SolveSAPHE
Reliable and Robust Carbonate System *p*H Calculations Made in Belgium

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Carbonate equilibria:

$$CO_2 + H_2O \longrightarrow HCO_3^- + H^+$$
$$HCO_3^- \longrightarrow CO_3^{2-} + H^+$$

4 unknowns and 2 equilibrium relationships

⇒ 2 additional measurables required

Currently available measurables:

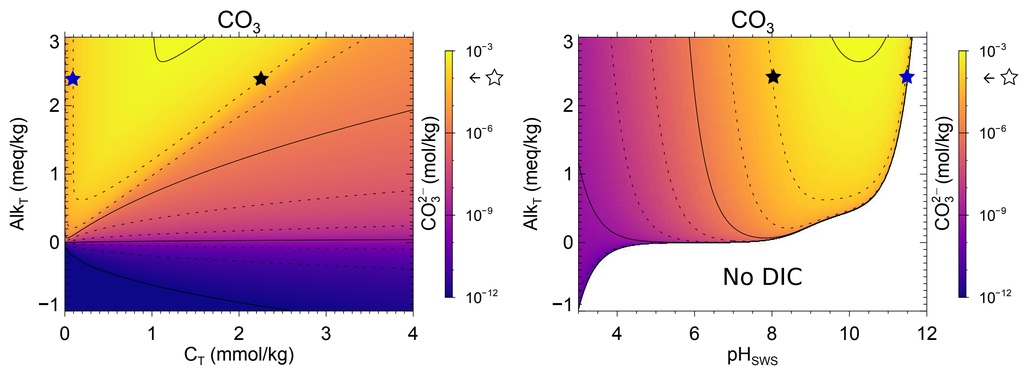
- DIC (C_T) } conservative
- Alk_T } (suitable for modelling)

- *p*H
- $pCO_{2(aq)}$ } non conservative
- CO_3^{2-}

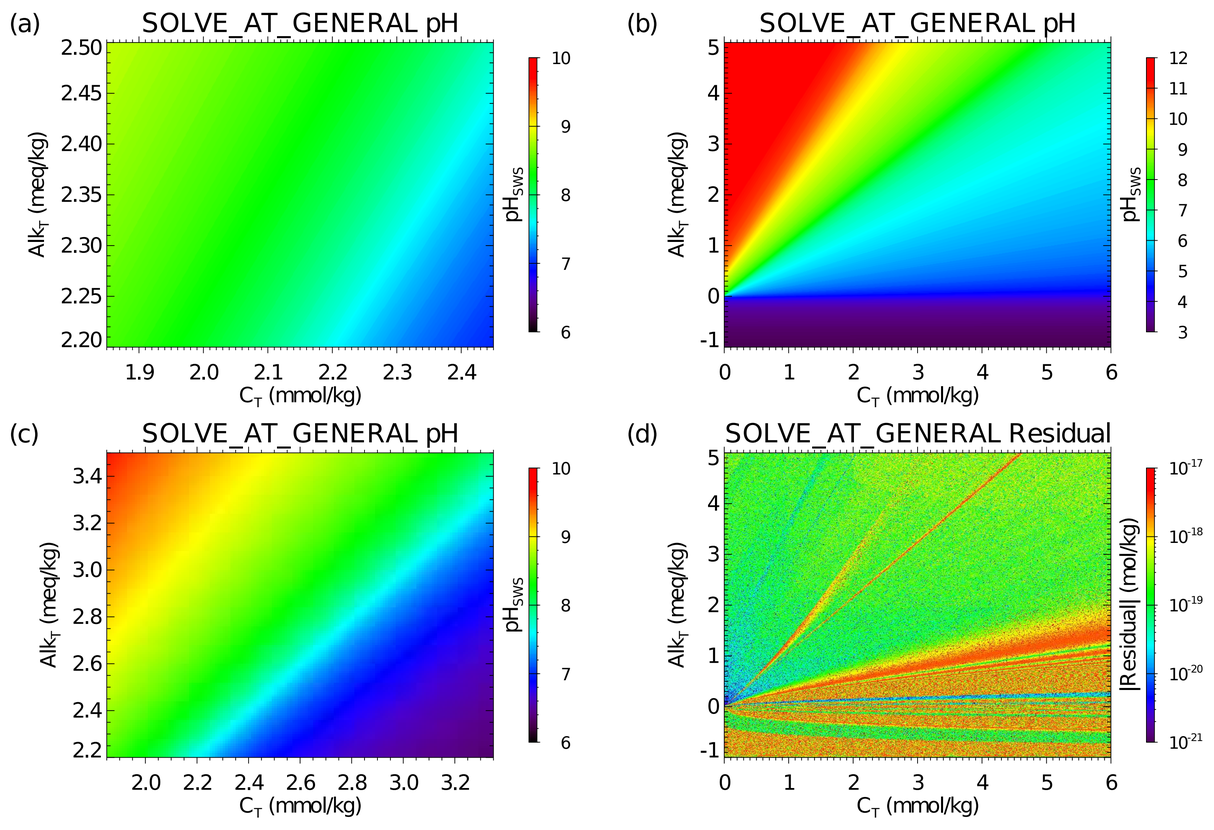
All pairs of measurables allow for an explicit speciation calculation, except for

