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Implementation of a Pitzer Activity Model into TOUGHREACT for Modeling Concentrated Solutions

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Abstract

TOUGHREACT (Xu et al., 2004) is a general-purpose reactive geochemical transport numerical simulator. It deals with multiphase flow, solute transport and geochemical reactions including aqueous complexation, mineral dissolution/precipitation and cation exchange. Making use of an extended Debye-Hückel ion activity model, this simulator can handle solutions concentrated to slightly above ~1 molal with caution, and only for NaCl-dominant waters at ionic strengths no greater than ~4 molal. However, brines produced under natural and artificial conditions are often more concentrated. To handle such brines, a Pitzer activity model was implemented in TOUGHREACT, based on the standard Harvie-Moller-Weare (HMW) formulation that accounts for all binary and ternary combinations of interaction terms. The vapor pressure lowering effect caused by the low water activity in brines was also taken into account. The code was verified and tested using published results of laboratory experiments and benchmarked against other computer codes. This new version of TOUGHREACT is being applied to the investigation of boiling and evaporation within and around proposed high-level nuclear waste emplacement tunnels at Yucca Mountain, Nevada. Example applications are presented, including boiling of pore water to near dryness, formation of highly concentrated brines, precipitation of deliquescent salts, and generation of acid gases.