UNIVERSITY OF LEEDS

Darcy’s Law, valid or not in a contaminant-impacted zone?

(Part 1: membrane porous media)

Dr Xiaohui Chen

Lecturer in Geotechnics

Academic Leader of BioSAS consortium (UoL, UoS, UoY)

Joint Leader of Nuclear Group at Civil (UoL)

UNIVERSITY OF LEEDS

Contents

Revisit Darcy’s Law (1856)

UNIVERSITY OF LEEDS

160 years, forming the basis of hydrogeology, cross-disciplinary used in geotechnics, geochemistry etc.

$$\mathbf{u} = \frac{k}{v} grad\ p$$

Note: The pictures taken from internet are only used to demonstrate the research idea. These pictures will not be used for publication or commercial purpose

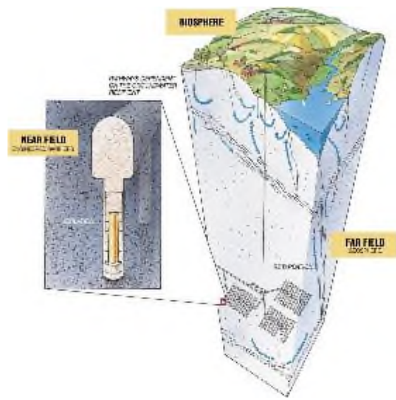
World has changed, and is changing

UNIVERSITY OF LEEDS

Nuclear: Fukushima (2011)

Landfill example

Waste Geological Disposal

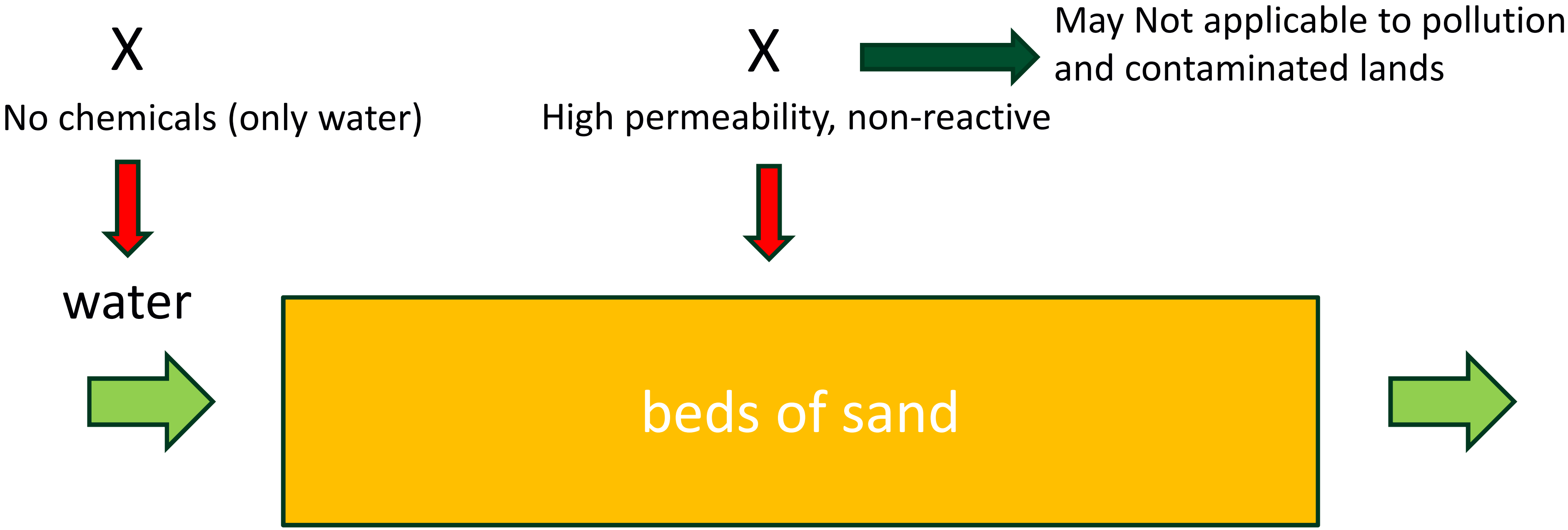


Note: The pictures taken from internet are only used to demonstrate the research idea. These pictures will not be used for publication or commercial purpose

Revisit Darcy's Law (1856)…needs to be changed

UNIVERSITY OF LEEDS

Assumption of Darcy's Law



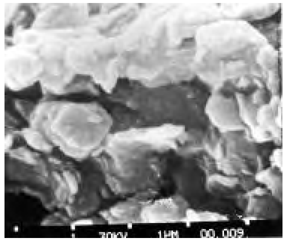
$$\mathbf{u} = \frac{k}{v}\, grad\ p$$

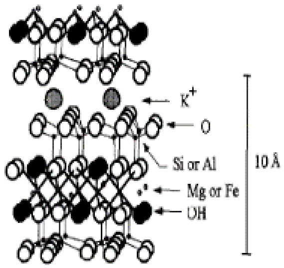
Darcy, H. (1856). *Les fontaines publiques de la ville de Dijon*. Paris: Dalmont.

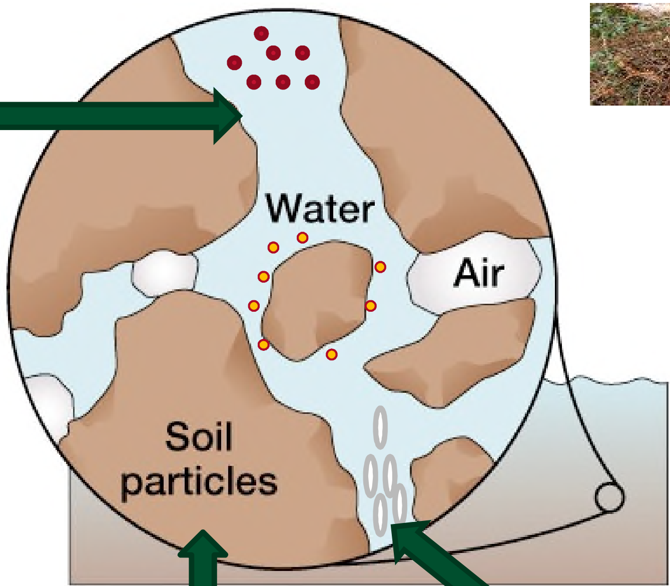
Molecular-scale coupled influence?

