Groundwater Chemistry

Module Handbook 2012/13

Course number CEG8522

School of Civil Engineering and Geosciences

Newcastle University

Module Aims and Outcomes

Details at http://www.ncl.ac.uk/module-catalogue/module.php?code=CEG8522

Whom is this module for?

This module is aimed at Environment Agency staff whose role requires them, or may in future require them, to have an understanding of groundwater chemistry. This may be in connection with a wide range of activities, including the following:

- Evaluating, reviewing and interpreting groundwater chemistry data for the purposes of the Water Framework Directive
- Devising, implementing, analysing or evaluating hydro-chemical investigations
- Understanding contaminant transport and implementing the source –pathway-receptor relationship
- Processing of applications and the evaluation of technical reports related to waste disposal, groundwater quality consents and notices, and PPC.

Pre-requisites

Pre-requisites for the module are:

- Competency in maths and chemistry above GCSE level (through undergraduate or work-based training/experience if not at AS or A-level), and
- some prior background in basic groundwater hydraulics, such as recharge processes, hydraulic conductivity, transmissivity, groundwater flow patterns (as covered in the Agency's T317 Groundwater Hydraulics module).

Newcastle University have developed pre-requisite self learning materials in maths and chemistry which are available to EA staff

Module Tutors

The Module Leader is Dr Geoff Parkin
Email: geoff.parkin@ncl.ac.uk

Other lecturers on the course are:

- Adam Jarvis
- Dave Banks (visiting presenter)
- Neil Gray
- David Werner
- Rick Brassington (visiting Professor)

Method of delivery and Time commitment

Details at **http://www.ncl.ac.uk/module-catalogue/module.php?code=CEG8522**

Pre-course preparation

In order to gain maximum benefit from this module, it is essential that you prepare yourself by undertaking at least the following pre-course activities:

- Revise specific concepts of basic mathematics and chemistry, if required. Under the *pre course reading* section of the Reading List (Appendix 1) reference is given to specific chapters in suitable chemistry texts that should be read prior to the course. The Newcastle University pre-requisite maths and chemistry self learning courses (and self assessment questions) are also available. These can be found on the GW quality community pages. https://www.ea-training.org/communities/gwaterqual/resources.html?folder=21.
  All of the self learning chemistry course is relevant preparation, as is Part A of the Maths course, especially section 2.6 on logarithms.
- Revise the content of the Groundwater Hydraulics module (see Pre-requisites, above), or equivalent material
- Read and become familiar with the book chapters on general groundwater issues cited in *Pre-course reading* section of the Reading List (Appendix 1)

Syllabus for residential course

Monday

0900-10:30: Course overview and objectives, hydrogeological context

- Groundwater in the hydrological cycle
- The surface water – groundwater continuum
- The influence of groundwater on surface water chemistry under various scenarios
- The hyporheic zone
- Residence times of groundwater and the influences of geology and hydrology

11:00-12:30: Basic chemical principles

- Solid-liquid interactions and chemical equilibria
- Law of Mass Action
- Chemical activity and activity coefficients
- The formation of ion complexes
- Calculation of saturation state

13:30-15:00: Basic chemical principles: Tutorial

15:30-17:00: Controls on groundwater chemistry I: Dissolution and precipitation

- Physical controls on the rate of dissolution
- Conditions favouring precipitation
- An example of dissolution and precipitation: The oxidative dissolution and
- precipitation of the mineral pyrite

Tuesday

0900-10:30: Controls on groundwater chemistry II: pH, acids & bases

- Effect of pH on speciation in solution
- Bronsted-Lowry definition, pK and the strength of acids
- Calculating the speciation of polyprotic acids in solution
- pH buffering and the importance of the carbonate system

11:00-12:30: Controls on groundwater chemistry III: Sorption, complexation & ion exchange

- Introduction to adsorption, absorption and ion exchange reactions
- Equilibrium constant for ion exchange
- Clay minerals and the cation exchange capacity (CEC)
- Surface complexation principles and the point of zero charge (PZC)

