RGC Ref.: N_HKUST603/16
NSFC Ref. : 51661165015
(please insert ref. above)

The Research Grants Council of Hong Kong
NSFC/RGC Joint Research Scheme
Joint Completion Report

(Please attach a copy of the completion report submitted to the NSFC by the Mainland researcher)

Part A: The Project and Investigator(s)

1. Project Title

Environmental Behaviors of Arsenic-loaded Zero-Valent Iron Nanoparticles in Subsurface Systems
地下系統中砷負載零價鐵納米顆粒的環境行為

2. Investigator(s) and Academic Department/Units Involved

	Hong Kong Team	Mainland Team
Name of Principal Investigator *(with title)*	Prof. Irene Man Chi LO	Prof. Liming HU
Post	Chair Professor	Professor
Unit / Department / Institution	Civil and Environmental Engineering, The Hong Kong University of Science and Technology	Geo-Environmental Research Centre/ Department of Hydraulic Engineering/ Tsinghua University
Contact Information	cemclo@ust.hk	gehu@tsinghua.edu.cn
Co-investigator(s) *(with title and institution)*	N/A	Prof. Xiaofeng WU, Professor, Tsinghua University Dr. Xiaoli LIU, Associate Professor, Tsinghua University Dr. Hui WU, Research Associate, Tsinghua University

3. Project Duration

	Original	Revised	Date of RGC/ Institution Approval *(must be quoted*)
Project Start date	1/1/2017		
Project Completion date	31/12/2020		
Duration *(in month)*	48		
Deadline for Submission of Completion Report	31/12/2021		

Part B: The Completion Report

5. Project Objectives

5.1 Objectives as per original application

1. Examine the stability of original nZVI and As-loaded nZVI in groundwater under different geochemical conditions in terms of aggregation and sedimentation of particles;
2. Investigate the immobilization and remobilization of original nZVI and As-loaded nZVI on soils, the adsorption of arsenic by nZVI immobilized soils, and the desorption of arsenic from As-loaded nZVI and As-loaded nZVI immobilized soils under different geochemical conditions by batch experiments.
3. Study the transport of original nZVI and As-loaded nZVI in different porous media, and the potential release of arsenic during the process by performing column experiments.
4. Perform large-scale 2D and 3D physical modelling to investigate the transport and fate of nZVI and As-loaded nZVI in soils under different geochemical conditions.
5. Develop a novel mathematical model with numerical simulation to mimic the environmental behaviors of nZVI and As-loaded nZVI in subsurface during in-situ remediation of arsenic-contaminated groundwater. The environmental risk will be evaluated based on the simulation results from the numerical modelling.

5.2 Revised Objectives

Nil

Date of approval from the RGC: _____

Reasons for the change: _____

_____

1.
2.
3. ....

6. Research Outcome

Major findings and research outcome
(maximum 1 page; please make reference to Part C where necessary)

To my knowledge, this is the first study that utilized plant biosensors (i.e., Arabidopsis) to investigate the toxicities of As(V) and nZVI in terms of Pi and ATP levels in plant tissues. We obtained high quality findings and thus successfully published our findings in the very prestigious journal, Environmental Science and Technology (IF 9.028).

The roles of surface modification and As loading on the transport of the As-loaded nZVI particles were examined. This study discovered that surface modification and As loading play critical roles in the mobility and transport of the As-loaded nZVI in quartz sand. The transport mechanisms were found to be the ripening and sedimentation, indicated by the Tufenkji- Elimelech equation and the HYDRUS-1D model. Therefore, for As remediation of groundwater, the injected nZVI is recommended to be modified by polymers. Moreover, in order to produce a higher As loading, an appropriate dosage of nZVI is preferable to be injected into the As-contaminated groundwater plume.

Our batch test results also show that the nZVI has high removal capacity on different types of contaminant such as phosphate. Under higher ionic strength and lower pH conditions, the aggregation tendency of nZVI is higher which affects the mobility of nZVI. In order to obtain good mobility of nZVI, an alkaline and low ionic strength condition is needed. However, to achieve high removal capacity, the pH condition should be controlled as a weakly acidic or neutral condition.

Results of 1D and 2D model tests show that due to the higher negative surface potential, the transport capacity of nZVI was enhanced after the adsorption of phosphate. The mobility of phosphate-sorbed nZVI is affected by the pore-structure and particle surface characteristics of soils.

