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Numerical investigation of nanoparticles transport in anisotropic porous media

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Abstract

In this work the problem related to the transport of nanoparticles in anisotropic porous media is investigated numerically using the multipoint flux approximation. Anisotropy of porous media properties are an essential feature that exist almost everywhere in subsurface formations. In anisotropic media, the flux and the pressure gradient vectors are no longer collinear and therefore interesting patterns emerge. The transport of nanoparticles in subsurface formations is affected by several complex processes including surface charges, heterogeneity of nanoparticles and soil grain collectors, interfacial dynamics of double-layer and many others. We use the framework of the theory of filtration in this investigation. Processes like particles deposition, entrapment, as well as detachment are accounted for. From the numerical methods point of view, traditional two-point flux finite difference approximation cannot handle anisotropy of media properties. Therefore, in this work we use the multipoint flux approximation (MPFA). In this technique, the flux components are affected by more neighboring points as opposed to the mere two points that are usually used in traditional finite volume methods. We also use the experimenting pressure field approach which automatically constructs the global system of equations by solving multitude of local problems. This approach facilitates to a large extent the construction of the global system. A set of numerical examples is considered involving two-dimensional rectangular domain. A source of nanoparticles is inserted in the middle of the anisotropic layer. We investigate the effects of both anisotropy angle and anisotropy ratio on the transport of nanoparticles in saturated porous media. It is found that the concentration plume and porosity contours follow closely the principal direction of anisotropy of permeability of the central domain.

Keywords: Nanoparticles transport, anisotropic porous media, filtration theory, Multipoint flux approximation.

1. Introduction

Nanomaterials (Auffan et al. 2009) have emerged to our environment without being alerted to their environmental impacts or even get prepared to, legislatively, dealing with

their emergence. These materials have been in production for decades and therefore parts of their volume have eventually reached our disposal facilities and start to transport in our different environmental compartments (Air, Water and Soil), Lin et al. 2010. In countries, where significant amount of nano-materials (e.g., Silver oxide, Zinc oxide nanoparticles) are produced for their production of household appliances (e.g., washing machines, purifiers, cosmetics, etc.), concerns were raised about the fate of these materials in their local environment. Zinc oxide nanoparticles, for example, have been extensively used in electronics, cosmetics (e.g., sunscreens, tooth paste, deodorants) and many other industries, Moezzi et al., 2012, Kurlanda-Witek et al., 2014. Zinc oxide, like Silver oxide, has antimicrobial effects which favor its use in cosmetic industries. Ma et al., 2013, have studied the toxicity of exposure of living organism to ZnO nanoparticles and reported that even low level exposure may be toxic to many species including plants, animals and bacteria. Therefore, concerns have risen about their probable effects on several useful bacteria (e.g., used in activated sludge) that are part of our eco-system. No wonder, therefore, the many recent studies on the mechanisms controlling the transport of nanoparticles and their fate, Klaine et al. 2008, Phenrat et al. 2010, Abraham et al. 2013, Goldberg et al. 2014, Sygouni et al. 2014, Sygouni and Chrysikopoulos 2015, and many others.

On the other hand, nanomaterials have been extensively used in petroleum-related industries. They have been applied to reservoir exploration, drilling and completion, production and improved oil recovery as well as refinery (Evdokimov et al., 2006, Pourafshary et al., 2009; Kong et al., 2010, Friedheim et al. 2012, El Amin et al., 2012). In reservoir exploration, nano-sensors and nano-composites can provide more accurate measurement of reservoir conditions (Prodanović et al., 2010, Alaskar et al., 2014). In upstream petroleum industry, functionalized nanomaterials have been introduced to subsurface reservoirs to alter wettability conditions of the host rock to facilitate displacing more oil. Nanoparticles have also been used as tracers to test and manage oil field operations. They have been introduced to cement materials used during drilling and completion, to increase compressive and flexural strength and decrease the weight (Xu et al., 2003). In shale gas technology, nanoparticle coated proppant used in hydraulic fracturing can successfully reduce fines migration in reservoirs near production wells.

All this and many others suggest that serious investigations on the fate and transport of nanoparticle in the environment need to be carried out. Despite the large number of research works that have been conducted to study transport of nanoparticles in porous media, they mostly abide to homogeneous, isotropic materials. Although this may give us a clue on the movement of nanomaterials in the subsurface, they hinder important effects related to the fact that naturally occurring porous media are in most cases anisotropic. In other words, correct understanding of the transport of nanomaterials in porous media

