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Peridynamic modelling of coupled hydro-chemical processes in clay erosion

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ABSTRACT

Hydro-chemical interactions at the interface between host rock and clay buffer in geological disposal facility for nuclear waste can lead to buffer erosion. The erosion of clay buffer can induce loss of a critical component of the engineered barrier system and migration of highly hazardous radionuclides into the environment. Classical local continuum formulations based on partial differential equations that have been used for modelling the hydro-mechanical behavior of soils are not suitable for analysis of this discontinuous physical phenomenon, whereas non-local formulations offered by peridynamics (PD) provide clear advantages. In this study, a bond-based PD formulation of coupled clay extrusion and sol transport in a fracture is presented. Pyramid, the PD model used in this study, accounts for the effect of van der Waals forces, repulsive electrostatic double layer forces, and friction forces between the particles on clay extrusion. A 2D case study of clay extrusion and erosion under water flow in a fracture is presented. The case study is compared with experimental results of erosion of compacted MX-80 bentonite reported in the literature to demonstrate the accuracy of formulations and the Pyramid model. This validation shows the potential applications and prediction capability of the Pyramid model for evaluating the erosion of clay buffer under geological disposal conditions.

Keywords: clay erosion, hydro-chemical coupling, peridynamics, swelling

1 INTRODUCTION

The clay buffer is a key component of the geological disposal concept in crystalline rocks and plays a critical role in the safe isolation of high-level radioactive waste (HLW). The clay buffer and backfill can be eroded by the hydro-chemical interactions at the rock interface, resulting in a potential loss of a critical component of the engineered barrier system. The clay particles generated by erosion in the colloid regime possess a very strong adsorption capacity, which facilitates migration of highly hazardous radionuclides into the environment (Neretnieks et al., 2009). Developing a sound predictive capability of erosion and erosion-assisted phenomena is therefore important for assessing the safety of the bentonite buffer and the long-term repository performance (Eriksson and Schatz, 2015).

Previous studies on clay erosion modelling have been based on continuum local formulations, which represent erosion of clay as a diffusion process of particles detached from the swelled porous medium of clay (Neretnieks et al., 2009). However, the detachment of clay particles at the boundary between solid and sol clay is a discontinuous process. The local continuum theories, i.e. those based on partial differential equations, offer limited capability to fully capture the processes involved in the erosion process. Therefore, in this paper, a non-local formulation, known as peridynamics (PD) will be introduced to address problems with discontinuous systems and heterogeneities (Silling, 2000). The theory of peridynamics presents a set of equations of continuum mechanics to overcome the limitations of the classical local theory in solving problems with discontinuities. A major development in this theoretical framework is that the partial differential equations of the classical local theory are replaced with a set of integral-differential equations, providing a mathematically consistent formulation, even where strong discontinuities appear due to fracturing and fragmentation of the material (Bobaru and Duangpanya, 2010).

This paper focuses on the development of the PD theory, formulation, computation and application for coupled water flow, clay expansion and clay sol transport in a fracture. The PD model of clay erosion takes into account the van der Waals forces, repulsive electrostatic double layer forces and friction forces between the particles. A new detachment model is introduced in our PD formulation to solve the discontinuous process at the boundary between solid and sol. The proposed peridynamics model known as Pyramid is tested against experimental bench marks to ensure accurate derivation and implementation of the formulations. An application of the performance of bentonite barrier will be further investigated by the

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proposed model.

2 FORMULATIONS OF CLAY EROSION

We present a set of formulations for the coupled process governing the clay erosion which includes clay expansion, water flow and sol/gel migration of the clay in fracture. The bentonite expansion is described by a dynamic force balance model (Liu et al., 2008). The mass balance equation for the clay expansion is given as follow:

$$\frac{\partial\phi}{\partial t} = \nabla\cdot\left(\frac{\chi}{f_r}\nabla\phi\right) + \overrightarrow{F_s}\nabla\left(\frac{\phi}{f_r}\right) \tag{1}$$

where ϕ is volume fraction of clay and t is time, χ is the sum of the energy of particles, f_r is friction coefficient between particles and water, and $\overrightarrow{F_s}$ accounts for the gravitational force and buoyant force.