UNIVERSITY OF LEEDS

Environmental geochemistry







Environmental mineralogy

Geomicrobiology

Fe2+, Mg, Na, Mn, SO4, K, NH_4, Ni, Cd, Cr and Zn

Geomechanics

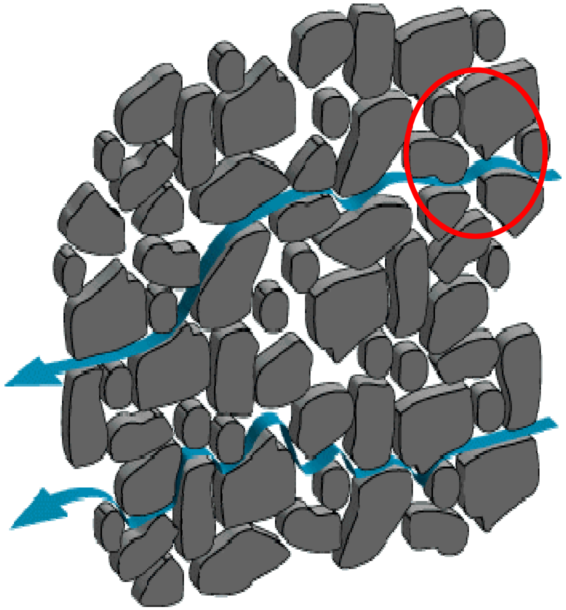
Soils/Rocks system

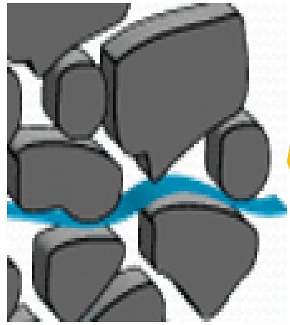
Question: how to incorporate such coupled influence into theoretical prediction?

Note: The pictures taken from internet are only used to demonstrate the research idea. These pictures will not be used for publication or commercial purpose

Conceptual model?