must consider anisotropy of media properties. In fact, Cullen et al. (2010) pointed out that much of the simulation work that has been done to date on the transport of nanoparticles in porous media has focused on one-dimensional investigations. They considered the simulation of the transport of carbon nanoparticles in two-dimensional, layered heterogeneous domain. Clearly, however, to account for full permeability tensor in the simulation of nanoparticles transport poses difficulties to numerical schemes and a search for a robust technique is still ongoing. Although the popular finite elements and finite volume methods can generally handle anisotropy of permeability field, they are relatively complex to formulate. On the other hand, two point flux finite difference approximation, which is the simplest of all, cannot handle but diagonal permeability tensor. In order to extend the use of cell-centered finite difference to encounter full permeability tensor a number of heuristic approaches have been assumed. Only recently that a rigorous derivation of finite difference approximation to fluxes have been developed based on the multipoint flux approximations. Two approaches have been suggested the first has been based on defining interacting sub-volumes and the second is based on the mixed finite element formulation using BDM spaces. In this case the flux vector at the center of each cell face is affected by six neighboring pressure values in 2D problems and eighteen pressure values in 3D case. The evaluation of the finite difference stencil for this case requires determining 6 coefficients in 2D problems (18 in 3D), which is a cumbersome task. Lately, Sun et al. 2012, and Salama et al., 2014, developed a technique whereby these coefficients are determined automatically by the solving local problems over each single cell. Solving multitude of local problems is by far much simpler than constructing the complex stencil such that the global system of equations is obtained. This technique has been used with success to study different problems related to single and two-phase flows in porous media.

The general framework of the theory of filtration has been suggested as appropriate to study transport of nanomaterial in the environment. In this theory, three patterns of flow conditions have been proposed. In the first, the sizes of particles are comparable to or larger than the size of the grains of porous media. In this case, particles will build a filter cake at the medium surface resulting in the permeability of the medium to significantly reduce. In the second flow pattern, particles are of medium sizes, i.e., not much smaller than the media grain. In this case, particles will be removed mechanically by straining at smaller pore throats. Likewise, this results in reduction of the permeability of the medium, albeit, less drastic as compared to that of filter cake. In the third regime, particles sizes are several orders of magnitude smaller than media grains. In this case, only physicochemical processes can retain the particles. Such processes include, for example, surface roughness of soil grain collectors, interfacial dynamics of double-layer in particle-particle and particle-collector interactions, surface charge heterogeneity of nanoparticles and soil grain collectors, and many others. In addition, nanoparticles are manufactured with different properties (i.e., size, shape, and agglomeration state) which definitely influence their

transport, Petosa et al. (2010), Ryan and Elimelech (1996). During physicochemical filtration, the interactions between neighboring nanoparticles and between particles and medium surfaces will determine particle stability and retention during transport. In this flow regime, the retained particles will not block any pore throat and the permeability reduction is negligible. In this work, we are particularly interested in investigating the transport of nanoparticles in porous media. We highlight the role of permeability anisotropy on the transport of nanoparticles. A number of numerical experiments are carried out.

2. Transport models of nanoparticles

Two approaches are commonly used to study the transport of nanoparticles in porous media. In the first approach (Lagrangian method) the particles are tracked and are coupled with the flow equations via interaction terms (Yao et al., 1971; Rajagopalan and Tien, 1976; Logan et al., 1995; Cushing and Lawler, 1998; Tufenkji and Elimelech, 2004). In the other approach (Eulerian methods) the nanoparticles are not tracked and a balance equation for the mass of the particles is derived. A filtration term is added to the advection-dispersion equation to account for nanoparticle transport and deposition process. Since, in this work, we are following the Eulerian approach more detail about the filtration model is given, for the sake of completion.

2.1 Review of filtration theory

Several models have been developed by several authors to study transport of nanoparticles in saturated porous media including Johnson and Elimelech 1995, Tufenkji and Elimelech 2004, 2005, Schijven et al. 2002, Bradford et al. 2003, 2004, 2012, Foppen et al. 2007, Kasel et al. 2013, Gargiulo et al. 2007. Goldberg et al. (2014) have recently reviewed a number of these models. They categorized them according to the mechanisms involved in the transport processes, including deposition (fast and slow), remobilization, blocking, etc. These models vary in their complexity according to the assumptions considered. Goldberg et al. (2014) indicated that, complex models do not necessarily imply better predictive capabilities than simpler ones. The mechanisms affecting the transport of nanoparticles in porous media, in addition to the conventional advection-dispersion mechanism, include retardation, detachment, site blocking, and a combination of them. The general advection-dispersion equation in porous media may be written as:

$$\phi \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c - \mathbf{D}\nabla c) = R + q_c \quad (1)$$

where c is the concentration of nanoparticles, $\mathbf{u}$ is Darcy velocity, ϕ is the porosity, $\mathbf{D}$ is the dispersion tensor, R accounts for mass insertion or depletion due to chemical reaction, and q_c is a source/sink term. In filtration theory the migration of fines is accompanied by

deposition and is incorporated into the governing balance equation by adding the rate at which the mass is deposited to the mass accumulation term (Bedrikovetsky et al., 2003, Benamar et al., 2007), such that:

$$\frac{\partial c}{\partial t} + \frac{\rho_b}{\phi} \frac{\partial s}{\partial t} = -\nabla \cdot (\mathbf{uc} - \mathbf{D}\nabla c) + R + q_c \quad (2)$$

where ρ_b is the solid bulk density, s is the concentration at the surface. Such deposition rate is modeled as

$$\frac{\rho_b}{\phi} \frac{\partial s}{\partial t} = k_{dep} c \quad (3)$$

where k_d is particle deposition coefficient [1/T] which depends on the flow velocity. In this approach, the deposition is assumed irreversible and s can grow indefinitely. Many authors have used this approach. To account or possible retardation of nanoparticles, He et al., 2009, proposed a model of the form:

$$\left(1 + \frac{\rho_b k_d}{\phi}\right) \frac{\partial c}{\partial t} = -\nabla \cdot (\mathbf{uc} - \mathbf{D}\nabla c) - k_{dep} c \quad (4)$$

where k_d [L³/M] is the distribution coefficient.

