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Numerical Simulation of Solute Transport in Fractured Rock with Particle Tracking Method

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Abstract—**In this work an open source scientific software platform OpenGeoSys (OGS) was utilized for the simulation of fluid flow and solute transport in fractured porous media. A particle based method was proposed which takes use of velocities calculated by finite element method (FEM) to obtain flow patterns, and in which the distribution of the solute mass is represented by particle plume and can be quantitatively obtained by counting the number of particles. Two benchmarks were developed in order to verify the proposed method: one was to simulate solute transport in two dimensional steady flow through infinite fractured porous media with one single crack; the other was to simulate solute transport in an artificial rock fracture in novaculite under laboratory conditions. The simulation results showed that the proposed particle tracking method agreed well with the classical FEM simulation methods. The particle plume could exhibit the flow pattern, as well as the detailed channeling effects and accelerations or decelerations in some regions. This method can be applied as a tool to observe the detailed structure of evolving contaminant plumes in fractured rock.**

Keywords-fractured porous media; particle tracking; solute transport; OpenGeoSys (OGS); dual-porosity/permeability; single fracture

I. INTRODUCTION

Groundwater flow and solute transport in fractured rocks is of great interest in the study of hydrogeology. The complexity of fracture structures leads to great difficulties in the investigation of flow patterns and contamination distributions within the fractured rocks. Numerous studies have been carried out in this area by means of both laboratory experiments and numerical simulations ([1]-[4]). It has been proved that varies of factors, e.g., the surface roughness and fracture aperture statistics may have some influences on the groundwater flow and solute transport processes during the numerical simulation ([5]-[7]). In these studies fractures are treated in several different ways: some researchers studied the seepage flow in single rock fracture ([8]-[13]); some considered the fracture and the matrix as a continuum ([14]-[16]); some developed the models under the consumption of dual-porosity/permeability ([17]-[20]); and some utilized the fracture network system to generate stochastic fracture models ([21]-[25]). All these methods are based on assumptions to some extent, and the selection of different methods depends on the specific circumstance.

For the numerically simulation of solute transport in porous media, particle tracking method ([26]-[28]) is an alternative of the classical finite element method (FEM). One of the main advantages of the particle tracking method is that the Peclet constraint on the grid spacing does not apply. The stochastic nature of this method makes it easily keeps away from suffering the pain of numerical dispersion or artificial oscillations, which in the FEM has to be achieved by maintaining fine grids or small time step sizes. Another advantage of the particle tracking method is that it may not require the solution of large system of equations. The computation time is proportional to the number of particles used. As the particles are independent of each other, this calculation can be parallelized. And a further advantage of the particle tracking method is that the velocity distribution used for moving the particles can be obtained from other method (e.g. FEM), thus this method is relatively easy to be combined with flow models.

Therefore, the combination of particle tracking with groundwater flow model in fractured rock was a meaningful attempt. It is difficult to fully describe the solute displacement in fractured rocks because of the randomness and irregularity of the fracture and matrix structure, but the particle tracking method provides a way to consider all possible displacement of the solute due to the statistical nature of the method that the particles can randomly move around to some extent. Some approaches have been devised for using particle tracking method in the simulation of solute transport in fractured rock. Some researchers utilized the particle tracking method in the continuum model ([29]-[31]); some developed the particle tracking method within the fracture-matrix system [32]; and some studied the fracture network system with particle tracking method ([33]-[35]).

In this work, a particle based method was developed for the simulation of velocity distribution of the fluid flow and the concentration distribution of the solute transport in fractured porous media. For the groundwater flow simulation, both dual-porosity/permeability model and single fracture model could be accomplished. For the solute transport simulation, particle tracking method was utilized. The calculation of the flow velocity and the simulation of solute displacement could be combined within one model that the particles took use of the velocity distribution to move in the fractured porous media.

II. NUMERICAL IMPLEMENTATION

This work was carried out on a scientific software platform OpenGeoSys (OGS) which is an open source initiative for numerical simulation of thermo-hydro-mechanical-chemical (THMC) processes in porous and fractured media ([36]-[39]). OGS is designed as an object-oriented platform and the source code is written in C++. Finite Element Method is utilized as a basic concept for most of the problems that OGS can solve.

