

Chlorella vulgaris cultivation under super high light intensity: a tentative photobioreactor design

Supplementary materials

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1. Fluid dynamics model

The hydrodynamic model features three different phases: the culture medium, considered as a continuum, the bubbles, considered as a dispersed gaseous phase, and the microalgae, considered as a dispersed solid phase. The dispersed phases are both described as Lagrangian particles.

1.1. Continuum description

The liquid flow is modeled using classical incompressible Navier-Stokes equations, considering the culture medium as a Newtonian fluid.

Bubbles are contributing to the continuum motion in a two-way coupling. Therefore, as they are traced using a Lagrangian approach (Sec. 1.2), the forces they apply on the liquid are directly accounted for in the momentum balance equation ($\frac{1}{V_c} \sum_{i=1}^n \sum_{i=1}^m \vec{F}_t^i$).

Overall, the continuum motion is governed by the following equation:

$$\begin{aligned} \frac{\partial}{\partial t}(\rho_f \vec{u}_f) + \nabla \cdot (\rho_f \vec{u}_f \vec{u}_f) = \\ - \nabla p + \nabla \cdot \left[\mu \left(\nabla \vec{u}_f + \nabla \vec{u}_f^T \right) \right] \\ - \frac{1}{V_c} \sum_{i=1}^n \sum_{i=1}^m \vec{F}_t^i + \rho_f \vec{g} \quad (1) \end{aligned}$$

1.2. Lagrangian phases description

Dispersed phases (bubbles and microalgae) motion is described using a Lagrangian approach. With this method, the tracer trajectories are the results of a force balance. This balance sums the contribution of: virtual mass, drag, and buoyancy (Eq. 2).

$$\begin{aligned} \rho_p V_p \frac{d\vec{u}_p}{dt} = \sum_{j=1}^m \vec{F}_p^j = \\ + \frac{1}{2} \rho_f C_d S_p \|\vec{u}_f - \vec{u}_p\| (\vec{u}_f - \vec{u}_p) \\ - C_m \rho_f V_p \frac{d\vec{u}_p}{dt} + V_p \vec{g} (\rho_f - \rho_p) \quad (2) \end{aligned}$$

whence C_m is the virtual mass coefficient (value of 0.5 for both bubbles and microalgae), C_d is the drag coefficient, expressed with Eq. 3 for microalgae (1) and Eq. 4 for bubbles (2).

$$\frac{24}{Re} (1 + 0.152 Re^{0.677}) + \frac{0.417}{1 + 5070 Re^{-0.940}}, \quad Re < 2 \cdot 10^5 \quad (3)$$

$$\frac{24}{Re} (1 + 0.15 Re^{0.687}), \quad Re < 1000 \quad (4)$$

Potential tracers-wall collisions are described using an elastic shock model with no energy dissipation. The same description is used for cell-cell collisions.

1.3. Conjugate Heat Transfer

Computing the temperature field across solid and fluid domains was done by solving coupled equations, each dedicated to a type of domain. In the fluid regions, the total energy (internal energy, simplified as enthalpy, and kinetic energy) is solved using Eq. 5. The solid regions were governed by Eq. 6. In both cases, Fourier's law was used to describe the conductive heat fluxes. The coupling between the regions was modeled using temperature and heat flux continuity.

$$\begin{aligned} \frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho \vec{u}_f h) + \frac{\partial}{\partial t}(\rho k) + \nabla \cdot (\rho \vec{u}_f k) = \\ - \nabla \cdot \left(-\frac{\kappa}{\rho C_p} \nabla h \right) + \frac{\partial}{\partial t} p - \rho \vec{g} \cdot \vec{u}_f + \nabla \cdot (\vec{\tau} \cdot \vec{u}_f) + r \quad (5) \end{aligned}$$

$$\frac{\partial}{\partial t}(\rho h) = - \nabla \cdot \left(-\frac{\kappa}{C_p} \nabla h \right) \quad (6)$$

1.4. Partial validation of the model

Partial validation of the model components was resorted to as no benchmark allowing for the validation of the workflow as a whole (thermal aspects, fluid flow, and light/dark cycles) exists. The specific components that were validated are the Conjugate Heat Transfer model and the fluid flow model.

1.4.1. Conjugate Heat Transfer validation. The Conjugate Heat Transfer part of the workflow was validated against the

canonical case introduced by Suscec in 1973. In this work, the author considered the 2D case of a laminar slug flow of a hot fluid sweeping the upper face of a thin layer of highly conductive solid material while its lower face is cooled down convectively (Fig. 1). Assuming an inviscid fluid, a low Biot number of the solid body, a high Péclet number, and constant physical properties, Suscec has been able to derive an analytical solution for the fluid temperature over time, anywhere in the domain:

$$\frac{\theta}{\theta_c} = 1 + U(\tau - 1)(-1 + \operatorname{erfc}(Y) - \exp(2\eta Y + \eta^2)\{\operatorname{erf}(\epsilon(\tau - 1) + \eta + Y)b - \operatorname{erf}(\eta + Y)\}) \quad (7)$$

