CrunchFlow numerical issue in advection

We did not use the CrunchFlow built-in function to describe fluid advection due to a significant numerical dispersion in CrunchFlow. This numerical issue is confirmed both by CrunchFlow developer (Steefel, personal communication) and also the tests we performed. Here we compared two simulations done by the CrunchFlow built-in function for advection (the "Erosion/burial" function) and our MATLAB routine to demonstrate this numerical issue. Both simulations were done assuming a 4-meter sediment column. Constant porosity of 0.68 throughout the core was used. We turned off all reactions and diffusion; only advection of fluid was allowed. Fixed concentrations for the upper boundary condition was used; a no flux lower boundary condition was adopted. Three lengths of simulation time were chose: 20, 80 and 140 years. The maximum allowed time step in CrunchFlow was set to be 0.02 years. An even smaller time step (0.002 years) was used for the CrunchFlow simulation but no noticeable difference in results was observed. For the MATLAB routine, advection is evaluated every 0.2 years, a smaller time step is possible with longer computing time. The same *Darcy* velocity 0.01 $m^3/m^2/yr$ (or 0.0147 m/yr for fluid velocity assuming 0.68 porosity) was used in both simulations. Two cases were simulated: a fluid with high concentration of chloride advects downward (Figure S2A) and a high chloride concentration pulse being transported by the advected fluid (Figure S2B).

It is obvious from Figure S2A that the advection simulation done by CrunchFlow shows significant numerical dispersion as the edges of the square function are gradually smeared with time. On the contrary, the square functions were better preserved in the simulations done by the MTALAB routine. In the other case, where a pulse of Cl-rich fluid is transported by the advected fluid (Figure S2B), the peak heights in the simulations done by CrunchFlow were reduced by 9.7%, 18%, and 20% comparing to the original peak height. For the simulations done by MATLAB, the peak heights were only 3.6% reduced at most after simulating the flow for 140 years. The reduced peak height and gradually spreading peak are clear characteristics of numerical dispersion during the simulation of advection. This comparison justifies our decision not to use the built-in function of CrunchFlow to simulate advection. Our MATLAB routine provides a more accurate and numerically stable alternative for this purpose.

Figure S2: Comparison of fluid advection simulated by CrunchFlow built-in function and our MATLAB routine. Grey dashed lines and blue solid lines are the results from CrunchFlow and our MATLAB routine, respectively. The red solid and dashed lines in (B) mark the initial concentration of Cl. As we included only fluid advection in both models, there should be no concentration reduction during fluid transport. The reduction between the model results and the initial Cl concentration, as shown by the percentages (the blue arrow in (B)), is solely due to numerical dispersion in both models. Our MATLAB routine provides more accurate model results with less numerical dispersion.