



Nano zero valent iron (nZVI) remediation: A COMSOL modelling approach

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ABSTRACT

Remediation using nanoscale zerovalent iron (nZVI) is a promising in situ technology that can convert toxic groundwater contaminants into environment-friendly compounds. Despite its promising characteristics, field scale implementation of nZVI technology has faced major challenges due to poor subsurface mobility, limited longevity and well clogging, all leading to a smaller travel distance. A greater travel distance is preferable since it can reduce the total time of remediation and provide a cost-effective solution. There are several factors that may affect nZVI travel distance such as rapid aggregation, settling, straining, unwanted oxidation, nZVI injection method, pore water velocity, lag phase (time duration when injection of nZVI is stopped), viscosity of solution, concentration of solution and heterogeneity of subsurface. Although various studies have been performed to investigate the effect of some of these parameters, no studies have investigated the role that soil heterogeneity plays on the efficiency of nZVI technology. Such a study may bridge the gap in fundamental understanding of nZVI transport in groundwater and help in overcoming the implementation challenges at the field scale. To examine the possible effects of soil heterogeneity on nZVI transport, a three-dimensional model has been developed using COMSOL, by modifying the colloid filtration theory (CFT) and verified with a previous field validated model.

RÉSUMÉ

La réhabilitation à l'aide de nanoparticules de fer zérovalentes (nZVI) est une technologie in situ prometteuse qui peut convertir les contaminants toxiques des eaux souterraines en composés respectueux de l'environnement. Malgré ses caractéristiques prometteuses, la mise en œuvre à grande échelle de la technologie du NZVI a été confrontée à des défis majeurs en raison de la faible mobilité souterraine, de la longévité limitée et du colmatage du puits, conduisant à une plus faible distance. Une plus grande distance de déplacement est préférable car elle peut réduire le temps total d'assainissement et fournir une solution rentable. Plusieurs facteurs peuvent affecter la distance de déplacement du NZVI: agrégation rapide, décantation, déformation, oxydation non désirée, méthode d'injection de nZVI, vitesse de l'eau interstitielle, phase de latence (durée d'arrêt de l'injection de nZVI), viscosité de la solution et l'hétérogénéité de la subsurface. Bien que diverses études aient été effectuées pour étudier l'effet de certains de ces paramètres, aucune étude n'a examiné le rôle de l'hétérogénéité du sol sur l'efficacité de la technologie du zona. Une telle étude peut combler le fossé dans la compréhension fondamentale du transport de NZVI dans les eaux souterraines et aider à surmonter les défis de mise en œuvre à l'échelle du terrain. Pour examiner les effets de l'hétérogénéité du sol sur le transport du NZVI, un modèle tridimensionnel a été développé en utilisant COMSOL, en modifiant la théorie de la filtration colloïdale (CFT) et vérifié avec un modèle antérieur validé sur le terrain.

1 INTRODUCTION

Groundwater contamination can be caused when chemicals such as heavy metals and chlorinated solvents make their way to underlying aquifers. If such aquifers are used for drinking water, these spills can result in health issues and damage to the environment (Harr 1996). In addition, once contaminated, remediation technologies are needed to treat the aquifer, preferably at the source zone. Remediation using nanoscale zerovalent iron (nZVI) is a promising in situ technology that can reduce groundwater contaminants leading to cleaner aquifers (O'Carroll et al., 2013, Mondal et al. 2017).

nZVI remediation works because the zero valent iron (Fe^0) releases an electron when it is oxidized. These electrons can then reduce toxic groundwater contaminants, converting them into environmentally friendly compounds (Li et al. 2006, O'Carroll et al. 2013). For example, trichloroethylene (TCE, C_2HCl_3) can be reduced to ethane which poses little toxicological risk (Li et al. 2006).

