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Inclusion of MyAMI-derived Mg / Ca corrections to the marine carbonate system in the cGENIE.cookie Earth system model (v.0.91)

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Table S1: Empirical approximations of apparent equilibrium constants in the default cGENIE carbonate system solver. T stands for in situ temperature, S for in situ salinity, I for in situ ionic strength after Millero [1982] and ION for in situ ionic strength after Zeebe and Wolf-Gladrow [2001].

Dissociation constant	Approximation	Reference
pK_1	$-(3670.7/T - 62.008 + 9.7944 \cdot \ln(T) - 0.0118 \cdot S + 0.000116 \cdot S^2)$	Mehrbach [1973], Dickson & Millero [1987]
pK_2	$-(1394.7/T + 4.777 - 0.0184 \cdot S + 0.000118 \cdot S^2)$	Mehrbach [1973], Dickson & Millero [1987]
pK_B	$148.0248 + 137.194 \cdot S^{0.5} + 1.62247 \cdot S + (-8966.90 - 2890.51 \cdot S^{0.5} - 77.942 \cdot S + 1.726 \cdot S^{1.5} - 0.0993 \cdot S^2)/T + (-24.4344 - 25.085 \cdot S^{0.5} - 0.2474 \cdot S) \cdot \ln(T) + 0.053105 \cdot S^{0.5} \cdot T$	Dickson [1990]
pK_W	$148.9802 - 13847.26/T - 23.6521 \cdot \ln(T) + (-5.977 + 118.67/T + 1.0495 \cdot \ln(T)) \cdot S^{0.5} - 0.01615 \cdot S$	Millero [1992]
pK_{Si}	$117.40 - 8904.2/T - 19.334 \cdot \ln(T) + (3.5913 - 458.79/T) \cdot I^{0.5} + (-1.5998 + 188.74/T) \cdot I + (0.07871 - 12.1652/T) \cdot I^2$	Yao & Millero [1995]
pK_{HF}	$1590.2/T - 12.641 + 1.525 \cdot ION^{0.5}$	Dickson & Riley [1979]
pK_{HSO_4}	$141.328 - 4276.1/T - 23.093 \cdot \ln(T) + (324.57 - 13856.0/T - 47.986 \cdot \ln(T)) \cdot I^{0.5} + (-771.54 + 35474.0/T + 114.723 \cdot \ln(T)) \cdot I - 2698.0/T \cdot I^{1.5} + 1776.0/T \cdot I^2$	Dickson [1990]
pK_{P1}	$115.54 - 4576.752/T - 18.453 \cdot \ln(T) + (0.69171 - 106.736/T) \cdot S^{0.5} + (-0.01844 - 0.65643/T) \cdot S$	Yao & Millero [1995]
pK_{P2}	$172.1033 - 8814.715/T - 27.927 \cdot \ln(T) + (1.3566 - 160.340/T) \cdot S^{0.5} + (-0.05778 + 0.37335/T) \cdot S$	Yao & Millero [1995]
pK_{P3}	$-18.126 - 3070.75/T + (2.81197 + 17.27039/T) \cdot S^{0.5} + (-0.09984 - 44.99486/T) \cdot S$	Yao & Millero [1995]
$pK_{sp,calc}$	$-171.9065 - 0.077993 \cdot T + 2839.319/T + 71.595 \cdot \log(T) + (-0.77712 + 0.0028426 \cdot T + 178.34/T) \cdot S^{0.5} - 0.07711 \cdot S + 0.0041249 \cdot S^{1.5}$	Mucci [1983]
$pK_{sp,arag}$	$-171.945 - 0.077993 \cdot T + 2903.293/T + 71.595 \cdot \log(T) + (-0.068393 + 0.0017276 \cdot T + 88.135/T) \cdot S^{0.5} - 0.10018 \cdot S + 0.0059415 \cdot S^{1.5}$	Mucci [1983]
pK_{HS}	$225.838 - 13275.3/T - 34.6435 \cdot \ln(T) + 0.3449 \cdot S^{0.5} - 0.0274 \cdot S$	Millero [1988]
pK_{NH_4}	$-6285.33/T + 0.0001635 \cdot T - 0.25444 + (0.46532 - 123.7184/T) \cdot S^{0.5} + (-0.01992 + 3.17556/T) \cdot S$	Yao & Millero [1995]

Tab S2: Parameters used to calculate pressure corrections for apparent equilibrium constants in the default cGENIE carbonate system solver.