To account for site blocking, Cullen et al., 2010 suggested that the rate of nanoparticles deposition takes the form:

$$\frac{\rho_b}{\phi} \frac{\partial s}{\partial t} = k_{dep} \left(1 - \frac{s}{s_{max}}\right) c \quad (5)$$

where s_{max} is the maximum retention capacity. To account for detachment of particles, Bradford et al. (2002) suggested

$$-\frac{\partial \rho_b s}{\partial t} = -\phi k_{att} c + \rho_b k_{det} s \quad (6)$$

k_{att} [T⁻¹] is the first order colloid attachment coefficient, k_{det} is the first-order colloid detachment coefficient.

2.2 Transport of nanoparticles in anisotropic porous media

In this work, we investigate the transport of nanoparticles in anisotropic porous media. Anisotropy of porous media is ubiquitous in almost all subsurface formations due to the several physiochemical and mechanical processes that took place over the longer geologic time scale, Fig. 1. Anisotropy in porous media manifests itself through the relationship between the flux and the pressure gradient vectors which are no longer coincident, Fig. 2.

As stated earlier, Cullen et al. 2010 investigated the transport of carbon nanoparticles in a two dimensional heterogeneous porous medium rectangular domain. They also considered a special case of anisotropy where the coordinate system aligns with the principle direction of anisotropy. In this case, the permeability tensor is diagonal and even the simple two-point flux approximation can be used. To account for the cross flow potential arisen from the off diagonal terms of the permeability tensor, a more sophisticated algorithms need to be devised, Arnaldsson et al., 2014, including the multipoint flux approximation as will be explained later.

The governing equations that describe flow and transport in porous media are based on the foundations of the continuum hypothesis in which macroscopic field variables are continuous functions of space and time, Salama and Van Geel (2008a, b). This allows the governing balance equations to be described in the form of differential equations. Therefore, we have

Mass conservation:

$$\nabla \cdot \mathbf{u} = 0 \quad (7)$$

Darcy's law:

$$\mathbf{u} = -\frac{\mathbf{K}}{\mu}(\nabla p - \rho \mathbf{g}) \quad (8)$$

where $\mathbf{K}$ is the permeability tensor, μ is the fluid viscosity, ρ is the fluid density and $\mathbf{g}$ is the gravity. The transport of nanoparticles in size interval i is governed by, (Ju et al., 2002, Ju and Fan, 2009, Liu and Civan, 1994, El-Amin et al., 2012a,b, 2013, 2015),

$$\phi \frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{u} c_i - \phi \tau \mathbf{D} \nabla c_i) = R_i + Q_{c_i}, \quad i = 1, 2, \dots, n \quad (9)$$

Here c_i is the concentration of nanoparticles in interval i , $\mathbf{D} = \mathbf{D}^{\text{disp}} + D^{Br}$ is a second order tensor that accounts for both hydrodynamic dispersion, $\mathbf{D}^{\text{disp}}$, and Brownian diffusion, D^{Br} (Zhang, 2012), such that

$$\mathbf{D}^{\text{disp}} = d_{t,w} |\mathbf{u}| \mathbf{I} + (d_{l,w} - d_{t,w}) \frac{\mathbf{u} \mathbf{u}}{|\mathbf{u}|} \quad (10)$$

and

$$D_i^{Br} = \frac{k_B T}{3\pi \mu d_{p,i}} \quad (11)$$

R_i is the net rate of loss of nanoparticles in interval i . In this model we follow the model of Gruesbeck and Collin (1982) of in which the rate of loss of nanoparticles:

$$R_i = \frac{\partial s_{1i}}{\partial t} + \frac{\partial s_{2i}}{\partial t} \quad (12)$$

Modified Gruesbeck and Collin's model for the surface deposition:

$$\frac{\partial s_{1i}}{\partial t} = \begin{cases} \gamma_{di} |\mathbf{u}| c_i, & |\mathbf{u}| \leq u_c \\ \gamma_{di} |\mathbf{u}| c_i - \gamma_{ei} (|\mathbf{u}| - u_c) s_{1i}, & |\mathbf{u}| > u_c \end{cases} \quad (13)$$

