

Independent Modelling Project

This Independent Modelling Project is designed for you

1. to practice with the geochemical code **PHREEQC** and to learn how to use the manual
2. to practice writing and running input files and producing output files, including Excel sheets
3. to learn more about adsorption as a key geochemical process affecting environmental contaminants, especially arsenic. We learnt about adsorption isotherms in the lecture - now we learn about surface complexation models.

Process

I outline the project steps.

1. The instructions for the modelling exercise will be uploaded unto ESEESIS and Git Hub by Sunday evening (15 February 2026). The folder is titled *Surface Complexation Model*. See Figure 1.
2. The exercise should take no more than three hours. You may complete the work anytime; however, the scheduled slot is Tuesday, 9 am to 12 pm.
3. The TAs and I are available to assist with any technical or content-related questions. Please use Microsoft Teams for communication and arranging meetings.
4. The GitHub repository contains model solutions for input and output files, including Excel files. If you encounter difficulties in (i) running the code or (ii) producing output files, please use the model answers.

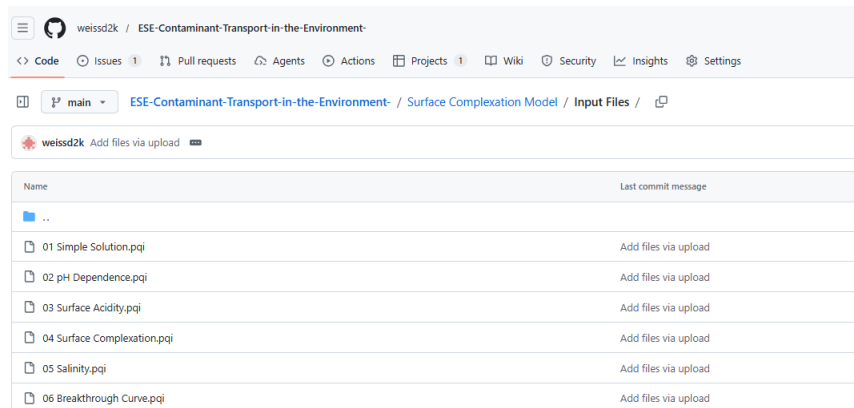


Figure 1: Location of input files

5. We will hold an online session on Tuesday, 17 February 2026, from 09:00 to 10:00 to answer any questions you might have.

Name	Last commit message
..	
Ignore	Add files via upload
01 Simple Solution.pqo	Add files via upload
01 Simple Solutionv2.pqo	Add files via upload
02 pH Dependence.pqo	Add files via upload
02 pH Dependence.xlsx	Add files via upload
03 Surface Acidity.pqo	Add files via upload
03 Surface Acidity.xlsx	Add files via upload
04 Surface Complexation.pqo	Add files via upload
04 Surface Complexation.xlsx	Add files via upload
05 Salinity.xlsx	Add files via upload
06 Breakthrough Curve.xlsx	Add files via upload
Student data v1 200414.xlsx	Add files via upload

Figure 2: Location of output files

6. You must write a short report (maximum 10 pages) detailing your modelling process and results. The report should follow the standard structure of a scientific paper, including:
 - Title
 - Abstract
 - Introduction
 - Results and Discussion
 - Conclusion
7. Submit the report by 09:00 on 2 March 2026, as a single PDF via email to d.weiss@imperial.ac.uk. You will receive feedback within two weeks. Submission is mandatory, but the report will not be graded.

Recommended Reading

Supporting documents are added to the repository for your reference:

1. Zhu, C. and Anderson, G. (2002). “Modelling Surface Adsorption”, Chapter 7 in *Environmental Applications of Geochemical Modelling*. Cambridge: Cambridge University Press, pp. 133–156. This chapter provides an overview of surface adsorption modelling and is useful for understanding relevant PHREEQC keywords, including SURFACE_MASTER_SPECIES and

SURFACE_SPECIES [1].

2. A paper on the experiments you will conduct was recently published in the *Journal of Chemical Education* [2].
3. The PHREEQC manual is available on GitHub [3]. Please review the sections relevant to surface modelling, including:
 - SURFACE_SPECIES (p. 229)
 - SURFACE_MASTER_SPECIES (p. 227)
 - SURFACE (p. 213)
 - SOLUTION (p. 189)
 - SOLUTION_MASTER_SPECIES (p. 196)
 - SOLUTION_SPECIES (p. 199)

References

1. Zhu, C. & Anderson, G. *Environmental Applications of Geochemical Modeling* (Cambridge University Press, 2002).
2. Bullen, J. C., Landa-Cansigno, O. & Weiss, D. J. Teaching adsorption chemistry by constructing surface complexation models (SCM) in PHREEQC. *Journal of Chemical Education* **101**, 1914–1924 (2024).
3. Parkhurst, D. L. & Appelo, C. A. J. *Description of Input and Examples for PHREEQC Version 3—A Computer Program for Speciation, Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations Techniques and Methods* 6-A43 (Reston, Virginia, 2013).