13:30-15:00: Organic solutes and colloids and their transport

- Dissolution of organic compounds from organic liquids (NAPL): equilibrium considerations
- Dissolution of organic compounds from organic liquids (NAPL): kinetic considerations
- Sorption of organic compounds to natural organic matter
- Sorption of organic compounds to mineral surfaces
- The role of dissolved organic matter and inorganic colloids in pollutant transport

15:30-17:00: Controls on groundwater chemistry IV: biogeochemical influences

- Chemical transformation of organic compounds in groundwater
- Biological transformation of organic compounds in groundwater
- Sorption and retardation of organic compounds in groundwater

Wednesday

09:00-10.30: Controls on groundwater chemistry: Tutorial

11:00-12:30: Controls on groundwater chemistry V: Redox reactions

- Definitions and guide to balancing redox reactions
- Quantifying redox reactions: the redox potential (Eh)
- The Nernst equation and the relationship between pe and Eh
- Spontaneity of redox reactions
- Measured versus computed Eh of groundwater: general controls on the redox state
- of groundwater

13:00-15:00: Controls on groundwater chemistry: Tutorial

15:30-17:00: Groundwater microbiology and vulnerability

- *Is groundwater sterile?*
    - The occurrence of bacteria in the geosphere and their evolutionary significance
    - Biofilms
- *Microbiological contaminants*
    - bacteria
    - viruses
    - protozoa
- *Vulnerability to microbiological contamination*
- examples
- *Models for assessing vulnerability*
    - DRASTIC
    - EA/SEPA approaches
    - Irish approaches

Thursday

0900-10:30: Sampling and analysis of groundwaters, and design of monitoring schemes

- *Design of monitoring schemes:*
    - defining why we are monitoring
    - frequency of monitoring (space and time)
    - the importance of the third dimension (wells and piezometers)
- *Sampling:*

    - Preparation for sampling; purging
    - field determinations
    - sampling for inorganic parameters
    - sampling for organic parameters
    - QA (to include blank/duplicate/spiked samples)
- *Analysis of groundwaters:*
    - alkalinity
    - ICP methods (ICP-OES / ICP-MS)
    - ion chromatography
    - gas chromatography (to include GC-MS)
    - IR spectrophotometry
    - reporting and non-detects: some common errors

11:00-12:30: Representation, interpretation and interrogation of groundwater chemistry

- *Some basic checks:*
    - ion balance error
    - solubility
    - total vs dissolved metals
- *Databasing chemical data*
- *Visualising chemical data*
    - Mapping and contouring (examples from UK, Scandinavia, Bangladesh)
    - Pie diagrams
    - Kurlov formula
    - Piper and Durov diagrams
- *Hydrochemical facies and evolution of groundwater chemistry*

13:30-17:00: Practical exercises in representation, interpretation and interrogation of groundwater chemistry (desk-based and Phreeqe)

- *Interpreting groundwater chemical data. Examples from Norway*
    - Converting units (require Excel)
    - Plotting pie diagrams (require Excel)
    - Plotting Durov diagrams (require template)
- *Speciation and saturation indices.*
    - Modelling using PHREEQCI (require PHREEQCI) of Norwegian samples
    - Mixing waters
    - Forward and reverse modelling
    -

Friday

0900-10:30: Effect of metal precipitation on borehole yields

- Why metals may precipitate
- Bacterial action
- Collecting and interpreting field evidence
- Impact on yields
- What can be done about it?
- Case histories

11:00-12:30: Saline groundwater

- Sea water intrusion
- Deep-seated saline groundwater
- Collecting and interpreting field evidence
- The significance on groundwater resource management

- Case histories (most examples will be from NW England and Harrogate)

13:30-15:00: Principles and application of environmental tracers

- uses of environmental tracers for groundwater dating, recharge assessment etc
- basic assumptions, end-members, mixing, advection/dispersion, residence times
- sources and properties of historical tracers: ^{3}H, $^{3}H/^{3}He$, ^{36}Cl, CFC's, SF_6, ^{85}Kr, $\delta^{18}O$, $\delta^{2}H$
- appropriate tracer selection, sampling, data interpretation
- case study examples
- limitations, uncertainty, comparison with other methods