In Eq. 13 γ_{di} and γ_{ei} are rate coefficients for surface retention and entrainment of nanoparticles in interval i , respectively. In this model, when the magnitude of the velocity is less than a predefined critical value, the nanoparticles deposits over the pore space. It also manifests the fact that the deposition increases with the increase of the velocity magnitude as long as it is less than the critical velocity. Rate of entrapment of the nanoparticles is calculated using:

$$\frac{\partial s_{2i}}{\partial t} = \gamma_{pt,i} |\mathbf{u}| c \quad (14)$$

Porosity variation:

$$\phi = \phi_0 - \sum \delta \phi_i \quad (15)$$

where $\sum \delta \phi_i = s_{1i} + s_{2i}$. Permeability variation is calculated using

$$\mathbf{K} = \mathbf{K}_0 \left[(1 - f) k_f + f \frac{\phi}{\phi_0} \right]^l \quad (16)$$

where $\mathbf{K}_0$ and ϕ_0 are initial permeability and porosity, f is called flow efficiency factor and is calculated as

$$f = 1 - \gamma_f s_2 \quad (17)$$

3. Numerical algorithm

Since, in this work, the permeability is considered full tensor, we use the multipoint flux approximation which is suited to handle full permeability tensor. We also adapt the experimenting field approach developed by Sun et al. (2012) which solves a set of local problems and construct the global system automatically, Salama et al. 2014. This scheme has been rigorously tested against a number of cases in both single and two-phase systems including anisotropy, e.g., Osman et al. 2012, Salama et al. 2013, Negara et al. 2013, 2015, Salama et al. 2015. Multipoint flux approximation has grown following two independent routes. The first route is based on control volume approximation by further dividing each finite volume cell into a number of interacting volumes by bisecting each edge (in 2D problems) and assign flux vector to each portion of the edge. This has been the approach

adapted by Aavatsmark et al. 1998, Aavatsmark 2002 and many others. The second route has been based on mixed finite element settings on BDM space, Brezzi et al. 1985, Wheeler et al. 2006 and many others. By adapting certain quadrature rules to approximate integrals, an equivalent MPFA stencil could be obtained. Utilizing this technique over structured grid generates MPFA which is suited to cell-centered finite difference approximation. However, the MPFA stencil is quite complicated to obtain. For example, the stencil for flux approximation and for divergence calculations in 2D involves 6 and 9 neighboring points, respectively. Figure 3 shows the 6 points associated with the calculations of the flux in 2D domain. In this case the x-component of the flux, for example, may be expressed in the form:

$$v_x = a_1 p_1 + a_2 p_2 + a_3 p_3 + a_4 p_4 + a_5 p_5 + a_6 p_6 \quad (18)$$

where the coefficients in the above equation include both the discretization and the permeability information. It is worth mentioning, however, that it is relatively cumbersome to derive expression for these coefficients. In the experimenting field approach, such coefficients are calculated by solving multitude of local problems which is much easier. To calculate such coefficients a set of predefined experimenting pressure fields are used. Such fields are designed such that when operating over the local problems, the global matrix coefficients are obtained. The local problem for the multipoint flux is defined for each node of the Cartesian grid as shown in Fig. 4, therefore, for the node i,j (Fig. 4) it may be written as

$$A[v_x^-, v_y^+, v_x^+, v_y^-]^T = B[p_1, p_2, p_3, p_4]^T \quad (19)$$

where

$$[A]_{ij} =$$

$$\frac{1}{4} \begin{bmatrix} \frac{k_{yy}^{E_1}}{\det E_1} A^{E_1} + \frac{k_{yy}^{E_2}}{\det E_2} A^{E_2} & -\frac{k_{xy}^{E_2}}{\det E_2} A^{E_2} & 0 & -\frac{k_{xy}^{E_1}}{\det E_1} A^{E_1} \\ -\frac{k_{xy}^{E_2}}{\det E_2} A^{E_2} & \frac{k_{xx}^{E_2}}{\det E_2} A^{E_2} + \frac{k_{xx}^{E_3}}{\det E_3} A^{E_3} & -\frac{k_{xy}^{E_3}}{\det E_3} A^{E_3} & 0 \\ 0 & -\frac{k_{xy}^{E_3}}{\det E_3} A^{E_3} & \frac{k_{yy}^{E_3}}{\det E_3} A^{E_3} + \frac{k_{yy}^{E_4}}{\det E_4} A^{E_4} & -\frac{k_{xy}^{E_4}}{\det E_4} A^{E_4} \\ -\frac{k_{xy}^{E_1}}{\det E_1} A^{E_1} & 0 & -\frac{k_{xy}^{E_4}}{\det E_4} A^{E_4} & \frac{k_{xx}^{E_1}}{\det E_1} A^{E_1} + \frac{k_{xx}^{E_4}}{\det E_4} A^{E_4} \end{bmatrix} \quad (20)$$

and

$$[B]_{ij} = \frac{1}{2} \begin{bmatrix} \Delta y_{E_1} & -\Delta y_{E_1} & 0 & 0 \\ 0 & \Delta x_{E_2} & -\Delta x_{E_2} & 0 \\ 0 & 0 & -\Delta y_{E_3} & \Delta y_{E_3} \\ \Delta x_{E_4} & 0 & 0 & -\Delta x_{E_4} \end{bmatrix} \quad (21)$$

Here A^{E_i} , Δx_{E_i} and Δy_{E_i} are the area, the horizontal and vertical length of cell E_i , respectively, and det is the determinant of the hydraulic conductivity tensor of each cell. This generates a system of algebraic equations in the pressure which can be written in a matrix form as

$$Cp=b \quad (22)$$

where C is the matrix of coefficients, p is the vector of the unknown pressure field and b is the right hand side vector which includes the source term and the boundary condition. Figure 5 shows flow chart of the solution steps using the experimenting pressure field approach to calculate the pressure and velocity fields.

