Supplement to: Substantial inter-model variation in OAE efficiency between the CESM2/MARBL and ECCO-Darwin ocean biogeochemistry models

1 Alkalinity injection locations used in this study

Name	Average Latitude	Average Longitude	Polygon index
Alaska	58.2	213.2	180
Brazil	1.9	311.8	29
East Coast USA	41.1	290.6	17
Gulf of Mexico	27.1	268.7	87
Hawai‘i	18.4	206.8	157
Iceland	61.7	340.7	32
Japan	32.3	136.5	158
Kerguelen	-49.3	72.0	363
Norway	65.3	5.8	99
Oman	24.2	59.5	437
West Coast USA	30.6	241.3	214
Western Sahara	24.1	341.9	27
East Coast USA (Offshore)	35.2	294.0	134
Oman (Offshore)	14.8	64.1	592
West Coast USA (Offshore)	27.3	235.2	345
Western Sahara (Offshore)	24.6	330.6	111

Table S1. Summary of the twelve main alkalinity injection locations and the four additional offshore locations used in this study together with the geographical location of their center. The polygon index refers to the numbering scheme used in Zhou et al. (2024) and the exact area definitions can be found therein. See also Fig. S1.

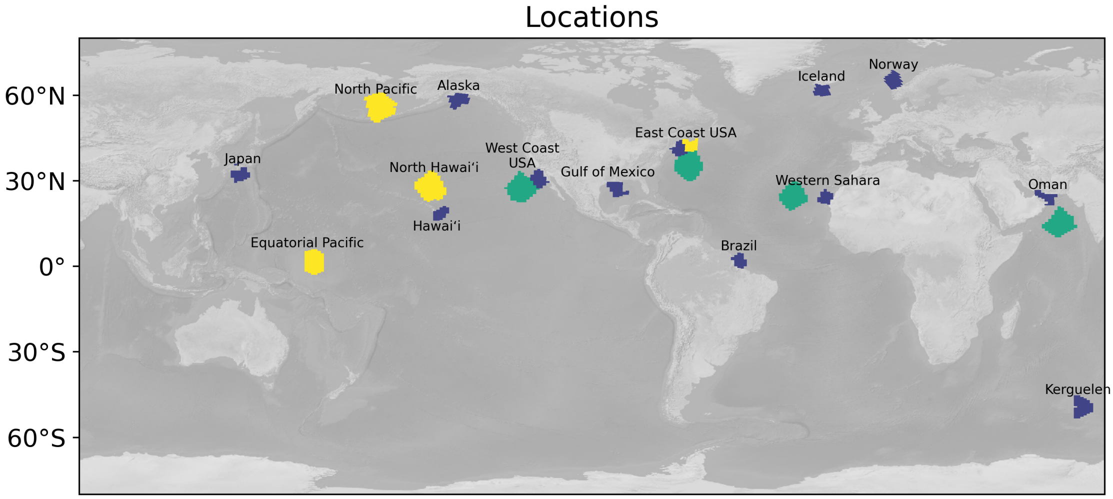

Figure S1. Locations selected for inter-model comparison. The twelve main locations investigated here are shown in blue. In four cases (green) a nearby area further offshore was also examined. In yellow are shown four locations from Yankovsky et al. (2025), which were compared to equivalent injection years in ECCO-Darwin. See also Tables S1 and S2.

Name	**Latitude**	**Longitude**	**Polygon index**
East Coast USA	42.5	294.6	72
North Hawai‘i	27.7	203.4	157
North Pacific	55.9	185.6	305
Equatorial Pacific	1.5	162.4	334

Table S2. Alkalinity injection locations used in the comparison of interannual variability together with the geographical location of their center. The polygon index refers to the numbering scheme used in Yankovsky et al. (2025). See also Fig. S1.