UNIVERSITY OF LEEDS

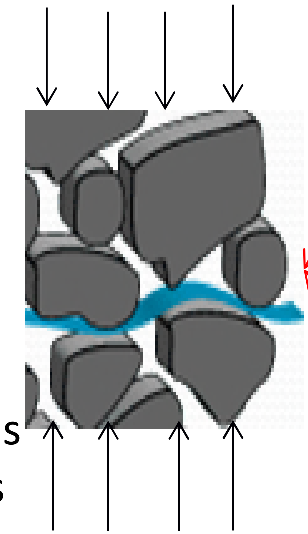




Multiple minerals transfer

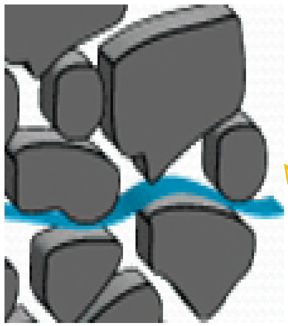
Multiple chemicals reaction

Multiple microbes process



Gas/CO2/Oil interactions with water

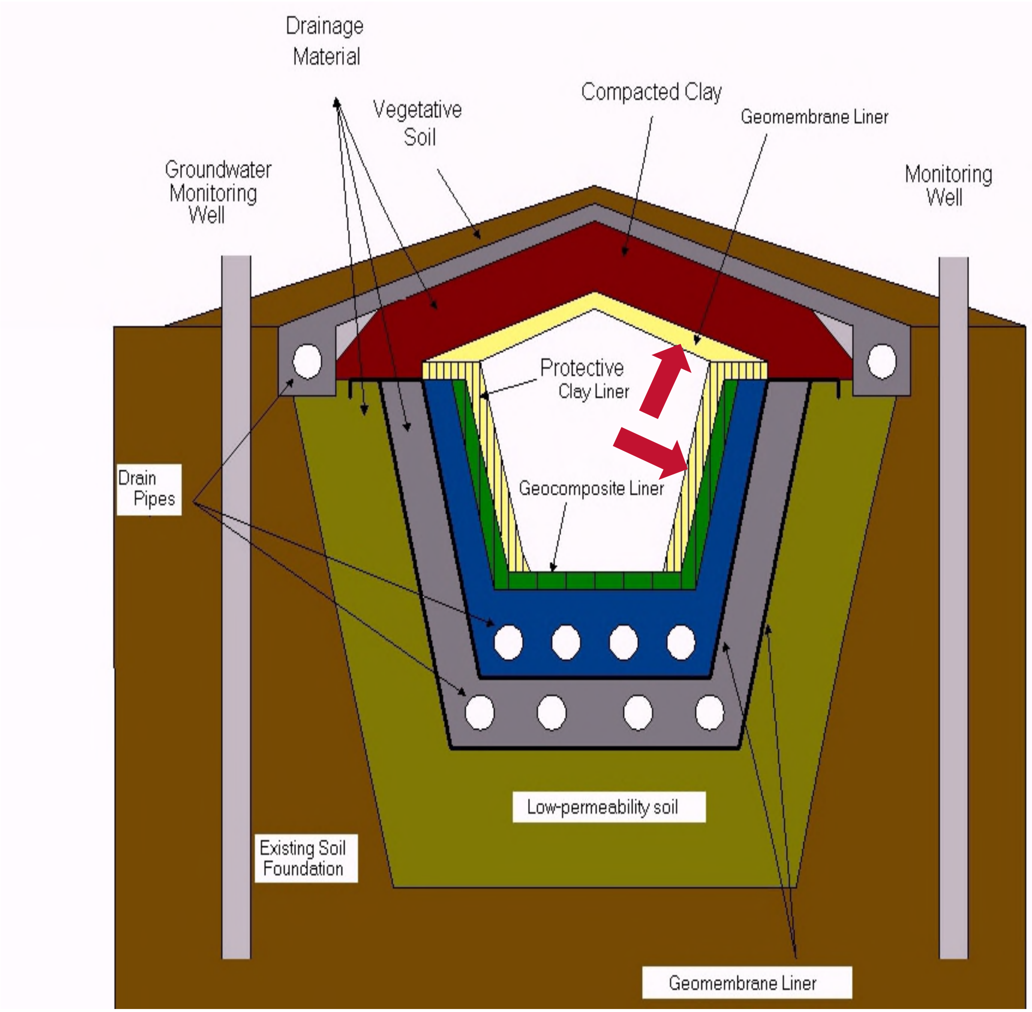
Soil/rock particles deformation



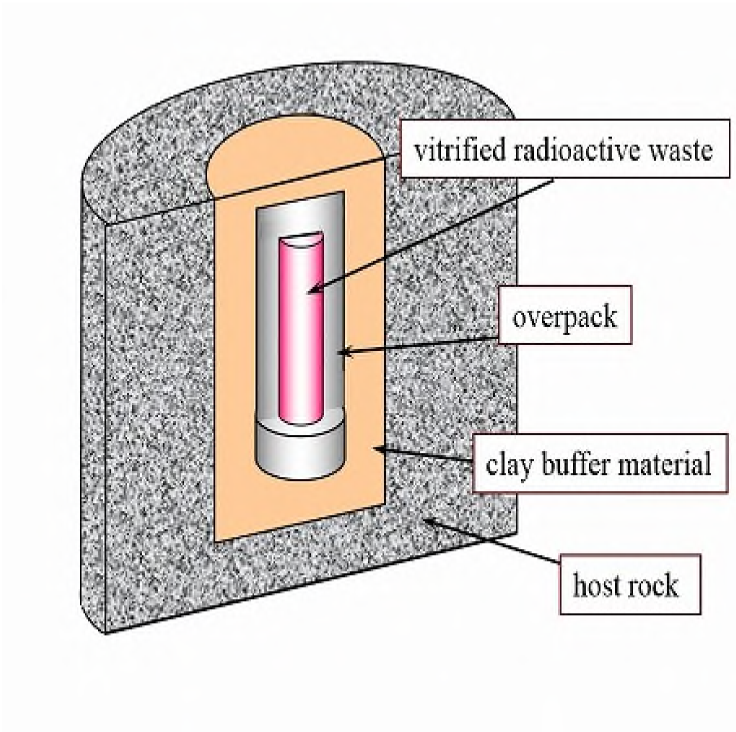
Chemical Osmosis
Thermal Osmosis

Why low permeability matters?

UNIVERSITY OF LEEDS



http://www.keepoklahomabeautiful.com/21st-century-landfills

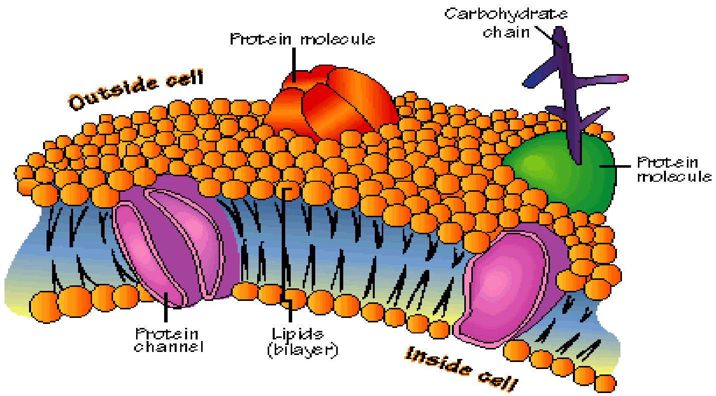


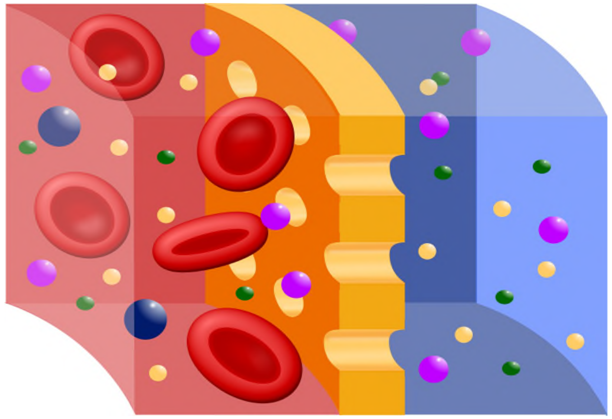
http://nucl-mater.eng.hokudai.ac.jp/overview-en/theme-en/

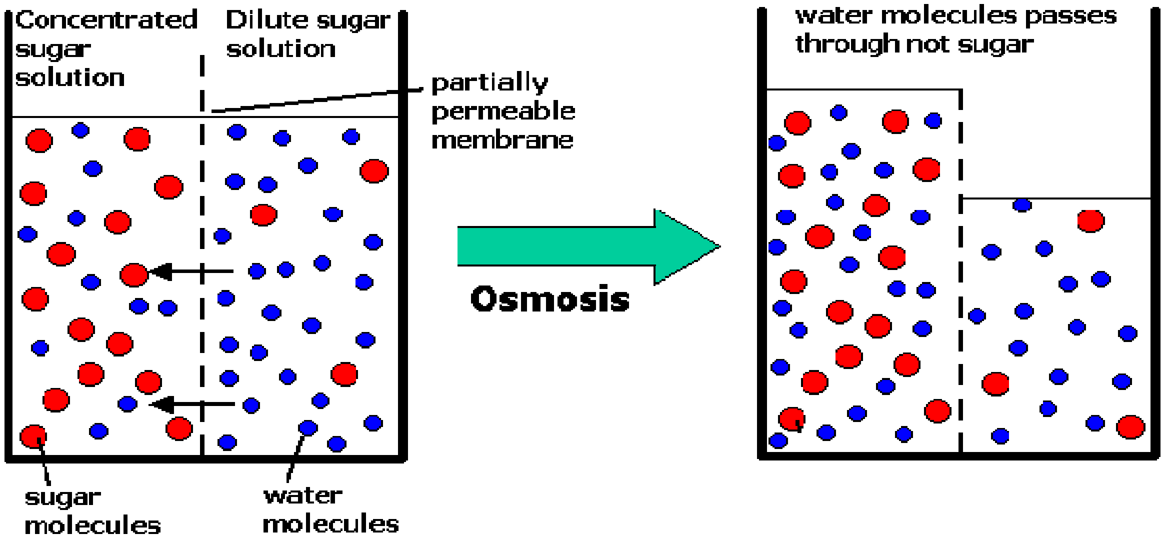
Note: The pictures taken from internet are only used to demonstrate the research idea. These pictures will not be used for publication or commercial purpose