4. Numerical examples

To investigate the effects of anisotropy on the transport of nanoparticles, we consider a set of 2D numerical experiments. A rectangular domain consisting of three zones, with the middle zone considered anisotropic, is studied. A number of scenarios of anisotropy inclination of the middle layer are considered; including 30°, 45°, 60° and 135°, Fig. 6. Nanoparticles are introduced to the domain within the middle layer as a source term of intensity 10^{-6} 1/s for single size particles and four different source intensities for the multiple size nanoparticles, as given in Table 2. The left boundary is assigned velocity boundary condition of 10^{-6} m/s, the right boundary is assigned pressure boundary condition of 1 bar and the top and bottom boundaries are considered no flow. Table 1 lists the values of the parameters considered in this research. A set of verification examples on the use of the multipoint flux technique in anisotropic media can be found elsewhere (e.g., Salama et al., 2013, and Salama et al., 2015).

5. Results and discussion

In this work, nanoparticles are injected in the middle domain (Fig. 6) at constant rate. The system is forced to flow by imposing velocity boundary condition at the left boundary. Initially the permeability field is given such that the middle layer is anisotropic with the principal axis direction and anisotropy ratio predefined. The nanoparticles are assumed not affecting the flow field allowing, thereby, the decoupling of flow and transport equations. As a result of nanoparticles deposition, the volume of the void space available for flow decreases with time and therefore, the permeability also decreases. Since the velocity is set constant at the left boundaries, the average pressure changes as a consequence of both anisotropy and the decrease of permeability with time. The

anisotropy of the middle layer has interesting consequence on the flow, pressure, concentration, and porosity fields. In this section we highlight these effects on the different scenarios. We consider two parameters defining the anisotropy; namely the angle the principle direction of anisotropy is making with the x-axis and the anisotropy ratio, which is the ratio between the anisotropy components in the principle directions (i.e. $\pi = k_{11}/k_{22}$). The different anisotropy angles considered in this work are 30°, 45°, and 60°. It is noteworthy that scenarios with angles 150°, 135° and 120° will generate exactly same results imaged across the x-axis. We also consider two different anisotropy ratios; namely 4 and 10. To account for the fact that nanoparticles are composed of a range of sizes rather than single size particles, we consider a combination of 4 different sizes. The presentations of results include highlighting the effect of the different anisotropy angles on the contours of pressure, porosity, concentration and the permeability fields. In all these cases we compare these profiles together with the isotropic scenario. Furthermore, we also consider comparisons between two anisotropic scenarios with and without effects on porosity and permeability fields.

5.1 Single size nanoparticles

5.1.1 Effects of anisotropy angle

In the isotropic scenario the whole domain is considered isotropic and homogeneous with respect to the permeability and porosity fields. It is clearly expected that at the start of simulation, uniform pressure and velocity fields is obtained. As the deposition starts to accumulate nanoparticles in the pore space and both the porosity and permeability deteriorate, the pressure and velocity fields slightly deform as depicted in Fig. 7-a. This figure shows an update of the pressure and velocity fields after 1 day of simulation time. At that time the porosity has dropped, approximately 12% which show slight change in the pressure and velocity fields. For all the anisotropic scenarios the pressure fields distort with the direction of anisotropy, Fig. 7-a. Moreover the pressure field at the inlet changes from being uniform along the left boundary as will be explained later. The anisotropic middle region also distorts the velocity fields inside the domain. In particular, velocity vectors align more along with the direction of anisotropy as also depicted in Fig. 7-a. After 1 day of nanoparticles injection, the concentration, porosity and permeability fields closer to the injection source change. That is the increased deposition of nanoparticles into the pore space decreases the porosity and likewise the permeability. This effect results in an increase of the required pressure to maintain the same velocity at the inlet as will be highlighted later.

Figure 7-b shows the contours of concentration of nanoparticles for the different scenarios after 1 day of injection. For the isotropic case, the nanoparticles plume is elongated along the direction of the flow compared with that normal to the flow as a result of dispersion. For the anisotropy scenarios where the principal direction of the permeability is inclined off the x-axis, the flow in the middle layer changes from being uniform to being inclined following the direction of anisotropy. This clearly derives concentration plume to become

inclined along the anisotropy direction. Furthermore, the inclination of the plume increases with the increase of the anisotropy angle. Porosity contours follow similar behavior for the different scenarios as depicted in Fig. 7-c. It is worthy to indicate that the minimum porosity in the middle of the domain decreases with the increase of anisotropy angle.

