Supplemental information to 'Quantifying the effect of salinity stratification on phytoplankton density patterns in estuaries'

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This document contains additional results of phytoplankton density (P) patterns for different boundary conditions and model parameters. In each experiment, one boundary condition or the value of one parameter is changed based on the setting of DF-W/DF-S (the default case for weakly/strongly stratified conditions). In all these experiments, Preaches equilibrium states within one week. Results are mainly presented by the values of ϕ_z and ϕ_x (defined in Eq. (20) and (21) of the main text), which quantify the overall vertical and along-estuary gradient of P at equilibrium, respectively.

⁸ S1 Setup of experiments

⁹ S1.1 Along-estuary turbulent diffusivity

A spatially constant longitudinal turbulent diffusivity κ_h was used in DF-W and DF-S. 10 To examine the influence of the magnitude of κ_h on the values of ϕ_z and ϕ_x , experiments 11 were conducted with the value of κ_h being halved and doubled, respectively, with respect 12 to that of default cases. Moreover, experiments were further carried out with along-13 estuary varying κ_h , as shown in Fig. S1, to investigate the influence of the shape of 14 κ_h on P pattern. Here, the values of κ_h were derived from the data of MacCready 15 and Banas (2011), in which κ_h was treated as a fitting parameter to obtain the best 16 representation of the measured tidal salt transport. Note that the data in MacCready 17 and Banas (2011) are only available in the area $0 \le x \le 30$ km. In this area, the profiles 18

were obtained by interpolating the data (open circles) of MacCready and Banas (2011). 19 In the area $30 < x \leq 45$ km, the values of κ_h were obtained by extrapolating the data 20 of MacCready and Banas (2011) with the constraint that $\kappa_h|_{x=45 \text{ km}} = 2600 \text{ m}^2 \text{ s}^{-1}$. 21 Here, the value $\kappa_h|_{x=45 \text{ km}} = 2600 \text{ m}^2 \text{ s}^{-1}$ is chosen such that the along-estuary diffusive 22 length scale $\sqrt{\kappa_h/\mu_{max}}$ is shorter than 15 km. This choice guarantees that the spatial 23 distribution of P in $0 \le x \le 30$ km (within which area P patterns are presented and field 24 data are available) is determined by internal dynamics rather than riverine boundary 25 conditions. 26

$\mathbf{S1.2}$ Tidally-averaged friction velocity and parameter A_S

In both DF-W and DF-S, the same value of the tidally-averaged friction velocity u_* was 28 used as input in Eq. (8) for vertical eddy viscosity A_v . To investigate the sensitivity 29 of the values of ϕ_z and ϕ_x to the value of this parameter, experiments were conducted 30 with u_* reduced by a factor of 0.8 and increased by a factor of 1.2, respectively, with 31 respect to its default value. The reason that u_* was not halved or doubled, as was done 32 to other parameters, is because the amplitude of the density-driven flow u_d is inversely 33 proportional to the overall intensity of A_v (see Eq. (3) and (4)). Halving u_* results in the 34 magnitude of the subtidal current to be above 1 m s^{-1} under both weakly and strongly 35 stratified conditions, which is unrealistic. 36

In the default cases DF-W and DF-S, the values of parameter A_S , which is proportional to the values of A_v and vertical eddy diffusivity κ_v at the water surface, has been tuned such that the amplitude and vertical structure of subtidal current are comparable to the field data of Chawla et al. (2008). Experiments were carried out with the value of A_S halved and doubled, respectively, with respect to those in the default cases.

42 S1.3 Bottom roughness length and river flow

The amplitude of the subtidal current decreases with increasing bottom roughness length z_0 . The depth-averaged river flow U_r represents the river discharge, whose time series exhibit fluctuations as shown in Roegner et al. (2011). Here, experiments were conducted with the value of these two parameters halved and doubled, respectively, with respect to those in the default cases.

