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Geoscientific Model Development Discussions

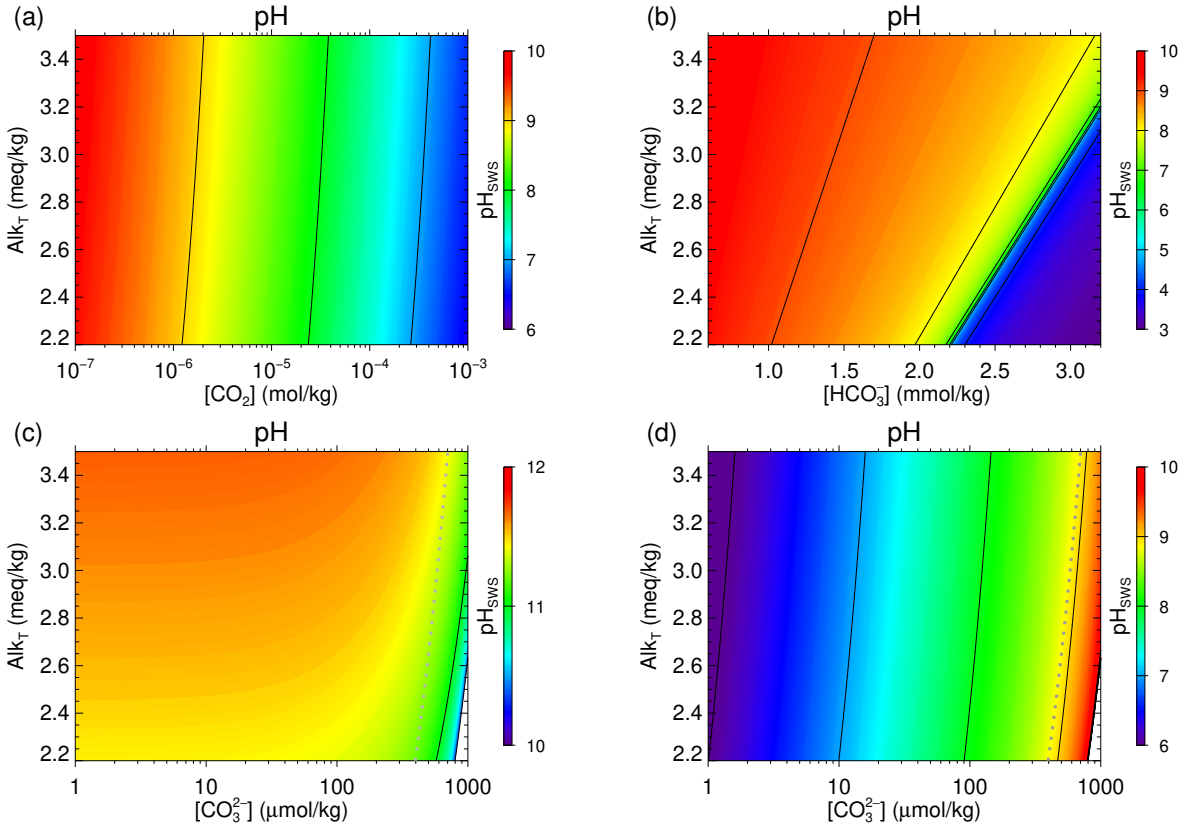

Figure 4. pH distributions for the SW2 test case under cold surface conditions ($T = 273.15\,\mathrm{K}$, $S = 35$ and $P = 0\,\mathrm{bar}$), obtained with `solve_at_general2_sec`: (a) $\mathrm{Alk_T}$ & $\mathrm{CO_2}$; (b) $\mathrm{Alk_T}$ & $\mathrm{HCO_3^-}$; (c) the lower $[\mathrm{H^+}]$ root (higher pH root) of $\mathrm{Alk_T}$ & $\mathrm{CO_3^{2-}}$; (d) the greater $[\mathrm{H^+}]$ root (lower pH root) of $\mathrm{Alk_T}$ & $\mathrm{CO_3^{2-}}$. The thick grey dashed line in (c) and (d) shows the critical limit above which the $\mathrm{Alk_T}$ & $\mathrm{CO_3^{2-}}$ always has two roots. Below this limit further calculations are required to determine the number of solutions. More details are given in the text and in the Supplement. Please notice the different scales on the horizontal axes and for the pH colour coding in the four panels.

3.2.2 Results

While all the test cases have their specific relevance, we are going to focus on SW2 for most of our discussion here. SW2 covers currently observed sea-water samples, thus encompassing SW1, and conditions expected to occur over the next 50,000 years as derived from simulation experiments carried out with MBM-MEDUSA (Munhoven, 2009). A wider selection of results also for the other cases presented in the *Additional Results* in the Supplement. pH distributions for the SW2 test case are shown on Fig. 4.

The difficulties posed by $\mathrm{Alk_T}$ & $\mathrm{CO_2}$ that were at the origin of most of the amendments to the solver algorithms show up in the histograms for the number of iterations required to reach convergence shown on Fig. 5 for `solve_at_general` which