The water flow in the fracture is described by (Biot, 1941):

$$S\frac{\partial p}{\partial t} - \nabla\cdot\left(T_f\nabla p\right) = 0 \tag{2}$$

where p is the fluid pore pressure, S is the specific storage, and T_f is the transmissivity of a fracture which is described by (Neretnieks et al., 2009):

$$T_f = T_w\frac{\eta_w}{\eta(\phi)} \tag{3}$$

where T_w is the fracture transmissivity for water, η_w is the viscosity of water, and $\eta(\phi)$ is the viscosity of clay sol/gel. Sol and gel are two different clay colloidal states. The distinction between the gel and sol phases can be made on the base of previous studies on smectite rich clays (Abend and Lagaly, 2000.). It has been shown that at solid contents below 2 to 4% and ionic strengths below 10 mM, the clay exhibits the properties of sol, that is susceptible to erosion by water flow (Neretnieks et al., 2009).

The viscosity of the sol/gel is a function of the clay volume fraction and the cation concentration in the water. A relationship developed using the concept of the co-volume as defined by Neretnieks et al. (2009) is as follow:

$$\eta(\phi) = \eta_w\left[1 + 1.022\phi_{cov} + 1.358{\phi_{cov}}^3\right] \tag{4}$$

where ϕ_{cov} is the co-volume fraction.

The diffusion-advection equation is used to model clay sol migration in the fracture as follow:

$$\frac{\partial\phi}{\partial t} = \nabla\cdot\left(D(\phi)\nabla\phi\right) + v(\phi)\nabla\phi \tag{5}$$

where $D(\phi)$ is the diffusion coefficient, and $v(\phi)$ is fluid velocity in the fracture.

The inter-dependencies of the fields and the constitutive relations are summarized in Figure 1. The model consists of field variables ϕ (volume fraction of clay) and p (pressure). The inter-dependencies are built through the water velocity, diffusivity function, viscosity of sol/gel and clay volume fraction.

3 PERIDYNAMICS FORMULATIONS FOR CLAY EROSION

A bond-based PD formulation is presented in this paper for aforementioned equations describing clay expansion, water flow and clay sol transport. In order to simulate the clay particle detachment at the boundary of solid and fluid, a new detachment function is introduced to the peridynamic formulations.

3.1 PD formulations for the clay expansion

In the PD approach a body occupying a region (***R***) is considered, as illustrated in Fig. 2. The material point ***x*** interacts with (and is connected to) all materials points ***x`*** within a certain finite region ***H_x***, where ***H_x*** is defined as the horizon of material point ***x***, and the radius of the horizon is denoted by ***δ***. The transfer of mass between

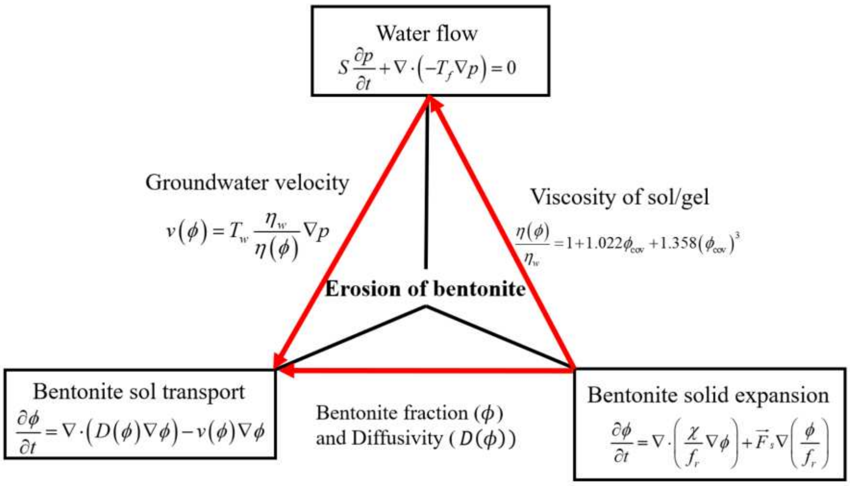

Fig. 1. Coupled processes and key variables describing the erosion of clay in the Pyramid model.

two interacting material points $\boldsymbol{x}$ and $\boldsymbol{x}$\` is called the 'mass bond' or 'm-bond'. The peridynamics mass flux per unit volume along a 'm-bond' is dependent on the distance between the material points $\boldsymbol{x}$ and $\boldsymbol{x}$\`.