- Alk_T & C_T
- Alk_T & $CO_{2(aq)}$
- Alk_T & HCO_3^-
- Alk_T & CO_3^{2-}

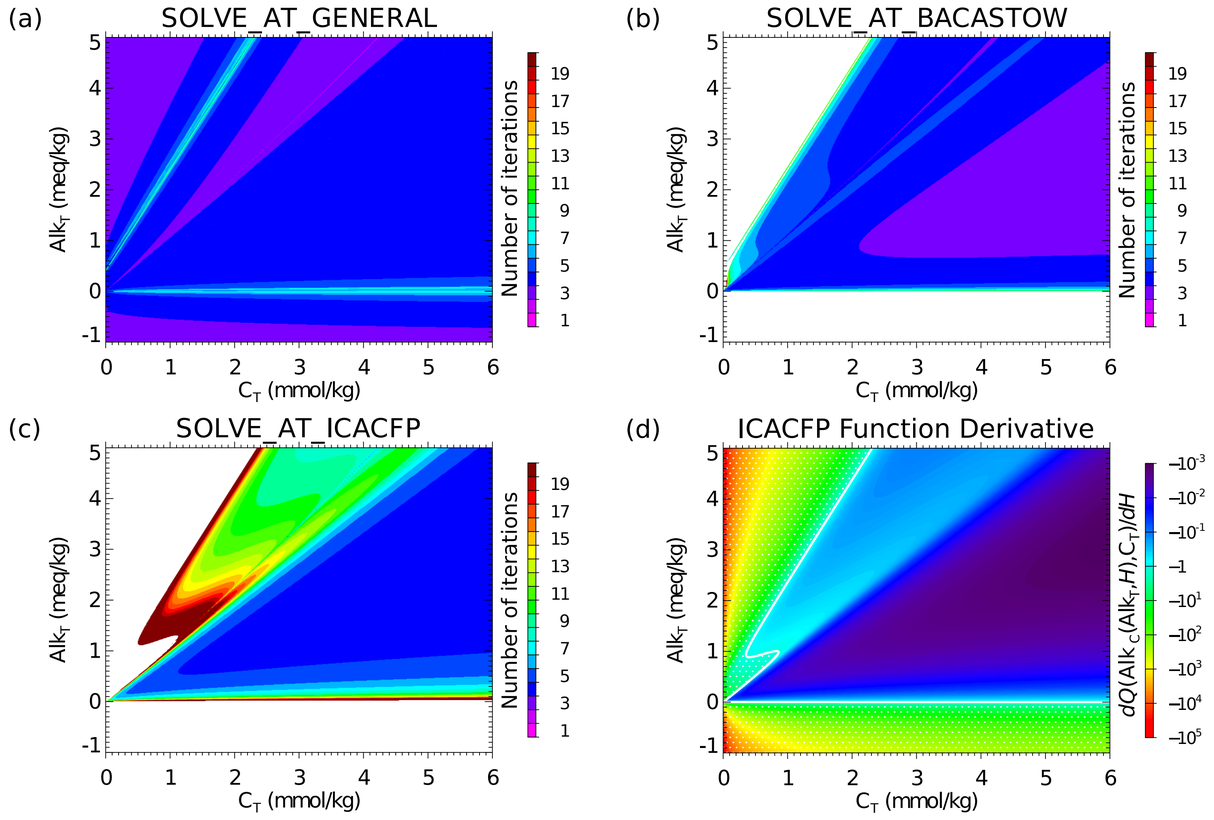
which require iterative approaches. The Alk_T & CO_3^{2-} pair presents the further complication that it may have zero, one or two solutions. SolveSAPHE offers robust self-starting algorithms to reliably solve these four pairs.



Alk_T & CO_3^{2-} problem: locations of 0, 1 and two possible *p*H solutions.



(a)-**(c)**: pH distributions calculated for three different Alk_T-C_T test cases with the standard SolveSAPHE-v1 solver SOLVE_AT_GENERAL; **(d)** equation residual for test case (c).



Numbers of iterations required to convergence with by **(a)** SOLVE_AT_GENERAL and two popular methods: **(b)** Bacastow with secant iterations on $[H^+]$ and an Iterative Carbonate Alkalinity Correction Fixed-Point (ICACFP) method. White areas indicate convergence failures. **(d)** Derivative of the recurrence function underlying ICACFP.

SolveSAPHE-v1 (Munhoven, GMD 2013)

Alk_T & C_T

Self-starting iterations, with guaranteed and *fast* convergence

SolveSAPHE-v1

SolveSAPHE-v1 is the solver engine in *mocsy 2.0*, the standard chemistry package for the CMIP6 Ocean Model Intercomparison Project (OMIP).

SolveSAPHE-v1 used in

- ORCA25-PISCES (IPSL)
- Delft3D (DELTARES)
- iLoveclim (LSCE, VU Amsterdam)
- Biogeochemical Flux Model (BFM)
- Bottom RedOx Model (BROM v.1.1)
- MITgcm (in package dic)
- CESM (MARUM Bremen)
- BICYCLE (AWI Bremerhaven)

SolveSAPHE-r2 (Munhoven, GMD 2021)

Alk_T & $CO_{2(aq)}$

Alk_T & HCO_3^-

Alk_T & CO_3^{2-}

Self-starting iterations, with guaranteed convergence

Complete characterisation of the Alk_T & CO_3^{2-} problem (number of solutions, brackets)

SolveSAPHE-r2

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