Constant	P1	P2	P3	P4	P5
K_1^*	-2.550E+1	+1.271E-1	+0.000E+0	-3.080E+0	+8.770E-2
K_2^*	-1.582E+1	-2.190E-2	+0.000E+0	+1.130E+0	-1.475E-1
K_B^*	-2.948E+1	+1.622E-1	+2.608E-3	-2.840E+0	+0.000E+0
K_W^*	-2.002E+1	+1.119E-1	-1.409E-3	-5.130E+0	+7.940E-2
$K_{HSO_4}^*$	-1.803E+1	+4.660E-2	+3.160E-4	-4.530E+0	+9.000E-2
K_{HF}^*	-9.780E+0	-9.000E-3	-9.420E-4	-3.910E+0	+5.400E-2
$K_{sp,cal}^*$	-4.876E+1	+5.304E-1	+0.000E+0	-1.176E+1	+3.692E-1
$K_{sp,arg}^*$	-4.596E+1	+5.304E-1	+0.000E+0	-1.176E+1	+3.692E-1
K_{P1}^*	-1.451E+1	+1.211E-1	-3.210E-4	-2.670E+0	+4.270E-2
K_{P2}^*	-2.312E+1	+1.758E-1	-2.647E-3	-5.150E+0	+9.000E-2
K_{P3}^*	-2.657E+1	+2.020E-1	-3.042E-3	-4.080E+0	+7.140E-2
$K_{H_2S}^*$	-1.107E+1	-9.000E-3	-9.420E-4	-2.890E+0	+5.400E-2
$K_{NH_4}^*$	-2.643E+1	+8.890E-2	-9.050E-4	-5.030E+0	+8.140E-2
K_{Si}^*	-2.948E+1	+1.622E-1	+2.608E-3	-2.840E+0	+0.000E+0

