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, $P$ reaches equilibrium states within one week. Results are mainly presented by the values of $\phi_z$ and $\phi_x$ (defined in Eq. (20) and (21) of the main text), which quantify the overall vertical and along-estuary gradient of $P$ at equilibrium, respectively.

S1 Setup of experiments

S1.1 Along-estuary turbulent diffusivity

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

In the area $30 < x \leq 45$ km, the values of $\kappa_h$ were obtained by extrapolating the data of MacCready and Banas (2011) with the constraint that $\kappa_h|_{x=45 \text{ km}} = 2600 \text{ m}^2 \text{ s}^{-1}$.

Here, the value $\kappa_h|_{x=45 \text{ km}} = 2600 \text{ m}^2 \text{ s}^{-1}$ is chosen such that the along-estuary diffusive length scale $\sqrt{\kappa_h/\mu_{max}}$ is shorter than 15 km. This choice guarantees that the spatial distribution of $P$ in $0 \leq x \leq 30$ km (within which area $P$ patterns are presented and field data are available) is determined by internal dynamics rather than riverine boundary conditions.

### 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 used as input in Eq. (8) for vertical eddy viscosity $A_v$. To investigate the sensitivity of the values of $\phi_z$ and $\phi_x$ to the value of this parameter, experiments were conducted with $u_*$ reduced by a factor of 0.8 and increased by a factor of 1.2, respectively, with respect to its default value. The reason that $u_*$ was not halved or doubled, as was done to other parameters, is because the amplitude of the density-driven flow $u_d$ is inversely proportional to the overall intensity of $A_v$ (see Eq. (3) and (4)). Halving $u_*$ results in the magnitude of the subtidal current to be above 1 m s$^{-1}$ under both weakly and strongly stratified conditions, which is unrealistic.

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 $\kappa_v$ 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.
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.

S1.4 Boundary conditions at the estuary mouth, phytoplankton and 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 $\phi_z$ and $\phi_x$, experiments were conducted with the second derivatives of $P$ and $N$ with respect to $x$ being zero at $x = 0$:

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

To examine the influence of riverine phytoplankton and nutrient availability on the values of $\phi_z$ and $\phi_x$, 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.

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

In the main text, the sensitivity of the values of $\phi_z$ and $\phi_x$ 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 $\phi_z$ and $\phi_x$ pattern to other biological parameters was investigated. To be specific, values of the following parameters were both halved and doubled with respect to those of default cases: the sinking velocity $v$ of phytoplankton, the maximum specific growth rate $\mu_{max}$ of phytoplankton, the half-saturation constant of nutrient-limited growth $H_N$, the half-saturation constant of light-limited growth $H_I$, the light extinction coefficient $k_{bg}$ due to background turbidity, the incident light intensity $I_{in}$, the light absorption coefficient $k$ of phytoplankton, the nutrient amount $\alpha$ in each phytoplankton cell and the proportion $\epsilon$ of respired/grazed phytoplankton that is subsequently recycled.

**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.
S2 Results and discussion

S2.1 Along-estuary turbulent diffusivity

Figure S2 shows the values of $\phi_z$ and $\phi_x$ for different values of spatially constant along-estuary turbulent diffusivity $\kappa_h$ and for the along-estuary varying $\kappa_h = \kappa(x)$ (whose profiles are plotted in Fig. S1). Under weakly stratified conditions, $\phi_z$ hardly changes and $\phi_x$ slightly decreases with the magnitude of $\kappa_h$. 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 $\kappa_h$, and $\phi_x$ decreases accordingly.

Similarly, under strongly stratified conditions, $\phi_x$ slightly decreases with the magnitude of $\kappa_h$. However, the range over which $\phi_x$ 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).

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

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

The values of $\phi_z$ and $\phi_x$ 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 S5.
Section 4.2.2. Thus, the values of $\phi_z$ decrease and those of $\phi_x$ increase.

**S2.3 Bottom roughness length and river flow**

Figure S4(a) shows values of $\phi_z$ and $\phi_x$ for different values of the bottom roughness length $z_0$. Under both weakly and strongly stratified conditions, the values of $\phi_z$ and $\phi_x$ hardly change with $z_0$ because halving or doubling the value of $z_0$ with respect to its default value causes only small changes in the amplitude of the subtidal current.

Figure S4(b) shows values of $\phi_z$ and $\phi_x$ for different depth-averaged velocities $U_r$ of river flow. During both weak and strong stratification, the value of $\phi_x$ decreases with increasing $U_r$ because elevated $U_r$ results in shorter time for phytoplankton being advected to the estuary mouth. Under strongly stratified conditions, the value of $\phi_z$ increases with increasing $U_r$ because phytoplankton in the upper layer is subject to shorter period of sinking processes, as is discussed in Section 4.2.1.