Despite its promising characteristics, field scale implementation of nZVI technology has faced major challenges due to poor subsurface mobility, limited longevity (O'Carroll et al. 2013, Kocur 2015) and well clogging (Elliott and Zhang 2001), all leading to a smaller travel distance. A greater travel distance is preferable since it can reduce the total time of remediation and provide a cost-effective solution.

There are several factors that may affect nZVI travel distance including rapid aggregation, settling, straining, unwanted oxidation, nZVI injection method, groundwater/pore water velocity, lag phase (time duration when injection of nZVI is stopped), concentration/density of solution, viscosity of solution, and heterogeneity of subsurface (Bennett et al. 2010, Krol et al. 2013, Raychoudhury et al. 2014, Kocur et al. 2014).

Aggregation may occur due to particle-particle interaction (Petosa et al. 2010) and settling occurs due to gravitational forces (Phenrat et al. 2007). Straining occurs due to entrapment of particles on thin water films around the soil particles (Shangping et al. 2006). These three factors affect nZVI travel distance by reducing the amount

of nZVI particles available for transport (O'Carroll et al. 2013, Raychoudhury et al. 2014, Kocur 2015).

Unwanted oxidation of nZVI with oxidants (i.e. dissolved oxygen (DO), water, natural oxidants) is responsible for limited longevity/lifetime of nZVI in groundwater (Su et al. 2013, Kocur 2015). In this case, instead of reacting with contaminants, nZVI is oxidized mostly by DO in groundwater which eventually forms various iron products (magnetite and other iron oxides) (Su et al. 2013) and results in nZVI loss. Therefore, this factor affects travel distance of nZVI by reducing the active iron content.

The method of nZVI injection may also influence nZVI travel distance. Different types of injection strategies can be used for nZVI remediation. These include pneumatic injection, direct injection, pressure pulse injection, gravity feed injection etc. (Su et al. 2013, Kocur et al. 2014). While gravity fed injection generally maintains a constant head at the injection well, other injection methods depend on injecting flux in the porous media. Krol et al. (2013) considered both constant flux (CF) and constant head (CH) injections from field injection data of Bennett et al. (2010) in a three dimensional model and found a higher travel distance in the case of a CF injection.

Laumann et al. (2013) conducted a column experiment for nZVI transport and suggested that doubling the injection velocity increased nZVI transport. According to Kocur et al. (2014), field travel distance and longevity of nZVI can be achieved with very high pore water velocity and highly stable nZVI suspension. Alternatively, lag phase during successive Injection of nZVI can lead to deposition of nZVI in porous media due to low pore water velocity (Bennett et al. 2010, Kocur et al. 2014) and make nZVI immobile (Krol et al. 2013).

Travel distance of nZVI can also be influenced by the solution viscosity (Krol et al. 2013, Chowdhury et al. 2015). nZVI solution viscosity and stability can be increased by adding different types of polymer such as carboxymethyl cellulose (CMC) (Li et al. 2015). Li et al. (2015) observed greater travel efficiency by adding 2 g/L CMC at a fixed nZVI concentration. Higher nZVI recovery was observed from the experimental sand tank as CMC concentration was increased from 1 g/L to 2 g/L. However, increasing solution viscosity decreased the hydraulic conductivity lowering the travel velocity.

nZVI concentration in the injected solution can also affect nZVI travel distance. Laboratory experiments showed a higher fraction of nZVI was recovered by injecting lower concentrations (Phenrat et al. 2010, Li et al. 2016). However, the length in the sand-tank was fixed during the experiment which may affect travel distance of nZVI directly and cannot represent a field aquifer.