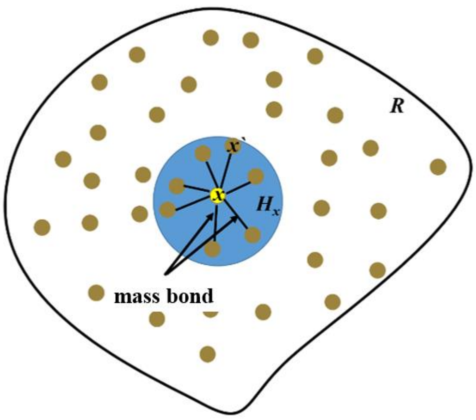

Fig. 2. Illustration of peridynamic horizon and mass-bonds.

The clay solid fraction difference at the two end points of a bond is assumed to cause the clay to expand along the bond. The peridynamics formulation for the expansion of clay can be expressed as follows (Bobaru and Duangpanya, 2010):

$$\frac{\partial\phi(\boldsymbol{x},t)}{\partial t} = \int_{H_x} d(\boldsymbol{x},\boldsymbol{x}',t)\frac{\phi(\boldsymbol{x}',t)-\phi(\boldsymbol{x},t)}{\|\boldsymbol{\xi}\|^2}dV_{x'} \qquad (6)$$

where, $\phi(\boldsymbol{x}',t)$ and $\phi(\boldsymbol{x},t)$ are clay volume fractions at material points $\boldsymbol{x}'$ and $\boldsymbol{x}$, respectively, $\boldsymbol{\xi}$ represents the distance vector between the two material points $\boldsymbol{x}$ and $\boldsymbol{x}'$, i.e. $\boldsymbol{\xi} = \boldsymbol{x}' - \boldsymbol{x}$, and $d(\boldsymbol{x},\boldsymbol{x}',t)$ is peridynamic microscopic (local) diffusivity.

3.2 PD formulations for water flow in the fracture

Similar to Eq. 6, mass conservation equation, Eq. 2, for the bond between material points can be written within the PD framework as follows (Katiyar et al., 2014):

$$\frac{\partial\theta_l(\boldsymbol{x},t)}{\partial t} = \int_{H_x} \bar{\kappa}(\boldsymbol{x},\boldsymbol{x}',t)\frac{H(\boldsymbol{x}',t)-H(\boldsymbol{x},t)}{\|\boldsymbol{\xi}\|^2}dV_{x'} \qquad (7)$$

where $\theta_l(\boldsymbol{x},t)$ is the water content, $H(\boldsymbol{x},t)$ and $H(\boldsymbol{x}',t)$ are the hydraulic potentials at material point $\boldsymbol{x}$ and $\boldsymbol{x}'$, respectively, and $\bar{\kappa}(\boldsymbol{x},\boldsymbol{x}',t)$ is the average hydraulic conductivity of the flow bond given as follows:

$$\bar{\kappa}(\boldsymbol{x},\boldsymbol{x}',t) = \frac{\kappa(\boldsymbol{x},t)+\kappa(\boldsymbol{x}',t)}{2} \qquad (8)$$

3.3 PD formulations for the clay sol transport in the fracture

The peridynamics formulation for sol transport in the fracture can be written as follows:

$$\frac{\partial\phi(\boldsymbol{x},t)}{\partial t} = \int_{H_x}\left(\begin{matrix} d(\boldsymbol{x},\boldsymbol{x}',t)\dfrac{\phi(\boldsymbol{x}',t)-\phi(\boldsymbol{x},t)}{\|\boldsymbol{\xi}\|^2} \\ -v(\boldsymbol{x},\boldsymbol{x}',t)\dfrac{\phi(\boldsymbol{x}',t)-\phi(\boldsymbol{x},t)}{\|\boldsymbol{\xi}\|}\end{matrix}\right)\frac{\boldsymbol{\xi}}{\|\boldsymbol{\xi}\|}dV_{x'} \qquad (9)$$

where $v(\boldsymbol{x},\boldsymbol{x}',t)$ is the micro advection coefficient.

The newly derived peridynamics formulations for clay solid extrusion, water flow and clay sol transport (i.e. Eqns. 6, 7 and 9), do not involve partial derivatives and therefore can be applied in all practical cases, including those involving spatial discontinuities and/or heterogeneities as well as discontinuities and or heterogeneities of material properties.