In the OGS simulation, the basic steps of the solution procedure are independent of the specific processes (defined as PCS in OGS). Several processes can be coupled for solving complex problems. For the simulation of groundwater flow in porous media (PCS named GROUNDWATER_FLOW), Darcy’s law and the law of conservation of mass are considered. And the calculation result of groundwater flow velocity can be utilized for the simulation of mass transport in groundwater (PCS named MASS_TRANSPORT), where the advection-dispersion equation is utilized as control equation.

In this work, an alternative method for solving the solute transport problem in groundwater is presented, which is based on the random walk particle tracking concept. This method does not solve the advection-dispersion equation directly; instead, a finite number of particles are utilized to represent the distribution of the solute in the groundwater. The particles are moved through the domain according to the velocity distribution obtained from the GROUNDWATER_FLOW process. The introduced process is named RANDOM_WALK in OGS simulation ([40],[41]). The RANDOM_WALK process includes several steps, which will be descripted in details below.

A. Information Read in

For the RANDOM_WALK process, an input file named “*.pct” is utilized to set up the properties of the particles, such as the way to generate the random series, the total number of the particles, the initial element index number of the particles, the initial position of the particles, the identity of the particles, the release time of the particles, the initial velocity of the particles, etc.

The details of the input file setting are as follows: there are two ways to generate the random series, “0” stands for different pseudo-random series and “1” stands for same pseudo-random series. The total number of the particles defines how many particles will be utilized in the simulation. The element index number of the particles illustrates in which mesh element the particles are located. The position of the particles is expressed as x-, y-, and z-coordinate in the coordinate system. The identity of the particles is set to be 0 when the particles are free to move in groundwater, 1 when the particles are temporarily absorbed by the porous media, and 2 when the particles are retarded. The release time of the particles defines when the particles are released to the system. The initial velocity of the particles is expressed as v_x, v_y, and v_z in a three dimensional system.

Another input file named “*.mcp” involves other information of the particles, such as the name of the particles and the mobility of the particles. Particles with different names can represent different kind of solute in groundwater. The particles can be defined as immobile when they are utilized to represent the background concentration; otherwise they are defined as mobile.

Note that all the particles are utilized together to represent the solute in groundwater, that the number of the particles can be converted to the solute concentration, and the position of the particles can represent the solute distribution, but the particles are independent from each other that in the numerical calculation each particle is looped over separately.

In the RANDOM_WALK process, firstly the information of the particles is read in from the input files. For each particle, if it is defined as mobile and its release time is smaller than or equal to the current calculation time step, this particle is considered to be released and can be involved in the next calculation steps. The initial properties of the released particles are retrieved.

B. Displacement Calculation

The RANDOM_WALK process takes use of the velocity distribution obtained from the GROUNDWATER_FLOW process to convey the particles. The control equation in this process is not the advection-dispersion equation, but an equation to calculate the particles’ displacement, which can be derived from the stochastic physics in the following way.

The stochastic differential equation can be expressed as [42]

$$x(t_i) = x(t_{i-1}) + v(x(t_{i-1}))\Delta t + Z\sqrt{2D(x(t_{i-1}))\Delta t} \qquad (1)$$

where x is the coordinates of the particle (L), v is the velocity of the particle (ML^{-1}), Δt is the calculation time step (T), D is the hydrodynamic dispersion tensor (L^2T^{-1}), and Z is a random number with a mean of 0 and unit variance.

This equation is equivalent to an expression that is slightly different from the advection-dispersion equation. To be equivalent to the advection-dispersion equation, the velocity should be modified and can be expressed as [43]

$$v_i^* = v_i + \sum_{j=1}^{3} \frac{\partial D_{ij}}{\partial x_j} \qquad (2)$$

with dispersion tensor [44]

$$D_{ij} = \alpha_T |v| \delta_{ij} + (\alpha_L - \alpha_T)\frac{v_i v_j}{|v|} + D_{ii}^d \qquad (3)$$

where δ_{ij} is the Kronecker symbol, α_L is the longitudinal dispersion length (L), α_T is the transversal dispersion length (L), D_{ij}^d is the tensor of molecular diffusion coefficient (L^2T^{-1}), and v_i is the component of the mean pore velocity in the *i*th direction (ML^{-1}).