2 Approximations and parameter dependence for $\partial[DIC]/\partial[Alk]$

The quantity $\eta_{max} = \frac{\partial[\mathrm{DIC}]}{\partial[Alk]}$ determines the maximal amount of additional CO_2 that can be taken up by a water parcel following the addition of a small quantity of alkalinity and therefore effectively determines the maximal efficiency of OAE at full equilibration. It is the reciprocal of the "isocapnic quotient" introduced by (Humphreys et al., 2018). In principle, it is dependent on all the carbonate system parameters and can be calculated exactly using a carbonate system solver such as PyCO2SYS (Humphreys et al., 2020). An exact analytical formula has also been given by (Humphreys et al., 2018):

$$1/\eta_{max} = \frac{(K_1hs + 4K_1K_2s + K_wh + h^3)(K_B + h)^2 + K_BB_Th^3}{K_1s(h + 2K_2)(K_B + h)^2}, \tag{1}$$

where h is the $[H^+]$ concentration, s is the $[CO_2]$ concentration, B_T is the total borate concentration and K_1,K_2,K_w and K_B are the equilibrium constants of the carbonate and borate equilibria. An approximation was also given as

$$1/\eta_{max} = \left(1 + \frac{2K_2[DIC]}{K_1[CO_2]}\right)^{-1} \tag{2}$$

For more detail on the derivation and the approximation, see Humphreys et al. (2018). By dividing denominator and numerator by the factor $h^2(K_B + h)^2$ and replacing the terms with the equivalent concentration terms, this expression can be expressed exactly in terms of the concentrations of species contributing to the carbonate equilibrium. This can be useful for practical purposes.

$$1/\eta_{max} = \frac{[HCO_3^-] + 4[CO_3^{2-}] + [OH^-] + [H^+] + [B(OH)_4][B(OH)_3]/([B(OH)_4] + [B(OH)_3]}{[HCO_3] + 2[CO_3^{2-}]} \tag{3}$$

Figure S2 plots values of η_{max} calculated using PyCO2SYS Humphreys et al. (2020) for a full parameter scan over the values of $[DIC]$, $[Alk]$ and T (temperature). $[Alk]$ was varied from 1600μmol/L to 6000μmol/L in 15 logarithmically spaced steps, $[DIC]$ was varied from 1900μmol/L to 3500μmol/L in logarithmically spaced steps. For each pair of values, η_{max} was calculated at T=0°C and T=30°C and also for $B_T = 0$ and B_T=415μmol/L, the default PyCO2SYS value. All other parameters (salinity etc) were also set to typical ocean values (default PyCO2SYS values were used).

When plotted against $[DIC]/[Alk]$, as shwon in Figure S2a, all the points lay almost perfectly along a monotonously increasing line (Fig. S2). In other words, η_{max} appears to be almost purely a function of $[DIC]$/$[Alk]$. Temperature does not appear to strongly affect the value for most of the $[DIC]$/$[Alk]$ ratio, except around $[DIC]/[Alk]$ ≈1.0, where a small temperature dependence is observed. This suggests that there should be simple approximations for η_{max} as a function of $[DIC]/[Alk]$ for convenient calculation of this quantity without the need to compute the entire carbonate system. A very simple approximation was given by (Tyka et al., 2022):