⁴⁸ S1.4 Boundary conditions at the estuary mouth, phytoplankton and ⁴⁹ nutrient availability at the riverine boundary

In the default cases DF-W and DF-S, zero diffusive flux conditions have been imposed for P and N at the estuary mouth x = 0 (see Eq. (19)). A zero diffusive flux condition forces the along-estuary advection term to become zero at x = 0, as is shown in Fig. 8(g) and 8(h). To investigate the impact of this boundary condition on the values of ϕ_z and ϕ_x , experiments were conducted with the second derivatives of P and N with respect to x being zero at x = 0:

$$\frac{\partial^2 P}{\partial x^2}\Big|_{x=0} = 0, \quad \frac{\partial^2 N}{\partial x^2}\Big|_{x=0} = 0.$$
(S1)

To examine the influence of riverine phytoplankton and nutrient availability on the values of ϕ_z and ϕ_x , the density $P|_{x=L}$ and the nutrient concentration $N|_{x=L}$ at the riverine boundary x = L were halved and doubled, respectively, with respect to their values in default cases.

⁶⁰ S1.5 Parameters related to the loss rate, other than m_0

In the main text, the sensitivity of the values of ϕ_z and ϕ_x to the value of loss rate m_0 of phytoplankton in salt water, which parameterises the osmotic stress, has been presented and discussed. Here, sensitivity experiments concerning the other parameters in the parameterisation of the specific loss rate m (see Eq. (17)) are carried out. Specifically, The values of m_L (the value of loss rate of phytoplankton in fresh water), s_c (the salinity where $m = (m_0 + m_L)/2$) and s_δ (the salinity scale over which m varies) are halved and doubled, respectively, with respect to their values in default cases.

S1.6 Parameters that are not related to the loss rate in the biological module

The sensitivity of the values of ϕ_z and ϕ_x pattern to other biological parameters was 70 investigated. To be specific, values of the following parameters were both halved and 71 doubled with respect to those of default cases: the sinking velocity v of phytoplankton, 72 the maximum specific growth rate μ_{max} of phytoplankton, the half-saturation constant 73 of nutrient-limited growth H_N , the half-saturation constant of light-limited growth H_I , 74 the light extinction coefficient k_{bg} due to background turbidity, the incident light inten-75 sity I_{in} , the light absorption coefficient k of phytoplankton, the nutrient amount α in 76 each phytoplankton cell and the proportion ϵ of respired/grazed phytoplankton that is 77 subsequently recycled. 78

⁷⁹ S1.7 Effect of net growth of phytoplankton on *P* patterns

Finally, experiments were carried out in which the net growth of phytoplankton is completely switched off, that is, $(\mu - m) = 0$. These experiments were designed to test whether it is appropriate to treat phytoplankton as a tracer.

83 S2 Results and discussion

⁸⁴ S2.1 Along-estuary turbulent diffusivity

Figure S2 shows the values of ϕ_z and ϕ_x for different values of spatially constant alongestuary turbulent diffusivity κ_h and for the along-estuary varying $\kappa_h = \kappa(x)$ (whose profiles are plotted in Fig. S1). Under weakly stratified conditions, ϕ_z hardly changes and ϕ_x slightly decreases with the magnitude of κ_h . This is because the along-estuary turbulent diffusion positively contributes to the accumulation rate of P in the lower reach (0 < x < 10 km), as is shown in Fig. 9(a). Thus, P in the lower reach increases with κ_h , and ϕ_x decreases accordingly.

Similarly, under strongly stratified conditions, ϕ_x slightly decreases with the magnitude of κ_h . However, the range over which ϕ_x varies is smaller compared to that during strong stratification because the along-estuary turbulent diffusion term is small, as is shown in Fig. 9(b).

⁹⁶ When the along-estuary varying κ_h , which exhibits substantial fluctuations along ⁹⁷ the estuary (Fig. S1), is employed, ϕ_x slightly increases under both weakly and strongly ⁹⁸ stratified conditions. This is because the along-estuary diffusive transport is much weaker ⁹⁹ than the longitudinal advective transport induced by subtidal current, as is discussed in ¹⁰⁰ Section 4.1.