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

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

Figure S5(b) shows values of $\phi_z$ and $\phi_x$ for different imposed values of phytoplankton density $P|_{x=L}$ at the riverine boundary. Under strongly stratified conditions, the value of $\phi_z$ decreases and that of $\phi_x$ increases with $P|_{x=L}$. As $P|_{x=L}$ increases, $P$ in the interior of the estuary increases. Since high values of $P$ occur in the upper layer during strong stratification, light is more limited for phytoplankton growth for larger $P|_{x=L}$. Hence, the specific net growth rate $(\mu - m)$ of phytoplankton in the upper layer generally decreases with increasing $P|_{x=L}$. As a result, $P$ in the upper layer decreases, and accordingly the value of $\phi_z$ decreases with $P|_{x=L}$. Moreover, a decrease of $(\mu - m)$ further results in a faster decrease of $P$ towards the estuary mouth, which leads to an increase of $\phi_x$. Under weakly stratified conditions, the values of $\phi_z$ and $\phi_x$ hardly vary with $P|_{x=L}$. This is because $P$ is vertically almost uniformly distributed rather than concentrated in the upper layer. Consequently, $(\mu - m)$ in the upper layer is hardly affected by the changes of light intensity due to varied $P|_{x=L}$ compared to that for strongly stratified conditions.

Figure S5(c) shows the values of $\phi_z$ and $\phi_x$ for different imposed nutrient concentrations $N|_{x=L}$ at the riverine boundary. Under strongly stratified conditions, the value of $\phi_z$ increases and that of $\phi_x$ decreases with $N|_{x=L}$. Similar to the spatial distribution of $P$ at equilibrium, that of $N$ (Fig. S6(b)) also shows a two-layer structure. In the upper layer, $N$ is lower than $N|_{x=L}$ and generally decreases towards the estuary mouth due to consumption by phytoplankton. In the lower layer, $N$ is much larger than $N|_{x=L}$ due to recycling of nutrient in dead phytoplankton cells. The $N$ pattern indicates that nutrients are not efficiently exchanged between the upper and the lower layer. Hence, if the riverine nutrient availability is elevated, $N$ in the upper layer in the interior of the estuary increases. As a result, $(\mu - m)$ in the upper layer becomes larger, which leads to an increase of $\phi_z$ and decrease of $\phi_x$, as is discussed in the previous paragraph. Under
weakly stratified conditions, the values of $\phi_z$ and $\phi_x$ 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 $\phi_z$ and $\phi_x$.

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

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

Figure S7(b) and S7(c) show the values of $\phi_z$ and $\phi_x$ for different values of $s_c$ and $s_\delta$, respectively. As $s_c$ increases, for both weak and strong stratification, the value of $\phi_z$ hardly changes and that of $\phi_x$ slightly decreases. The changes in $\phi_x$ 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 $\phi_z$ and $\phi_x$ hardly change for different values of $s_\delta$ within the range explored in this study.

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

Figure S8 shows the values of $\phi_z$ and $\phi_x$ for different sinking velocity $v$ of phytoplankton. Under strongly stratified conditions, the value of $\phi_z$ decreases and that of $\phi_x$ increases.
with increasing $v$. An increased $v$ leads to the decrease of $P$ in the upper layer, as is illustrated by Fig. 8(h) and discussed in Section 4.1, and $\phi_z$ therefore decreases. Furthermore, along the estuary, $P$ decreases faster towards the estuary mouth due to sinking processes, which results in the increase of $\phi_x$. In the case of weakly stratified conditions, the ranges over which $\phi_z$ and $\phi_x$ vary are much smaller. This is because the sinking of phytoplankton has little impact if the vertical turbulent mixing is strong, as illustrated by Fig. 8(g). Note that $\phi_z$ falls below zero for $v = 2$ m day$^{-1}$, that is $P$ at the estuary mouth attains higher values in the lower layer than in the upper layer.

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

Figures S9(b) and S9(c) show the values of $\phi_z$ and $\phi_x$ for different values of half-saturation constant of nutrient-limited growth $H_N$ and half-saturation constant of light-limited growth $H_I$, respectively. By increasing $H_N$ ($H_I$), the specific growth rate $\mu$ of phytoplankton decreases. As a result, when increasing $H_N$ ($H_I$), $P$ patterns behave similar as those for decreasing $\mu$.

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

Figure S10(c) contains the values of $\phi_z$ and $\phi_x$ for different light absorption coefficient
of phytoplankton. Similar to increasing background turbidity $k_{bg}$, increasing $k$ also leads to decrease of light intensity in the water column. Thus, $\phi_z$ decreases and $\phi_x$ increases with $k$.

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

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).

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

Figure S2: Scatter plot of $\phi_z$ and $\phi_x$ for different values of spatially constant along-estuary turbulent diffusivity $\kappa_h$, and also for along-estuary varying $\kappa_h$ as shown in Fig. S1. Here, open circles indicate results for weakly stratified $\kappa_h$ 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 $s_\delta$ (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 $\mu_{\text{max}}$ 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 $\alpha$ in each phytoplankton cell and (b) for different values of the nutrient recycling coefficient $\epsilon$. 

S17
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.