

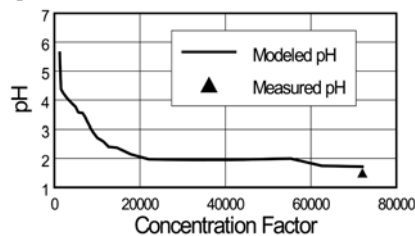
## Reactive transport modeling of acid gas generation and condensation

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Pulvirenti et al. (2004) recently conducted a laboratory evaporation/condensation experiment on a synthetic solution of primarily calcium chloride. This solution represents one potential type of evaporated pore water at Yucca Mountain, Nevada, a site proposed for geologic storage of high-level nuclear waste. These authors reported that boiling this solution to near dryness (a concentration factor  $>75,000$  relative to actual pore waters) leads to the generation of acid condensate (pH  $<1.5$ ) presumably due to volatilization of HCl (and minor HF and/or  $\text{HNO}_3$ ). To investigate the various processes taking place, including boiling, gas transport, and condensation, their experiment was simulated by modifying an existing multicomponent and multiphase reactive transport code (TOUGHREACT). This code was extended with a Pitzer ion-interaction model to deal with high ionic strength. The model of the experiment was set-up to capture the observed increase in boiling temperature ( $143^\circ\text{C}$  at  $\sim 1$  bar) resulting from high concentrations of dissolved salts (up to 8 m  $\text{CaCl}_2$ ). The computed HCl fugacity ( $\sim 10^{-4}$  bars) generated by boiling under these conditions is not sufficient to lower the pH of the condensate (cooled to 80 and  $25^\circ\text{C}$ ) down to observed values unless the  $\text{H}_2\text{O}$  mass fraction in gas is reduced below  $\sim 10\%$ . This is because the condensate becomes progressively diluted by  $\text{H}_2\text{O}$  gas condensation. However, when the system is modeled to remove water vapor, the computed pH of instantaneous condensates decreases to  $\sim 1.7$ , consistent with the experiment (Figure 1). The results also show that the HCl fugacity increases, and calcite, gypsum, sylvite, halite,  $\text{MgCl}_2 \cdot 4\text{H}_2\text{O}$  and  $\text{CaCl}_2$  precipitate sequentially with increasing concentration factors.

Figure 1. pH of the condensate



### Reference

Pulvirenti, A.L., K.M. Needham, M.A. Adel-Hadadi, A. Barkatt, C.R. Marks, and J.A. Gorman, (2004), *Corrosion 2004, NACE International*, New Orleans.

## Hydrodynamic and thermodynamic modelling of the formation of the Yuzhna Petrovitsa hydrothermal Pb-Zn ore deposit, Madan, Bulgaria

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Coupled fluid flow and speciation computations in reactive transport modelling are feasible on normal workstation computers for low temperature environments, because of their simple (if any) P-T dependence of fluid properties. Realistic modelling of high-temperature ore forming processes, however, requires orders of magnitude larger computational resources because of the much more complex equations governing multiphase flow of compressible fluids with highly nonlinear P-T-X dependencies of density, viscosity, and thermochemical properties of the solvent and dissolved minor components. This has severely limited the application to ore-forming hydrothermal systems using a realistic degree of geometric as well as chemical complexity.

Here we demonstrate how a careful combination of fluid inclusion-derived thermal and chemical data (Kostova et al., 2005) with hydrodynamic simulations provides a framework that allows decoupling of the hydrodynamic and speciation calculations. The data set comprises ore fluid compositions derived from LA-ICPMS analyses of fluid inclusions from early to late mineralization stages over a vertical interval of 500 m in the main vein of the Oligocene Yuzhna Petrovitsa Pb-Zn-Cu deposit in Bulgaria. Fluid inclusion data and  $f_{\text{S}_2}$  and pH constraints from mineral buffers are the main input to a moderate number of stand alone speciation calculations. The latter provide a full quantitative picture of the chemical evolution and predict the correct depth distribution of Pb precipitated as galena in response to cooling of a low salinity,  $>320^\circ\text{C}$  input fluid with less than 10 ppm Pb. Precipitation and a transient dissolution stage seen in the ore textures are correctly predicted from the combination of this chemical modelling with the physical modelling of advective fluid and heat transport within the vertically extensive vein system.

### Reference

Kostova B., Pettke T., Driesner T., Heinrich C.A. and Petrov, P. (2005), *Schweizer. Miner. Petr. Mitt.*, in press