Thus the equivalent stochastic differential equation to the advection-dispersion equation in three dimensional problems can be written as ([45],[46])

$$
\begin{aligned}
x_{t+\Delta t} &= x_t + \left(v_x(x_t, y_t, z_t, t) + \frac{\partial D_{xx}}{\partial x} + \frac{\partial D_{xy}}{\partial y} + \frac{\partial D_{xz}}{\partial z} \right)\Delta t + \sqrt{2D_{xx}\Delta t}Z_1 + \sqrt{2D_{xy}\Delta t}Z_2 + \sqrt{2D_{xz}\Delta t}Z_3 \\
y_{t+\Delta t} &= y_t + \left(v_y(x_t, y_t, z_t, t) + \frac{\partial D_{yx}}{\partial x} + \frac{\partial D_{yy}}{\partial y} + \frac{\partial D_{yz}}{\partial z} \right)\Delta t + \sqrt{2D_{yx}\Delta t}Z_1 + \sqrt{2D_{yy}\Delta t}Z_2 + \sqrt{2D_{yz}\Delta t}Z_3 \\
z_{t+\Delta t} &= z_t + \left(v_z(x_t, y_t, z_t, t) + \frac{\partial D_{zx}}{\partial x} + \frac{\partial D_{zy}}{\partial y} + \frac{\partial D_{zz}}{\partial z} \right)\Delta t + \sqrt{2D_{zx}\Delta t}Z_1 + \sqrt{2D_{zy}\Delta t}Z_2 + \sqrt{2D_{zz}\Delta t}Z_3
\end{aligned}
\tag{4}
$$

Within one calculation time step, the displacement of the released particle is calculated. It can be seen that the displacement of the particle includes two sections, one is a certain distance caused by advection and dispersion, the other is a “random walk” caused by the method’s intrinsic stochastic nature.

Considering equation (4) together with equation (3), the spatial derivatives of the dispersion coefficients can be expressed as a function of the derivatives of velocity. It can be seen that the calculation of groundwater flow velocity is crucial to this random walk particle tracking method. Especially that, to obtain the derivatives of velocity, velocity has to be continuous mathematically. This is achieved by the way that velocity at any location in an element is interpolated from the known velocity at the element nodes. Note that as previously mentioned, the processes are independent with each other in the OGS simulation, thus the RANDOM_WALK process can be coupled with processes other than GROUNDWATER_FLOW.

C. Boundary Control

After one calculation time step, the new x-, y- and z-coordinate of the particles are obtained from equation (4). Because of the “random walk”, there’s a chance that some particles are on the outside of the calculation domain. In this case, a boundary control is necessary in order to “drag” the particles back in.

To achieve this goal, the first step is to check if one particle has gone outside, which can be implemented with search algorithms. Secondly, regarding the particles which are outside of the calculation domain, an intersection point between the particle’s path line and the domain surface is calculated. Thirdly, the intersection point’s x-, y- and z-coordinate will be assigned to the particle and thus the particles are dragged back to the surface of the calculation domain.

The properties of the particles, e.g., the element index number, the position, and the velocity, will be updated in the memory after the displacement calculation and boundary control. Loop over all the particles and proceed all the calculation time steps, the final information of the particles can be obtained.

III. BENCHMARKS AND SIMULATION RESULTS

A. Strack’s Experiment

Strack [47] developed a numerical model to simulate two dimensional steady flow through infinite fractured porous media with one single crack. The numerical experiment was utilized to verify the flow patterns in a dual-porosity/permeability model with simplified assumptions. In this work, a benchmark was developed according to Strack’s numerical experiment.

The calculation domain is a quadrilateral with constant hydraulic head on the inflow (left) and outflow (right) boundary and with a single line inside to represent the crack which has an angle of 45°with the hydraulic gradient. The numerical solution was computed using FEM to solve steady state liquid flow problem in the dual-porosity/permeability model. The relevant parameters are listed in Table 1.

TABLE I. MODEL PARAMETERS FOR STRACK’S EXPERIMENT

Parameters	***Value***	***Unit***
Porosity of the continuum	0.2	-
Permeability of the continuum	1E-12	m^2
Length of the fracture	2	m
Thickness of the fracture	0.05	m
Porosity of the fracture	0	-
Permeability of the fracture	1E-10	m^2