Lastly, subsurface heterogeneity can affect nZVI travel distance, for example, more nZVI can be transported in coarse sands than in fine sands (Yang et al. 2007, Phenrat et al. 2010, Raychoudhury et al. 2014, Li et al. 2016). During field injection, subsurface heterogeneity strongly hindered flow (Kocur et al. 2014) and distribution of nZVI (Henn and Waddill 2006). Preferential flow caused by subsurface heterogeneity negatively impacted the remediation goal as nZVI failed to reach the target contaminant (He et al. 2010, Velimirovic et al. 2014),

daylighting of injected solution (solution shows up on surface) was also observed in field study (Su et al. 2013). In addition, phenomena such as aggregation and straining are greatly influenced by soil particle size. As natural aquifer are heterogeneous in nature (variable permeability distribution in every layer of soil profile), modeling studies should incorporate heterogeneity to investigate the effect and optimize nZVI technology. However, few studies exist examining nZVI distribution in a heterogeneous permeability field representing a typical groundwater aquifer.

Such a study may bridge the gap in fundamental understanding of nZVI transport in groundwater and help in overcoming the implementation challenges at the field scale. To examine the effects of soil heterogeneity on nZVI transport, a three-dimensional model has been developed using COMSOL, by modifying the colloid filtration theory (CFT) and verifying it with a field validated model of Krol et al. (2013).

2 COMSOL MODELLING APPROACH

COMSOL Multiphysics is a software platform based on finite elements for modelling and simulating physics-based problems. It is defined as a "Multiphysics" platform because it can deal with various types of physical phenomena such as fluid flow, heat transfer, pore scale flow, etc. (COMSOL User's Guide 2017). Various types of physics are built into COMSOL modules, with appropriate characteristic equations and fundamental features. These modules can be linked together, as well as, modified with additional user-defined equations (COMSOL User's Guide 2017). For this work, the Transport of Diluted Species (TDS) Module and the Darcy's Law (DL) Module were used.

2.1 Model Development for nZVI Transport

To model nZVI transport, a three dimensional (3D) modelling approach described by Krol et al. (2013) was used. Krol et al. (2013) simulated a field study (Bennett et al., 2010) in which CMC-coated nZVI was injected in a shallow granulated aquifer. Krol et al (2013) used CompSim, a 3D finite difference, three-phase, simulator developed by Sleep and Sykes (1993). The results of the CompSim was used to verify the model developed in this study to ensure that the transport of CMC-nZVI was correctly implemented using COMSOL.

2.2 Numerical Approach

The DL module defines Darcy's law in COMSOL by:

$$\frac{\partial n}{\partial t} + \nabla \cdot (\rho q) = Q_m \quad [1]$$

Where q is the Darcy velocity ($m \cdot s^{-1}$) and $q = -\frac{K_p \nabla P}{\mu}$; K_p is the permeability (m^2), ∇P is the pressure head gradient (m/m) and μ is viscosity ($Pa \cdot s$). $\nabla P = \rho g \nabla h$, where ∇h is hydraulic gradient. A 3D Darcy velocity field is created in the DL module which is transferred to the TDS module.

The transport of polymer coated nanoparticles in a porous media is described by the TDS module:

$$\frac{\partial(nC)}{\partial t} - \nabla \cdot (nD \cdot \nabla C) + \nabla \cdot (Cq) = -nK_{att}C \quad [2]$$

Where C is the aqueous solute concentration ($\text{mol} \cdot \text{m}^{-3}$), n is the soil porosity ($-$), D is the effective hydrodynamic dispersion tensor. Attachment rate coefficient K_{att} (s^{-1}) is defined by the CFT (Tufenkji and Elimelech 2004) and expressed as:

$$K_{att} = \frac{3(1-n)\alpha\eta u}{2d_c} \quad [3]$$

Where α is the attachment efficiency ($-$), η is the single collector contact efficiency ($-$), d_c is the collector (soil grain) diameter (m). The term ($u = q/n$) is the pore water velocity ($\text{m} \cdot \text{s}^{-1}$) or average linear groundwater velocity through the pores. It is to be noted that the term K_{att} (s^{-1}) is applied for nanoparticle transport or nZVI transport only. The polymer (CMC) is considered a conservative species, and therefore the attachment rate for polymer is zero.