3.4 Detachment model

One question with respect to the erosion of clay barrier material in the repository environment is the extent to which the mass loss mechanism will involve the removal of clay particles by shear stress. Flowing water is known to impose a shear stress on the particle-particle bond in gel-shaped clay. This shear stress can be related to the flow velocity by Stoke's law

$$\tau_f = \frac{6\pi\eta a v}{S_p} \qquad (10)$$

where τ_f is the shear stress, η is viscosity of fluid, a is bentonite particle diameter, and v is water flow velocity.

Here, the concept of yield stress is adopted for describing the detachment processes (Laxton and Berg, 2006). The density of clay decreases after deposition as the clay swells further into the fracture and undergoes phase changes from a hydrated solid to a swelling paste, to a gel. The gel finally disperses as colloidal sol. Previous studies have shown that at solid contents and ionic strengths below 2%-4% and 10mM, respectively, the sodium bentonite has the properties of sols, which are most susceptible to erosion by flowing water (Michot et al., 2004). When the shear stress is greater than the yield stress, bentonite particles behave like a fluid. If the shear stress is less than the yield stress, the behavior of bentonite tends towards that of a solid material. The interactions between bentonite particles in different phases including liquid-liquid bonds, solid-solid bonds and interfacial bonds are illustrated in Fig. 3.

In this study, the detachment of clay particles is assumed to take place when shear stress induced by the water flow at the solid and fluid boundary exceeds the yield stress as described by the following detachment function:

$$\mu(\boldsymbol{x},\boldsymbol{x}',t) = \begin{cases}1, & \tau_y < \tau_f \\ 0, & \tau_y \geq \tau_f\end{cases} \qquad (11)$$

where τ_f is the yield stress.

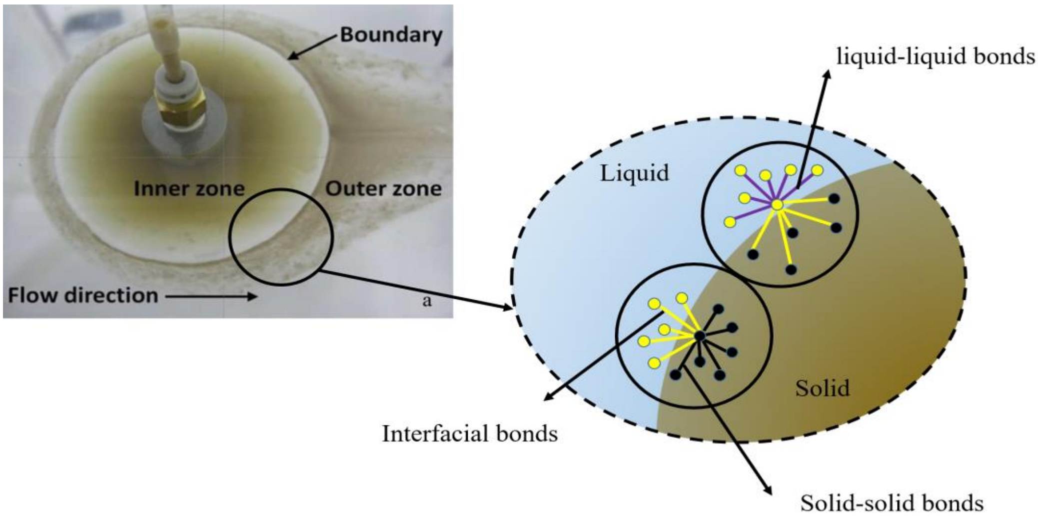

Fig.3 Bentonite particles detachment in peridynamic models (modified from Eriksson and Schatz, 2015).

Incorporating the detachment function $\mu(\boldsymbol{x},\boldsymbol{x}',t)$into PD formulations of clay expansion and sol transport, the peridynamic formulations for clay expansion and sol transport can be written by

$$\frac{\partial\phi(\boldsymbol{x},t)}{\partial t} = \int_{H_x}\left(d(\boldsymbol{x},\boldsymbol{x}',t)\frac{\phi(\boldsymbol{x}',t)-\phi(\boldsymbol{x},t)}{\|\xi\|^2} - \mu(\boldsymbol{x},\boldsymbol{x}',t)v(\boldsymbol{x},\boldsymbol{x}',t)\frac{\phi(\boldsymbol{x}',t)-\phi(\boldsymbol{x},t)}{\|\xi\|}\right)\frac{\boldsymbol{\xi}}{\|\xi\|}d\boldsymbol{V}_{x'} \tag{12}$$

4 Model Application and Validation

The validation exercise presented focuses on testing the PD model for clay expansion in a stagnant water system. The results with the PD model are obtained with Δ = 1.5 mm and horizon size of 4.5 mm. The results of simulations are compared with experimental data reported by Schatz et al. (2013).