$$1/\eta_{max} \approx 3 - 2[DIC]/[Alk]. \tag{4}$$

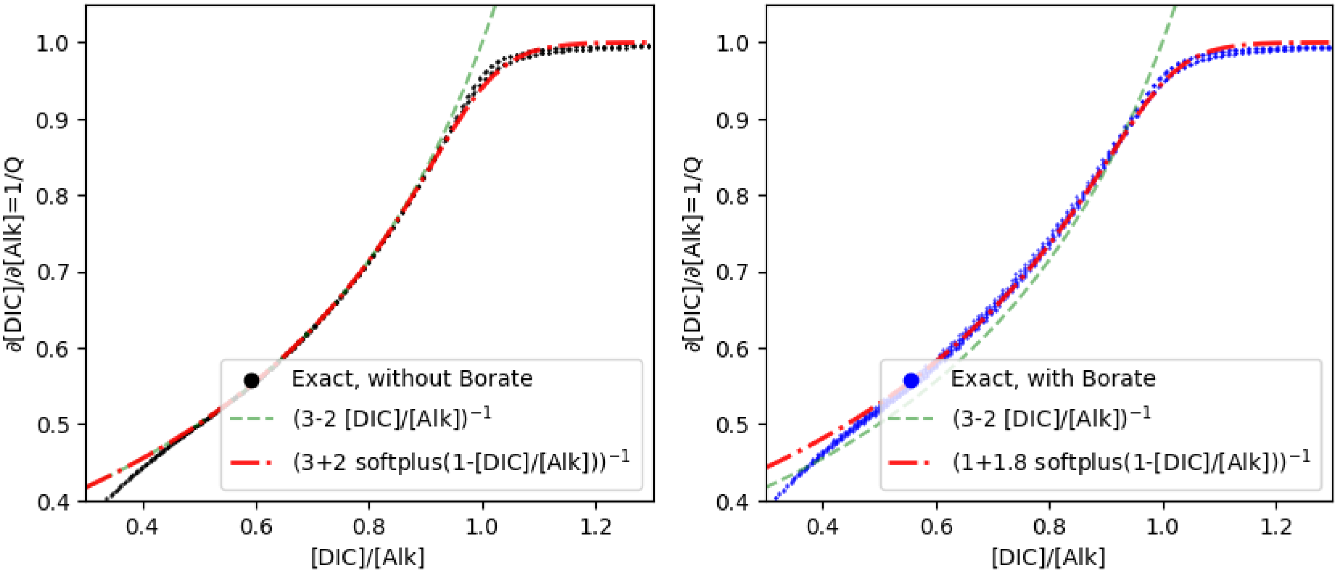

Figure S2. η_{max} as a function of [DIC]/[Alk] for carbonate systems with and without borate present. The approximation (Tyka et al., 2022) is shown as a dashed line. The superior approximation from Equation 5 is shown as a dash-dot line.

This approximation is shown as a dashed line in Figure S2 and is surprisingly good between $[DIC]$/$[Alk]$=0.45 and $[DIC]$/$[Alk]$=0.95, but fails to account for more alkaline and more acidic extremes. Its advantage is that it is easy and fast to calculate because it is not necessary to solve the carbonate system (i.e. there's no need to determine the value of pH, $[CO_2]$ or $[HCO_3^-]$, etc which are needed for the exact expression Eq. 3).

At values of $[DIC]/[Alk]$ greater than 0.9 the approximation begins to strongly diverge from the real value of η_{max}, which cannot exceed 1.0. The value of the approximation, however, continues beyond 1.0 because the term $3-2[DIC]/[Alk]$ continues to decrease below 1 (and eventually below 0), yielding nonsensical values. Here, we introduce an improvement on Eq. , which can be achieved by clipping $[DIC]/[Alk]$ above 1.0. If a simple truncation $\min(1,[DIC]/[Alk])$ were used, the result would be a sharp kink at $[DIC]/[Alk]=1.0$ and a poor fit in its vicinity. Instead, a much better result is obtained if one uses a softplus function, such as $\ln(\exp(\gamma x)+1)\gamma^{-1}$, where γ is an empirical sharpness parameter.

This yields an easy to compute, yet excellent approximation for almost all practically relevant values of $[DIC]/[Alk]$:

$$1/\eta_{max} = 1 + 2\gamma^{-1}\ln\{1+\exp(\gamma-\gamma[DIC]/[Alk])\}, \tag{5}$$

with γ set to ≈ 22, which leads to about the right curvature around $[DIC]/[Alk]=1.0$. This approximation is shown in Figure S2a as a dash-dot line.

2.1 Borate

When the effect of typical ocean borate concentrations are included in the calculation, η_{max} is somewhat increased and a small temperature dependence is now evident across the entire $[DIC]$/$[Alk]$ range Fig.S2b). The earlier approximation is now a little too low (by around 0.03) compared to the accurate value of η_{max} due to the additional buffering provided by the borate system. This can be empirically corrected by adjusting Equation 5 slightly:

$$1/\eta_{max} = 1 + 1.8\gamma^{-1}\ln\{1 + \exp(\gamma - \gamma[DIC]/[Alk])\} \tag{6}$$

The comparison to the exact values calculated with PyCO2SYS is shown in Figure S2b.

2.2 Other approximations

Other, less empirical, approximations can be constructed starting from Equation 3 by making some increasingly simplifying assumptions, which we note here for completeness. Some of them are extremely accurate, but generally require knowing the value of $[CO_2]$ or $[HCO_3]$.

