Selenium (Se) is an essential micronutrient for humans and animals, although elevated concentrations and bio-accumulation can prove detrimental to aquatic habitats and to health. During the recent decades, either deficient or elevated concentrations of Se in soil water, groundwater, surface waters, and associated cultivated crops has emerged as a serious concern in regions around the world. Regardless of the nature of concern regarding Se, there is a basic need for the development of numerical simulation tools that allow for the assessment of baseline conditions and possible mitigation scenarios in hydro-systems.

In this study we present the development of a Se reaction module for the newly-developed numerical model RT3D-AG, which was originally developed for the reactive transport of nitrogen (N) species in variably-saturated agricultural groundwater systems. The Se module, similar to the cycling of carbon and N species already included in RT3D-AG, includes organic matter decomposition and mineralization, oxidation-reduction reactions, and sorption. An accounting of the mass of Se species entering/exiting the system via irrigation water, canal seepage, fertilizer and manure, dead root mass and after-harvest stover mass, discharge to surface water bodies, crop uptake, and groundwater pumping also is included. Of particular importance is autotrophic oxidation, in which reduced Se from outcropped and bedrock shale is released into the aquifer through oxidation by dissolved oxygen (O2) and nitrate (NO3), as well as the influence of both O2 and NO3 in inhibiting the chemical reduction of toxic Se species.

We also present preliminary results of calibrating and applying the model to a 50,400-ha regional study site within the Lower Arkansas River Valley in southeastern Colorado, where elevated concentrations of Se have been monitored in both groundwater and surface water during the recent decade. The study site includes the Arkansas River as well as six un-lined irrigation canals. Main crops include alfalfa, corn, sorghum, onions, and melons. The model is run for the 2006-2008 time period, with initial conditions provided by spin-up simulations. Initial results compare favorably with field observations. Future implementation includes sensitivity analyses, refined calibration, and scenario testing to investigate best-management practices.