2.3 Boundary Condition

Figure 1 represents the boundary conditions (BC) and characteristics of half of a 3D domain. Since this model represents a remediation scenario, a cylindrical injection well has been defined in the middle of domain which injects CMC-coated nZVI solution into the subsurface. The initial concentration of solution is defined as zero in the domain and the direction of groundwater flow (Q_m) is from left to right due to "hydraulic head" BC.

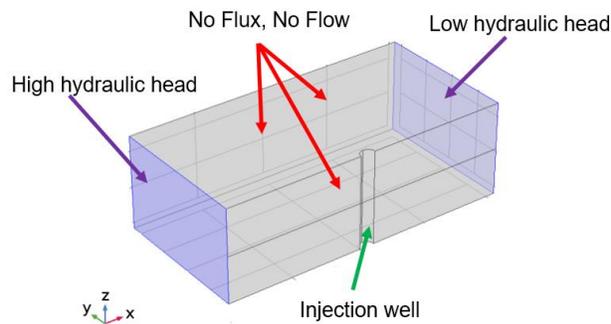


Figure 1. Boundary condition for half of a 3D domain.

"No flow" and "no flux" BC have been defined at the upper, lower and side boundaries. The injection well can be used for defining a mass flow rate of water ($\text{kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$) in the DL module and constant flux of nZVI ($\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$) in the TDS module. A symmetry BC has been used along the XZ plane through the injection well to split the domain into half and minimize computations.

2.4 Parameters and Variables

To simulate the Krol et al (2013) domain, the same parameters were used and are summarized in Table 1.

Table 1. Basic simulation parameters (adapted from Krol et al (2013))

Name	Symbol	Value
Length of domain	L	4 (m)
Radius of injection well	R_i	0.05 (m)
Density of porous media	ρ_P	1250 ($\text{kg} \cdot \text{m}^{-3}$)
Porosity	n	0.36 ($-$)
Density of nZVI solution	ρ_F	1000 ($\text{kg} \cdot \text{m}^{-3}$)
Diameter of nZVI	d_p	1.40×10^{-7} (m)
Diameter of collector	d_c	2×10^{-4} (m)
Hamker constant	A	3×10^{-21} (J)
Boltzmann constant	k	1.4×10^{-23} (J/k)
Temperature	T	293 K
Diffusion coefficient (nZVI)	D_{FN}	3×10^{-9} ($\text{m}^2 \cdot \text{s}^{-1}$)
Diffusion coefficient (polymer)	D_{FP}	1×10^{-9} ($\text{m}^2 \cdot \text{s}^{-1}$)
Permeability	K_P	3.6×10^{-11} (m^2)
Hydraulic gradient	∇h	0.0142 (m/m)
Attachment efficiency coefficient	α	0.02
CMC molecular weight		90K (g/mol)
CMC percentage		0.8%
nZVI injection concentration		0.96 (g/L)

2.4.1 Colloidal Filtration Theory

To simulate the transport of nZVI, the transport equation (Equation 1) was modified with the CFT. Single collector contact efficiency (η), a variable in CFT equation requires calculation of several parameters. While some values are fixed at the start of a model, other values vary with time and space, for example pore water velocity, producing a non-linear system which is sensitive to initial conditions and can result in numerical convergence challenges. Single collector contact efficiency (η) can be determined by the following equation (Tufenkji and Elimelech 2004)

$$\eta = 2.4 A_S \frac{1}{N_r} N_r^{-0.081} N_{Pe}^{-0.715} N_{vdw}^{0.052} + 0.55 A_S N_r^{1.675} N_a^{0.125} + 0.22 N_r^{-0.24} N_G^{1.11} N_{vdw}^{0.053} \quad [4]$$

where, A_S is called the porosity dependent parameter, N_r is the aspect ratio, N_{Pe} is the Peclet number, N_{vdw} is the Van der Waals number, N_a is the attraction number and N_G is the gravity number. A_S and N_{vdw} are fixed parameters. N_{Pe} depends on both pore water velocity (u) and bulk diffusion coefficient (D_B). Both N_a and N_G depend on pore water velocity and subsurface viscosity (μ_{sub}). N_r varies with collector diameter (d_c) therefore for heterogeneous domain it can be calculated using the Kozeny-Carman equation (Kozeny 1927, Carman 1937, 1956).