¹⁰¹ S2.2 Tidally-averaged friction velocity and parameter A_S

The values of ϕ_z and ϕ_x for different values of tidally-averaged friction velocity u_* and for different values of parameter A_S are shown in Fig. S3(a) and S3(b), respectively. If u_* is increased, the intensity of turbulence is increased. When the value of parameter A_S is increased, the values of vertical eddy viscosity and eddy diffusivity in the upper layer increases. Both the above changes amplify the negative contribution of the vertical turbulent diffusion to the accumulation rate of P in the upper layer, as is discussed in ¹⁰⁸ Section 4.2.2. Thus, the values of ϕ_z decrease and those of ϕ_x increase.

¹⁰⁹ S2.3 Bottom roughness length and river flow

Figure S4(a) shows values of ϕ_z and ϕ_x for different values of the bottom roughness 110 length z_0 . Under both weakly and strongly stratified conditions, the values of ϕ_z and 111 ϕ_x hardly change with z_0 because halving or doubling the value of z_0 with respect to 112 its default value causes only small changes in the amplitude of the subtidal current. 113 Figure S4(b) shows values of ϕ_z and ϕ_x for different depth-averaged velocities U_r of river 114 flow. During both weak and strong stratification, the value of ϕ_x decreases with increas-115 ing U_r because elevated U_r results in shorter time for phytoplankton being advected to 116 the estuary mouth. Under strongly stratified conditions, the value of ϕ_z increases with 117 increasing U_r because phytoplankton in the upper layer is subject to shorter period of 118 sinking processes, as is discussed in Section 4.2.1. 119

S2.4 Boundary conditions at the estuary mouth, phytoplankton and nutrient availability at the riverine boundary

Figure S5(a) contains values of ϕ_z and ϕ_x for the experiments in which the second 122 derivatives of P and N with respect to x vanish at the estuary mouth (see Eq. (S1)) 123 and for those where zero along-estuary diffusive fluxes of P and N are imposed at the 124 seaward boundary (see Eq. (19) for the default cases DF-W and DF-S). Under weakly 125 stratified conditions, when Eq. (S1) is used, the value of ϕ_x slightly decreases compared 126 to that for DF-W. This is because in the former case, the positive contribution of the 127 along-estuary advection of P by subtidal current extends to the seaward boundary. As 128 a result, P in the vicinity of the estuary mouth increases and the value of ϕ_x therefore 129 decreases. During strong stratification, when Eq. (S1) is used, the value of ϕ_z slightly 130 increases. This is because the positive contribution of the along-estuary advection term 131 leads to the increase of P at the vicinity of the seaward boundary. However, the increase 132

of P in the upper layer is much larger than that in the lower layer due to loss and sinking processes in the aphotic zone. Hence, the difference of P between the upper and the lower layer, as is measured by ϕ_z , is larger than that for DF-S.