Fig. 7-d shows the x-component permeability field in the domain. In the isotropic scenario, the permeability field is uniform except where the plume exists. In the three anisotropic scenarios the whole middle strip has been considered anisotropic. In these scenarios the permeability in the center of the domain reduces as a result of the deposition of nanoparticles. Also the permeability decreases with the increase of anisotropy angle.

On comparing the evolution of the average pressure at the inlet for the different anisotropy cases ($\pi = 10$) with time, (Fig. 8), one notices two things; first the average pressure at the inlet at the start of simulations is larger the larger the anisotropy angle which is a manifestation of the decrease of effective permeability. Second, the average inlet pressure increases with time because of the decrease of permeability and to maintain the constant flux condition. Figure 9 shows the evolution of minimum porosity with time for the different anisotropy scenarios. It is clear from this figure that the minimum porosity decreases with time as a consequence of the increase of deposition of nanoparticles. Furthermore, the minimum porosity curves are different for different anisotropy conditions (smaller the larger the anisotropy). This is also manifested in Fig. 10 which shows profiles of porosity along the height of the middle domain after 1 day of simulation time. In this figure, the porosity is the least the larger the anisotropy. Figure 11, on the other hand, shows comparisons of the concentration profiles along the middle layer height. Based on this figure, the concentration is higher for the isotropic scenario and decreases with the increase of anisotropy. These behaviors (Figs. 10 and 11) may possibly be described by exploring velocity profiles as shown in Fig. 12 and 13. Figure 12 shows a comparison between the x-component velocity along the height of the middle layer for the different anisotropy scenarios and it is clear that in the middle of the middle layer, the x-component velocity drops because of the decrease in permeability. On comparing the magnitude of velocity along the middle layer height, Fig. 13, it is clear that velocity magnitude is generally larger the larger the anisotropy. This explains the behavior of both the concentration and the porosity in the middle layer, which is manifested by the fact that increasing the velocity increases the dispersion and deposition rate. On the other hand, the profile of the pressure at the inlet for the different scenarios shows interesting patterns, Fig. 14. The pressure generally increases with the increase of anisotropy and it is not constant along the height. Figure 15 shows permeability component in the x-direction and it is apparently smaller the larger the anisotropy and it also gets smaller in the middle layer as a consequence of nanoparticles deposition.

5.1.2 Effects of anisotropy ratio

As indicated earlier, the anisotropy ratio represents the ratio between the permeability values in the principle directions, Fig. 16. Therefore, for the same permeability component,

k_{11} , higher anisotropy ratio implies lower k_{22} and vice versa. This, as will be seen, has interesting implications on the transport of nanoparticles in these systems. In this work, we examine two anisotropy ratios; namely 4 and 10 for the 60° anisotropy angle. Apparently for the same k_{11} , $K_{22}=0.25 K_{11}$ when $\pi = 4$ and $K_{22}=0.1 K_{11}$ when $\pi = 10$. In the case when $\pi = 4$, Fig. 17-a, velocity vectors are less inclined in the anisotropic region. Whereas, when $\pi = 10$, velocity vectors are aligned more towards the upward direction, Fig. 17-b. This is a manifestation of the lower k_{22} component which directs the fluid to follow the path of lower resistance along the K_{11} direction. This clearly influences the porosity contours which are more skewed for the larger anisotropy ratio scenario as depicted in Fig. 18-a,b.

5.2 With and without porosity and permeability changes

In this case, we would like to single out the influence of porosity and permeability changes when anisotropy exists. For this case we simulate the 30° scenario, with anisotropy ratio of 4. We consider two cases, in the first case the injection of nanoparticles affects both porosity and permeability and in the second case both porosity and permeability are not affected. Contours of pressures, concentration, porosity and permeability for the two cases are shown in Figs. 19-21 after 2.5 days of simulation time. It is clear in these figures the significance of considering both porosity and permeability changes. Fig. 19-a shows pressure contours for the case with porosity and permeability changes. It is clear that the pressure field is highly getting distorted and the velocity vectors largely direct in such a way that it tries to avoid the central region where the permeability gets smaller. Figure 19-b, on the other hand, does not show such effects in the central region as the porosity and permeability never change. Figure 20-a,b shows concentration contours for the two cases. The interesting thing is that with porosity and permeability changes, the plume seems to be much more skewed upwards (Fig. 20-a) than it is when both porosity and permeability remains constant. This behavior is also noticed for the porosity and permeability contours as depicted in Figs. 21 and 22. Profiles of different parameters for the anisotropic cases with and without porosity and permeability changes are shown in Fig. 23. Fig. 23-a shows porosity profiles along the mid vertical line. From this figure, one notices that porosity profile is uniform for the scenario in which porosity do not change. When porosity is allowed to change, the porosity for the anisotropic scenario drops in the middle region due to the deposition of nanoparticles. Pressure profiles along the mid vertical line is depicted in Fig. 23-b. In this figure, for the anisotropic scenario without change of porosity the pressure along the mid vertical line is generally larger than the isotropic scenarios and also is not uniform, which is attributed to the effect of anisotropy. When porosity and consequently permeability change, pressure profile along the vertical line further increase in accordance with the changes in permeability. Velocity profiles in the x-direction along the mid vertical line for the different scenarios are shown in Fig. 23-c. It is clear that, for the isotropic scenario without porosity changes, the velocity is uniform, whereas it decreases in the middle region when porosity changes are considered. In the anisotropic scenario without porosity changes the velocity is almost uniform except at the edges which