$$d_c = \sqrt{\frac{(K_p (1-n)^2 180)}{n^3}} \quad [5]$$

2.4.2 Molar Fraction of nZVI and Polymer

COMSOL solves two dependent variables for the aqueous concentrations of nZVI and polymer, (C_N) (mol. m^{-3}) and (C_P) (mol. m^{-3}) respectively. In COMSOL, the unit (mol. m^{-3}) represents the moles of species per unit of total volume. However, typically field nZVI injections are given in terms of mole fractions therefore the concentrations are related as follows:

$$X_N = \left(\frac{C_N x_{ni}}{n C_{in}} \right) \quad [6]$$

$$X_P = \left(\frac{C_P x_{pi}}{n C_{ip}} \right) \quad [7]$$

where x_{ni} , x_{pi} and x_w are the initial mole fractions of nZVI, polymer and water respectively and C_{in} and C_{ip} are initial concentration of nZVI and polymer respectively. n is soil porosity and the mole fraction of nZVI and polymer are X_N and X_P , respectively. These mole fractions vary in each node of the model as concentration varies with time.

2.4.3 Subsurface Viscosity

To calculate the viscosity of the injected solution the Grunberg and Nissan equation was used (Grunberg and Nissan 1949) :

$$\log(\mu_{sol}) = x_{pi} \log(\mu_p) + x_{ni} \log(\mu_{nf}) + x_w \log(\mu_{wf}) \quad [8]$$

Where μ_{sol} is the solution viscosity determined from experiments. While initial mole fractions and viscosity of nZVI (μ_{nf}) and water (μ_{wf}) are known, viscosity of polymer (μ_p) is difficult to determine from experiments. So, $\log(\mu_p)$ is determined from Equation 8 in following way

$$\log(\mu_p) = \frac{\log(\mu_{sol}) - x_{ni} \log(\mu_{nf}) - x_w \log(\mu_{wf})}{x_{pi}} \quad [9]$$

When the CMC-nZVI solution is injected into the subsurface, the solution viscosity is calculated at every node since the mole fraction of nZVI and polymer (i.e. X_N and X_P) changes. The equation for calculating subsurface viscosity (μ_{sub}) of the solution is:

$$\mu_{sub} = 10^{X_P \log(\mu_p) + X_N \log(\mu_{nf}) + x_w \log(\mu_{wf})} \quad [10]$$

This uses the X_N and X_P in each node of the model domain, thereby varying the subsurface viscosity accordingly.

2.4.4 Molar Flux for Injection Well

The molar flux of nZVI or polymer can be computed from the multiplication of mass flow rate per unit area (M_{fa}) ($\text{kg. m}^{-2}. \text{s}^{-1}$) and molar rate of injection of nZVI and polymer (I_{MNP}) (mol. kg^{-1}) and dividing them by porosity (n).

$$F_{NP} = \frac{M_{fa} I_{MNP}}{n} \quad [11]$$

If the mass concentration of the total solution is defined by C_M (kg. m^{-3}), the percentage of nZVI or polymer in total solution by P_t , Molecular weight of nZVI or polymer by M_W (kg. mol^{-1}) and density of water by ρ_F (kg. m^{-3}), (density of nZVI solution also), then a general equation for finding molar rate of injection of nZVI and polymer (I_{MNP}) (mol. kg^{-1}) is

$$I_{MNP} = \frac{C_M P_t}{M_W \rho_F} \quad [12]$$

3 VERIFICATION OF MODEL RESULTS

The COMSOL model was verified using the Krol et al. (2013) study. Figures 2 and 3 compare nZVI concentration and subsurface viscosity of the COMSOL and CompSim models respectively for 1 and 20 hours of constant injection. Figure 2 compares a one dimensional (1D) plot of nZVI concentration from these two studies showing good agreement of the COMSOL model with previous work of Krol et al. (2013).