Figure S5(b) shows values of ϕ_z and ϕ_x for different imposed values of phytoplankton 136 density $P|_{x=L}$ at the riverine boundary. Under strongly stratified conditions, the value of 137 ϕ_z decreases and that of ϕ_x increases with $P|_{x=L}$. As $P|_{x=L}$ increases, P in the interior 138 of the estuary increases. Since high values of P occur in the upper layer during strong 139 stratification, light is more limited for phytoplankton growth for larger $P|_{x=L}$. Hence, the 140 specific net growth rate $(\mu - m)$ of phytoplankton in the upper layer generally decreases 141 with increasing $P|_{x=L}$. As a result, P in the upper layer decreases, and accordingly the 142 value of ϕ_z decreases with $P|_{x=L}$. Moreover, a decrease of $(\mu - m)$ further results in a 143 faster decrease of P towards the estuary mouth, which leads to an increase of ϕ_x . Under 144 weakly stratified conditions, the values of ϕ_z and ϕ_x hardly vary with $P|_{x=L}$. This is 145 because P is vertically almost uniformly distributed rather than concentrated in the 146 upper layer. Consequently, $(\mu - m)$ in the upper layer is hardly affected by the changes 147 of light intensity due to varied $P|_{x=L}$ compared to that for strongly stratified conditions. 148 Figure S5(c) shows the values of ϕ_z and ϕ_x for different imposed nutrient concentra-149 tions $N|_{x=L}$ at the riverine boundary. Under strongly stratified conditions, the value of 150 ϕ_z increases and that of ϕ_x decreases with $N|_{x=L}$. Similar to the spatial distribution of 151 P at equilibrium, that of N (Fig. S6(b)) also shows a two-layer structure. In the upper 152 layer, N is lower than $N|_{x=L}$ and generally decreases towards the estuary mouth due 153 to consumption by phytoplankton. In the lower layer, N is much larger than $N|_{x=L}$ 154 due to recycling of nutrient in dead phytoplankton cells. The N pattern indicates that 155 nutrients are not efficiently exchanged between the upper and the lower layer. Hence, if 156 the riverine nutrient availability is elevated, N in the upper layer in the interior of the 157 estuary increases. As a result, $(\mu - m)$ in the upper layer becomes larger, which leads to 158 an increase of ϕ_z and decrease of ϕ_x , as is discussed in the previous paragraph. Under 159

weakly stratified conditions, the values of ϕ_z and ϕ_x hardly vary with $N|_{x=L}$. This is because during weak stratification, N is vertically mixed and generally increases towards the estuary mouth (see Fig. S6(a)), which indicates that N is sufficient for phytoplankton growth. Thus, increasing $N|_{x=L}$ results in little changes in $(\mu - m)$ and therefore negligible changes in the values of ϕ_z and ϕ_x .

165 S2.5 Parameters related to the loss rate, other than m_0

Figure S7(a) shows the values of ϕ_z and ϕ_x for different values of the loss rate m_L of phy-166 toplankton in fresh water. Under strongly stratified conditions, the value of ϕ_z decreases 167 and that of ϕ_x increases with increasing m_L . Values of P in the upper layer decrease 168 with increasing m_L because an increase of the latter parameter results in a decrease of 169 the net specific growth rate $(\mu - m)$ in the surface fresh water. As a consequence, ϕ_z 170 decreases. The decreased $(\mu - m)$ in the surface fresh water further causes an increase 171 of ϕ_x , as is discussed in Section S2.4. Under weakly stratified conditions, ϕ_z and ϕ_x 172 hardly change with m_L . This is because m_L affect the loss rate in the fresh water area 173 is $27 \le x \le 45$ km, whereas ϕ_z and ϕ_x quantify the characteristics of P pattern in the 174 area $0 \le x \le 30$ km. 175

Figure S7(b) and S7(c) show the values of ϕ_z and ϕ_x for different values of s_c and s_{δ} , respectively. As s_c increases, for both weak and strong stratification, the value of ϕ_z hardly changes and that of ϕ_x slightly decreases. The changes in ϕ_x are because higher s_c values lead to smaller areas of high loss rates (see Eq. (17)), which results in less loss of P as phytoplankton are transported through the domain. The values of ϕ_z and ϕ_x hardly change for different values of s_{δ} within the range explored in this study.

¹⁸² S2.6 Biological parameters that are not related to the loss rate

Figure S8 shows the values of ϕ_z and ϕ_x for different sinking velocity v of phytoplankton. Under strongly stratified conditions, the value of ϕ_z decreases and that of ϕ_x increases

with increasing v. An increased v leads to the decrease of P in the upper layer, as 185 is illustrated by Fig. 8(h) and discussed in Section 4.1, and ϕ_z therefore decreases. 186 Furthermore, along the estuary, P decreases faster towards the estuary mouth due to 187 sinking processes, which results in the increase of ϕ_x . In the case of weakly stratified 188 conditions, the ranges over which ϕ_z and ϕ_x vary are much smaller. This is because the 189 sinking of phytoplankton has little impact if the vertical turbulent mixing is strong, as 190 illustrated by Fig. 8(g). Note that ϕ_z falls below zero for $v = 2 \text{ m day}^{-1}$, that is P at 191 the estuary mouth attains higher values in the lower layer than in the upper layer. 192

Figure S9(a) shows the values of ϕ_z and ϕ_x for different values of maximum specific growth rate μ_{max} . As defined in Eq. (15), the specific growth rate μ of phytoplankton increases with μ_{max} . Thus, according to the discussion in Section S2.4, ϕ_z increases and ϕ_x decreases with μ_{max} under both weakly and strongly stratified conditions.