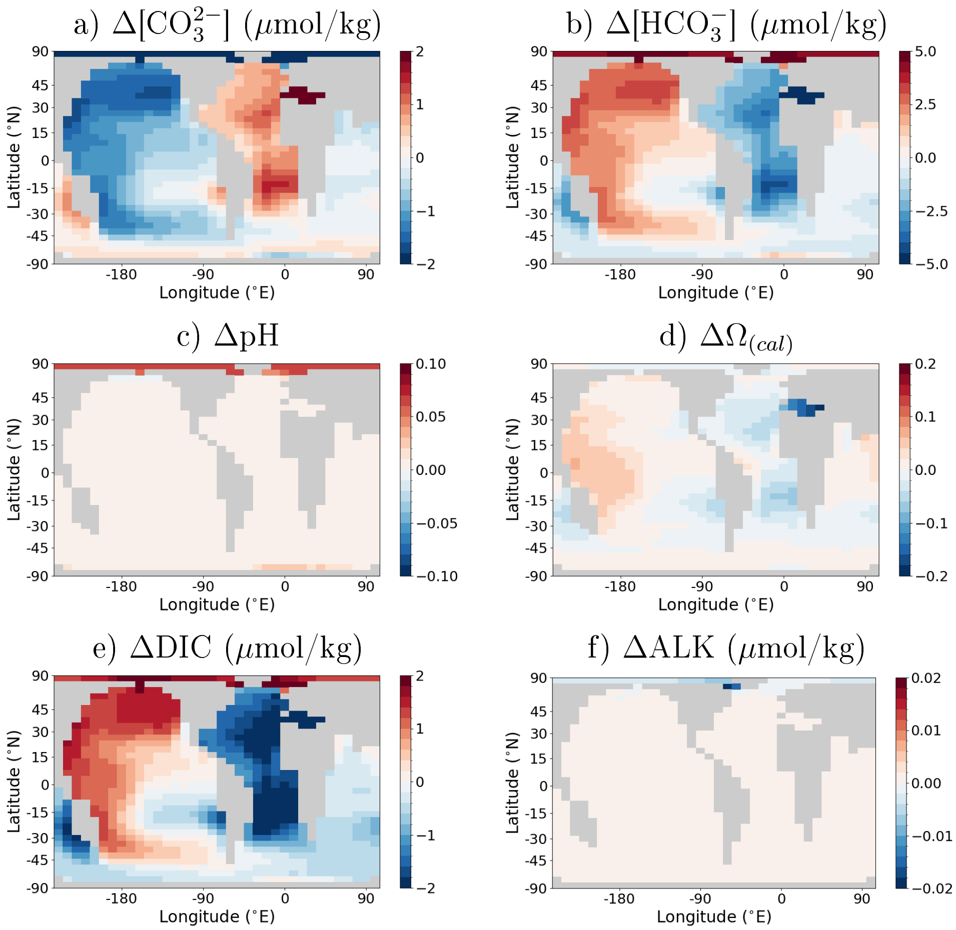

Fig. S1: Differences of the simulated carbonate system in the surface ocean between default cGENIE and cGENIE+MyAMI with pre-industrial Mg/Ca (simulations PI-C-ocean minus PI-B-ocean).

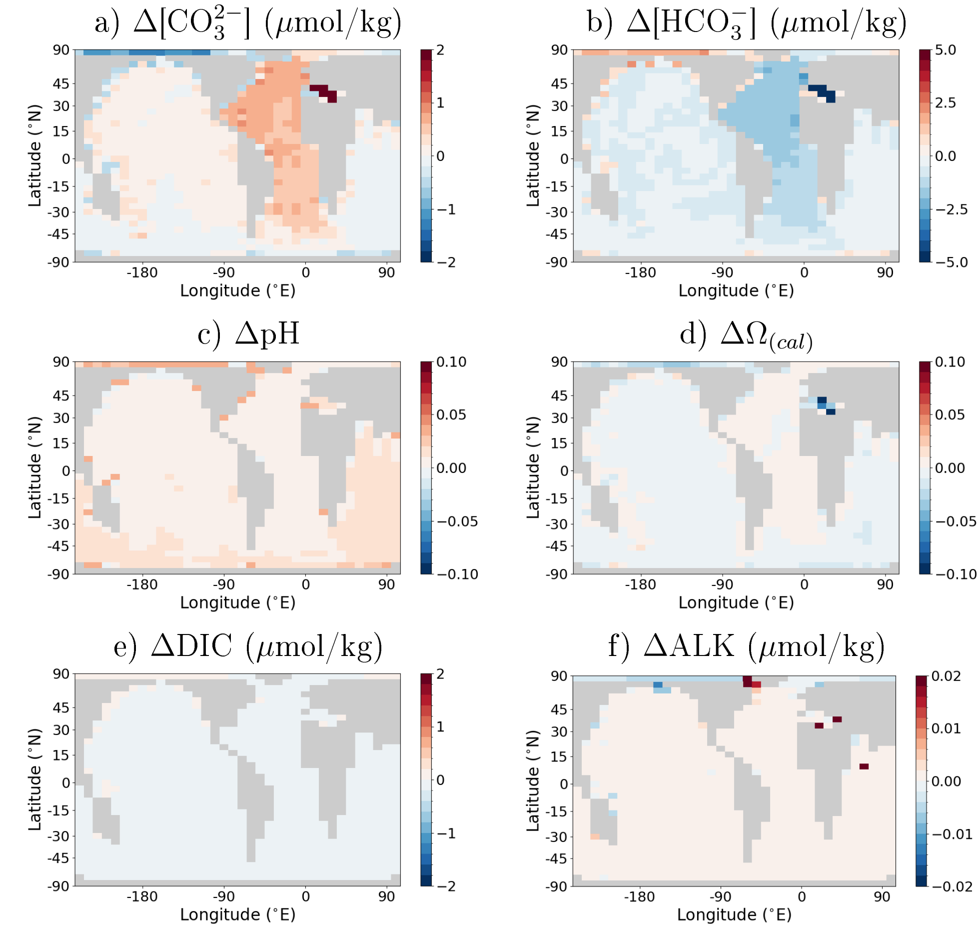

Fig. S2: Differences of the simulated carbonate system in the benthic ocean between default cGENIE and cGENIE+MyAMI with pre-industrial Mg/Ca (simulations PI-C-ocean minus PI-B-ocean).