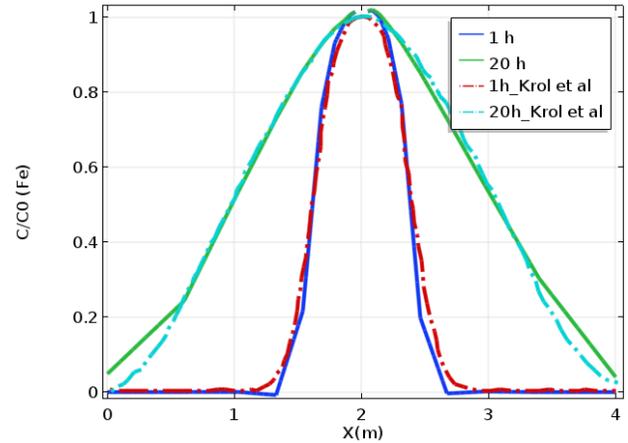


Figure 2. Comparison of nZVI concentration with time.

Figure 3 shows a 1D plot of subsurface viscosity for both plots showing good agreement of the COMSOL model with previous work of Krol et al. (2013).

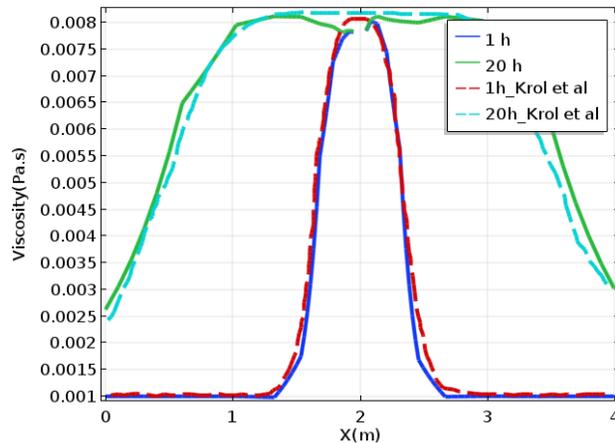


Figure 3. Comparison of subsurface viscosity with time.

To rule out mesh and time size dependence, a mesh convergence study was performed for various mesh size (i.e. coarser to extremely fine mesh). The result for different mesh sizes were quite similar therefore the solution was found to be mesh independent. A time convergence study was also performed and the solution was found to be time independent.

4 3D NZVI TRANSPORT IN POROUS MEDIA

nZVI injection into the subsurface is typically performed using an injection well. To better depict and predict remediation scenarios and to study the effect of various parameters, a 3D model is needed. Figure 4 represents a simulated 3D domain showing nZVI spread from a constant flux injection well after 20 hours of injection into a homogeneous domain.

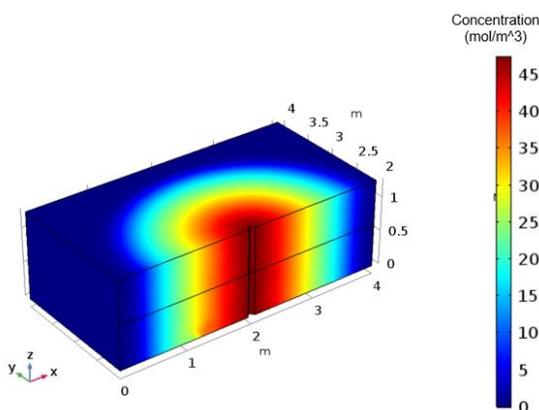


Figure 4. nZVI spread after 20 hours of injection

5 CONCLUSIONS

In this paper, COMSOL Multiphysics has been used to simulate a constant nZVI flux injection in a homogeneous

3D domain representing a remediation scenario. The model modifies the transport equation by CFT and uses a field-validated model from Krol et al. (2013) to verify the nZVI transport. Good agreement between the COMSOL and CompSim (Krol et al. (2013) models was found. In addition, the COMSOL model was found to be mesh and time dependent. The newly developed model will be used to examine various parameters affecting nZVI remediation including subsurface heterogeneity which has not been studied in depth to date.

