

## Supplementary Material



**Supplementary Figure 1.** Modeled CO<sub>2</sub> concentration at the cell surface as a function of cell diameter under low-CO<sub>2</sub> (LC) (blue) and high-CO<sub>2</sub> (HC) (red) conditions.



**Supplementary Figure 2.** Diel cycle of instantaneous maximal growth rate (blue line) of model phytoplankton cells as a result of changing light. The black dotted line represents the daily average maximal growth rate set by the model parameter  $g_0$ .



**Supplementary Figure 3.** The response of the modeled energy consumption for  $HCO_3^-$  acquisition to parameter changes as function of cell diameter. (A) Cell membrane permeability to  $CO_2$  (P) increases by 50%, and (B) CO<sub>2</sub> leakage fraction ( $l_k$ ) reduces by 50%. The energy for  $HCO_3^-$  acquisition is shown as the fraction of total cellular energy under the low-CO<sub>2</sub> (LC) (blue) and high-CO<sub>2</sub> (HC) (red) conditions, as well as the saved energy in  $HCO_3^-$  acquisition when the condition changed from LC to HC (black). The solid and dashed lines represent model results under the default and changed parameter values, respectively.



**Supplementary Figure 4.** Original reported experiment GRR and the GRR adjusted to the same CO<sub>2</sub>-enrichment factor of 2. The inset is zoomed in to a cell range of  $1-20 \ \mu m$ .



**Supplementary Figure 5.** Model experiments in which the daily maximal growth rate  $(g_0)$  decreases with cell size. (A) Modeled growth rate under the low-CO<sub>2</sub> (LC) (blue) and high-CO<sub>2</sub> (HC) (red) conditions, and (B) the corresponding growth rate response (GRR). The magenta dashed line and number in (B) represent the optimal cell diameter at peak GRR.



**Supplementary Figure 6.** Model experiments of extracellular carbonic anhydrase (eCA). (A) The modeled GRR with different eCA enhancement factors; note that the GRR lines approximately overlap when the cell size is smaller than 10  $\mu$ m. (B) The comparison of GRR between the standard model without eCA (black line) and the experiment (red line) using a linearly increasing eCA with cell size (see texts).



**Supplementary Figure 7.** Impact of diffusion coefficient (*D*) and combined rate constant (*k'*) on the model. (**A**) Model sensitivity tests of peak GRR (black) and optimal cell diameter ( $\mu$ m; blue) as a function of parameters of *D* and *k'* (see main text for its definition). (**B**) Modeled growth rate and (**C**) GRR versus cell size at 15 °C ( $D = 1.45 \times 10^3 \mu m^2 s^{-1}$ ,  $k' = 0.018 s^{-1}$ , according to Wolf-Gladrow and Riebesell 1997) and 25 °C ( $D = 1.45 \times 10^3 \mu m^2 s^{-1}$ ,  $k' = 0.018 s^{-1}$ , according to Wolf-Gladrow and Riebesell 1997). Blue and red lines in (**B**) are for low-CO<sub>2</sub> (LC) and high-CO<sub>2</sub> (HC) conditions.