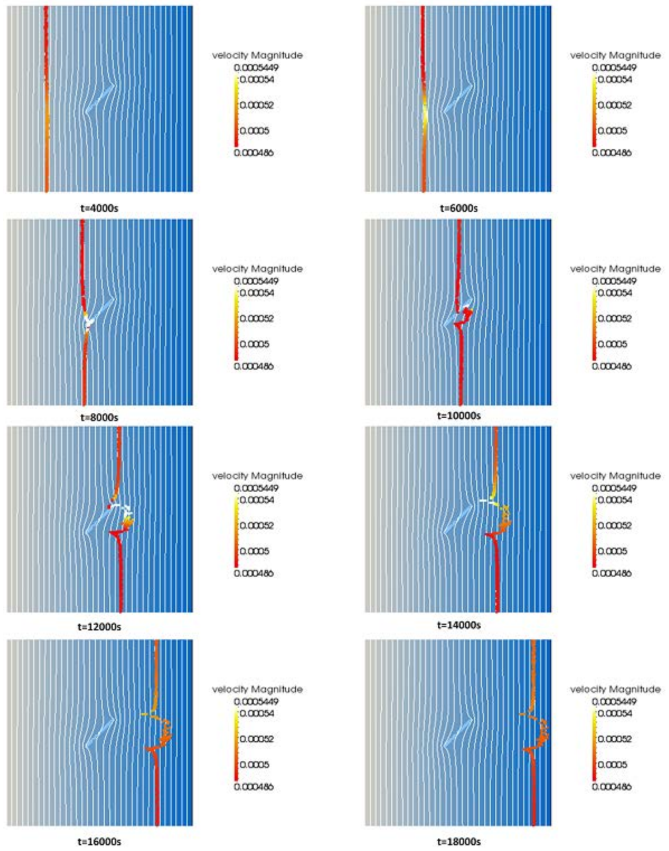

FIGURE I. PARTICLE PLUME DISTRIBUTION IN THE FRACTURED MEDIUM OVER TIME. THE DOTS INDICATE THE POSITION OF PARTICLES AND THE COLORS OF THE DOTS REPRESENT THE VELOCITY OF THE PARTICLES. THE WHITE CURVES AND BACKGROUND COLORS SHOW THE CONTOUR OF THE PRESSURE GRADIENT.

Particles were injected from a thin belt shaped area very close to the inflow (left) boundary to indicate the flow pattern within the domain. The total number of the particles was 500. In the very beginning of the simulation (t=0) all the particles were released at once and the simulation continued for several time steps. The simulation results are shown in Figure 1.

The white curves are the piezometric contours and the dots are the particles. The color of the dots represents the velocity of the particles. It can be seen that the particles moved along the calculation domain according to the velocity distribution. At an early stage of the simulation (Figure 1a-1c), the particles formed a line that is nearly straight. As the particles approaching to the fracture (Figure 1d), a velocity acceleration occurred in the fracture area. This trend became more obvious when the particles passed through the fracture area completely (Figure 1e-1g), and the particles formed a w-shaped plume. At a later stage of the simulation (Figure 1h-1j) the shape of the particle plume didn't change much.

B. Yasuhara's Experiment

In this section a benchmark test was established in order to verify a laboratory experiment operated by Yasuhara ([48],[49]), in which an artificial fracture sample of novaculite was injected with water for a flow-through experiment.

In Yasuhara's experiment, the novaculite sample was split open and the fracture surfaces were profiled. Then the two parts of the rock were mated together again under moderate effective stresses. The fracture structure could be obtained by simply point-by-point subtraction of the upper and lower surfaces, but since these two surfaces were measured separately in an open-book format, it was difficult to match them precisely. Thus in this work, the fracture was defined through geostatistical reproduction by giving a desired mean and standard deviation of the aperture, which can be utilized directly in the hydraulic simulations.

Under the assumption of laminar flow in the fractured rock, permeability is a function of the fracture aperture,

$$k=b^2/12 \tag{5}$$

where k is permeability (L^2) and b is fracture aperture (L).

The fracture aperture model was established by using geostatistical Gaussian simulation method. The mean aperture was 18.5μm in the beginning of the experiment. It was assumed that the aperture probability distribution follows log normal distribution. An exponential type Variogram model was used and the range and sill were obtained by trial and error.

In the numerical mesh, aperture information was assigned to each grid. A series of steady state hydraulic simulations were conducted on the mesh domain by fixing the pressure (345kPa) on the outlet boundary and inflow rate (1mL/min) on the inlet boundary. By comparing the pressure distribution on the inlet boundary with the observation from the experiment (402.02kPa), the best fitted aperture distribution was with range of 6 mm and sill 0.5mm. Relative parameters are listed in Table 2 and the aperture distribution is shown in Figure 2.