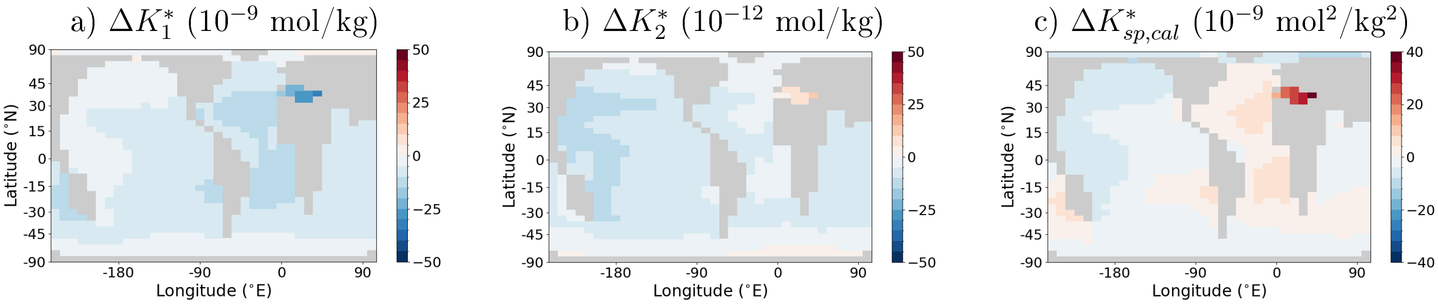

Fig. S3: Differences in K_1^*, K_2^*, $K_{sp,cal}^*$ and K_B^* between default cGENIE and cGENIE+MyAMI solutions for the pre-industrial carbonate system of the surface ocean with the same temperature limitations as those applied in default cGENIE (simulations PI-C2-ocean minus PI-B-ocean).

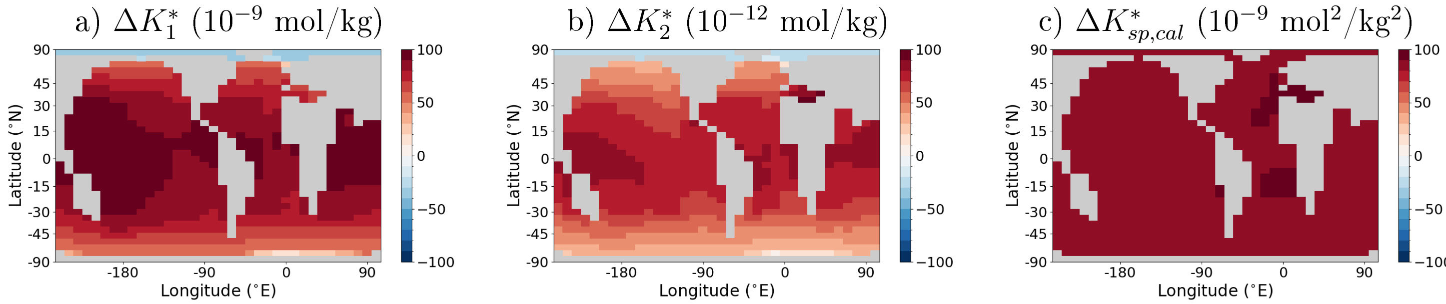

Fig. S4: Differences in K_1^*, K_2^*, $K_{sp,cal}^*$ and K_B^* between default cGENIE and cGENIE+MyAMI solutions for the carbonate system of the surface ocean with Eocene-like Mg/Ca (simulations EE-C-open minus EE-B-open).

