



## **Numerical validation of first order theory in bimodal porous formations**

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Solute transport in heterogeneous formations is controlled by hydraulic and geochemical property variations over many spatial scales. Detailed studies of the variability of sedimentary formations have revealed a hierarchical structure in which several modes and correlation lengths combine to create a more complex and heterogeneous structure. Such complexity is created by the arrangement of lithofacies units, with sizes, granulometric and textural properties dependent upon the energy of the depositional environment. Multi-indicator geostatistical models provide a useful way to model such complexity. As an example of such a class of models we consider the bimodal model discussed by Rubin (1995), which is formed by inclusions implanted in a formation characterized by variability acting on a larger scale. Two important cases can be distinguished depending if the mean hydraulic conductivity of the inclusions is larger or smaller than the mean hydraulic conductivity of the background, and are discussed in this work. Furthermore, to our knowledge most of the work that has been done so far is for transport of non-reactive tracers.

In this work we extend the first-order solution to reactive solutes undergoing non-equilibrium reversible adsorption, and assess its applicability by means of accurate numerical simulations. We used a first-order perturbation method to develop closed-form approximations for the displacement moments as a function of time. Similar comparisons for the case of multi-Gaussian log-conductivity distribution have been extensively presented in the literature, but to our knowledge, there are no published works analysing the applicability of the first-order theory for bimodal formations. We

compare the first two spatial moments computed numerically throughout Monte Carlo simulations with the first-order solution. Specifically, we have analyzed both conservative and reactive solutes for inclusions with contrast between the mean hydraulic conductivity of the two modes of variability alternatively smaller and larger than one. The first-order approximation predicts a symmetric behaviour of the dispersion coefficient with respect to the contrast in the mean hydraulic conductivity, but the numerical simulations show that this is actually the case only for small contrasts, when the hydraulic conductivity of the inclusions differs slightly from the background conductivity. The results for the reactive case show that the performance of the analytical solution improves as the reaction rate decreases.