6 REFERENCES

- Bennett, P., he, F., Zhao, D., Aiken, B., and Feldman, L. 2010. In situ testing of metallic iron nanoparticle mobility and reactivity in a shallow granular aquifer. *Journal of contaminant hydrology*, 116: 35–46.
- Carman, P.C. 1937. Fluid flow through granular beds. *Transactions, Institution of Chemical Engineers (London)*, 15: 150–166.
- Carman, P.C. 1956. *Flow of gases through porous media*. London : Butterworths Scientific.
- Chowdhury, A.I.A., Krol, M.M., Kocur, C.M., Boparai, H.K., Weber, K.P., Sleep, B.E., and O'Carroll, D.M. 2015. nZVI injection into variably saturated soils: Field and modeling study. *Journal of Contaminant Hydrology*, 183: 16–28.
- COMSOL User's Guide. 2017. *Introduction to COMSOL Multiphysics*.USA.
- Elliott, D.W., and Zhang, W. 2001. Field Assessment of Nanoscale Bimetallic Particles for Groundwater Treatment. *Environmental Science & Technology*, 35(24): 4922–4926.
- Grunberg, L., and Nissan, A.H. 1949. Mixture Law for Viscosity. *Nature*, 164(4175): 799–800.
- Harr, J. 1996. *A civil action*. Vintage Books, New York.
- He, F., Zhao, D., and Paul, C. 2010. Field assessment of carboxymethyl cellulose stabilized iron nanoparticles for in situ destruction of chlorinated solvents in source zones. *Water Research*, 44(7): 2360–2370.
- Henn, K.W., and Waddill, D.W. 2006. Utilization of nanoscale zero-valent iron for source remediation—A case study. *Remediation Journal*, 16(2): 57–77.
- Kocur, C. 2015. *Field Scale Application of Nanoscale Zero Valent Iron: Mobility, Contaminant Degradation, and Impact on Microbial Communities*. Electronic Thesis and Dissertation Repository, Canada.
- Kocur, C.M., Chowdhury, A.I., Sakulchaicharoen, N., Boparai, H.K., Weber, K.P., Sharma, P., Krol, M.M., Austrins, L., Peace, C., Sleep, B.E., and O'Carroll, D.M. 2014. Characterization of nZVI Mobility in a Field Scale Test. *Environmental Science & Technology*, 48(5): 2862–2869.
- Kozeny, J. 1927. *Ueber kapillare Leitung des Wassers im Boden*. *Sitzungsber Akad. Wiss, Wien*, 136(2a): 271–306.