15:00-15:30: Course wrap up

Independent learning

Following the residential teaching period, students should:

- review the material covered in the course
- read other material, including (but not limited to) the references given in Appendix 1. Note that award of higher marks in assessments depends in part on evidence of wider reading.
- complete and submit the coursework assignment
- work through example exam questions, which will be made available during the residential period

Assessment, Reassessment, Coursework submission

Refer to the Newcastle University Standalone Module Handbook

Module dates

Block module:
21st – 25th January, 2013
Coursework completion deadline:
8th March, 2013
Examination:
During the two-week period 20th May - 7th June, 2013 (inc. Saturdays 25th May and 1st June)

Appendix 1: Reading list

A note on the reading list

It is strongly recommended that course attendees read all of the pre-course reading below, particularly if you do not have a strong background in maths, chemistry or a basic understanding of the fundamentals of groundwater science. You will get far more from the course if you read and understand this material. Specific chapters have been cited below, but this is not to suggest that other sections of these texts are not worth reading (indeed, it may be necessary to refer back to preceding chapters).

The Newcastle University pre-requisite maths and chemistry self learning courses (and self assessment questions) are also available. These can be found on the GW quality community pages. https://www.ea-training.org/communities/gwaterqual/resources.html?folder=21

You may wish to also look at some of the further reading shown below before the course, but these texts are principally intended for use after the course, during Independent Learning (see above), to help review and strengthen the knowledge gained during the course.

Copies of the key reading material given below have been made available in a number of Area offices - please check with your colleagues in your office, and nearby areas as to their whereabouts and availability

Pre-course reading

Chemistry

Holum, J.R. 1998. Fundamentals of general, organic, and biological chemistry. 6th Edition. John Wiley & Sons, New York. ISBN 0-471-17574-9

- Especially Chapters 2, 3, and 4

Maths

For a basic description of the mathematical principles and techniques, a good introduction is given by:
Bostock, L. and Chandler, S. (1994). Core Maths for A-level (2nd Ed.). Thornes, Cheltenham. ISBN 0-7487-1779-X

For those students who already have a reasonable understanding of basic mathematics, a comprehensive textbook which includes a more advanced description of mathematical techniques (including the basic concepts) is:
Jordan, D.W. and Smith, P. (1997). Mathematical techniques : an introduction for the engineering, physical, and mathematical sciences (2nd Ed.). Oxford University Press, Oxford. ISBN 0-19-856461-9 (paperback edition)

Groundwater

Price, M. 1996. Introducing Groundwater. 2nd Edition. Chapman & Hall, London. ISBN 0-412-48500-1

- Especially Chapters 1-5 and 7

Younger, P.L. 2007. Groundwater in the Environment: An Introduction. Blackwell Publishing, Oxford. ISBN 1-4051-2143-2

- Especially Chapters 1 and 2

Further essential reading

Appelo C.A.J. and Postma D.H. 1993. Groundwater, Geochemistry and Pollution. 2nd Edition. Balkema. ISBN 04-1536-428-0

Further recommended reading

Price, M. 1996. Introducing Groundwater. 2nd Edition. Chapman & Hall, London. ISBN 0-412-48500-1

Younger, P.L. 2006. Groundwater in the Environment: An Introduction. ISBN 1-4051-2143-2

Further background reading

Brassington, R. 2006. Field Hydrogeology, 3rd Edition, John Wiley & Sons. ISBN 978-0-470-01828

Drever, J.I. 1998. The Geochemistry of Natural Waters. Prentice Hall. ISBN 0-13-272790

Hiscock, K. 2005. Hydrogeology: Principles and Practice. Blackwell Publishing, Oxford. ISBN 0-632-05763-7

Scwarzenbach, R.P., Gschwend, P.M., Imboden, D.M. 2003. Environmental organic chemistry. Wiley-Interscience. ISBN 0-471-35750-2

Stumm W. and Morgan J.J. 1996. Aquatic Chemistry: Chemical Equilibria and Rates in Natural Waters. 3rd Edition. Wiley. ISBN 0-471-51185-4