

## GEMS: Gibbs energy minimization software for geochemical modeling

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Geochemical modeling is relevant in ore geochemistry, CO<sub>2</sub>/radioactive/toxic waste disposal, cosmochemistry, petrology, and hydrogeochemistry. GEMS is an advanced software tool for modeling complex systems that involve non-ideal solid solutions, fluids and aqueous solutions, mineral phases metastability, adsorption, and ion exchange. GEMS (<http://gems.web.psi.ch>) comprises the GEM-Selektor code; default thermodynamic databases; the GEMS3K kernel code [1,2] included into the GEMSFIT code [3] and available open-source for coupling into reactive transport codes.

The GEM-Selektor v.3 is the main tool for interactive geochemical thermodynamic modeling. It integrates a multi-document graphical user interface with a built-in script interpreter, a database management system, and a context-driven help browser. These features support forward- or inverse modeling tasks, plotting or exporting results, and creating GEMS3K input files. The usage is focused around a *modeling project* database that accumulates all input data and results for a given application. Any project can be shared with others, which greatly facilitates the data exchange in teams. GEMS databases equally support thermochemical and reaction-based formats of standard-state thermodynamic data. Creation of new projects is facilitated by the supplied thermodynamic databases, derived from the PSI/Nagra 12/07 [4] and the SUPCRT92 [5] datasets. Third-party databases for specific application fields are also available in GEMS format.

Current development is focused on adding the kinetics of mineral-aqueous reactions and trace element uptake; implementing sorption models using a concept of linked phase metastability; improving GEM numerical algorithms; moving to industrial NoSQL database format in connection with the general parameter-fitting code GEMSFIT. Our goal is to make GEMS the software of choice for all kinds of geochemical modelling applications.

[1] Kulik *et al.* (2013) *Comput. Geosci.* **17**, 1-24. [2] Wagner *et al.* (2012) *Can. Mineral.* **50**, 701-723. [3] Hingerl *et al.* (2013) *Comput. Chem. Eng.* (submitted). [4] Thoenen *et al.* (this conference). [5] Shock *et al.* (1997) *Geoch. Cosmoch. Acta* **61**, 907-950.

## Southward transport of the Fukushima-derived radiocesium due to the subtropical mode water

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### Fukushima-derived Radiocesium

The massive Tohoku earthquake and consequent giant tsunami of March 11, 2011 resulted in releases of radiocesium from the Fukushima Dai-ichi nuclear power plants. The total amount of the radiocesium derived from the direct discharge into the North Pacific Ocean was estimated to be about 4 PBq for Cs-137 [1, 2]. However, that from the atmospheric deposition contains large uncertainty mostly due to the restriction of available data in the open ocean.

### Sample Collection and Radiocesium Analysis

We measured the radiocesium in seawaters from surface to 800-m depth at stations along approx.149°E line more than hundreds km away from the plants in the western North Pacific Ocean in January and February 2012. Radiocesium in the seawater was concentrated onto ammonium molybdophosphate and then measured using a gamma-spectrometry with Ge detectors.

### Results and Discussion

Cs-134 was found in surface waters at all the stations from 20°N to 42°N. Activity of Cs-134 in the surface mixed layer was highest (~ 20 Bq m<sup>-3</sup>) in the transition area between the subarctic and subtropical regions, which was due to the direct discharge into the transition area. Below the surface mixed layer Cs-134 activity decreased sharply and was not detected in deeper layers than 400-m depth in the subarctic region and transition area. However, in the subtropical region we observed Cs-134 maxima just below the mixing layer that corresponds to about 25.3 sigma-theta, implying that the Cs-134-rich waters in the transition area have been transported southwardly to the subtropical region due to formation of the subtropical mode water.

[1] Kawamura *et al.* (2011) *J. Nucl. Sci. Technol.* **48**, 1349-1356. [2] Tsumune *et al.* (2012) *J. Environ. Radioactiv.* **111**, 100-108, doi:10.1016/j.jenvrad.2011.10.007.