

Science gateway of online geochemical programs for modeling CO₂-water-mineral-H₂S reactions from ambient to deep crustal temperature and pressure conditions

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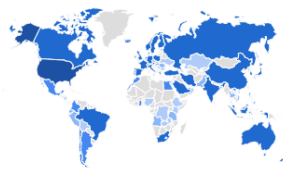
Thanks to the bright and responsible computer science undergrads Ranvir, Kevin, and Rob, the geochemical community now has a science gateway for geochemical modeling at <https://models.earth.indiana.edu/>, (and upcoming: geochemsim.org). About ~7000 users/visitors from 89 countries used these programs in the past two years for teaching and research.

The gateway hosts programs SUPCRTBL [1], Online PHREEQC, CO₂ Solubility Calculator, Reaction Rate Calculator, and H₂S Solubility Calculator. Notably, the Online PHREEQC program together with our customized databases now allows speciation and solubility and reaction path modeling to temperatures up to 1000 °C and pressure up to 5000 bars [2]. Recently, an internally consistent thermodynamic database for rare earth element crystalline solids with 155 end-members for phosphates [3], oxides, hydroxides, chlorides, fluorides, carbonates, hydrous carbonates, and ferrite are added to SUPCRTBL and PHREEQC.

The science gateway is hosted on Indiana University's high-performance computers. The format of open-source and science gateway technologies answers the call from the U.S. National Science Foundation's FAIR guiding principles (Findability, Accessibility, Interoperability, and Reuse).

1. Zimmer, K., et al., *Computers & Geosciences*, 2016. **90, Part A**: p. 97-111.
2. Zhang, G.R., et al., *Computers & Geosciences*, 2020. **143**.
3. Pan, R., et al., *Minerals*, 2024. **14(3)**: p. 305.

Users by Country ID



COUNTRY	USERS
United States	1.6K 1142...
Japan	220 1124...
United Kingdom	153 1150...
Canada	143 1138...
France	140 1125...
Germany	137 190.3%
China	111 1200...

Last year

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