is manifestation of anisotropy. When porosity changes are considered, the velocity is decreased in the middle region and increases in the top and bottom region. The profiles of the y-component velocity along the mid vertical line for the different scenarios are depicted in Fig. 23-d. In the isotropic scenario without porosity change the y-component velocity is zero whereas it alternate between negative and positive profile in the case when porosity changes. On the other hand, for the anisotropic case without change of porosity the y-component velocity increases and when porosity changes are accounted for, it further increases. The permeability component, k_{xx} , also is affected by both the anisotropy and porosity changes. In general, k_{xx} gets smaller with both anisotropy and with porosity change, Fig. 23-e. The peak concentration reaches maximum when both anisotropy and porosity changes are accounted for, Fig. 23-f. The history of the minimum porosity in the domain with time is depicted in Fig. 23-g. From this figure, it is clear that the porosity is smaller in the anisotropic case with porosity change. Furthermore, the average pressure at the inlet increases with time and it is more pronounced when porosity changes are taken into consideration, Fig. 23-h.

5.3 Multiple size nanoparticles

To account for the fact that nanoparticles are not of one size we also consider the case when there exist multiple sizes of nanoparticles. For the sake of illustration, we consider 4 sizes with parameters as depicted in Table 2. Clearly, based on the rate of injection, these extra sizes will generally affect the change of porosity and permeability. For the sake of showing concentration contours of the 4 sizes, we consider the scenario 45° anisotropy scenario with anisotropy ratio of 10. Fig. 24-a-d shows the concentration contours for the four nanoparticle sizes after 1 day injection time. The plumes of the four sizes are similar but the peak concentrations are different because of the different injection rates. The concentration profiles along the mid vertical line for different nanoparticle sizes, Fig. 25. In this figure the concentration of particle size 1 is larger and the smallest is the concentration of particle size 4. This is because the injection rate of particle size 1 is the largest. Comparisons of the x-component permeability profiles along the mid vertical line for the case of single and multiple size nanoparticles are shown in Fig. 26. It is clear that for all the anisotropic cases, the 4 sizes nanoparticles injection results in more decrease in permeability because of the extra deposition of nanoparticles. Also the time history of the minimum porosity for different anisotropy scenarios indicates that the extra sizes nanoparticles decrease the porosity even further as depicted in Fig. 27.

Conclusion

In this work, flow and transport of nanoparticles in porous media is considered numerically using the multipoint flux approximation. A source term in the middle of anisotropic domain is used to introduce nanoparticles to the domain. Several scenarios of anisotropy are considered including different anisotropy angles and ratios. It is found that anisotropy has significant effect on the velocity and pressure field of the system. When nanoparticles are deposited into the pore space, they deteriorate both the velocity and

permeability fields. Pressure and velocity fields change in response to the change in permeability. When anisotropy is large, it is found that both the peak concentration and the minimum porosity decrease. This is a manifestation of the increase of the magnitude of velocity when anisotropy is large which increases dispersion and deposition of nanomaterials. We also compared the case when porosity changes are taken into consideration versus when it has been ignored. The investigations show that porosity changes have significant effect of the behavior of the system.

Nomenclature:

Symbol	Unit	Definition
c		Fluid concentration
s_1		Volume concentration of the nanoparticles in contact with water phase deposited on the surfaces per unit bulk volume concentration of the porous medium
s_2		Volume concentration of the nanoparticles entrapped in pore throats from the water phase per unit bulk volume of porous medium due to plugging and bridging
$d_{l,w}$	m	Longitudinal dispersion
$d_{t,w}$	m	Transverse dispersion
d_p	m	Particle diameter
D	$m^2 s^{-1}$	Hydrodynamic dispersion
D^{disp}	$m^2 s^{-1}$	Mechanical dispersion
D^{Br}	$m^2 s^{-1}$	Brownian diffusion
f		Flow efficiency factor
g	$m s^{-2}$	Gravitational acceleration
k_B	$m^2 kg s^{-2} K^{-1}$	Boltzmann constant
k_f		Constant fluid seepage allowed by the plugged pores
K	m^2	Permeability
p	Pa	Pressure
q_c	s^{-1}	Rate change of particle volume belonging to a source/sink term
R	s^{-1}	Rate of loss of nanoparticles
t	s	Time
T	K	Absolute temperature
u	$m s^{-1}$	Darcy velocity
u_c	$m s^{-1}$	Critical velocity of water
z	m	Depth