Moreover, pore-network models are established to simulate colloid transport and retention. The influence of nanoscale roughness, chemical heterogeneity, and microscopic roughness on the transport and retention of colloids with different particle sizes was investigated under conditions of different pore water velocity. The retention of nZVI is mainly controlled by hydrodynamic bridging and straining. The retention of phosphate-sorbed nZVI is also influenced by surface deposition besides hydrodynamic bridging and straining.

From this project, we have published 8 top international journals based on the findings from our in-depth fundamental understanding of nZVI in subsurface remediation. In addition, we also received 2 major awards: (1) 2019 Natural Science Award, and (2) 2019 top 10% of the papers published in *Environmental Science-Water Research & Technology.* Details of these 2 awards are mentioned in the section “Other Impacts”.

Potential for further development of the research and the proposed course of action
(maximum half a page)

Since the fundamental understanding of the arsenic removal mechanisms of nZVI and its application with the potential risk have been developed from this project, we would like to further investigate the potential of recovering the nZVI from the subsurface to the above ground using magnetic field for recycling and reuse. It is because nZVI has its natural magnetic property and should be able to

recover by applying magnetic field. If this research idea is feasible, it can further reduce its potential risk to the ecosystem and minimize the cost of site remediation.

7. The Layman's Summary

(describe in layman's language the nature, significance and value of the research project, in no more than 200 words)

Nanoparticles are promising materials for environmental remediation, and nanoscale zero-valent iron (nZVI) in particular has been extensively studied for the in-situ remediation of pollutants such as chlorinated organic compounds, metal ions, and arsenic. This project provides scientific study to assess the transport and fate of original and As-loaded nZVI in various environmental conditions. A mathematical modelling with numerical simulation was developed to simulate the transport and fate of nZVI and thereby predict the potential environmental risk of using nZVI for subsurface remediation. The findings significantly increase our understanding of the environmental behavior of nZVI in the subsurface, which is essential for the responsible application of nZVI in groundwater remediation, and the appropriate assessment of the potential risks. The results also provide a knowledge base to assess the efficacy of in-situ application of nZVI in groundwater remediation.

Part C: Research Output

8. Peer-reviewed journal publication(s) arising directly from this research project

(Please attach a copy of each publication and/or the letter of acceptance if not yet submitted in the previous progress report(s). All listed publications must acknowledge RGC's funding support by quoting the specific grant reference.)

The Latest Status of Publications				Author(s) *(**bold** the authors belonging to the project teams and denote the corresponding author with an asterisk*)*	Title and Journal/ Book *(with the volume, pages and other necessary publishing details specified)*	Submitted to RGC *(indicate the year ending of the relevant progress report)*	Attached to this report *(Yes or No)*	Acknowledged the support of this Joint Research Scheme *(Yes or No)*	Accessible from the institutional repository *(Yes or No)*
Year of publication	Year of Acceptance *(For paper accepted but not yet published)*	Under Review	Under Preparation *(optional)*						
2018				**W Zhang**, **Irene M.C. Lo***, **L Hu**, CP Voon, BL Lim, WK Versaw	Environmental Risks of Nano Zerovalent Iron for Arsenate Remediation: Impacts on Cytosolic Levels of Inorganic Phosphate and MgATP2– in Arabidopsis thaliana. *Environmental Science & Technology* 52 (7), 4385-4392	2019	No	Yes	Yes

2019				**Z. Yu**, **L Hu**, **Irene M. C. Lo***	Transport of the arsenic (As)-loaded nano zero-valent iron in groundwater-saturated sand columns: Roles of surface modification and As loading. Chemosphere, 216, 428-436.	2019	No	Yes	Yes
2019				**Z. Yu, J. Huang, L. Hu, W. Zhang*, Irene M. C. Lo***	Effects of geochemical conditions, surface modification, and arsenic (As) loadings on As release from As-loaded nano zero-valent iron in simulated groundwater. Environmental Science: Water Research & Technology, 5 (1), 28-38.	2021	Yes	Yes	Yes
2019				**J. Huang,** S. Yi, C. Zheng, **Irene M. C. Lo***	Persulfate activation by natural zeolite supported nanoscale zero-valent iron for trichloroethylene degradation in groundwater. Science of The Total Environment. 684, 351-359.	2021	Yes	Yes	Yes
2020				**D. Lin; L. Hu*; Irene M.C. Lo.; Z. Yu**	Size Distribution and Phosphate Removal Capacity of Nano Zero-Valent Iron (nZVI): Influence of pH and Ionic Strength, Water, 12, 2939.	2021	Yes	Yes	Yes

