

Assessment of predictive uncertainty in coupled groundwater reactive transport modeling

M. YE^{1*}, D. LU¹, G. MILLER¹, G.P. CURTIS²,
P.D. MEYER³ AND S.B. YABUSAKI³

¹Department of Scientific Computing, Florida State University, Tallahassee, FL 32306, USA
(*correspondence: mye@fsu.edu)

²Water Resources Division, US Geological Survey, Menlo Park, CA 94025, USA (gpcurtis@usgs.gov)

³Hydrology Technical Group, Pacific Northwest National Laboratory, Richland, WA 99352 (Philip.Meyer@pnl.gov and yabusaki@pnl.gov)

Bayesian Model Averaging Method

Groundwater reactive transport simulations provide a systematic framework for integrating hydrologic and biogeochemical conceptual process models into a quantitative description of subsurface behaviors. However, subsurface environments are open and complex and subject to multiple interpretations and conceptualizations given available data and information. Model uncertainty is quantified using the Bayesian Model Averaging method (BMA), in which multiple plausible reactive transport models are postulated and calibrated against observations. Instead of making predictions based on a single model, predictions of groundwater fate and transport are made using the calibrated model ensemble, and BMA jointly assesses parametric uncertainty and model uncertainty.

Application to Surface Complexation Models

The BMA methodology is applied to a set of surface complexation models of varying complexity developed for simulating U (VI) transport in columns packed with well-characterized quartz [1]. Model probabilities, measures of plausibility of the models, are calculated using the Maximum Likelihood version of BMA (MLBMA [2, 3]) based on model calibration results, and used as model averaging weights. Monte Carlo simulations are also used to calculate the probabilities to evaluate accuracy of MLBMA. Model uncertainty significantly exceeds parametric uncertainty even in these well-controlled laboratory experiments and model averaging give significantly superior predictions relative to any single model.

[1] Kohler *et al.* (1996) *Water Resour. Res.* **32**, 3539–3551.

[2] Neuman (2003) *Stochast. Environ. Res. Risk Assess.* **17**, 291–305. [3] Ye *et al.* (2004) *Water Resour. Res.* **40**, doi: 10.1029/2003WR002557.

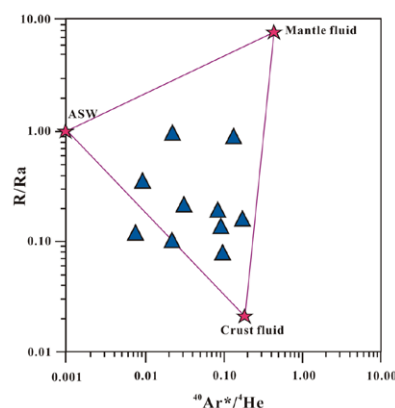
The helium and argon isotopic compositions in the minerals from the Qulong porphyry copper deposit, Tibet, SW, China

X.R. YE¹ J.R. TANG¹ M.X. TAO² L. DU¹

¹Key Laboratory of Petroleum Resources Research, Institute of Geology and Geophysics, CAS, Lanzhou 730000, P. R. China (xrye287@163.com)

²Environment School, Beijing Normal University, Beijing 100875, P. R. China (Mxtao@ires.cn)

The helium and argon isotopic compositions in the minerals from the Qulong porphyry copper deposit, Tibet, NW China, have been determined using MM5400 mass spectrometry. The $R (=^3\text{He}/^4\text{He})$ values in the chalcopyrites and molybdenites were between 0.815Ra and 0.894Ra with an average of 0.854Ra (Ra is the atmospheric $^3\text{He}/^4\text{He}$ value), and the helium contents were lower. It suggested the effect from mantle fluids. The R values in the chalcopyrite-vein quartzs and chalcopyrite-vein anhydrites were between 0.1002Ra and 0.3284Ra with an average value of 0.2026Ra, much higher than the typical R value in crust fluids. The R values in two granodiorites from the country rock were respectively 0.1815Ra and 0.2026Ra, and closed to the R values in the chalcopyrite-vein quartzs. In a chalcopyrite-vein anhydrite, it was observed that the R value (0.854Ra) in the chalcopyrite was much higher than one (0.136) in the anhydrite. It indicated that the ore-forming fluids of the Qulong porphyry copper deposit had been dominated by mantle fluids in the prior period and by crust fluids in the late period. All of the $^{40}\text{Ar}/^{36}\text{Ar}$ values were slightly higher than the atmospheric. The highest value of 864.5 was found in a granodiorite, a country rock. It was the result from radiogenic ^{40}Ar . In the $R-^{40}\text{Ar}^*/^4\text{He}$ diagram, the data points were plotted into a triangle formed by ASW (air-saturated water), mantle fluids and crust fluids. It is surmisable that the sources of ore-forming fluids are various.



This work was supported by NSFC (Grant No. 40873033 and 40573012).