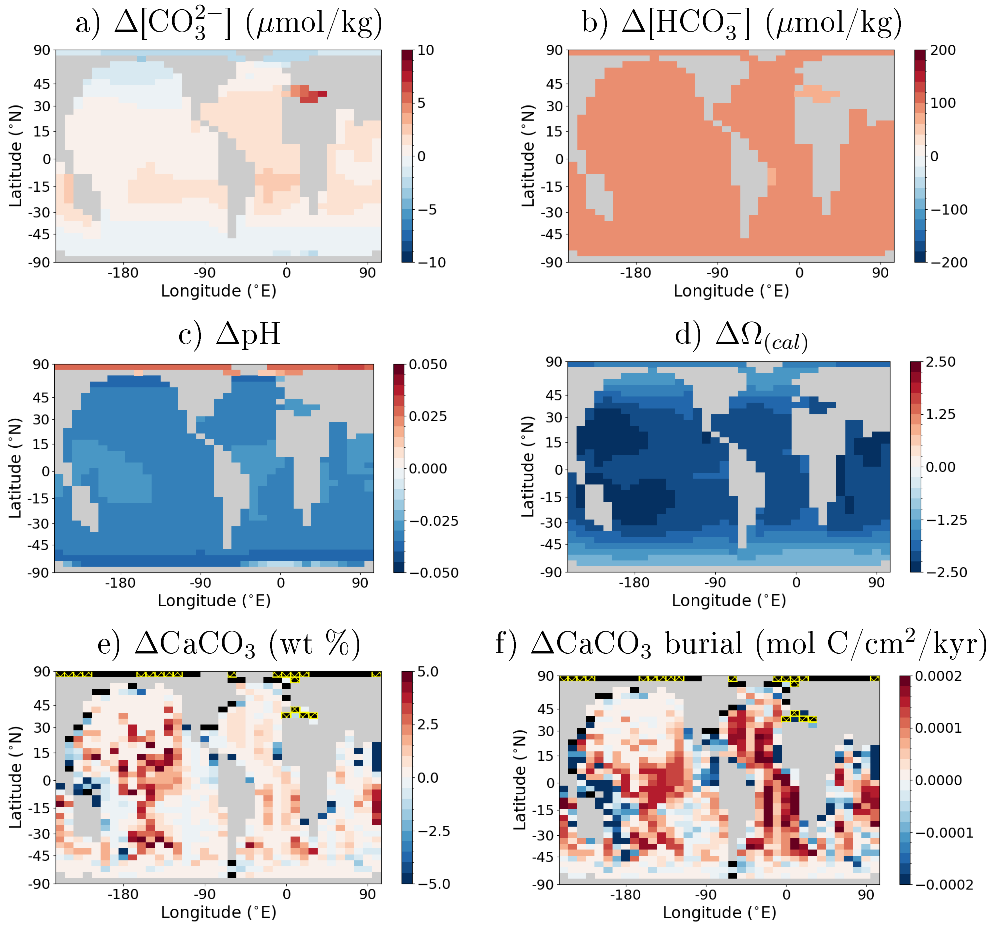

Fig. S5: Differences of the simulated carbonate system in the surface ocean, carbonate content in marine sediments and burial rates between cGENIE with default Mg/Ca corrections and cGENIE+MyAMI with Eocene-like Mg/Ca (simulations EE-C-open minus EE-B-open). A comparison of the respective absolute values in the two simulations is provided in Fig. S7 and spatial patterns of the absolute values in simulation EE-C-open are shown in Fig. S8. Pacific depth transects of these differences are shown in Fig. S6. Sediments shallower than 1000 m are masked in black and locations where the sedimentary carbonate system could not be solved dynamically and was instead replaced by a lookup table value is hatched in yellow.