With this aperture distribution, steady state groundwater flow distribution can be obtained and the simulation result is shown in Figure 3.

TABLE II. PARAMETERS FOR THE FRACTURE APERTURE MODEL

Parameters	***Value***	***Unit***
Length of mesh domain	89.5	mm
Width of mesh domain	50	mm
Resolution of mesh domain	1	mm
Mean of aperture	18.5	μm
Range of aperture distribution	6	mm

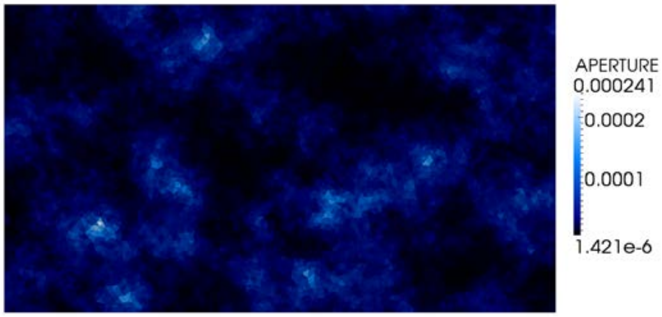

FIGURE II. THE BEST FITTED APERTURE DISTRIBUTION FOR YASUHARA'S EXPERIMENT.

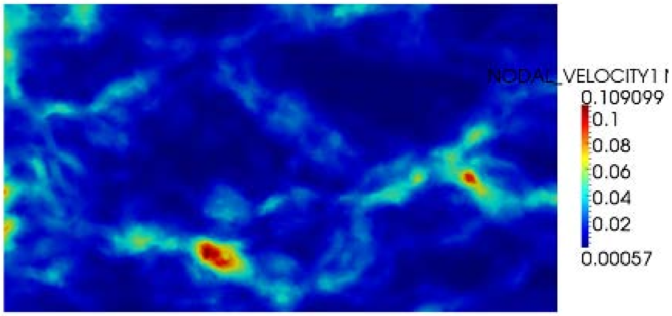

FIGURE III. THE STEADY STATE GROUNDWATER FLOW VELOCITY DISTRIBUTION WITHIN THE FRACTURE.

Based on this fixed steady state hydraulic simulation, the solute transport in the fracture can be simulated. In order to compare the performance of proposed particle tracking method with classical FEM which solves the advection-dispersion equation, two simulations were conducted separately. The simulation results overlaid each other and are shown in Figure 4.

The background color represents the solute concentration and the red dots represent the particles. Comparison between FEM and RWPT shows a good agreement and indicates that the later one allows accounting for realistic features of the transport process.

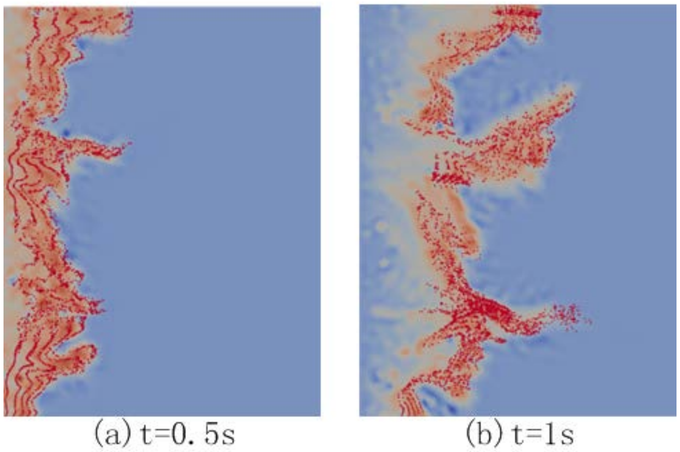

FIGURE IV. COMPARISON OF SIMULATION RESULT OF PARTICLE PLUME OBTAINED BY RWPT (RED DOTS) WITH CONCENTRATION OBTAINED BY FEM (BACKGROUND COLOR GRADIENT)

In the particle tracking simulation, particles were injected from the inlet (left) boundary to simulate the solute transport process in the fracture. The total number of particles injected was 10000 and the particles were injected for a constant time period of 1s.The simulation results of particles plume over time are shown in Figure 5.