μ	Pa s	Fluid viscosity
ρ	kg m ⁻³	Fluid density
γ_d	m ⁻¹	Rate coefficients for surface retention of the nanoparticles
γ_e	m ⁻¹	Rate coefficients for entrainment of the nanoparticles
γ_f	m ⁻¹	Coefficient of flow efficiency for the particles
γ_{pt}		Pore throat blocking constants
ϕ		Porosity
ϕ_0		Initial porosity

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Table 1. Simulation domain and single nano-size parameters

Parameter	Value
$L_x \times L_y$	$5\text{m} \times 5\text{m}$
$n_x \times n_y$	30×30
ϕ_0	0.3
$\mathbf{K}_0$:	
Isotropic	$\mathbf{K} = \begin{bmatrix} 9.869 & 0 \\ 0 & 9.869 \end{bmatrix} \times 10^{-14} \text{ m}^2$
Anisotropic layer:	
$\theta = 30^\circ$	$\mathbf{K} = \begin{bmatrix} 7.649 & 3.846 \\ 3.846 & 3.208 \end{bmatrix} \times 10^{-14} \text{ m}^2$
$\theta = 45^\circ$	$\mathbf{K} = \begin{bmatrix} 5.428 & 4.441 \\ 4.441 & 5.428 \end{bmatrix} \times 10^{-14} \text{ m}^2$
$\theta = 60^\circ$	$\mathbf{K} = \begin{bmatrix} 3.208 & 3.846 \\ 3.846 & 7.649 \end{bmatrix} \times 10^{-14} \text{ m}^2$
D^{Br}	$2 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$
μ	10^{-3} Pa s
γ_d	5 m^{-1}
γ_{pt}	1 m^{-1}
γ_f	0.01 m^{-1}
k_f	0.6
c_0	0
c_{s1}	0
c_{s2}	0
q_c	10^{-6} s^{-1}
$t^{\text{simulation}}$	86400 s
Δ_t	4.7 s

Table 2. Simulation values for multiple nanoparticles parameters

Parameter	d (nm)	Q_{ci}	γ_{di}	$\gamma_{pt,i}$	γ_{fi}	γ_{ei}	u_{ci}
C_1	40	10^{-6}	2.15	1	0.011	3.1	4.6×10^{-6}
C_2	80	5×10^{-7}	3.23	0.82	0.0225	2.4	5.8×10^{-6}
C_3	100	2×10^{-7}	4.1	0.67	0.033	1.3	9.2×10^{-6}
C_4	200	1×10^{-7}	5.15	0.43	0.0445	1.22	1.6×10^{-5}

Fig. 1 Anisotropic rock mass systems are ubiquitous in subsurface formations (Wikipedia)

Fig. 2 The flux vector is not coincident with the pressure gradient vector in anisotropic media

Fig. 3 Six pressure values contribute to flux calculations in multipoint point flux approximation

Fig. 4 The four velocity components and four pressure values constituting the local problem.

Fig. 5 Flow chart of the solution using the experimenting pressure field approach to calculate the velocity field

Fig. 6 Schematic of the 2D computational domain

Fig. 7 Contours of pressure, porosity, concentration, permeability in the x-direction after 1 day for different anisotropy angle with anisotropy ratio (k_{11}/k_{22}) of 4.

Fig. 8 comparison of the average pressure profile at the inlet for the different anisotropy scenarios

Fig. 9 Comparison of the minimum porosity profile for the different anisotropy scenarios

Fig. 10 Porosity profiles along the middle layer for the different anisotropy scenarios.

Fig. 11 concentration profile along the middle layer for different anisotropy scenarios

Fig. 12 Velocity profile along the middle layer for the different anisotropy scenarios

Fig. 13 Velocity magnitude along the height of the middle layer

Fig. 14 Pressure profiles along the middle region for different anisotropy scenarios.

Fig. 15 Permeability profiles along the height of the middle layer

Fig. 16 Illustration of the concept of anisotropy ratio

Fig. 17 Pressure contours for different anisotropy ratios for the 60° angle

Fig. 18 Porosity contours for different anisotropy ratios for the 60° angle

Fig. 19 Pressure contours

Fig. 20 Concentration contours

Fig. 21 Porosity contours

Fig. 22 K_{xx} contours

(a) porosity

(b) Pressure

(c) Velocity in the x-direction

(d) Velocity in the y-direction

(e) Permeability component in the x-direction

(f) Concentration

Fig. 23 Profiles of different parameters for the isotropic and anisotropic cases with and without porosity and permeability changes.

Fig. 24 Concentration profiles of the four species for the anisotropy scenario with angle 45° and anisotropy ratio of 10

Fig. 25 Concentration profile for the 4 nanoparticles sizes

Fig. 26 Comparisons of the x-component permeability for single size and multiple sizes nanoparticles after 1 day.

Fig. 27 Comparisons of minimum porosity evolution for single size and multiple sizes nanoparticles after 1 day

Highlights

- Numerical investigation of nanoparticles transport in anisotropic porous media is considered
- Multipoint flux approximation is used
- Anisotropy affects both pressure and velocity fields
- Deposition of nanoparticles deteriorates both porosity and permeability.