Osmosis

UNIVERSITY OF LEEDS





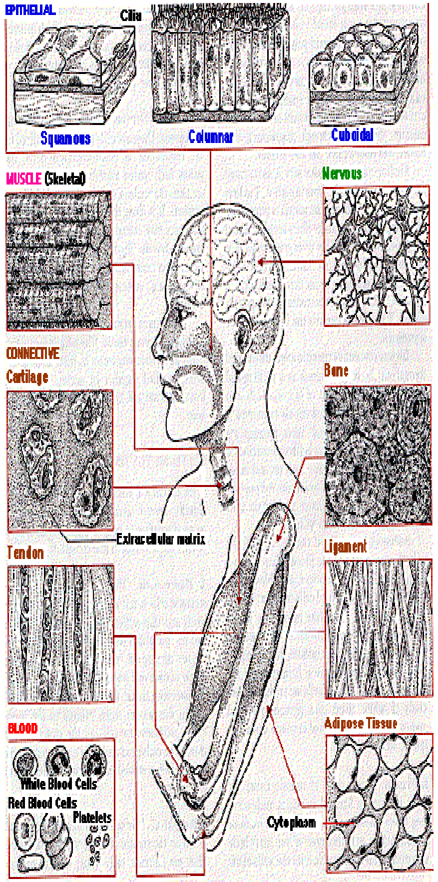


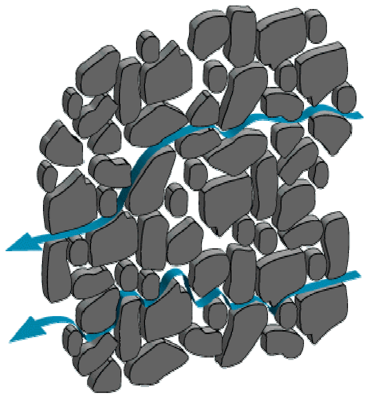
Note: The pictures taken from internet are only used to demonstrate the research idea. These pictures will not be used for publication or commercial purpose

UNIVERSITY OF LEEDS

Contents

Mixture Theory





Blood in tissues

≈

groundwater in soils/rocks

More realistic

More systematic

Mixture Coupling Theory

"a systematic approach...,which can help build coupled formulations based on a ***single unified theory***, between geophysics and geochemistry"

CHEN, X., PAO, W., THORNTON, S. & SMALL, J. 2016. Unsaturated hydro-mechanical–chemical constitutive coupled model based on mixture coupling theory: Hydration swelling and chemical osmosis. International Journal of Engineering Science (IF:3.165), 104, 97-109.

Entropy

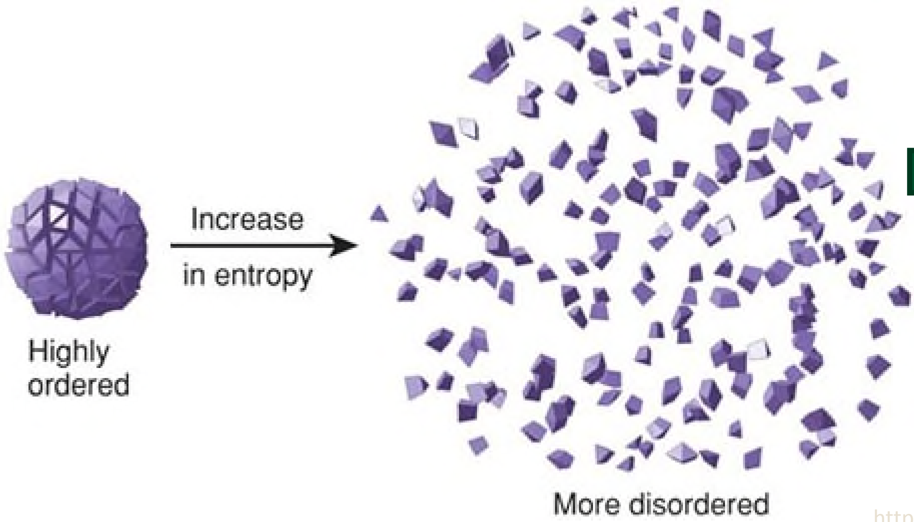
UNIVERSITY OF LEEDS

Second law of thermodynamics

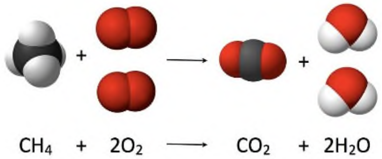
The entropy of an isolated system not in equilibrium will tend to increase over time, approaching a maximum value at equilibrium

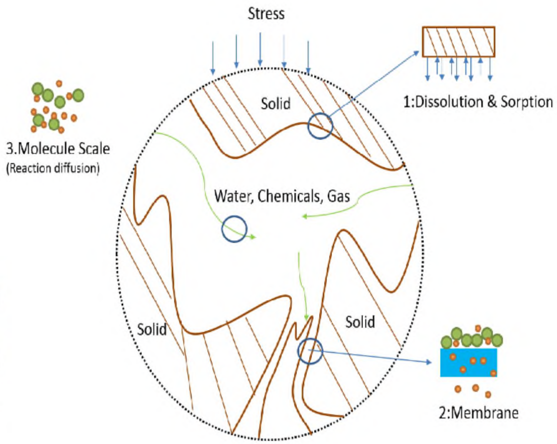
Professor Stephen Hawking: Black hole

Interpreted as the degree of disorder or randomness in the system



Freedom change





https://en.wikipedia.org/wiki/Chemical_reaction

http://www.michelecoscia.com/?p=1041

How to give the relationships between flows

the Fourth Law of Thermodynamics

- phenomenological equations:

A set of functions are used to express the linear dependence of these two flows on the corresponding forces.

$$J_1 = L_{11}F_1 + L_{12}F_2 + ... + L_{1k}F_k$$
$$J_2 = L_{21}F_1 + L_{22}F_2 + ... + L_{2k}F_k$$
$$J_k = L_{k1}F_1 + L_{k2}F_2 + ... + L_{kk}F_k$$