whence

$$\tau = \frac{u_\infty t}{x} \quad Y = \frac{y}{2} \sqrt{\frac{u_\infty}{a_f x}} \quad \eta = \frac{h_c}{k_f} \sqrt{\frac{a_f x}{u_\infty}} \quad \epsilon = \frac{\sqrt{\frac{x}{u_\infty a_f}}}{2r} \quad (8)$$

and U is the step function, $r = \frac{\rho_s C p_s b}{k_f}$, $\theta = T - T_\infty$, a_f is the fluid thermal diffusivity, b is the solid thickness, h_c is the cooling convective heat exchange coefficient on the bottom side of the solid, k_f is the fluid thermal conductivity, u_∞ is the fluid velocity, T_∞ is the hot temperature going to sweep the solid, T_c is the coolant temperature (and initial temperature of the domain).

Assuming the fluid to be water (flowing at 0.01 m/s) and the solid to be a 1 mm thick aluminum sheet (physical properties available in the manuscript body), and intense convective cooling (1000 W/m²/K), in a 10x100 mm² domain, one can compute several dimensionless numbers to corroborate the assumptions made to derive the analytical solution. For this setup, the Reynolds number reaches 200, which is congruent with a laminar flow in such a channel. The solid Biot number is $4.9 \cdot 10^{-3}$, far below the 0.1 limit conventionally used to validate thermal homogeneity. The fluid Péclet number (based on the domain length) in the fluid is 7 000, which validates that axial diffusivity is indeed negligible before convection. As a final check, the Péclet number was assessed, as the thermal conductivity in the aluminum is much greater than that in water. Its value turned out to be 11.7, which ensures that heat travels the fastest with the fluid anyway.

To ensure numerical convergence, two meshes (22 000 and 44 000 cells, fully hexahedral, refined where gradients are encountered) and two timesteps (2.5 ms, amounting to a Courant number of 0.05, and 0.25 ms, amounting to a Courant number of 0.005) were tested. The chosen outcomes to compare the simulations with the analytical solution were three probes placed within the thermal boundary layer at $x = 10, 50$, and 90 mm, and $y = 1$ mm.

Figure 2 offers a visualization of the excess temperature field at 0.5 dimensionless time (the heat wave traveled half of the solid length). The heat moved indeed faster in the fluid, and the solid is homogeneous thermally in its thickness. Moving to quantitative observations, Figure 3 displays the

temperature excess histories for the selected probe positions. As one can see, the workflow adequately predicts the dynamic and the final value of the water temperature. Furthermore, the simulations can be deemed numerically converged as the four tested numerical configurations yield extremely close predictions. The only discrepancy is the smoothing of the stepwise temperature increase (corresponding to when the hot air reaches the probe location). Yet, it echoes the challenge that represents conserving a shock with a numerical scheme (confirmed by visual observation on Fig. 2), which is fortunately not encountered in the intended application of the workflow.

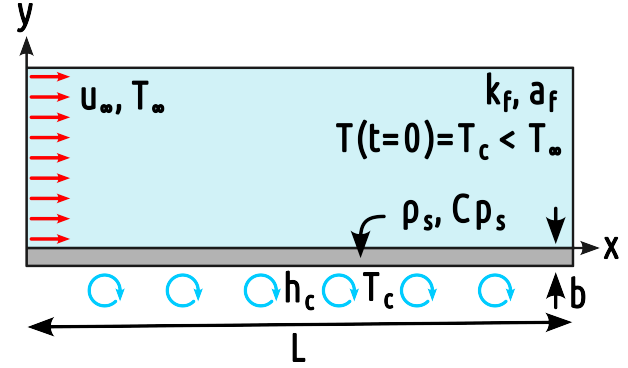


Fig. 1. Schematic of the setup for Conjugate Heat Transfer validation

1.4.2. Fluid flow validation. Validating the fluid flow prediction was carried out using experimental data obtained on an airlift reactor. This configuration was chosen as it corresponds to the advanced design proposed in the manuscript body. Yet, few authors have investigated airlift reactors with detailed analysis tools, such as Particle Image Velocimetry (a.k.a. PIV) or Laser Doppler Anemometry (a.k.a. LDA). Among them, the possibilities are further restricted by the fact that bubbles are assumed to be spherical and that gas is the only means to entrain the liquid. Finally, among the references identified (Liew *et al.*, 2017, and Qie *et al.*, 2015), only the work of Liew *et al.* provided sufficient details to ensure a reasonably faithful reproduction of the experimental device (Fig. 4). The setup is relatively simple with a sparger on one side of the reactor and a fixed baffle to separate the riser from the downcomer. Only one level of water filling (46 cm) and one gas flow rate (0.30 m³/h, assumed Nm³/h) were tested, while the outcomes were the velocity profile (using Laser Doppler Anemometry) on the symmetry plane of the reactor at three different heights. Finally, it is worth mentioning that the authors took care to add some salt to prevent bubble coalescence, but did not specify the average bubble diameter, though.