The background color represented the groundwater flow distribution and the dots represented the particles. The colors of the particles showed their velocities in groundwater. It can be seen that the complexity of groundwater flow and mass transport in fractured rock can be exhibited by the proposed simulation model. Particles released at different position in the simulation domain experienced very different processes during their journey to the downstream. The particle plume showed the flow pattern, as well as the detailed channeling effects and accelerations or decelerations in some regions. The dense particle plume showed the accumulation of solute mass in the fractured porous media. The tailing phenomenon is also well exhibited.

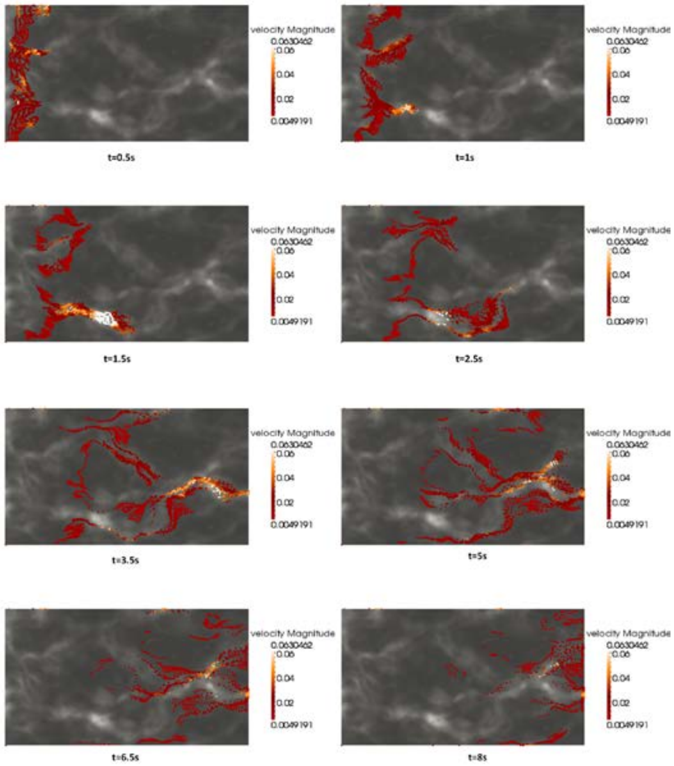

FIGURE V. PARTICLE PLUME DISTRIBUTION IN THE FRACTURE APERTURE OVER TIME. THE DOTS INDICATE THE POSITION OF PARTICLES AND THE COLORS OF THE DOTS REPRESENT THE VELOCITY OF THE PARTICLES

IV. CONCLUSION

The proposed particle tracking based method was numerically implemented in OGS, as a simulation process which is independent from the flow process. For both dual-porosity/permeability model and single fracture model, this method showed very good performance and adaption. Moderate number of particles was utilized in the implementation of two benchmarks. The computation process was not so expensive comparing to the classical FEM. No obvious numerical fluctuations were observed in the simulation.

This proposed method provides a way to consider all possible displacement of the contaminant in the fractures due to the statistical nature of the method that the particles can randomly move around to some extent. The method can be applied as a tool to observe the detailed structure of evolving contaminant plumes in fractured rock.

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REFERENCES

[1] Kalbacher T, Mettier R, McDermott C, Wang W, Kosakowski G, Taniguchi T, Kolditz O (2007) Geometric modelling and object oriented software concepts applied to a heterogeneous fractured network from the Grimsel rock laboratory. Comput Geosci 11(1):9–26

[2] Jaffre´J and Roberts JE (2012) Modeling Flow in Porous Media with Fractures: Discrete Fracture Models with Matrix-Fracture Exchange. Numerical Analysis and Applications 5(2): 162–167

[3] Marina S, Derek I, Mohamed P, Yong S, Imo-Imo EK (2015) Simulation of the hydraulic fracturing process of fractured rocks by the discrete element method. Environ Earth Sci 73(12): 8451-8469

[4] Martin L, Auli N, Chin-Fu T (2012) A study of flow-wetted surface area in a single fracture as a function of its hydraulic conductivity distribution. Water Resour Res 48(1):239-249

[5] Kristinof R, Ranjith PG, Choi SK (2010) Finite element simulation of fluid flow in fractured rock media. Environ Earth Sci 60(4):765-773

[6] Müller C, Siegesmund S, Blum P (2010) Evaluation of the representative elementary volume (REV) of a fractured geothermal sandstone reservoir. Environ Earth Sci 61(8):1713-1724

