the limestone rock matrix (Bear, 1979, p. 68).

3D P-FT simulation

P-FT simulations (Figure 5) were performed using a modified version of Particle3D software. Twelve backbone inlet nodes corresponding to the simulated injection well were injected with a total of 1440 particles to obtain the Particle3D solution. Consequently, 184 particles were collected at five outlet nodes of the monitoring well. The 3D solid zone depicted in Fig. 5 (indicated using a red shadow) outlines the spatial spreading of the 3D tracer in the groundwater rock block under investigation.

Figure 5. Modified Particle3D/ADFNE1.5 simulation results: 1440 particles were released into 12 backbone nodes of the injection well; 184 were collected at the five outlet nodes of the monitoring well. The 3D solid zone (indicated by the red shadow) outlines the spatial spreading of the tracer in the fractured aquifer.

Modification of the applied codes enabled us to include the individual revised particle travel time equation for each pathway segment, *ij,* using the following equation:

$t_{\mathrm{ij}} = \frac{L_{\mathrm{ij}}}{U_{\mathrm{ij}}}$ (5),

where L_{ij} represents the length of the pipe, with extremities i and j and cross-section $1 \times b_{ij}$; and U_{ij} denotes the flow velocity defined by the Hagen–Poiseuille equation utilizing a 3D block-centered grid (Masciopinto, 1999; Masciopinto et al., 2021), which is expressed as follows:

$U_{\mathrm{ij}} = -\gamma \ \left(b_{\mathrm{ij}}\right)^2 (12\mu)^{-1} \ \nabla \left(\varphi_i - \varphi_j\right)$ (6),

where (ML^{-3}) and ($\mathrm{ML}^{-1}\mathrm{t}^{-1}$) represent the specific weight and dynamic viscosity of the fluid, respectively, and $_{\mathrm{i}}$ denotes the groundwater pressure head (L) at the pipe extremity (or node) *i*.

The head gradient at the pipe intersection nodes was, thus, estimated by solving the linear system of equations obtained for every intersection node devoid of sources or sinks, using the following expression:

(7),

where M represents the number of all inflow and outflow channels for each channel intersection of the pipe network, determined using the 3D backbone topology of the DFN. The channel flow rate, Q_{ij}, is calculated using the cubic law equation by applying the Hagen–Poiseuille equation to every pipe with a cross-section of $1 \times b_{ij}$.

Results and discussion

Figure 6a shows the histogram for the predicted tracer concentrations (see Eq. 1) generated by the P-FT simulation, together with the channeling analytical solution (van Genuchten and Alves, 1982) (see Eq. 3) for the corresponding initial and boundary (see Eq. 3a–d) conditions. The solution for Equation (3) was based on the preliminary estimation of the dispersion coefficient from Equation (2), as a function of the groundwater flow velocity and parameters obtained from the exponential variogram model of the fracture apertures (i.e., $_{\mathrm{b}}{}^2$, correlation length, and scale). Specifically, most of the tracer particles in the observed groundwater exhibited a mean water velocity (U = 64.8 m/d) consistent with the pre-defined arrival time of 0.31 d (modal time), established by the histogram-based selection of concentrations generated using the P-FT code (see Fig. 6a). Moreover, using the spatial and directional variogram model (indicated using a solid line in Fig. 4b), we defined the variables, i.e., $\sigma_b =$ 0.3 and = 0.1, to determine the hydrodynamic dispersion coefficient, which was estimated to be 372 m^2/d. Figure 6b presents a comparison between the proposed combined solution and the BTC of the observed chlorophyll-A concentration in the groundwater flow that passed through the monitoring well. The concentration measurements corresponded accurately to the simulated solution combination. By comparing the tracer BTC (Fig. 6b) with the P-FT histogram illustrated in Fig. 6a, we can see that the portion of the histogram originally absent from the P-FT backbone simulations is highlighted, as only the preferential flow pathways are considered. Hence, the proposed combined solution essentially functions as a work-around method used to obtain a complete 3D advective–dispersive solution model, beginning with the backbone P-FT output and field fracture data. The 3D channeling solution obtained using the P-FT output was instrumental in inferring a complete solution for the spatial spread of the pollutant in the DFN representation. The combination model, i.e., the

Particle3D and channeling outputs, indicated appropriate values for the tracer velocity (64.8 m/d) and hydrodynamic dispersion coefficient (372 m^2/d) of the tracer spreading through the target aquifer. The positive verification of the proposed modeling approach was attributed to the strong link between the field aperture estimations and both the input of the P-FT code and the dispersion coefficient (2) applied to the analytical solution (3).

Fig. 6. **a)** Particle-following tracking (P-FT) histogram concentrations and the corresponding three-dimensional (3D) channeling analytical solution (indicated using a dashed line); **b)** combined 3D P-FT/channeling *model* solution (indicated using a solid line) overlapped with the tracer breakthrough curve (BTC) concentrations (indicated using solid triangles) above the background concentration (290 FU) from the monitoring well (L = 20 m).

The low Peclet number ($0.29 < 5$) highlighted the prevalent mixing of the tracer fluxes, with dispersion occurring predominantly at a macro-scale with respect to tracer advection. This corresponds to the predicted nature of hydrodynamic dispersion in limestone aquifer DFNs, in which the generation of a typically long BTC tail resulting from a high degree of tracer dispersion can be observed. The strong asymmetry of the expected tracer concentrations (see Fig 1) was attributed to the high heterogeneity of the fracture apertures, which indicated the high velocity assumed by the tracer particles along limited preferential pathways into the backbone pipes, as shown in Fig. 6a. The slow-velocity particles in the groundwater fracture network could be observed in the characteristic long tail exhibited by the tracer concentrations, which was not observed in the backbone P-FT output but was described using the proposed dispersion coefficient and groundwater flow velocities in the channeling solution.

