

IsoGem: An Isotope Geochemical Modeling Program

JÓHANN GUNNARSSON ROBIN¹, ANDRI STEFÁNSSON¹,
BARBARA KLEINE¹

¹Institute of Earth Sciences, University of Iceland, Sturlugata
7, 101 Reykjavík, Iceland (jog13@hi.is)

Stable isotopes are an important tool to trace the sources and processes of various elements and compounds. To model these sources and geochemical processes at low and hydrothermal temperatures, a computer program has been designed, named IsoGem (Isotope Geochemical Modelling).

IsoGem is used in conjunction with other programs like PHREEQC [1] and WATCH [2, 3] and involves thermodynamic, geochemical and equilibrium isotope calculations and simulations. A part of the program is a database for equilibrium fractionation factors (α). The modelling capabilities include, for example, multiple isotope sources, progressive water-rock interaction, temperature changes and boiling and phase separation. Over 400 aqueous and gaseous species and more than 100 minerals are included and the isotope ratios of these gases, aqueous species and minerals are calculated by the program. The isotope ratios already implemented in IsoGem are δD , $\delta^{18}\text{O}$, $\delta^{11}\text{B}$, $\delta^{13}\text{C}$ (CO_2 , C_{1-6}), $\delta^{25,26}\text{Mg}$, $\delta^{30}\text{Si}$, $\delta^{33,34,36}\text{S}$ (S^{II} and S^{VI}) and $\delta^{37}\text{Cl}$. The inputs of the program include the results of geochemical calculations, source constraints and equilibrium fractionation factors (α) for various reactions.

Examples will be presented, including (1) the effects on δD and ^{18}O isotope systematics upon adiabatic and isobaric boiling, (2) seawater-rock interaction between the oceanic crust and $\delta^{34}\text{S}$ and (3) ^{13}C isotope systematics of CO_2 and hydrocarbons upon water-rock interaction and boiling.

[1] Parkhurst and Appelo (2013) *USGS A43*. [2] Bjarnason (2010) *Isor Report*. [3] Arnórsson *et al.* (1982) *Geochim. Cosmochim Acta* **46**, 1513-1532.