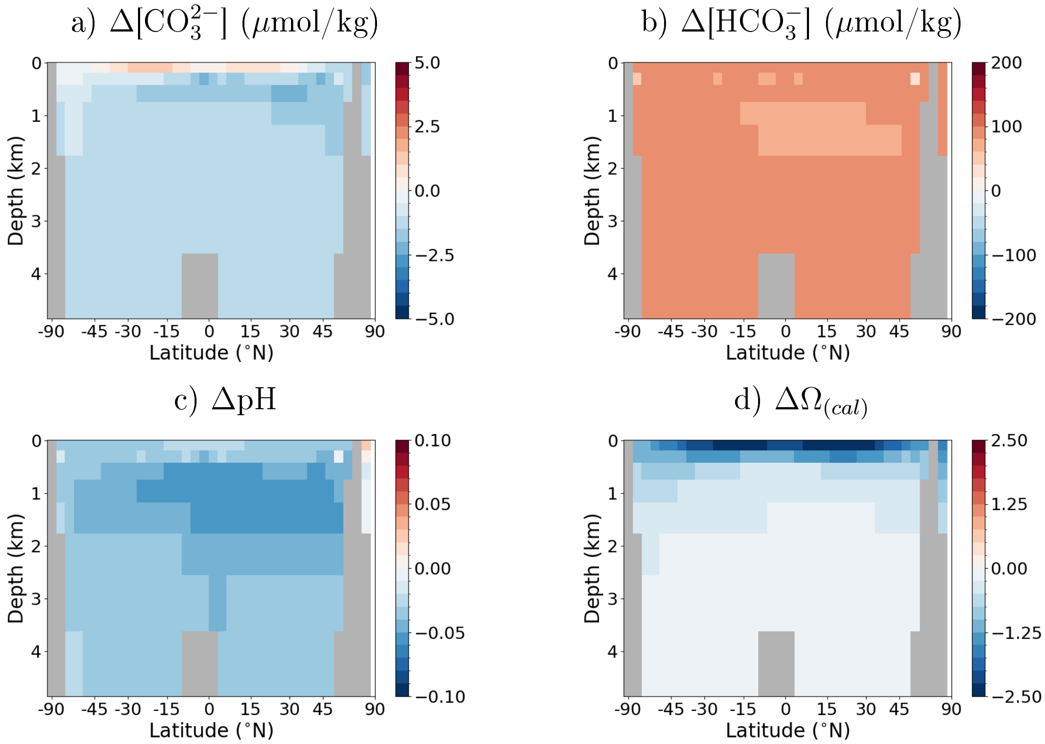

Fig. S6: Transects of differences of the simulated carbonate system between cGENIE with default Mg/Ca corrections and cGENIE+MyAMI with Eocene-like Mg/Ca (simulations EE-C-open minus EE-B-open) in the Pacific basin.

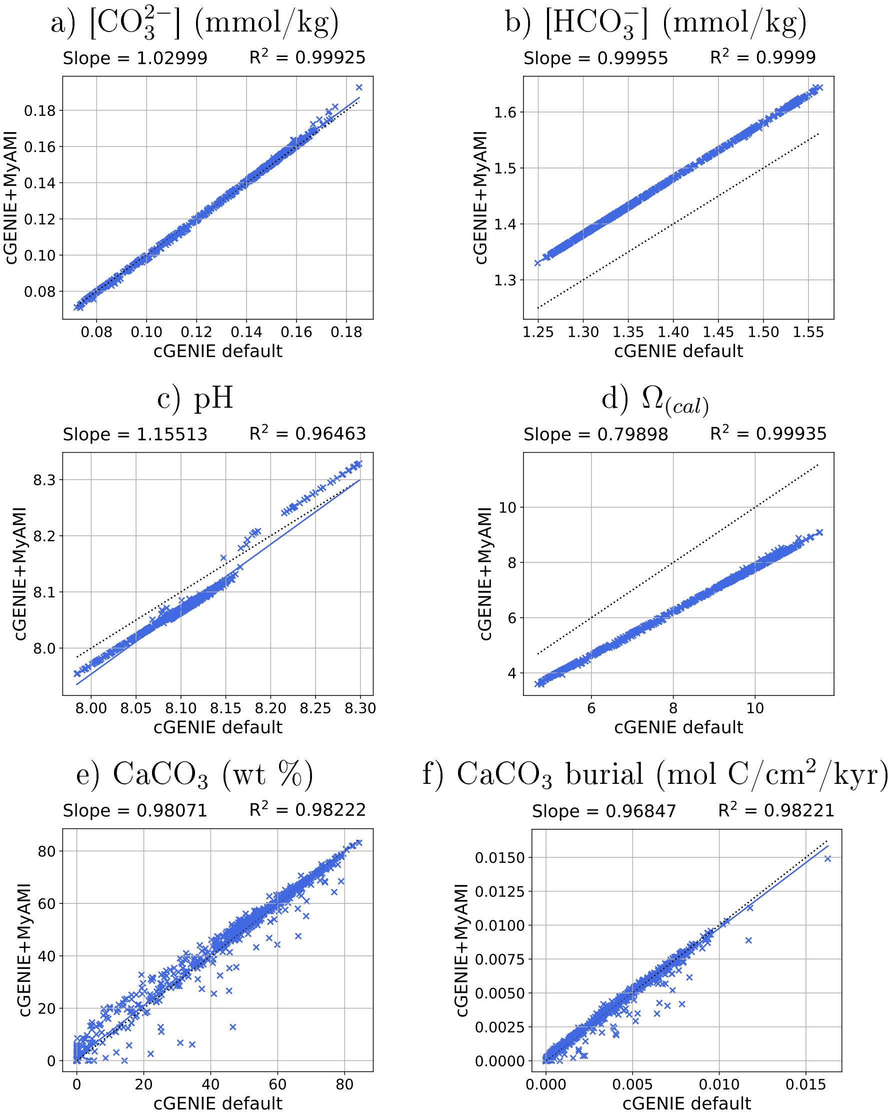

Fig. S7: Comparisons of absolute measures of the simulated carbonate system in the surface ocean, carbonate content in marine sediments and burial rates in simulations EE-B-open and EE-C-open.