Assuming the concentration of free $[H^+]$ is negligible and $B_T = 0$, Eq 3 simplifies to

$$1/\eta_{max} \approx \frac{[HCO_3^-] + 4[CO_3^{2-}] + [OH^-]}{[HCO_3] + 2[CO_3^{2-}]} \tag{7}$$

The assumptions above also imply, $[Alk] = [HCO_3^-] + 2[CO_3^{2-}] + [OH^-]$ as the contributions of the other ions is ignored. One can thus substitute the numerator and denominator as:

$$1/\eta_{max} \approx \frac{[Alk] + 2[CO_3^{2-}]}{[Alk] - [OH^-]} = \frac{[Alk] + ([Alk] - [OH^-] - [HCO_3^-])}{[Alk] - [OH^-]} = 1 + \frac{[Alk] - [HCO_3^-])}{[Alk] - [OH^-]} \tag{8}$$

If one further assumes that $[OH^-]$ is also relatively small compared to $[Alk]$ in the denominator, another approximation arises (Keeping in mind that $[DIC] = [CO_2] + [HCO_3^-] + [CO_3^{2-}]$):

$$\begin{aligned} 1/\eta_{max} &\approx \frac{[Alk] + 2[CO_3^{2-}]}{[Alk]} \\ &= \frac{Alk + 2([Alk] - [DIC] + [CO_2])}{[Alk]} \\ &= 3 - 2\frac{([DIC] - [CO_2])}{[Alk]} \end{aligned} \tag{9}$$

Finally, this approximation simplifies further at typical ocean pH of 8 where the concentration of free CO_2 is very small) and the earlier approximation from Tyka et al. (2022) is recovered ($1/\eta_{max} = 3 - 2DIC/Alk$).

Figure S3 shows these approximations against the exactly calculated values of η_{max} for both the borate free carbonate system and the more realistic carbonate system with borate, respectively. Remarkably, the approximation

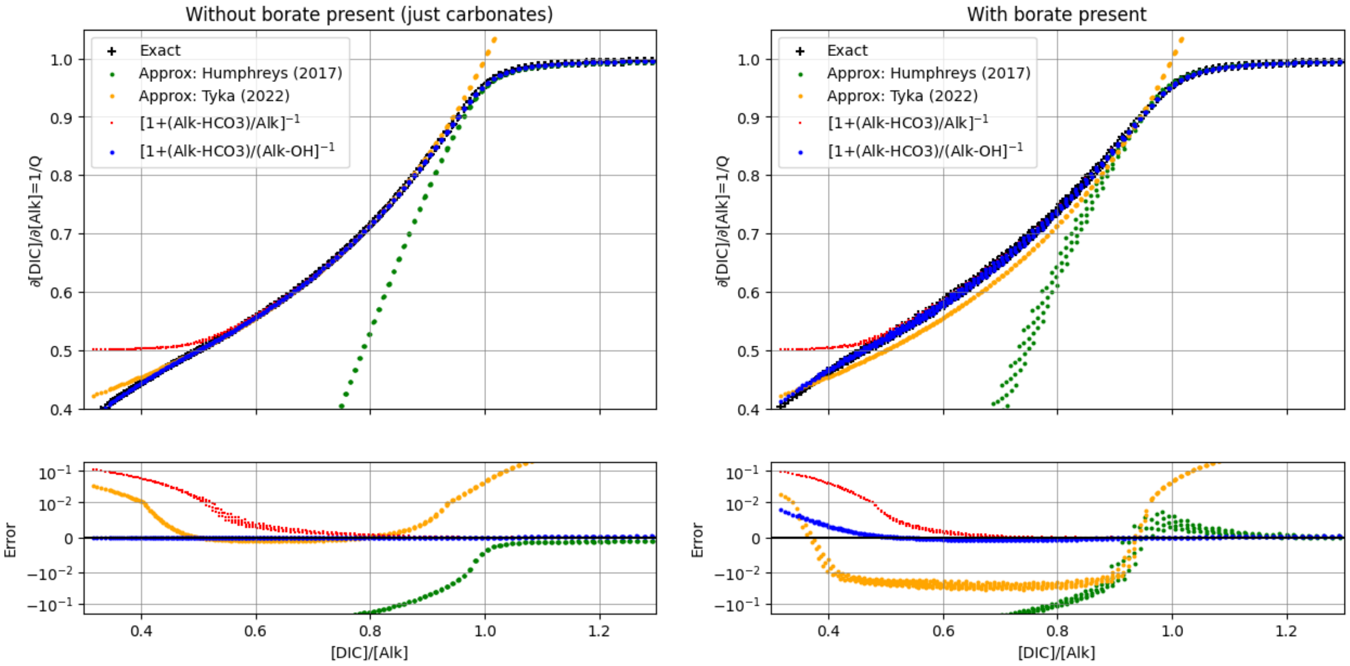

Figure S3. Various approximations to η_{max} discussed in the text. The approximations from (Humphreys et al., 2018) and from (Tyka et al., 2022) is also shown for comparison.

$$1/\eta_{max} \approx 1 + \frac{[Alk] - [HCO_3^-])}{[Alk] - [OH^-]} \tag{10}$$

and its slightly simpler relative

$$1/\eta_{max} \approx 1 + \frac{[Alk] - [HCO_3^-])}{[Alk]} \tag{11}$$

work extremely well even when borate is present, even though the approximations don't explicitly include the concentrations of borate (unlike the exact expression).