[7] McDermott C, Bond A, Harris AF, Chittenden N, Thatcher K (2015) Application of hybrid numerical and analytical solutions for the simulation of coupled thermal, hydraulic, mechanical and chemical processes during fluid flow through a fractured rock. Environ Earth Sci 74:7837–7854

[8] Tan Y, Zhou Z (2008) Simulation of solute transport in a parallel single fracture with LBM/MMP mixed method. Journal of Hydrodynamics 20(3):365–372

[9] Pan P, Feng X, Xu D, Shen L, Yang J (2011) Modelling fluid flow through a single fracture with different contacts using cellular automata. Computers and Geotechnics 38(8):959–969

[10] Chen Z, Qian J, Qin H (2011) Experimental study of the non-Darcy flow and solute transport in a channeled single fracture. Journal of Hydrodynamics 23(6):745–751

[11] Baykasoglu C, Mugan A (2012) Nonlinear fracture analysis of single-layer graphene sheets. Engineering Fracture Mechanics 96:241–250

[12] Li JC, Li HB, Zhao J (2014) Study on wave propagation across a single rough fracture by the modified thin-layer interface model. Journal of Applied Geophysics 110:106–114

[13] Zou L, Jing L, Cvetkovic V (2015) Roughness decomposition and nonlinear fluid flow in a single rock fracture. International Journal of Rock Mechanics and Mining Sciences 75:102–118

[14] Settgasta RR, Rashidb MM (2009) Continuum coupled cohesive zone elements for analysis of fracture in solid bodies. Engineering Fracture Mechanics 76(11):1614–1635

[15] Prabhakar P, Waas AM (2013) A novel continuum-decohesive finite element for modeling in-plane fracture in fiber reinforced composites. Composites Science and Technology 83:1–10

[16] Wassing BBT, van Wees JD, Fokker PA (2014) Coupled continuum modeling of fracture reactivation and induced seismicity during enhanced geothermal operations. Geothermics 52:153–164

[17] Neretnieks I (2007) Fast method for simulation of radionuclide chain migration in dual porosity fracture rocks. Journal of Contaminant Hydrology 88(3–4):269–288

[18] Ranjbar E, Hassanzadeh H, Chen Z (2011) Effect of fracture pressure depletion regimes on the dual-porosity shape factor for flow of compressible fluids in fractured porous media. Advances in Water Resources 34(12):1681–1693

[19] Guo J, Nie R, Jia Y (2012) Dual permeability flow behavior for modeling horizontal well production in fractured-vuggy carbonate reservoirs. Jour of Hydrol 464–465:281–293

[20] Fahs H, Hayek M, Fahs M, Younes A (2014) An efficient numerical model for hydrodynamic parameterization in 2D fractured dual-porosity media. Advances in Water Resources 63:179–193

[21] Jafari A and Babadagli T (2012) Estimation of equivalent fracture network permeability using fractal and statistical network properties. Journal of Petroleum Science and Engineering 92–93(4):110–123

[22] Reeves DM, Parashar R, Pohll G, Carroll R, Badger T, Willoughby K (2013) The use of discrete fracture network simulations in the design of horizontal hill slope drainage networks in fractured rock. Engineering Geology 163:132–143

[23] Benedetto MF, Berrone S, Pieraccini S, Scialò S (2014) The virtual element method for discrete fracture network simulations. Computer Methods in Applied Mechanics and Engineering 280:135–156

[24] Ezulike DO and Dehghanpour H (2014) A model for simultaneous matrix depletion into natural and hydraulic fracture networks. Journal of Natural Gas Science and Engineering 16:57–69

[25] Vujević K, Graf T, Simmons CT, Werner AD (2014) Impact of fracture network geometry on free convective flow patterns. Advances in Water Resources 71:65–80

[26] Prickett TA, Naymik TG, Lonnquist CG (1981) A “random-walk” solute transport model for selected groundwater quality evaluations. Illinois State Water Survey Bulletin 65, 103p

[27] Tompson AFB and Gelhar LW (1990) Numerical simulation of solute transport in three dimensional, randomly heterogeneous porous media. Water Resour Res 26(10):2541–2562

[28] LaBolle EM, Fogg GE, Tompson AFB (1996) Random-walk simulation of transport in heterogeneous porous media: Local mass-conservation problem and implementation methods. Water Resour Res 32(3):583–593