Figures S9(b) and S9(c) show the values of ϕ_z and ϕ_x for different values of halfsaturation constant of nutrient-limited growth H_N and half-saturation constant of lightlimited growth H_I , respectively. By increasing H_N (H_I), the specific growth rate μ of phytoplankton decreases. As a result, when increasing H_N (H_I), P patterns behave similar as those for decreasing μ .

The light extinction coefficient k_{bq} due to background turbidity and incident light 202 intensity I_{in} are two parameters that influence light intensity in the water column. 203 Fig. S10(a) shows the values of ϕ_z and ϕ_x for different values of k_{bg} . As k_{bg} increases, 204 underwater light intensity decreases, which results in a decrease of the net specific growth 205 rate $(\mu - m)$. Accordingly, under both weakly and strongly stratified conditions, ϕ_z 206 decreases and ϕ_x increases with k_{bg} , as discussed in Section S2.4. Similar to a increase 207 in k_{bg} , a decrease in incident light intensity I_{in} also cause stronger limitation on the 208 growth of phytoplankton. Accordingly, ϕ_z decreases and ϕ_x increases with I_{in} , as is 209 shown in Fig. S10(b). 210

Figure S10(c) contains the values of ϕ_z and ϕ_x for different light absorption coefficient

²¹² k of phytoplankton. Similar to increasing background turbidity k_{bg} , increasing k also ²¹³ leads to decrease of light intensity in the water column. Thus, ϕ_z decreases and ϕ_x ²¹⁴ increases with k.

Figure S11(a) and S11(b) show the values of ϕ_z and ϕ_x for different nutrient amount α 215 in each phytoplankton cell and nutrient recycling coefficient ϵ , respectively. Clearly, both 216 ϕ_z and ϕ_x hardly change with either α or ϵ . This is because during weak stratification, 217 the values of ϕ_z and ϕ_x are not sensitive to the changes of nutrient concentration N, 218 as is illustrated by Fig. S5(c) and discussed in Section S2.4. Under strongly stratified 219 conditions, for different values of α or ϵ used in this study, the values of N in the upper 220 layer changes in a small range such that the net specific growth rate $(\mu - m)$ is hardly 221 affected. 222

223 S2.7 Effect of net growth of phytoplankton on P patterns

Figure S12 shows the spatial distribution of P at equilibrium for the experiment in which the net growth of phytoplankton is switched off, i.e., $(\mu - m) = 0$. Clearly, under both weakly and strongly stratified conditions, P values are high in the domain and they increases towards the bottom. These patterns are markedly different from those of the default cases DF-W and DF-S, as well as from the observed P patterns shown by Roegner et al. (2011).

230 **References**

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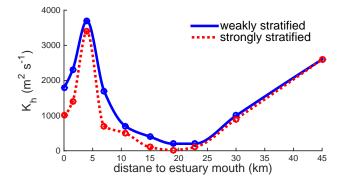


Figure S1: The along-estuary profiles of along-estuary turbulent diffusivity κ_h for weakly stratified conditions (solid line) and strongly stratified conditions (dotted line). In the area $0 \le x \le 30$ km, the profiles were obtained by interpolating the data (open circles) of MacCready and Banas (2011). In the area $30 < x \le 45$ km, the profiles were obtained by exterpolating the data of MacCready and Banas (2011) with the constraint that $\kappa_h|_{x=45 \text{ km}} = 2600 \text{ m}^2 \text{ s}^{-1}$

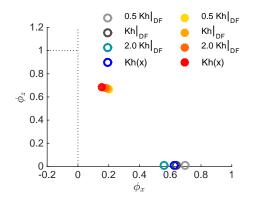


Figure S2: Scatter plot of ϕ_z and ϕ_x for different values of spatially constant alongestuary turbulent diffusivity κ_h , and also for along-estuary varying κ_h as shown in Fig. S1. Here, open circles indicate results for weakly stratified conditions, whereas full circles represent results for strongly stratified conditions.

