REGISTRATION INFORMATION

Participants may register until **April 30, 2019**.
For registration and further information please go to:
www.empa-akademie.ch/gems
Participants are kindly asked to indicate their areas of interest in thermodynamic modeling upon registration, so that we can design a program that matches the needs of the attendees as close as possible.

FEES AND PAYMENT

The workshop fee of CHF 600.– for PhD students is paid to cover lunch, conference dinner, get-together, refreshments during coffee breaks and printed course material. The payment must be made in advance upon receiving the invoice.

ACCOMMODATION

Overnight accommodation can be arranged at Hotel Sonnental for the special Empa rate of CHF 130.– or at Hotel Zwiback for CHF 120.– for a single room, including breakfast. Please arrange your room directly with Hotel Sonnental or Hotel Zwiback:

https://sorellhotels.com/en/sonnental/duebendorf
or
www.zwiback.ch

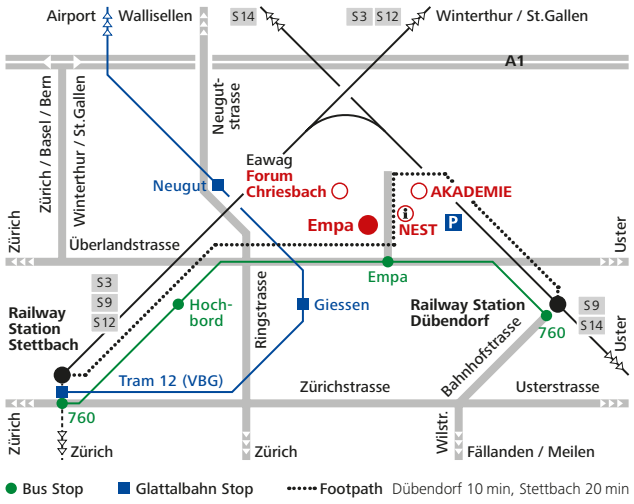
Please mention your participation at the **Empa GEMS workshop**.
The deadline for this offer is **April 30, 2019**.
Please only book your room through the above mentioned links.

LANGUAGE

The course will be held in English.

GENERAL INFORMATION

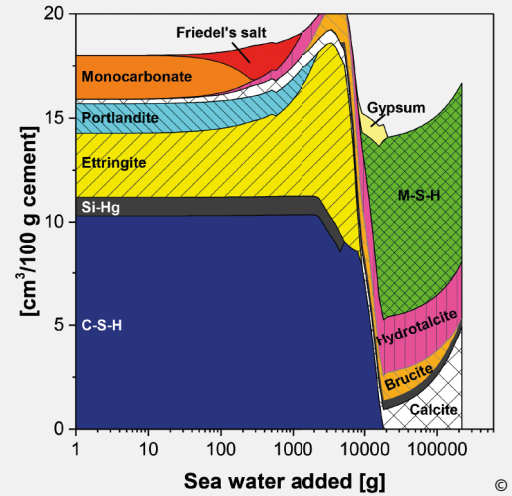
Location	Empa, Überlandstrasse 129, 8600 Dübendorf AKADEMIE
Costs	CHF 600.– (for four days)
Registration	www.empa-akademie.ch/gems
Registration deadline	April 30, 2019
Cancellation	For cancellations after April 30, 2019, 50% of the fee will be charged. In case of non appearance we will charge the full fee. A replacement will be accepted.
Organization	Empa **Barbara Lothenbach / Frank Winnefeld** Concrete & Construction Chemistry www.empa.ch/web/s308 NTNU **Barbara Lothenbach / Klaartje De Weerdt** Department of Structural Engineering www.ntnu.no/kt
Administrative	Empa **Barbara Gleich** Concrete & Construction Chemistry Phone +41 58 765 44 02 barbara.gleich@empa.ch
How to get here	Please do use public transport. There is only very limited parking available.



