Multicomponent inverse modelling in aquatic sediments

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A comprehensive understanding of chemical mass transfer in aquatic sediments requires a comprehensive tool capable of deconvoluting all major processes that are heavily interrelated. Multicomponent reactive transport modelling can be the comprehensive tool when reaction and transport parameters are adequately constrained through a sufficient number of observations and prior knowledge of their interdependency. In the present study, a multicomponent inverse model written in Matlab was applied to a saltmarsh environment heavily affected by vegetation and bioturbating organisms, located in Skidaway Island, Georgia, USA. Depth profiles of most major redox species were directly measured, and transport parameters were determined using porosity profiles (for diffusion coefficients) and the relationship between ^{35}S-determined sulfate reduction rates and pore water sulfate concentration profiles (for irrigation coefficients). Consequently, the multicomponent inverse model could be used to quantify the reaction rates. The results indicate that within the upper few millimetres of intertidal sediments, carbonate mineral precipitation takes place during the low tide periods generating small pH maxima in the immediate vicinity of sediment surface. The results also show that the *in situ* rates of iron (III) reduction determined through modelling are comparable to the rates obtained by the *ex situ* incubation procedures. Inverse modelling of reaction rates can be especially useful where forward modelling with *a priori* application of rates is difficult due to complex reaction geometry and/or rapid recycling of redox species.