REGISTRATION INFORMATION

Participants may register until **April 30, 2017**.
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

A Workshop fee of CHF 600.– (CHF 400.– for students) is payable to cover lunch, conference dinner, refreshments during coffee breaks and printed course material. For experienced users, it is possible to attend the second and third day only for CHF 400.–. Payment should be made in advance upon receipt of 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 that you participate at the
"Empa GEMS-Workshop".
The deadline for this offer is also **April 30, 2017**.

LANGUAGE

The course will be held in English.

CREDIT POINT

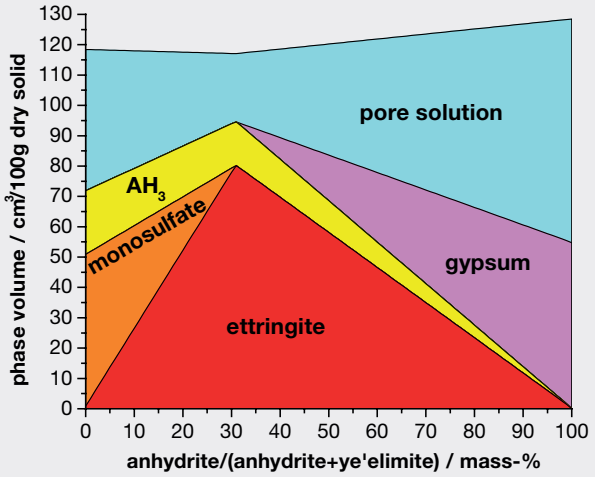
1 ECTS point can be certified when all workshop days are attended, and the practical training is successfully completed.

GENERAL INFORMATION

Location	Empa, Dübendorf, Überlandstrasse 129 Forum Chriesbach, Room C20
Costs	CHF 600.– (for three days) CHF 400.– (for PhD students) CHF 400.– (second and third day only, for advanced users)
Registration	www.empa-akademie.ch/gems
Registration deadline	April 30, 2017
Cancellation	For cancellations after April 30, 2017, 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
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

5th GEMS WORKSHOP

Thermodynamic Modeling of Cementitious Systems



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Empa, Dübendorf, Switzerland
May 30th to June 1st, 2017

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

SCOPE AND BACKGROUND

Hydraulic binders such as cement paste, mortar and concrete show a rapid and complex evolution of pore water composition and mineral assemblage during hydration. Thermodynamic equilibrium 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. Equilibrium calculations have been successfully used to compute the stable phase assemblages based on the solution composition as well as to model the stable phase assemblage in completely hydrated cements and thus to assess the influence of the chemical composition on the hydrate assemblage.

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 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 will be on practical hands-on simulations with GEMS. A first part is planned as hands-on tutorial for beginners and to introduce the theoretical background. Some simple exercises will be available before the course such that the participants can become familiar with the software. The second part will concentrate on applications in the context of cement hydration, effects of different raw materials and additives, calculation and interpretation of saturation indices and modelling of the interaction with the environment.

Learning outcomes:

- Mastering of simple and process calculations in GEMS
- Basic understanding of the chemistry of cements
- Effect of high pH on solubility
- Understanding and calculation of solubility products

TARGET AUDIENCE

Industrial and academic researchers who seek to relate cement chemistry to mineralogy, and more broadly, who seek to match cement mechanical properties and microstructure with chemistry.

PROGRAM

Day one is planned as hands-on tutorial for beginners and to introduce the theoretical background. Some simple exercises will be sent out before the course such that the participants could get more familiar with the software.

Day two and three will provide tutorials related to more advanced applications auf thermodynamic modeling to cement science.

Tuesday, May 30

Introduction to thermodynamic modelling
Single system calculation, input, output

- Examples: effect of sulfate
- Tutorial: effect of carbonate

Process calculations:

- Hydrated cements
- Tutorial: Effect of limestone

Thermodynamic database: overview

Wednesday, May 31

Solubility products, effect of pH on solubility of simple solids

- Tutorial: Calculation of speciation diagrams
- Tutorial: Solubility calculations for pure solids: portlandite,
- Solid solutions: effect on solubility, XRD, …
- Tutorial: Monocarbonate, monosulfate: calculate solubility, determine whether solid solution is present

Effect of temperature on solubility products

- Tutorial: effect of temperature on hydrated cement

Thursday, June 1

Process calculations:

- Blended cements
- Alternative cements: CSA
- alkali activated cements: composition, volume, strength

Dissolution/precipitation kinetic or interaction with the environment (sulfate, chloride, sea water, clay stone,...)

COURSE INFORMATION

The overall number of participants is limited to 40, thus 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