GEMS SELEKTOR · NTNU · Empa Akademie

6th GEMS WORKSHOP FOR PHD STUDENTS

Thermodynamic Modeling of Cementitious Systems



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A. Machner

Empa, Dübendorf, Switzerland
June 18 – 21, 2019

Online registration: *www.empa-akademie.ch/gems*

SCOPE AND BACKGROUND

Cementitious materials show a rapid and complex evolution of pore water composition and mineral assemblage during hydration. Thermodynamic equilibrium and mass balance calculations are a valuable tool to understand the different processes in cementitious systems. They can help to understand the consequences of different factors such as cement composition, hydration, leaching or temperature on the composition and the properties of a hydrated cementitious system on a chemical level.

In combination with a kinetic model, thermodynamic calculations can also be used to follow changes during hydration or, in combination with transport models, to calculate the interaction of cementitious systems with the environment.

In all these applications, thermodynamic equilibrium calculations have been a valuable addition to experimental studies deepening our understanding of the processes that govern cementitious systems and interpreting experimental observations.

The intention of this workshop is to give an introduction to use mass balance calculations as well as GEMS, a thermodynamic modelling software using free energy minimization developed at PSI, and its applications to cementitious systems. The theoretical background of GEM (Gibbs Energy Minimization) algorithms will be briefly discussed.

The focus of this workshop for PhD students will be on practical hands-on simulations with GEMS. It will comprise a hands-on tutorial for beginners, introduction to the theoretical background, applications in the context of cement hydration and effects of different raw materials and additives, calculations and interpretations of saturation indices, and modelling of the interaction with the environment.

Learning outcomes:

- Understanding of the principles of thermodynamic equilibrium and mass balance calculations
- Basic knowledge on thermodynamic data
- Ability to use ternary diagrams to calculate the hydrate composition of cementitious materials
- Ability to create single systems and process files in GEMS to calculate:
  - hydrate compositions of cementitious materials
  - saturation indices
  - chemical interactions of cementitious materials with the environment

TARGET AUDIENCE

PhD students who seek to relate cement chemistry and mineralogy to the properties of cementitious materials, such as mechanical properties, microstructure and durability.

PROGRAM

The course is planned as hands-on tutorial for beginners and those with intermediate knowledge. The theoretical background needed for mass balance calculations and thermodynamic modelling will shortly be introduced and discussed. The students are expected to come with laptop and preinstalled software (link for software installation will be sent out before the course).

Tuesday, June 18, start at 9 am

Introduction to thermodynamic modelling and cement chemistry

Single system calculation, input, output

- Examples: C_3A, effect of sulfate
- Excercise: effect of carbonate and CaO
- Student presentations

Get-together in the evening

Wednesday, June 19

Process calculations:

- Hydrated cements/overview thermodynamic database
- Solubility products, effect of pH on solubility of simple solids
- Exercise: process calculations
- Group work

Thursday, June 20

- Blended cements
- Interactions with the environment
- Group work

Get-together in the evening

Friday, June 21

- Presentations of group work

End: 3 pm

CREDIT POINTS

It is estimated that the PhD course will require 120 hours of work from the student including preparation of the students' presentations before the course, the 4 days intensive course, and the written report about applying GEMS, to be handed in within 3 months after the course. The PhD course is integrated in NTNU's doctoral courses. 5 ECTS points can be obtained when all workshop days are actively attended and the written report is handed in in time and accepted.

COURSE INFORMATION

The overall number of participants is limited to 30 and the number of participants from the same institute/company is limited to 2. A waiting list will be used in the case that more people register than there are places available.

Every attendee is asked to bring along his/her own notebook (note that Switzerland has different power outlets than EU or other countries).

Please, download and install the actual version of the GEM-Selektor code package and the Cemdata thermodynamic database at least 10 days prior to the Workshop

GEM-Selektor package:
http://gems.web.psi.ch/GEMS3

Cemdata thermodynamic database for cementitious materials:
http://www.empa.ch/cemdata