- Krol, M.M., Oleniuk, A.J., Kocur, C.M., Sleep, B.E., Bennett, P., Xiong, Z., and O'Carroll, D.M. 2013. A Field-Validated Model for In Situ Transport of Polymer-Stabilized nZVI and Implications for Subsurface Injection. *Environmental Science & Technology*, 47(13): 7332–7340.
- Laumann, S., Micić, V., Lowry, G.V., and Hofmann, T. 2013. Carbonate minerals in porous media decrease mobility of polyacrylic acid modified zero-valent iron nanoparticles used for groundwater remediation. *Environmental Pollution*, 179: 53–60.
- Li, J., Bhattacharjee, S., and Ghoshal, S. 2015. The effects of viscosity of carboxymethyl cellulose on aggregation and transport of nanoscale zerovalent iron. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 481:451-459.
- Li, J., Rajajayavel, S.R.C., and Ghoshal, S. 2016. Transport of carboxymethyl cellulose-coated zerovalent iron nanoparticles in a sand tank: Effects of sand grain size, nanoparticle concentration and injection velocity. *Chemosphere*, 150: 8–16.
- Li, X., Elliott, D.W., and Zhang, W. 2006. Zero-Valent Iron Nanoparticles for Abatement of Environmental Pollutants: Materials and Engineering Aspects. *Critical Reviews in Solid State and Materials Sciences*, 31(4): 111–122.
- Mondal, P.K., Furbacher, P.D., Cui, Z., Krol, M.M., and Sleep, B.E. 2017. Transport of polymer stabilized nano-scale zero-valent iron in porous media. *Journal of Contaminant Hydrology*, 1–13.
- O'Carroll, D., Sleep, B., Krol, M., Boparai, H., and Kocur, C. 2013. Nanoscale zero valent iron and bimetallic particles for contaminated site remediation. *Adv. Advances in Water Resources*, 51: 104–122.
- Petosa, A.R., Jaisi, D.P., Quevedo, I.R., Elimelech, M., and Tufenkji, N. 2010. Aggregation and Deposition of Engineered Nanomaterials in Aquatic Environments: Role of Physicochemical Interactions. *Environmental Science & Technology*, 44(17): 6532–6549.
- Phenrat, T., Cihan, A., Kim, H.-J., Mital, M., Illangasekare, T., and Lowry, G.V. 2010. Transport and Deposition of Polymer-Modified Fe₀ Nanoparticles in 2-D Heterogeneous Porous Media: Effects of Particle Concentration, Fe₀ Content, and Coatings. *Environmental Science & Technology*, 44(23): 9086–9093.
- Phenrat, T., Saleh, N., Sirk, K., Tilton, R.D., and Lowry, G.V. 2007. Aggregation and Sedimentation of Aqueous Nanoscale Zerovalent Iron Dispersions. *Environmental Science & Technology*, 41(1): 284–290.
- Raychoudhury, T., Tufenkji, N., and Ghoshal, S. 2014. Straining of polyelectrolyte-stabilized nanoscale zero valent iron particles during transport through granular porous media. *Water Research*, 50: 80–89.
- Shangping, X., Bin, G., and Saiers James E. 2006. Straining of colloidal particles in saturated porous media. *Water Resources Research*, 42(12).
- Sleep, B.E., and Sykes, J.F. 1993. Compositional simulation of groundwater contamination by organic compounds: 1. Model development and verification. *Water Resources Research*, 29(6): 1697–1708.
- Su, C., Puls, R.W., Krug, T.A., Watling, M.T., O'Hara, S.K., Quinn, J.W., and Ruiz, N.E. 2013. Travel distance and transformation of injected emulsified zerovalent iron nanoparticles in the subsurface during two and half years. *Water Research*, 47(12): 4095–4106.
- Tufenkji, N., and Elimelech, M. 2004. Correlation Equation for Predicting Single-Collector Efficiency in Physicochemical Filtration in Saturated Porous Media. *Environmental Science & Technology*, 38(2): 529–536.
- Velimirovic, M., Tosco, T., Uyttebroeck, M., Luna, M., Gastone, F., De Boer, C., Klaas, N., Sapion, H., Eisenmann, H., Larsson, P.-O., Braun, J., Sethi, R., and Bastiaens, L. 2014. Field assessment of guar gum stabilized microscale zerovalent iron particles for in-situ remediation of 1,1,1-trichloroethane. *Journal of Contaminant Hydrology*, 164: 88–99.
- Yang, G.C.C., Tu, H.-C., and Hung, C.-H. 2007. Stability of nanoiron slurries and their transport in the subsurface environment. *Separation and Purification Technology*, 58(1): 166–172.