[29] Ding J, Chen F, Wu SE (2012) A novel particle tracking scheme for modeling contaminant transport in a dual-continua fractured medium. Water Resour Res 48(10):130-140

[30] Grindrod P, Lee AJ (1997) Colloid migration in symmetrical non-uniform fractures: particle tracking in three dimensions. Journal of Contaminant Hydrology 27(3–4):157–175

[31] Hassan AE and Mohamed MM (2003) On using particle tracking methods to simulate transport in single-continuum and dual continua porous media. Jour of Hydrol 275:242–260

[32] Willmann M, Lanyon GW, Marschall P, Kinzelbach W (2013) A new stochastic particle-tracking approach for fractured sedimentary formations. Water Resour Res 49(1):352–359

[33] Roubinet D, Dreuzy JR, Tartakovsky DM (2013) Particle-tracking simulations of anomalous transport in hierarchically fractured rocks. Computers & Geosciences 50:52–58

[34] Zhao Z, Rutqvist J, Leung C et al (2013) Impact of stress on solute transport in a fracture network: A comparison study. Journal of Rock Mechanics and Geotechnical Engineering 5(2):110–123

[35] Stalgorova E, Babadagli T (2015) Modified Random Walk–Particle Tracking method to model early time behavior of EOR and sequestration of CO2 in naturally fractured oil reservoirs. Journal of Petroleum Science and Engineering 127:65–81

[36] Kolditz O and Bauer S (2004) A process-oriented approach to computing multi-field problems in porous media. Jour of Hydroinfor 6:225–244

[37] Kolditz O, Bauer S, Bilke L, Boettcher N, Delfs JO, Fischer T, Goerke UJ, Kalbacher T, Kosakowski G, McDermott CI, Park CH, Radu F, Rink K, Shao H, Shao HB, Sun F, Sun YY, Singh AK, Taron J, Walther M, Wang W, Watanabe N, Wu Y, Xie M, Xu W, Zehner B (2012a) OpenGeoSys: an open-source initiative for numerical simulation of thermo-hydro-mechanical/chemical (THM/C) processes in porous media. Environ Earth Sci 67(2):589–599

[38] Kolditz O, Goerke U, Shao H, Wang W (2012b) Benchmarks and examples for Thermo- Hydro-Mechanical-Chemical processes in porous media. Springer, Berlin

[39] Kolditz O, Shao H, Wang W, Bauer S, et al (2015) Thermo-Hydro-Mechanical-Chemical Processes in Fractured Porous Media: Modelling and Benchmarking. Springer, Switzerland

[40] Sun Y (2013) Water Quality Simulation with Particle Tracking Method. Dissertation, TU Dresden

[41] Sun Y, Park CH, Pichot G and Taron J (2015) RandomWalk Particle Tracking. In: Kolditz O et al (eds) Thermo-Hydro-Mechanical-Chemical Processes in Fractured Porous Media: Modelling and Benchmarking, Terrestrial Environmental Sciences, pp 153-184, DOI 10.1007/978-3-319-11894-9_6

[42] Ito K (1951) On stochastical differential equations. American Mathematical Society 4:289–302

[43] Kinzelbach W (1986) Groundwater Modelling. Elsevier, Amsterdam

[44] Bear J (1979) Hydraulics of groundwater. McGraw-Hill, New York

[45] Kinzelbach W (1988) The random-walk method in pollutant transport simulation. NATO ASI Ser, C224:227–246

[46] Hoteit H, Mose R, Younes A, Lehmann F, Ackerer Ph (2002) Three-dimensional modeling of mass transfer in porous media using the mixed hybrid finite elements and the random walk methods. Mathe Geology 34(4):435–456

[47] Strack ODL (1982) Assessment of effectiveness of geologic isolation systems: Analytic modeling of flow in a permeable fissured medium. Technical report, Pacific Northwest Lab, Richland, WA

[48] Yasuhara H, Polak A, Mitani Y, Grader A, Halleck P, Elsworth D (2006a) Evolution of fracture permeability through fluid-rock reaction under hydrothermal conditions. Earth and Planetary Science Letters 244:186-200

[49] Yasuhara H and Elsworth D (2006b) A numerical model simulating reactive transport and evolution of fracture permeability. Int J Numer Anal Meth Geomech 30:1039–1062