Erosion of compacted MX-80 bentonite in a square domain (240 mm×240 mm) is analyzed. The bentonite sample studied is a cylindrical sample with a 20 mm diameter, placed in the center of the domain. The coordinate system is attached to its center with axes parallel to the domain sides. The dry density if the sample is 1.6 Mg/m^3. The initial bentonite fraction in the domain outside of the sample is set to zero. Impervious boundary conditions are prescribed at the domain boundaries y=-120 mm and y=120 mm. No bentonite particles can exit the left border (x=-120 mm). The bentonite particles are allowed to leave through the right boundary (x=120 mm). The inner zone bentonite volume fraction was calculated by using the relationship $\phi = 1-\varepsilon$. ε is the porosity of bentonite. The bentonite volume fraction of the sample at inner zone is assumed to be maintained at 0.6 because the height of bentonite is 20 times larger than that of fracture thickness.

Figure 4 shows the comparison between results of the extrusion distance calculated by the PD model against the results obtained by the experiment reported by Schatz et al. (2013).

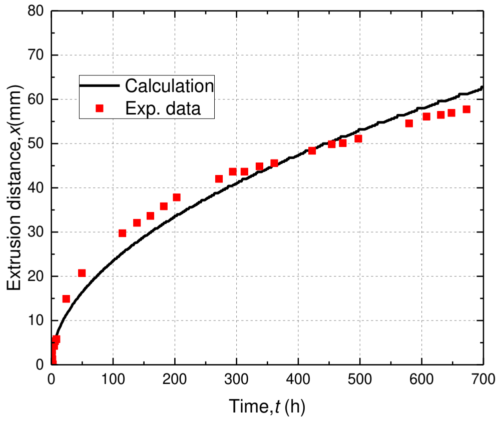

Fig.4. variations of extrusion distance with time for free swelling of MX-80 bentonite in stagnant water.

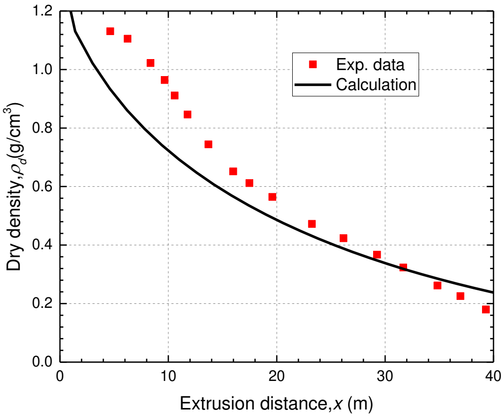

Fig.5. Variations of dry density with extrusion distance for free swelling of MX-80 bentonite in stagnant water.

Figure 5 shows the comparison of the PD bentonite dry density distribution along the extrusion distance with the experimental data. The close agreement between the experimental and modelling data in both Figs, 4 and 5 indicates that the developed implementation of the theoretical formulation of bentonite extrusion is robust and predictive.

5 CONCLUSIONS

Bond-based peridynamics modelling of coupled hydro-chemical effects on clay erosion in a fracture was proposed. The PD model of clay extrusion takes into account the van der Waals forces, repulsive electrostatic double layer forces, and friction forces between the particles. The water flow is coupled with the clay extrusion processes via an explicit numerical scheme to allow for solving coupled problems of practical importance.

A case study of two-dimensional modelling of bentonite extrusion and erosion in a fracture was presented to demonstrate the accuracy of formulations and the Pyramid model. The case study is based on experimental results of erosion of compacted MX-80 bentonite reported in the literature. The validation demonstrates the potential applications and prediction capabilities of the Pyramid model for evaluating the erosion of clay buffer under geological disposal conditions. Overall, the proposed nonlocal Peridynamics-based framework is efficient and effective in analysis of coupled hydro-chemical effects on bentonite erosion in a fracture.

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