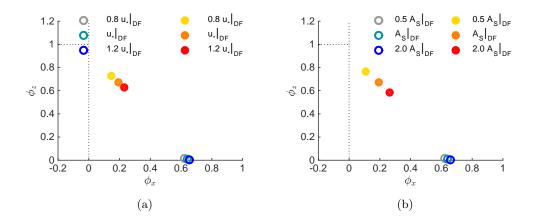


Figure S3: As Fig. S2, but (a) for different values of the tidally averaged friction velocity u_* and (b) for different values of parameter A_S (that is proportional to the values of vertical eddy viscosity and eddy diffusivity at the water surface)

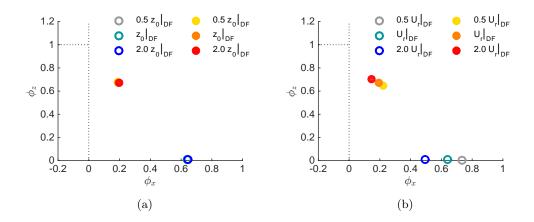


Figure S4: As Fig. S2, but (a) for different values of the bottom roughness length z_0 and (b) for different values of depth-averaged velocity U_r of river flow

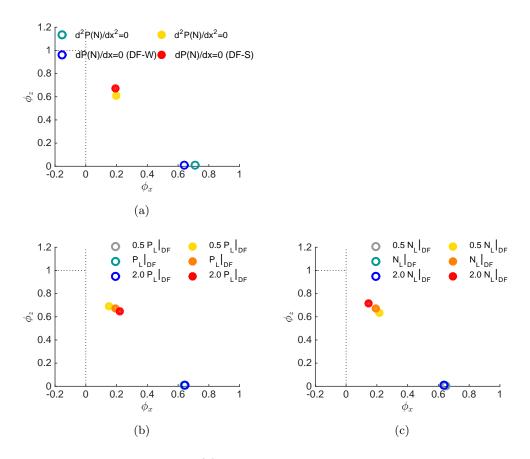


Figure S5: As Fig. S2, but (a) for different boundary conditions of P and N at the estuary mouth x = 0, (b) for different values of phytoplankton density $P|_{x=L}$ at the riverine boundary x = L and (c) for different values of nutrient concentration $N|_{x=L}$ at x = L

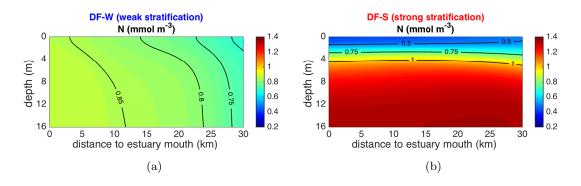


Figure S6: (a), (b): Spatial distribution of nutrient concentration N at equilibrium for DF-W and DF-S, respectively

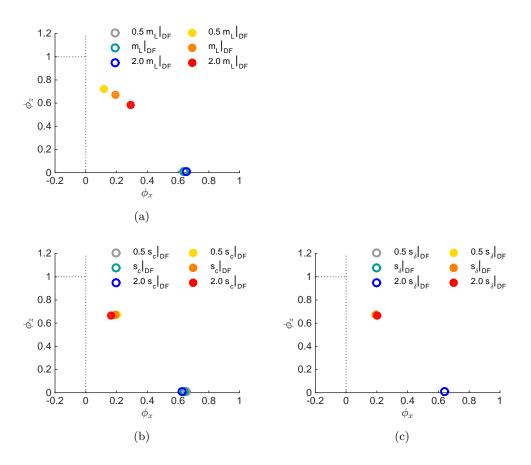


Figure S7: As Fig. S2, but (a) for different values of the loss rate m_L of phytoplankton in fresh water, (b) for different values of s_c (the salinity at which $m = (m_0 + m_L)/2$) and (c) for different values of s_δ (the salinity scale over which m varies)