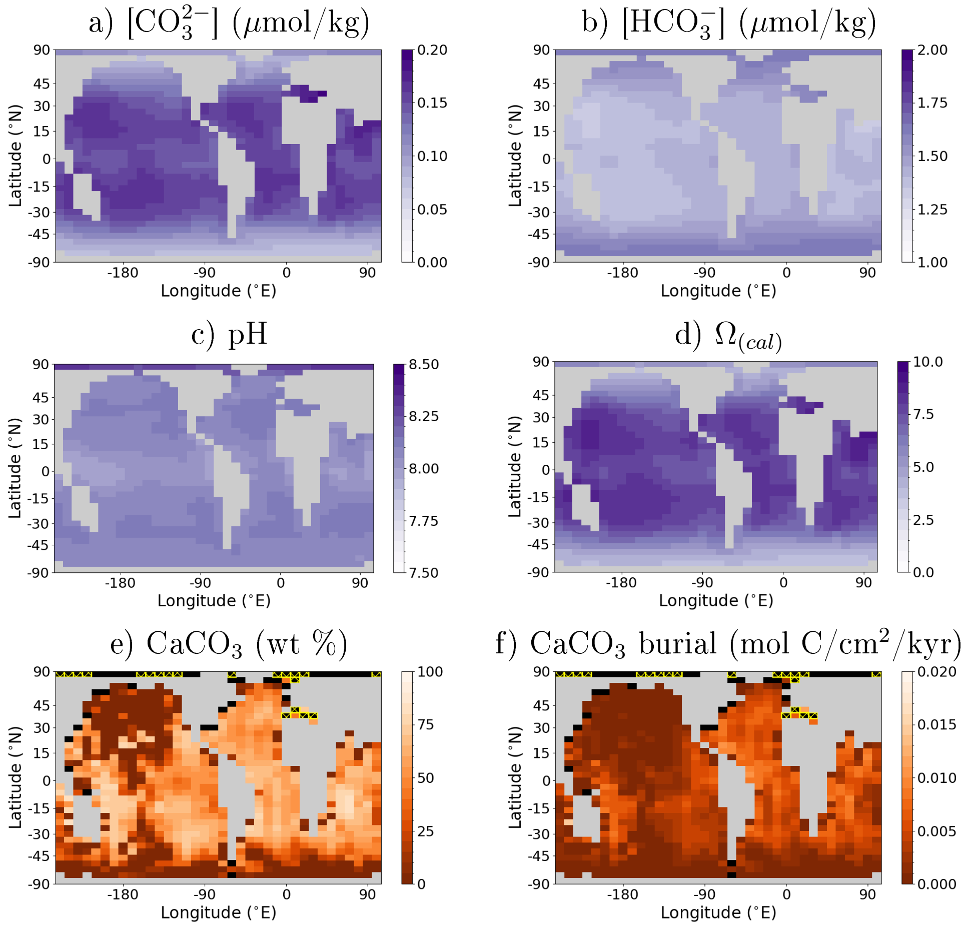

Fig. S8: Absolute measures of the simulated carbonate system in the surface ocean, carbonate content in marine sediments and burial rates in simulation EE-C-open. Sediments shallower than 1000 m are masked in black and locations where the sedimentary carbonate system could not be solved dynamically and was instead replaced by a lookup table value is hatched in yellow.