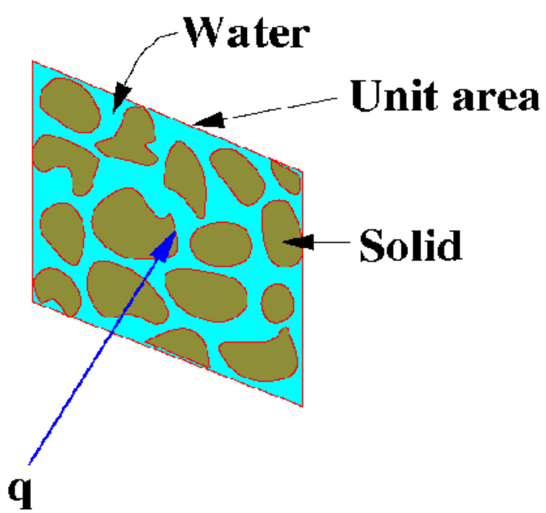
$$J_i = \sum_{k=1}^{n} L_{jk} F_k \quad (j = 1,2,3....n)$$

Lars Onsager

Nobel Prize in Chemistry in 1968

Contents

Solid and fluid



Dissipation generated by frictional resistance at solid and fluid interface

$$0 \le T\gamma = -\mathbf{I}^w \cdot \nabla \mu^w - \mathbf{I}^c \cdot \nabla \mu^c$$

Gibbs-duhem equation

$$0 \le T\gamma \ = -\mathbf{u} \cdot \nabla p - (\mathbf{J}^w \cdot \nabla \mu^w + \mathbf{J}^c \cdot \nabla \mu^c)$$

Note: Since the diffusion fluxes of the water and chemical relative to the barycentric motion can be written as

$$\mathbf{J}_\beta = \tilde{\rho}_\beta (\mathbf{v}_\beta - \mathbf{v}_f)$$

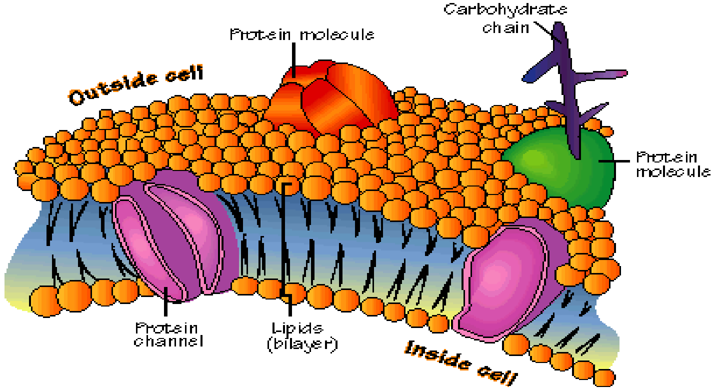
Extending of
Fick's diffusion law and Darcy's laws

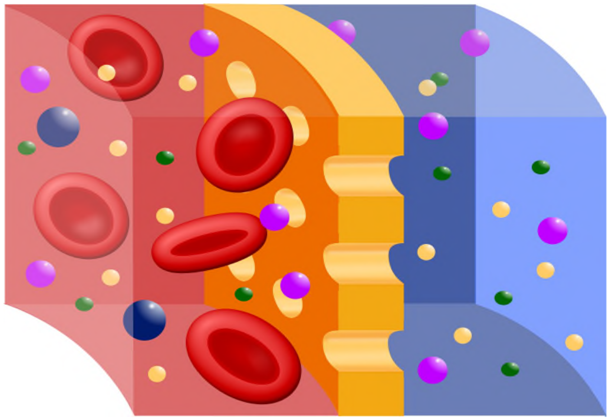
$$\mathbf{u} = -k\frac{k_{rw}}{\theta}(\nabla p - r\frac{\rho_t^f}{C^w}\frac{\partial\mu^c}{\partial C^c}\nabla C^c)$$

$$\mathbf{J}^c = L\rho_t^f\frac{\nabla p}{p} - \rho_t^f D\nabla C^c$$

where

$$k\frac{k_{rw}}{\theta} = \frac{L^{11}}{\left(\rho_t^f\right)^2} \qquad r = -\frac{L^{21}}{L^{11}} \qquad L = \frac{L^{21}p}{\left(\rho_t^f\right)^2} \qquad D = \frac{L^{22}}{C^w\left(\rho_t^f\right)^2}\frac{\partial\mu^c}{\partial C^c}$$





Note: The pictures taken from internet are only used to demonstrate the research idea. These pictures will not be used for publication or commercial purpose

Darcy's Law and Fick's Law

UNIVERSITY OF LEEDS

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{J}^s \end{pmatrix} = -\begin{bmatrix} \dfrac{k}{v} & \dfrac{kr_f \bar{\rho}_f}{vc_d} \dfrac{\partial \mu_s}{\partial c_s} \\ \dfrac{L\rho_f}{p} & \rho_f D \end{bmatrix} \begin{pmatrix} grad\ p \\ grad\ c_s \end{pmatrix}$$

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{J}^s \end{pmatrix} = -\begin{bmatrix} \dfrac{k}{v} & 0 \\ 0 & \rho_f D \end{bmatrix} \begin{pmatrix} grad\ p \\ grad\ c_s \end{pmatrix}$$

CHEN, X., PAO, W., THORNTON, S. & SMALL, J. 2016. Unsaturated hydro-mechanical–chemical constitutive coupled model based on mixture coupling theory: Hydration swelling and chemical osmosis. International Journal of Engineering Science (IF:3.165), 104, 97-109.

