Finite Element Solution to Groundwater Transport of Dissolved Contaminants Undergoing Decay and Non-Linear Sorption

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Abstract. Contaminants are often found in groundwater as a result of disposal or leakage of urban sewage and industrial wastes, surficial applications of pesticides and fertilizers used in agriculture, or accidental releases of chemicals on the ground surface. Once contaminants enter the subsurface, they may reach shallow aquifers, where they dissolve in water, and are transported downstream along flow pathways. This often poses serious risks for human health or ecosystems in general.

Dissolved contaminants typically experience complex physical and chemical processes such as advection, diffusion, chemical reactions, sorption, biodegradation and decay. Understanding and simulating these processes is crucial to predict the fate and transport of solutes in groundwater. The study of contaminant transport is further complicated by the limited ability to sufficiently characterize the inherent heterogeneities in the subsurface and the time scales at which transport processes occur.

Mathematical models of groundwater flow and reactive transport may provide an effective tool to study these processes when supported by consistent and reliable datasets. These models rely upon the numerical solution to the fundamental equations of mass conservation for the aquifer/contaminant system.

In this work, a finite element simulation model is presented that solves the contaminant transport equation for a solute undergoing advection, dispersion, first-order decay, and non-linear local-equilibrium sorption. The assumption of local equilibrium is valid provided that the sorption rates are much larger than the rates of advection and dispersion. Non-linear sorption introduces a source of non linearity in the transport partial differential equation, which is here tackled using a direct iterative approach based upon Picard linearization. This method is implemented using several types of sorption isotherms, which can be specified arbitrarily in however heterogeneous settings.