

CALPHAD 2026 - FactSage, CALPHAD Optimizer, and FactFlow Workshop

Workshop program

Workshop overview

This workshop will present practical and advanced uses of FactSage, CALPHAD Optimizer, and FactFlow for thermodynamic calculations and process simulation. The program is designed for CALPHAD participants and external attendees interested in applying thermodynamic data, phase-equilibrium calculations, database optimization, and process-oriented simulation to materials and industrial problems.

The workshop will begin with a concise introduction to FactSage, CRCT, and GTT-Technologies. It will then move to current FactSage 8.4 capabilities, CALPHAD Optimizer, ThermML, database optimization examples, advanced equilibrium calculations, and a FactFlow demonstration showing how equilibrium results can be used in a process-simulation workflow. A FactSage workshop version will be provided to registered workshop participants so that they can follow selected demonstrations on their own computers. The program will also include a short section on the new FactSage 9.0 installation approach and will close with discussion and attendee feedback.

General information

Item	Information
Event	CALPHAD 2026 - Pre-conference Workshop
Workshop	FactSage / CALPHAD Optimizer / FactFlow Workshop
Date	Sunday, June 7, 2026
Planned time	1:00 p.m. to 5:00 p.m.
Venue	Universite Laval, Pavillon Alphonse-Desjardins, Quebec City
Format	Technical presentations, demonstrations, and discussion
Recording / webcasting	Not currently planned
Software preparation	A FactSage workshop version will be provided to registered workshop participants. Installation instructions will be shared before the workshop.

Who should attend

- CALPHAD conference participants interested in software tools and practical applications.
- Thermodynamic database developers and users.
- Materials scientists working with phase equilibria, high-temperature processes, alloy design, or process chemistry.
- Process-modeling researchers and industrial users who want to connect thermodynamic calculations with process-level analysis.
- Students and new users who want a structured view of FactSage, Calphad Optimizer, and FactFlow, while moving quickly toward technical examples.

Program

Time	Section	Main contents	Lead
1:00-1:15	Opening	What FactSage, CRCT, and GTT are; workshop objective and structure	Jean-Philippe Harvey
1:15-2:15	FactSage today	Current capabilities in FactSage 8.4; relevant modules; practical workflows; selected demonstrations	Jean-Philippe Harvey
2:15-3:05	CALPHAD Optimizer, ThermML, and database optimization	CALPHAD Optimizer, database optimization examples, ThermML (XML database format)	Moritz to Baben/ Florian Tang / GTT
3:05-3:15	Break	Short break and transition	-
3:15-3:50	Advanced equilibrium calculation example	Equilib, Phase Diagram, database selection, phase selection, CST file generation, ChemApp for Python script generation; possible niobium-based example	Jean-Philippe Harvey / Florian Tang
3:50-4:30	FactFlow demonstration	Process simulation using the equilibrium example; possible niobium-based workflow; simple process with two reactors	Kyota Poëti / Kentaro Oishi
4:30-4:45	FactSage 9.0 - new installations	New FactSage 9.0 installation approach, including replacement of the former Standalone Single User, Network Server, and Network Client modes by the new Single Installation mode	Christopher W. Bale
4:45-5:00	General discussion and attendee feedback	Questions, comments, attendee feedback, future training needs, and possible next steps	All

What participants can expect

- A concise introduction to FactSage, CRCT, and GTT-Technologies.
- A technical overview of current FactSage 8.4 capabilities relevant to applied calculations.
- A section on CALPHAD Optimizer, ThermML, and database optimization examples.
- An advanced equilibrium calculation example showing database selection, phase selection, CST file generation, ChemApp for Python script generation, and interpretation of results.
- A FactFlow demonstration showing how equilibrium calculations can be extended toward process-level simulation.
- The possibility to follow selected demonstrations using a FactSage workshop version provided before the workshop.
- A short explanation of the new FactSage 9.0 installation approach.
- Discussion time for questions, attendee feedback, and future training needs.

Session description

The FactSage / CALPHAD Optimizer / FactFlow Workshop will present practical and advanced thermodynamic calculation workflows for CALPHAD users, materials scientists, database developers, and process-modeling researchers. The workshop will begin with a short orientation for participants who may not be regular FactSage users, followed by current FactSage 8.4 capabilities and a dedicated section on CALPHAD Optimizer, ThermML, and database optimization examples. The second half of the workshop will show how advanced equilibrium calculations can be connected to process simulation using FactFlow, with a possible niobium-based example linking Equilib, CST file generation, ChemApp for Python script generation, and a simple two-reactor process simulation. A FactSage workshop version will be provided to registered workshop participants so that they can follow selected demonstrations on their own computers. The workshop will also include a short section on the new FactSage 9.0 installation approach and will close with discussion and attendee feedback.

Participant preparation

A FactSage workshop version will be provided to registered workshop participants before the workshop. Participants who wish to follow selected demonstrations actively should bring their own laptop. Detailed installation instructions and any required preparation steps will be shared before the workshop. The workshop will also be accessible to participants who prefer to attend without running the software during the session.