Darcy’s Law and Fourier's law of heat conduction

UNIVERSITY OF LEEDS

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{q} \end{pmatrix} = -\begin{bmatrix} \frac{k}{v} & \frac{k r_q \bar{\rho}_f}{vT} \\ \frac{L_q \rho_f}{p} & \lambda \end{bmatrix} \begin{pmatrix} grad\ p \\ grad\ T \end{pmatrix}$$

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{q} \end{pmatrix} = -\begin{bmatrix} \frac{k}{v} & 0 \\ 0 & \lambda \end{bmatrix} \begin{pmatrix} grad\ p \\ grad\ T \end{pmatrix}$$

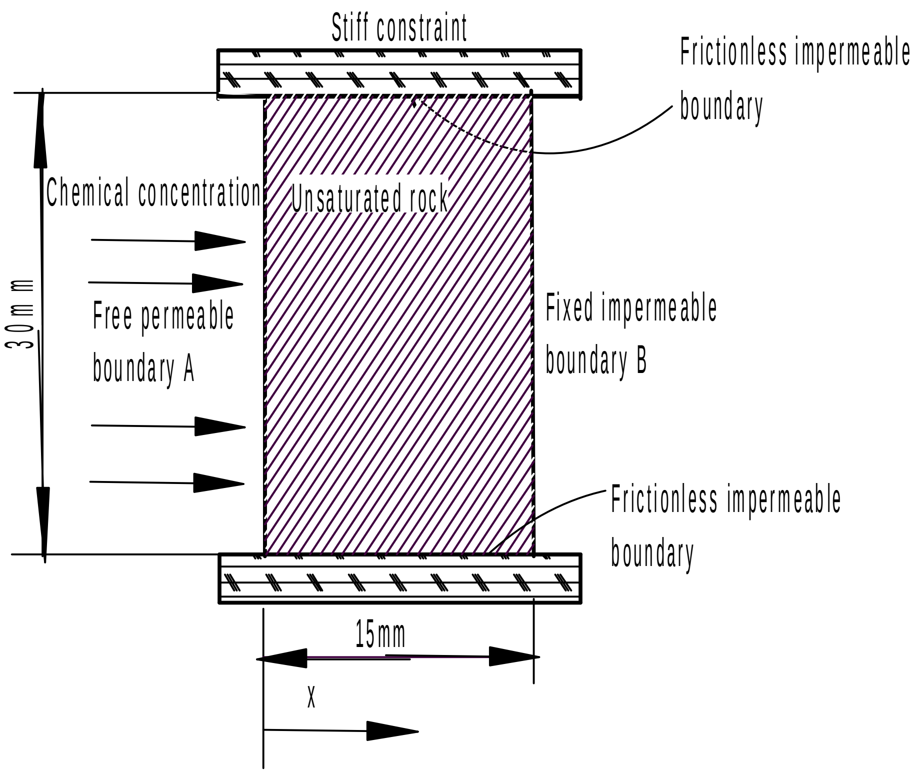
CHEN, X., PAO, W. & LI, X. 2013. Coupled thermo-hydro-mechanical model with consideration of thermal-osmosis based on modified mixture theory. *International Journal of Engineering Science,* 64**,** 1-13.

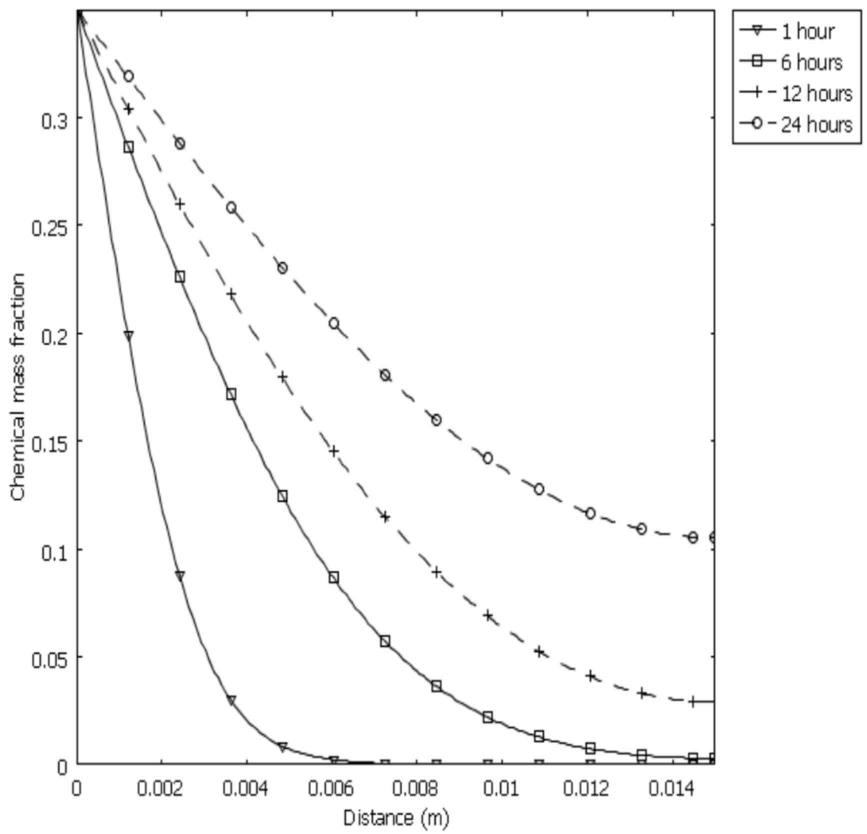
UNIVERSITY OF LEEDS

Contents

(Experiment set up + chemical transport)

Invalidate Darcy's Law (1: Chemical osmosis)





