Job vacancy (13 months-PostDoctoral Position)

Modelling metal binding to environmental humic nanoparticles: theory and application to data interpretation

Type. 13-Months Postdoctoral fellowship.

Start of the position. January-February 2023 (flexible)**.**

Location. Lorraine University, Interdisciplinary Laboratory for Continental Environments (LIEC), Group ''Physical Chemistry and Reactivity of Surfaces And interfaces'' (PhySI). Vandoeuvre-lès-Nancy (direct vicinity of Nancy), FRANCE. Web page: https://liec.univ-lorraine.fr/

Context.

Addressing metal toxicity towards biota in aquatic media within risk assessment studies requires the evaluation of metal speciation, which includes the estimation of the stability of complexes formed between metals and natural organic matter like (nano)particulate fulvics and humics (HNPs). To that end, the binding of metals to HNPs is commonly described using historical Windermere Humic Aqueous Model (WHAM) or Non-Ideal Competitive Adsorption (NICA) models. Both integrate however a crude Donnan-like electrostatic representation for HNPs, which may clearly bias the evaluation of HNPs reactivity towards protons and metals[1-3] and, thereby, question the applicability of commonly accepted ''generic parameters'' derived from NICA-Donnan modeling for the binding of protons and metals to HNPs. Following previous results from our group,[1-3] this postdoc position is concerned with theoretical developments on metal ion complexation by HNPs, especially with respect to proper integration of electrostatics via resolution of mean-field Poisson-Boltzmann equations for ion-permeable particles like HNPs.[4] Results will have a societal impact with respect to refinement brought in the interpretation of metal toxicity data in aquatic media.

[1] Rotureau et al. *Colloids and Surfaces A: Physicochemical and Engineering Aspects* **2022**, *645*, 128859.
[2] Pinheiro et al. *Journal of Colloid and Interface Science* **2021**, *583*, 642-651.
[3] Town et al. *Environmental Science & Technology* **2019**, *53*, 8516-8532.
[4] Duval et al. *Environmental Science & Technology* **2005**, *39*, 6435-6445.

Description.

The project focuses on the elaboration of a physicochemical model for metal ion binding to humic nanoparticles (HNPs) with account of electrostatic contribution beyond the representation classically assumed in the common metal speciation codes NICA-Donnan or WHAM. The model is based on the combination between (i) non-linear **P**oisson-**B**oltzmann **T**heory applied to **S**oft (ion-permeable) particles like HNPs (**SPBT**), and (ii) **N**on-**I**deal **C**ompetitive **A**dsorption (**NICA**) complexation formalism to capture the very chemical component of the binding. The project is organized according to 3 steps: writing a new computational software combining NICA and SPBT; developing a fitting toolbox to retrieve metal/HNPs binding parameters from NICA-SPBT -based analysis of metal-HNPs titration data with help of a freely available software for the adjustment and estimation of relevant model parameters (**PEST**). In turn, this will make it possible to reparametrize existing published metal/HNP datasets interpreted so-far with

considering Donnan electrostatics that is poorly applicable to nanoparticulate humics with size comparable to Debye layer thickness under practical ionic strength conditions. Depending on candidate's performance and time, we shall envisage -as an application of the theoretical modules elaborated above- the design of a new user-friendly metal speciation code able to predict metal complexation by HNPs in environmental systems.

Tasks of the successful candidate will consist in:

- Writing NICA-SPBT software for modelling metal complexation by HNPs.
- Developing a data fitting toolbox combining {NICA-SPBT} and the freely available parameter estimation PEST module to obtain metal/HNP binding parameters from analysis of existing metal-HNPs titration data.
- Re-evaluating metal-HNPs binding parameters from {NICA-SPBT-PEST}-based modeling of metal titration data published for different types of HNPs and metallic elements.
- And, depending on time, building a new user-friendly metal speciation toolbox to predict trace metal speciation in environmental systems using NICA-SPBT software and the newly established parameter database.

Recent references from our group related to the project

- Tesfa, M.; Duval, J.F.L.; Marsac, R.; Dia, A. and Pinheiro, J.P. Absolute and relative positioning of natural organic matter acid-base potentiometric titration curves: implications for the evaluation of density of charged reactive sites. *Environmental Science & Technology*, **2022**. In press.
- Rotureau, E.; Pinheiro, J.P. and Duval, J.F.L. On the evaluation of the intrinsic stability of indium-nanoparticulate organic matter complexes. *Colloids and Surfaces A: Physicochemical and Engineering Aspects* **2022**, *645*, 128859 (DOI: 10.1016/j.colsurfa.2022.128859).
- Pinheiro, J.P.; Rotureau, E. and Duval, J.F.L. Addressing the electrostatic component of protons binding to aquatic nanoparticles beyond the Non-Ideal Competitive Adsorption (NICA)-Donnan level: theory and application to analysis of proton titration data for humic matter. *Journal of Colloid and Interface Science* **2021**, *583*, 642-651 (DOI: 10.1016/j.jcis.2020.09.059).
- Town, R.M.; van Leeuwen, H.P. and Duval, J.F.L. Rigorous physicochemical framework for metal ion binding by aqueous nanoparticulate humic substances: implications for speciation modeling by the NICA-Donnan and WHAM codes. *Environmental Science & Technology* **2019**, *53*, 8516-8532.

To be successful, the candidate should demonstrate one or several of the following skills:

- Possess a strong background in physico-chemical modelling AND/OR applied mathematics (REQUIRED),
- Have a solid experience in programming with Fortran and Python or similar object-oriented languages (REQUIRED),
- Be results-driven, have a marked sense of autonomy while being eager to work in a dynamic team,
- Able to manage deadlines,
- Have good communication skills (both oral and written) in English (knowledge in French is not required).

Education/Experience:

- PhD in Physical-Chemistry or related-Engineering field with a solid background in theoretical Physical Chemistry and/or Applied Mathematics, and Programming.

Remuneration
ca. 2200 (net) €/year, depending on the experience of the candidate.

Applications to submit:
Candidates are requested to submit a written application comprising:

1. A letter that addresses one or several of the Selection Criteria set out in the Position Description.
2. An executive summary (no more than approximately 1000 words) that highlights your strengths and reasons why you should be appointed to the position.
3. Your CV.
4. Recommendations letters by at least two referees, including their contact details (emails and phone numbers) and positions.

Supervisors of the Post-Doctoral fellowship:

- Prof. José Paulo Pinheiro (https://scholar.google.fr/citations?hl=fr&user=PIEYMkAAAAAJ)
- Prof. Jérôme F.L. Duval (https://scholar.google.fr/citations?user=HiVen9QAAAAJ&hl=fr&oi=ao & https://duvaljfl.webnode.fr/), Group leader PhySI in LIEC.

Complete applications should be sent to Jerome F.L. Duval (**jerome.duval@univ-lorraine.fr**) ***and*** Jose-Paulo Pinheiro (**jose-paulo.pinhero@univ-lorraine.fr**) before **October 30th, 2022**. A first round of interviews for pre-selected candidates will take place before the end of November 2022.