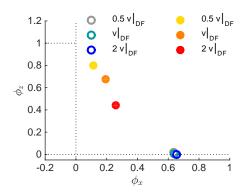


Figure S8: As Fig. S2, but for different values of the sinking velocity v of phytoplankton

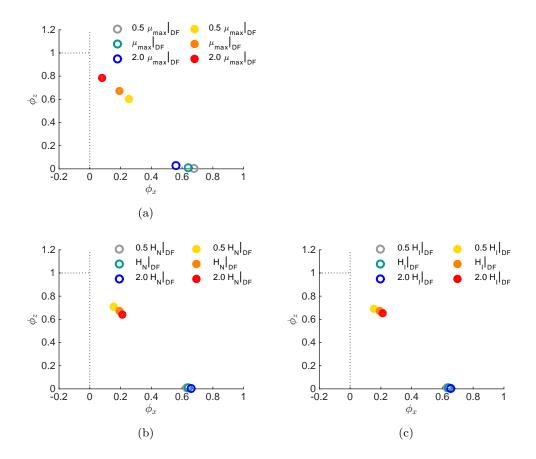


Figure S9: As Fig. S2, but (a) for different values of the maximum specific growth rate μ_{max} of phytoplankton, (b) for different values of the half-saturation constant H_N of nutrient-limited growth and (c) for different values of the half-saturation constant H_I of nutrient-limited growth

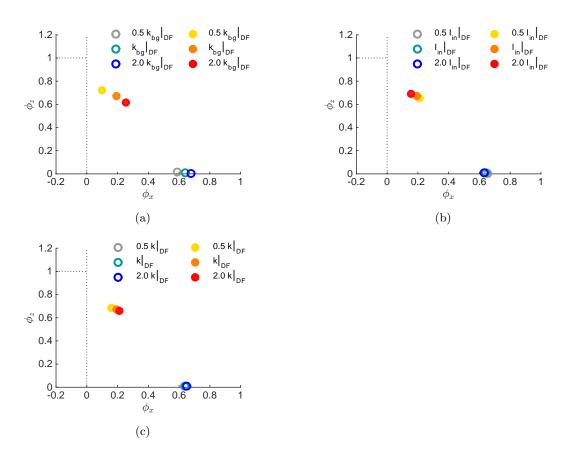


Figure S10: As Fig. S2, but (a) for different values of the light extinction coefficient k_{bg} due to background turbidity, (b) for different values of the incident light intensity I_{in} and (c) for different values of the light absorption coefficient k of phytoplankton

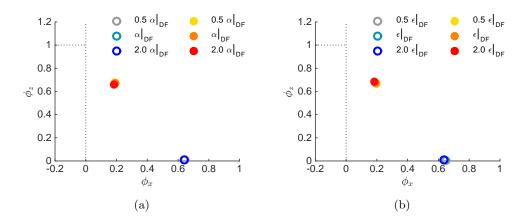


Figure S11: As Fig. S2, but (a) for different values of the nutrient amount α in each phytoplankton cell and (b) for different values of the nutrient recycling coefficient ϵ

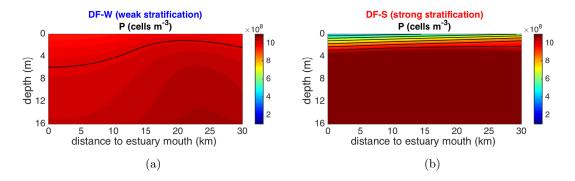


Figure S12: Spatial distributions of phytoplankton density P at equilibrium for the experiments, in which the net growth of phytoplankton is switched off, that is $(\mu - m) = 0$, under (a) weakly stratified conditions and (b) strongly stratified conditions