3 Analytical expression for $\partial[CO2]/\partial[DIC]$

An analytic expression for $\partial[CO2]/\partial[DIC]$ may be obtained using a similar approach to that used to derive $\partial[DIC]/\partial[Alk]$ by Humphreys et al. (2018). Beginning with their general expressions for alkalinity (A_T) and DIC (C_T)

$$\begin{aligned} A_T &= [HCO_3^-] + 2[CO_3^{2-}] + [B(OH)_4^-] + [OH^-] - [H^+] \\ &= K_1 s/h + 2K_1K_2 s/h^2 + K_B B_T/(K_B + h) + K_w/h - h \end{aligned} \tag{12}$$

$$\begin{aligned} C_T &= [CO_2] + [HCO_3^-] + [CO_3^{2-}] \\ &= s + K_1 s/h + K_1K_2 s/h^2 \end{aligned} \tag{13}$$

we calculate the two derivatives $\partial C/\partial h$ and $\partial s/\partial h$, both at constant alkalinity.

First expressing $s = [CO_2]$ in terms of A_T and h,

$$s = \frac{A_T - \frac{K_B B_T}{K_B + h} - \frac{K_W}{h} + h}{K_1/h + 2K_1K_2/h^2} \tag{14}$$

one can take its derivative with respect to h:

$$\frac{\partial s}{\partial h} = h\frac{(h+4K_2)(A_T - \frac{K_B B_T}{K_B+h} - \frac{K_W}{h} + h) + h(h+2K_2)(\frac{B_T K_B}{(h+K_B)^2} + \frac{K_W}{h^2} + 1)}{K_1(h+2K_2)^2} \tag{15}$$

Similarly, expressing C_T in terms of A_T and h,

$$C_T = \frac{(A - K_B B_T/(K_B+h) - K_W/h + h)(1 + K_1/h + K_1K_2/h^2)}{K_1/h + 2K_1K_2/h^2} \tag{16}$$

and differentiating with respect to h yields:

$$\frac{\partial C_T}{\partial h} = \frac{C_T}{hs}\left[\left(1 - \frac{K_1/h + 4K_1K_2/h^2}{(K_1/h + 2K_1K_2/h^2)^2}\right)\left(\frac{K_B B_T}{K_B + h} - A - h + \frac{K_W}{h}\right) + \frac{\frac{h}{h+K_3}\frac{K_B B_T}{K_B+h} + h + K_W/h}{K_1/h + 2K_1K_2/h^2}\right] \tag{17}$$

The sought-after derivative is then given by the quotient of these two derivatives:

$$\left.\frac{\partial C_T}{\partial s}\right|_{A_T} = \frac{\partial C_T}{\partial h} / \frac{\partial s}{\partial h} \tag{18}$$

After some simplification one obtains:

$$\begin{aligned} \left.\frac{\partial C_T}{\partial s}\right|_{A_T} &= s^{-1}\left[C_T - \frac{(K_1 s/h + 2K_1K_2 s/h^2)^2}{K_1 s/h + 4K_1K_2 s/h^2 + h + K_w/h + h/(h+K_B)\frac{K_B B_T}{K_B+h}}\right] \\ &= s^{-1}\left[C_T - \frac{([HCO_3^-] + 2[CO_3^{2-}])^2}{[HCO_3^-] + 4[CO_3^{2-}] + [OH^-] + [H^+] + [B(OH)_4][B(OH)_3]/([B(OH)_4] + [B(OH)_3])}\right] \end{aligned} \tag{19}$$

which can be further simplified by substituting η_{max} from Equation 3 to give

$$\left.\frac{\partial C_T}{\partial s}\right|_{A_T} = s^{-1}\left[C_T - \eta_{max}([HCO_3^-] + 2[CO_3^{2-}])\right] \tag{20}$$

This equation is very convenient for calculating the β factor using PyCO2SYS.

References

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