Conclusions

The positive benchmark case supports the application of the P-FT/channeling modeling approach to 3D DFN backbone networks at large scales, i.e., 1000 m, owing to its highly simplified computation method. At this scale, considering the high number of fractures (>20,000) and the unknown geometry of the fracture intersections at an actual site, simulating the PT of the DFN applying finite-volume computational methods to meshed domains for every fracture to determine the flow solution in the DFN, as required for DFNWORKS for instance, would result in very uncertain and tedious computations. At large scales PT or P-FT simulations should be based on the flow solution in DFN backbone pipe network provided by topology graph representation. The DFN input data representation could be obtained using a minimum number of field experimental estimations to ensure a good fit of the spatial covariance applied to the fractures parameters and reduce results uncertainty. The P-FT backbone simulation rendered a solid 3D representation of the spatial tracer spread during the well-to-well test conducted in the Bari fractured limestone aquifer.

The tracer BTC highlighted the portion that could not be generated by applying the P-FT method using DFN backbones from heterogeneous discrete fractured aquifers. Here, the proposed 3D P-FT method could not be used considering the slow pathways that characterized actual pollutant spreading, because backbone extraction algorithms could capture only the preferential flow and pollutant transport pathways in the DFN. Thus, in discrete fractured aquifers, further interpretation of the expected P-FT backbone outputs of pollutant concentrations at the observation wells is necessary to obtain a comprehensive advection–dispersion solution for pollutant transport. This study utilized the channeling modeling approach to predict accurate BTCs. The 3D P-FT backbone simulation output (depicted using a histogram) was used to determine only the modal tracer velocity and hydrodynamic dispersion coefficient of the tracer transport, factors that have been deemed necessary for the application of the known analytical solution (Eq. 3) for tracer advection and dispersion, as proposed in 3D channel modeling. Thus, the combined P-FT/channeling output provided comprehensive concentration trends with accurate time points that could finely overlay the collected measurements during the injection of the tracer compound into the fractured limestone aquifer of Bari. This was attributed to the fact that the proposed modeling approach was based on a strong association between the field fracture apertures and velocities (see Eq. 6) and both the input data of the P-FT code (fracture density, length, orientation, and apertures) and the dispersion coefficient applied to the channeling model solution. The obtained results support further field investigations for simulating large-scale pollutant pathway representations using the combined P-FT/channeling modeling approach.

List of symbols

b (L) mean fracture aperture;

$C,\ C_b,\ C_{T,}$

$C_m,\ C_0$ (M/L^3) dissolved concentration of the considered chemical;

D (L^2/t) hydrodynamic dispersion coefficient of the pollutant;

f($\mathbf{x}$) probability function defining the particle trajectory ($\mathbf{x}$);

g (L^2/t) acceleration of gravity;

K (L/t) single fracture hydraulic conductivity;

L (L) *distance* between two flow cross-sections in the DFN;

n (-) effective (i.e. secondary) rock formation porosity;

nc (-) number of clusters of particles having different travel times;

Q_{ij} water flowrate between the extremity pipe nodes i and j;

Greek symbols

(L) watertable drawdown (or mound);

(L) water-pressure head;

m_k (M) mass fraction of pollutant particles with same pathways;

(L) correlation length of the variogram of fractures aperture;

σ_b(L) standard deviation of the log-fracture apertures;

σ_b^2(L) variance of the log-fracture apertures;

$\frac{\mu}{\gamma}$ (L t) fluid viscosity/specific weight ratio;

σ^2_{logK} ($\mathrm{L}^2/\mathrm{t}^2$) variance of the log hydraulic fracture conductivities;

σ_t^2(t^2) second moment of the expected concentrations in fractures;

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Figure captions

Figure 1. Literature (Hyman et al., 2016; Painter et al., 2002) and proposed (blue text) computational methods for modeling the breakthrough curve (BTC), based on a tracer pulse injection into a 3D discrete fracture network (DFN) of a fractured aquifer. PT, particle tracking; P-FT, particle-following tracking.

Figure 2. a) Discrete fracture network (DFN) representation of a fractured aquifer and backbone; particle-following tracking (P-FT) outputs at two subsequent simulation times**: b**) 2979 s (49.7 min) and **c**) 4086 s (68.1 min). **d)** Typical histogram of the arrival times of the particle clusters at the outlets.

Figure 3. (Left) Map of the Bari aquifer contour head (m) (above sea level), showing flow velocity vectors (Masciopinto et al., 2010) and the area (yellow polygon) of the tracer test wells; and (right) fluorometer set-up used for chlorophyll-A concentration measurements (FU) into the groundwater flows

Figure 4. a) Three-dimensional (3D) model of the fractures and backbone obtained using MATLAB R2019b, and b) fitted exponential model of the experimental variogram (indicated using a dashed line) of the fractured limestone aquifer in Bari, Southern Italy.

Figure 5. Modified Particle3D/ADFNE1.5 simulation results: 1440 particles were released into 12 backbone nodes of the injection well; 184 were collected at the five outlet nodes of the monitoring well. The 3D solid zone (indicated

by the red shadow) outlines the spatial spreading of the tracer in the fractured aquifer.

Figure 6. a) Particle-following tracking (P-FT) histogram concentrations and the corresponding three-dimensional (3D) channeling analytical solution (indicated using a dashed line); b) combined 3D P-FT/channeling model solution (indicated using a solid line) overlapped with the tracer breakthrough curve (BTC) concentrations (indicated using solid triangles) above the background concentration (290 FU) from the monitoring well (L = 20 m).