



EU Horizon 2020 ENeRAG project  
Excellency Network Building for Comprehensive  
Research and Assessment of Geofluids

Online course “Improving skills in  
conservative and reactive transport modelling”

20 - 30 September 2021

Organized by



UNIVERSITÀ  
DEGLI STUDI  
DI MILANO

Key topics:

- ✚ Introduction to mathematical models for flow and transport in geological media.
- ✚ Stochastic transport modelling and risk assessment
- ✚ Use of multi-domain upscaling modelling tools.
- ✚ Applied reactive transport modelling using multicomponent geochemical systems.

Instructors

**Samrit Luoma**

Geologian tutkimuskeskus (GTK)  
Finland

**Muhammad Muniruzzaman**

Geologian tutkimuskeskus (GTK)  
Finland

**Daniele Pedretti**

Università degli Studi di Milano (UNIMI)  
Italy

*Invited lecturers:*

**Daniel Fernández-Garcia**

Universitat Politècnica de Catalunya –  
BarcelonaTech (UPC), Spain

**Chuanhe Lu**

University of Manchester, UK

**Henning Prommer**

Commonwealth Scientific and Industrial Research  
Organisation (CSIRO), Australia

For more information, please contact us ([daniele.pedretti@unimi.it](mailto:daniele.pedretti@unimi.it); [md.muniruzzaman@gtk.fi](mailto:md.muniruzzaman@gtk.fi))

**[Click here to register](#)**

Free of charge

Registration closes on **10 September 2021.**

A certificate of attendance will be issued after the completion of the school.



This course is organized as a winter school in the frame of the ENeRAG project a European Union's Horizon 2020 research and innovation project (grant agreement No 810980).



## Programme\* (CEST time zone)

### Week 1 (20-23 September 2021)

	<i>Monday 20</i>	<i>Tuesday 21</i>	<i>Wednesday 22</i>	<i>Thursday 23</i>
10:00-11:00	Welcome and introduction to week 1	Key concepts of solute transport modelling	Transport in heterogeneous media	Stochastic modelling and risk assessment
11:00-12:00	Basics of flow modelling in porous media	Key concepts of solute transport modelling	Transport in heterogeneous media	Stochastic modelling and risk assessment
12:00-13:00	Break	Break	break	Break
13:00-15:00	Practice	Practice	Practice	Practice

### Week 2 (27-30 September 2021)

	<i>Monday 27</i>	<i>Tuesday 28</i>	<i>Wednesday 29</i>	<i>Thursday 30</i>
9:00-10:00	Welcome and introduction to week 2	Principles of multicomponent RTM	Application of RTM: Case study 1	Application of RTM : Case study 2
10:00-11:00	Basics of reactive transport modelling			
11:00-12:00	Break	Break	break	break
12:00-14:00	Practice	Practice	Practice	Practice

*\*The organizers reserve the right to make minor changes in the program.*

The practice will be carried out using a public-domain Windows-based software.



# Course content \*

## *Week 1: Flow and conservative transport modelling*

### **Day 1 - Basics of flow modelling in porous media**

- Overview of the concepts of aquifers, hydraulic gradient, Darcy's law and hydraulic conductivity, flow conservation and the flow equation, concept of storativity and aquifer tests.
- Overview of mathematical models for the solution of the flow equation.
- Examples of analytical and numerical methods.

### **Day 2- Key concepts of solute transport modelling**

- Overview of the concepts of advection, diffusion and dispersion
- The concept of mass conservation and the solute transport equation
- Mathematical models for the solution of the transport equation.
- Examples of approaches that can be used to solve for the equation, analytical and numerical codes and some applications at different spatial scales.

### **Day 3 - Transport in heterogeneous media (Daniele Pedretti)**

- Effects of different geological structures of fluid flow
- Methods to reproduce solute transport heterogeneity
- Use of upscaling models to effectively reproduce solute transport in heterogeneous media

### **Day 4 - Stochastic modelling and risk assessment (Daniel Fernandez-Garcia)**

- Basics of stochastic modelling in hydrogeology
- Approaches and application on groundwaters
- Use of stochastic modelling for solute transport modelling
- Risk assessment and typical applications involving stochastic modelling

## ***Week 2: Reactive transport modelling***

### **Day 1 - Basics of reactive transport modelling**

- Overview of the key concepts of reactive transport modelling
- Overview of different geochemical processes (e.g., aqueous complexation/speciation, acid-base reactions, redox reactions, ion exchange, surface complexation, mineral dissolution/precipitation, redox reactions)
- Fundamentals of mathematical and numerical formulation for chemical reactions
- Overview of coupling techniques between transport and chemical reactions

### **Day 2 - Principles of multicomponent reactive transport modelling**

Key multicomponent reactive transport principles

- Brief introduction to PHREEQC keywords, datablocks, and input files
- Introduction to multicomponent diffusion
- Effects of charge interactions and uphill diffusion

### **Day 3 and Day 4- Applications of multicomponent reactive transport modelling**

- Case study 1: Quantifying groundwater quality impacts associated with managed aquifer recharge
- Case Study 2: Modelling the fate of arsenic across multiple length and time scales

*\* The organizers reserve the right to make changes regarding the topic and exercises in the program.*