2020				**D. Lin**; S. Bradford; **L. Hu*; Irene M. C. Lo**	Impact of phosphate adsorption on the mobility of PANI-supported nano zero-valent iron, Vadose Zone Journal, 2021, 20.	2021	Yes	Yes	Yes
2021				**D. Lin; L. Hu***; S. A. Bradford*; X. Zhang; **Irene M.C. Lo**	Simulation of Colloid Transport and Retention Using a Pore-Network Model with Roughness and Chemical Heterogeneity on Pore Surfaces, Water Resources Research, 2021, 57.	2021	Yes	Yes	Yes
2021				**D. Lin, L. Hu***, Scott Alan Bradford*, Xinghao Zhang, **Irene M.C. Lo**	Pore-network modeling of colloid transport and retention considering surface deposition, hydrodynamic bridging, and straining. Journal of Hydrology 603, 127020	2021	Yes	Yes	Yes

9. Recognized international conference(s) in which paper(s) related to this research project was/were delivered

(Please attach a copy of each delivered paper. All listed papers must acknowledge RGC's funding support by quoting the specific grant reference.)

Month/Year/ Place	Title	Conference Name	Submitted to RGC *(indicate the year ending of the relevant progress report)*	Attached to this report *(Yes or No)*	Acknowledged the support of this Joint Research Scheme *(Yes or No)*	Accessible from the institutional repository *(Yes or No)*
Nil						

Note: Due to the Covid 19, an abstract was submitted to World Nanotechnology International Conference in early 2019 (where I was invited to give a keynote speech on nZVI) but the conference was cancelled.

10. Student(s) trained

(Please attach a copy of the title page of the thesis.)

Name	Degree registered for	Date of registration	Date of thesis submission/ graduation

Zhigang YU	MPhil	1 Sept 2017	15 Aug 2018

Note: we had a Postdoctoral Fellow (Dr. Weilan Zhang) and a Research Assistant (Junyi Huang) working together with the MPhil student (Zhigang Yu) for this project. They are the co-authors of the first 4 publications.

11. Other impact *(e.g. award of patents or prizes, collaboration with other research institutions, technology transfer, etc.)*

Two awards are obtained as listed below.

1.Prof. Irene Lo received the 2019 Natural Science Award from the Ministry of Education of China. The award certificate is attached herein. Prof. Lo was the only HKUST lead applicant among the eleven awardees from all universities in Hong Kong. Her team has been studying the fundamentals of heavy metal pollution control using zero valent iron-based magnetic materials for the last two decades, and has recently turned the technical know-how into a pilot-scale application. Below is the award title in Chinese.

項目名稱： 鐵基磁性材料應用於重金屬污染控制的基礎研究.
教育部2019年度高等學校科學研究優秀成果獎 (二等獎)

2. The following journal paper was selected as one of the top 10% of the papers published in *Environmental Science-Water Research & Technology* by the editors based on the significance and impact of our journal paper. Please refer to the attached notification by the journal.

Yu Zhigang; Huang Junyi; Hu Liming; Zhang Weilan*; **Lo Irene M. C.*** Effects of geochemical conditions, surface modification, and arsenic (As) loadings on As release from As-loaded nano zero-valent iron in simulated groundwater, *Environmental Science-Water Research & Technology*, 2019, 5(1) 28-38.

12. Statistics on Research Outputs *(Please ensure the summary statistics below are consistent with the information presented in other parts of this report.)*

	Peer-reviewed journal publications	Conference papers	Scholarly books, monographs and chapters	Patents awarded	Other research outputs (Please specify)
No. of outputs arising directly from this research project [or conference]	8	0	0	0	項目名稱： 鐵基磁性材料應用於重金屬污染控制的基礎研究.. 教育部2019年度高等學校科學研究優秀成果獎 (二等獎)