Plan Overview

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Title: Multiscale Investigation of Reactive Biosurfactant/Nanoparticles for in Situ Remediation of Contaminated Groundwater

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Affiliation: University of Manchester

Funder: Natural Environment Research Council (NERC)

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Project abstract:

Contamination of groundwater and soil by chemical solvent and industrial waste has become a matter of increasing public concern. According to UK's parliament by June 2016, around 300,000 hectares of UK soil are known as the contaminated land with toxic elements including cadmium, arsenic, and lead. Where chemical solvent – e.g. Non-Aqueous Phase Liquid (NAPL) – is present, it represents a source of contamination that requires remediation. According to the UK Environment Agency, England and Wales suffer from these contaminations and ever-increasing demand for water. These contaminations also limit the applicability of produced geothermal water that could be considered for agriculture, industry, and drinking water. Consequently, soil and groundwater remediation are necessary to provide high quality and sustainable soil/groundwater.

In-situ flushing through biosurfactant/nanofluid-enhanced aquifer remediation (SNEAR) is one of the cost-effective and environmentally friendly novel technologies for soil/groundwater remediation. The study of SNEAR is challenging (little is known) as it needs to accurately represent the simultaneous occurring of dissolution, mobilisation, chemical and geochemical reactions, thermal effect, etc. Concurrently, the majority of bacteria live in porous environments and microorganisms are naturally present as a biofilm at the surface of the grains, i.e., it is not well understood about how these complex environments shape the composition of the microbial communities during SNEAR. While microorganisms and biosurfactants enhance bioremediation and dissolution, nanomaterials enhance remediation through the chemical oxidation of NAPL.

This proposal aims to investigate – experimentally and numerically – multiscale (pore and large scales) remediation of soil and groundwater using reactive biosurfactants and nanoparticles, i.e., overall aim of this proposal is to reduce empiricism and enhance predictive capacity for fate and transport of NAPL species in SNEAR processes. Accordingly, it is aims to develop numerical models and simulators (at both pore and large scales) for computational miscible interface and reactive fluid dynamics for SNEAR by simultaneously occurring dissolution, mobilisation, chemical and geochemical reactions, thermal effect, and bacterial evolution in the porous media. This proposal focuses on miscible dynamic interfaces with interphase mass transfer affected by the heterogeneity of subsurface. The numerical model will be incorporated into a meso- and macroscopic code for SNEAR operation, and devise a novel computationally efficient spatio-temporal adaptive multiscale apparatus to

account for micro- and macro-heterogeneities of porous media. Ultimately, it aims to study a field (pilot-scale) by developing a multiscale computational software for soil and water remediation.

Furthermore, microfluidics (micromodel) and x-ray microtomography experiments will be conducted for developing such phenomena of soil/groundwater remediation to be used in numerical modelling and simulator. These experiments provide useful information on the feasibility of biosurfactant and Nano-remediation together with the effect of surfactant/nanoparticle concentration, temperature, and heterogeneity on NAPL remediation. The final goal will be to address the discrepancy between overall NAPL removal efficiency between experimental observations and large-scale actual data, through a physically-based model of NAPL enhanced mobilisation and solubilisation.

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Multiscale Investigation of Reactive Biosurfactant/Nanoparticles for in Situ Remediation of Contaminated Groundwater - Outline DMP

Manchester Data Management Outline

1. Will this project be reviewed by any of the following bodies (please select all that apply)?

- Funder

2. Is The University of Manchester collaborating with other institutions on this project?

- Yes - Part of a collaboration and not handling data

3. What data will you use in this project (please select all that apply)?

- Acquire new data

4. Where will the data be stored and backed-up during the project lifetime?

- University of Manchester Research Data Storage Service (Isilon)

5. If you will be using Research Data Storage, how much storage will you require?

- 1 - 8 TB

6. Are you going to be receiving data from, or sharing data with an external third party?

- No

7. How long do you intend to keep your data for after the end of your project (in years)?

- 5 - 10 years

Guidance for questions 8 to 13

Highly restricted information defined in the Information security classification, ownership and secure information handling SOP is information that requires enhanced security as unauthorised disclosure could cause significant harm to individuals or to the University and its ambitions in respect of its purpose, vision and values. This could be: information that is subject to export controls; valuable intellectual property; security sensitive material or research in key industrial fields at particular risk of being targeted by foreign states. See more examples of highly restricted

information.

Personal information, also known as personal data, relates to identifiable living individuals. Personal data is classed as special category personal data if it includes any of the following types of information about an identifiable living individual: racial or ethnic origin; political opinions; religious or similar philosophical beliefs; trade union membership; genetic data; biometric data; health data; sexual life; sexual orientation.

Please note that in line with data protection law (the UK General Data Protection Regulation and Data Protection Act 2018), personal information should only be stored in an identifiable form for as long as is necessary for the project; it should be pseudonymised (partially de-identified) and/or anonymised (completely de—identified) as soon as practically possible. You must obtain the appropriate ethical approval in order to use identifiable personal data.

8. What type of information will you be processing (please select all that apply)?

- No confidential or personal data

9. How do you plan to store, protect and ensure confidentiality of any highly restricted data or personal data (please select all that apply)?

- Not applicable

10. If you are storing personal information (including contact details) will you need to keep it beyond the end of the project?

- Not applicable

11. Will the participants' information (personal and/or sensitive) be shared with or accessed by anyone outside of the University of Manchester?

- Not applicable

12. If you will be sharing personal information outside of the University of Manchester will the individual or organisation you are sharing with be outside the EEA?

- Not applicable

13. Are you planning to use the personal information for future purposes such as research?

- No

14. Will this project use innovative technologies to collect or process data?

- No

15. Who will act as the data custodian for this study, and so be responsible for the information involved?

Dr Morteza Aminnaji

16. Please provide the date on which this plan was last reviewed (dd/mm/yyyy).

24102021

Outline DMP

Project Title

Multiscale Investigation of Reactive Biosurfactant/Nanoparticles for in Situ Remediation of Contaminated Groundwater

Principal Investigator(s) / Grant Holder

Morteza Aminnaji

Will the grant produce data?

- Yes

Nominated Data Centre(s)

- Environmental Information Data Centre (EIDC)

Briefly list the datasets that the project will produce. If the total is likely to be larger than 1TB please indicate.

Data will comprise 3 main categories: (1) C++ codes for pore-scale (pore network) and large-scale (Darcy scale) modelling, (2) results of pore scale and large scale for soil and groundwater remediation including modelling/simulation results and field-scale studies, and (3) Microfluidics and X-ray microtomography data for soil and groundwater remediation studies.

All derived data will be deposited at the Environmental Information Data Centre (EIDC). An archive copy of raw data will be securely retained for 10 years in line with UK requirements (we will maintain a copy of all project data on the Manchester local servers). To ensure that other researchers benefit from this project, these data (methods, raw data, processed results) will be freely available upon the direct request of interested parties, and also, they will be published in peer-reviewed scientific journals. The C++ code will be also shared using some code sharing websites such as GitHub Gist.

Furthermore, some data for the field and pilot studies will be provided by the collaborators from the University of Sao Paulo, Brazil. These data include geochemistry, reservoir geology structure, well size, and screened length of the contaminated land/site.

The raw data for X-ray microtomography is likely to be larger than 1TB which needs to be processed using some software such as Avizo. The University of Manchester Research Data Storage Service (Isilon) will be used for storing these data.