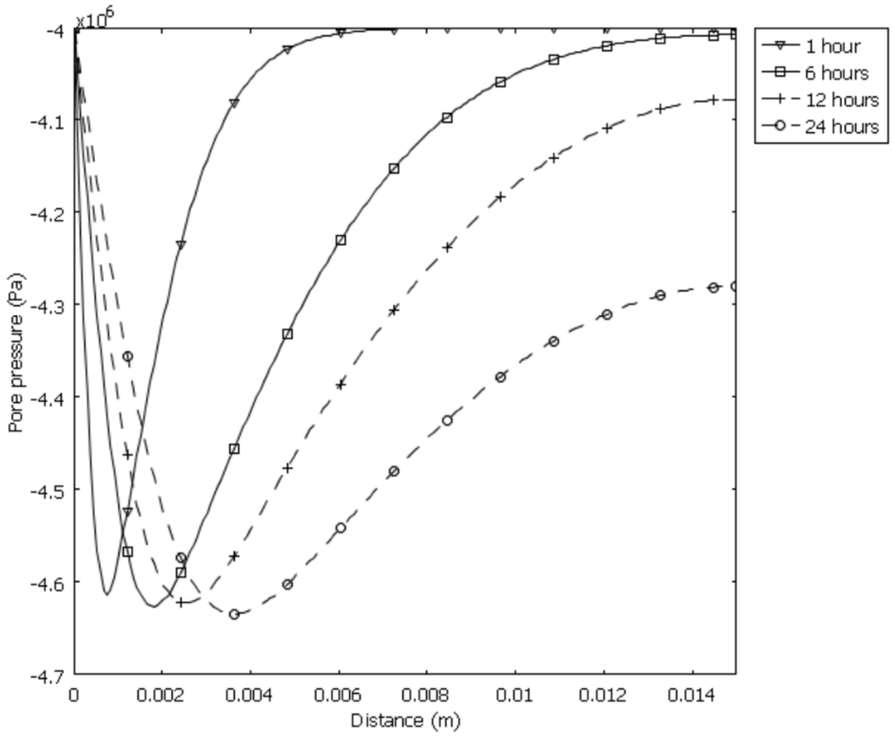


Fig. 3 Evolution of pore water pressure distribution with time during first day

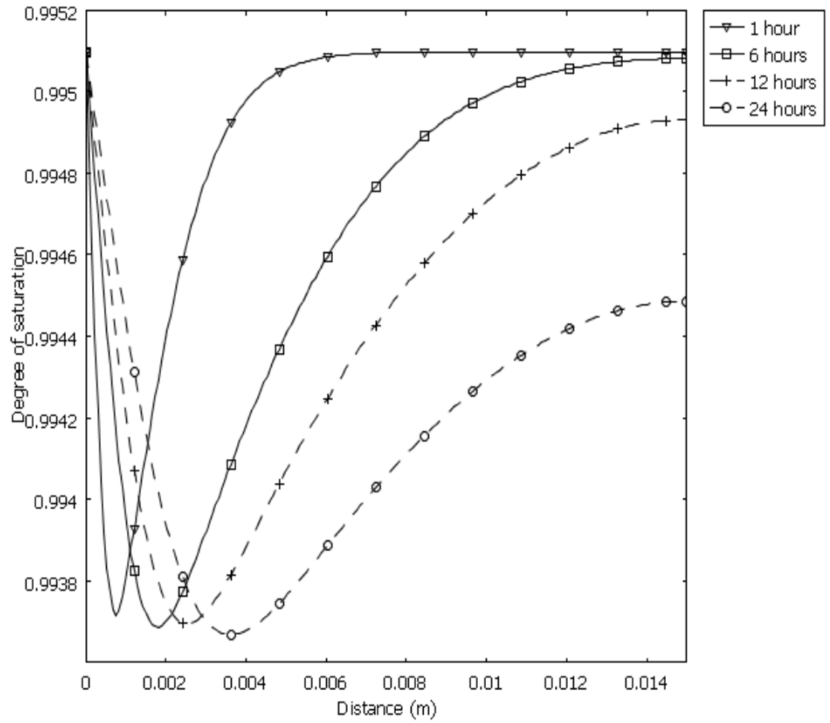


Fig. 4 Evolution of degree of saturation distribution with time during first day

Invalidate Darcy's Law (2: Thermo osmosis)

X. Chen et al./International Journal of Engineering Science 64 (2013) 1–13

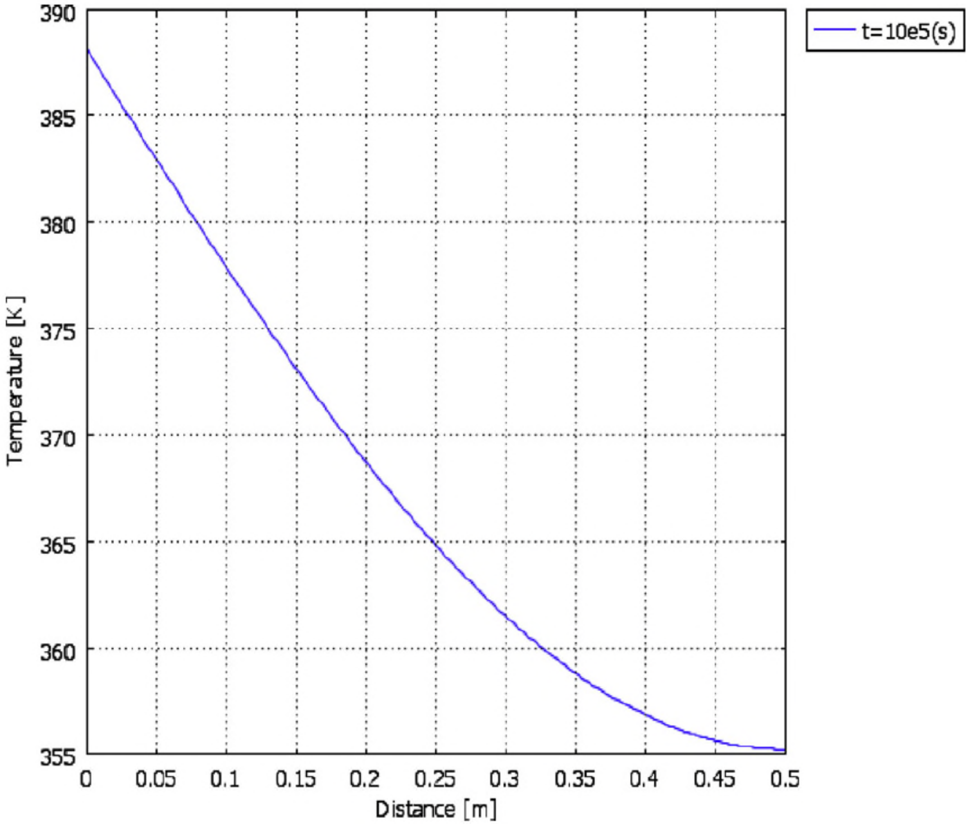
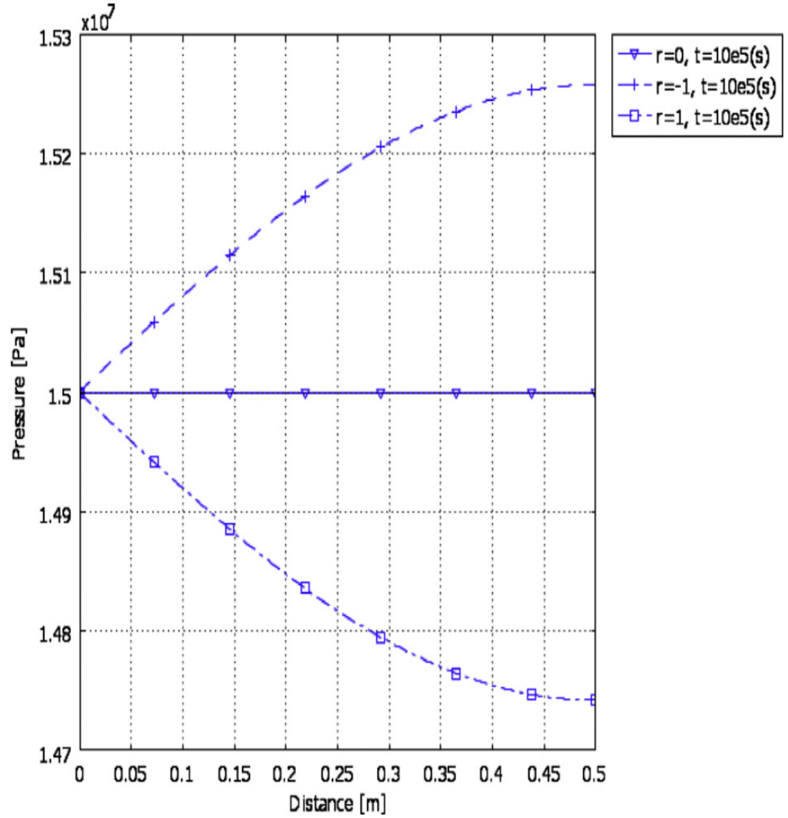