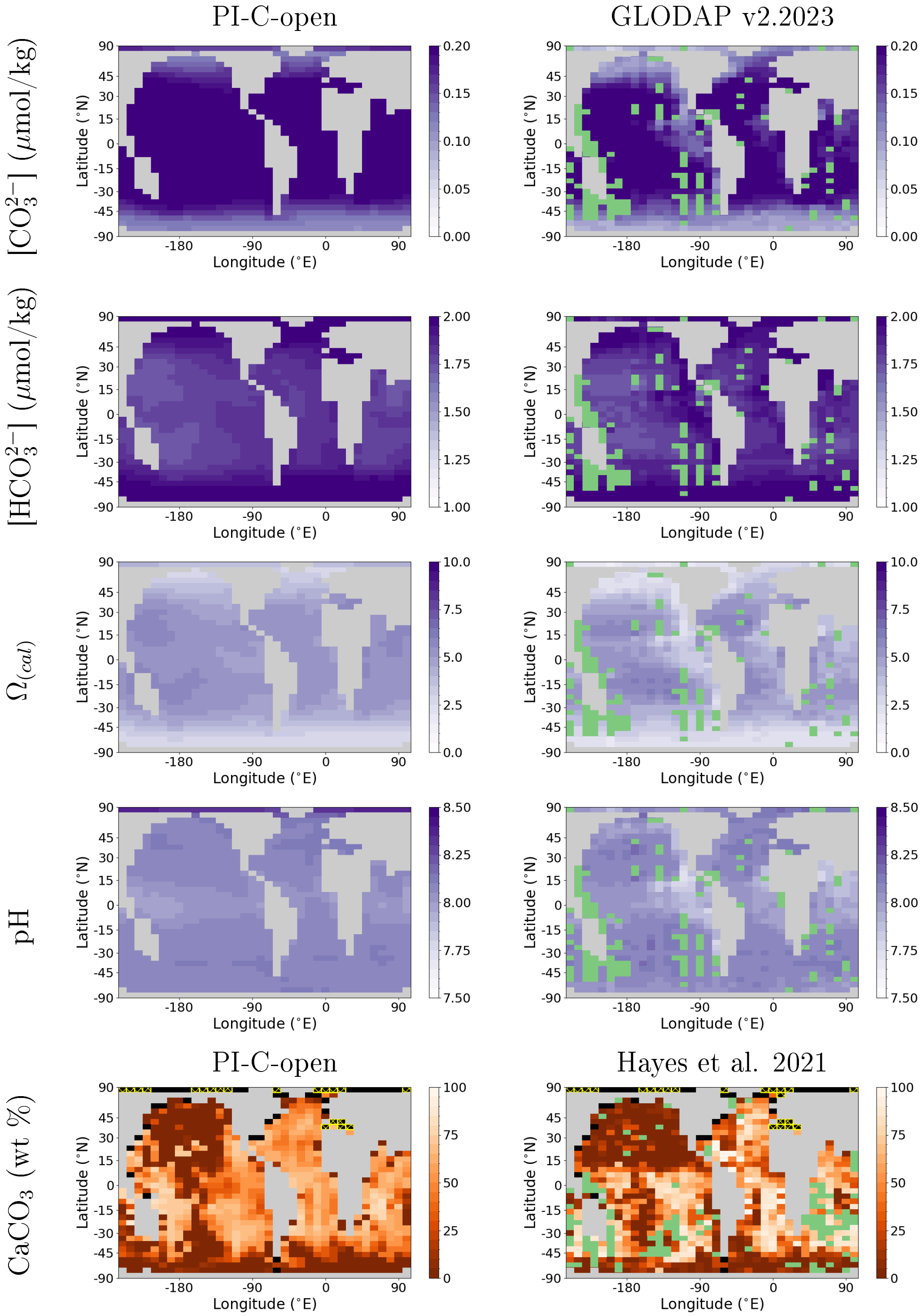

Fig. S9: Comparison of the simulated surface ocean carbonate system to variables calculated with PyCO2SYS (Humphreys et al. [2024]) from compiled observations in GLODAP v2.2023 (normalised to 2002, Olsen et al. [2016]) and carbonate content of marine sediments in simulation PI-C-open and the Holocene compilation from Hayes et al. [2021], all interpolated onto the cGENIE grid. Grid cells without observational data are marked in green. Sediments shallower than 1000 m are masked in black and locations where the sedimentary carbonate system could not be solved dynamically and was instead replaced by a lookup table value is hatched in yellow. The simulated carbonate system is the solution for the year 2002 in a historic simulation initialized with simulation PI-C-open and forced with CO_2 concentrations from Meinshausen et al. 2010. We note that the observations may contain seasonal signals that our annual means do not reflect and that the simulated sedimentary composition is the steady state solution after 100 kyr of equilibration time while less than 20 kyr have passed since the last major perturbation of real world sediments during the last deglaciation.

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