Fig. 5. Temperature distribution.

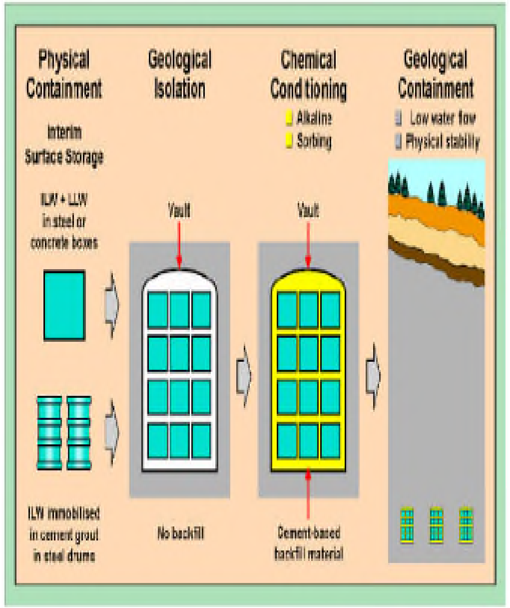


Contents

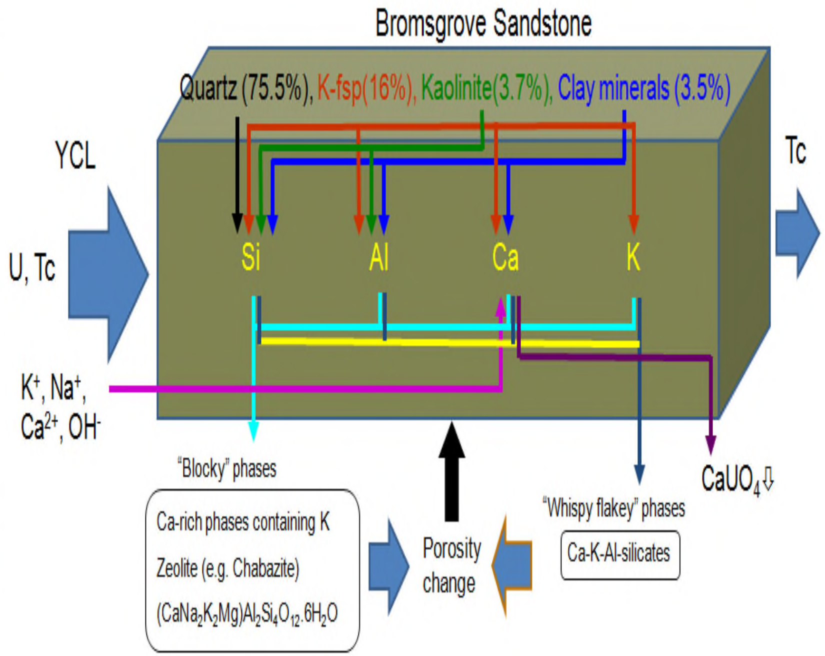
Intermediate/Low Level nuclear waste: Radionuclides transport through sandstone in groundwater

Darcy's Law, valid or not in a contaminant-impacted zone?

(Part 2: heavily reactive porous media)



Nuclear Waste Concept



(2) Conceptual model

Conclusion: multi-minerals dissolution strongly affects the pathway and chemistry of groundwater flow .

Corkhill, C; Bridge, J; **Chen, X**; Hillel, P; Thornton, S; Romero-Gonzalez, M; Banwart, S; Hyatt, N. (2013) Real-time gamma imaging of technetium transport through natural and engineered porous materials for radioactive waste disposal, *Environmental Science & Technology, 47(23): 13857-1864.*

Chen, X., Thornton, S. F. & Small, J. Influence of Hyper-Alkaline pH Leachate on Mineral and Porosity Evolution in the Chemically Disturbed Zone Developed in the Near-Field Host Rock for a Nuclear Waste Repository. *Transport in Porous Media* **107**, 489-505, doi:10.1007/s11242-014-0450-0 (2015).

Acknowledgement

UNIVERSITY OF LEEDS

New theory could boost engineering solutions/innovations…
… gap between theory and engineering application….

Geochemistry

Geomechanics

Groundwater

Nuclear Waste

Agriculture Soil

Available for consultancy;

Welcome industry partner to join our team to develop links with China industry and academy for applications to Innovate UK and Newton fund in the area of contaminated lands.

Contact information:
x.chen@leeds.ac.uk

Current funded project:
BioSAS consortium (around £580k)