The system was reproduced as a 3D transient case, for three different bubble diameters (1, 3, and 5 mm). In addition to this screening, mesh convergence was ensured using three different meshes (20 100, 66 365, and 144 200, hex-dominant, with close to the wall refinement, maximum Courant number set at 0.5). Figure 5 presents the results of the mesh convergence analysis. As one can see the medium and fine meshes yielded similar results, the medium was

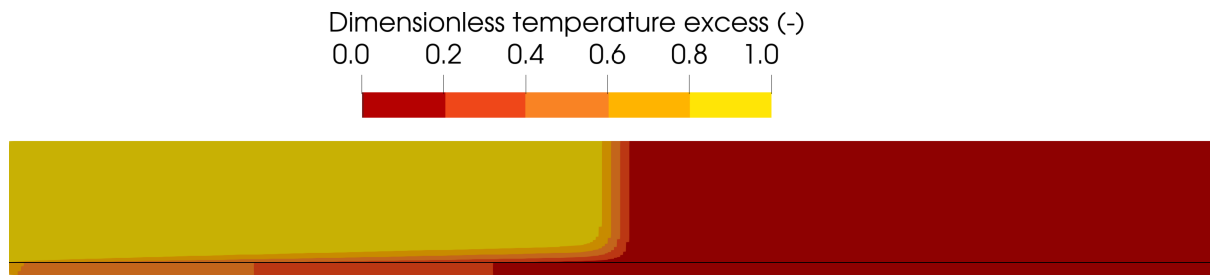


Fig. 2. Visualization of the domain after 0.5 dimensionless times. Black line - Delineation between the solid and the fluid

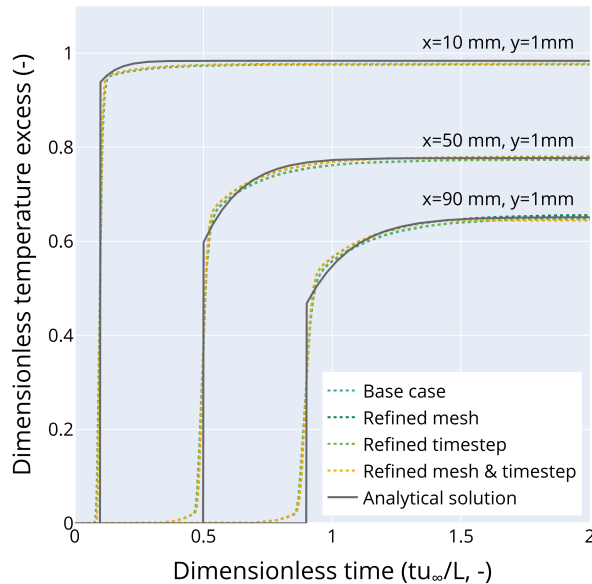


Fig. 3. Simulation results and analytical solution for the Conjugate Heat Transfer validation setup

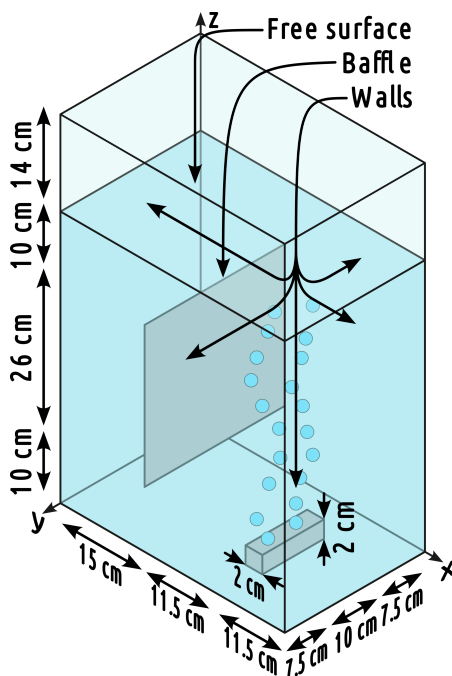


Fig. 4. Schematic of the setup for fluid flow validation

therefore retained for the rest of the study. Once numerical independence has been ensured, the next step was to robustify the data extraction process. Indeed, as the plume tends to oscillate, one has to ensure that the extracted data matches the experimental ones (averaged over 60 seconds). The first point is to confirm that a pseudo-steady state is reached, which is the case after about 10 seconds (Fig. 6). The second point is to ensure that the averaging time before data extraction is long enough to ensure the stability of the velocity profile. Figure 7 illustrates the velocity profiles obtained at different times after pseudo-steady state is reached. Each of the ten profiles is averaged over 20 seconds. As one can see, they exhibit quite a high dispersion. Increasing the time-averaging window (from 20 to 200 seconds) allowed to stabilize the results (Fig. 8, where averaging increases as line opacity increases).

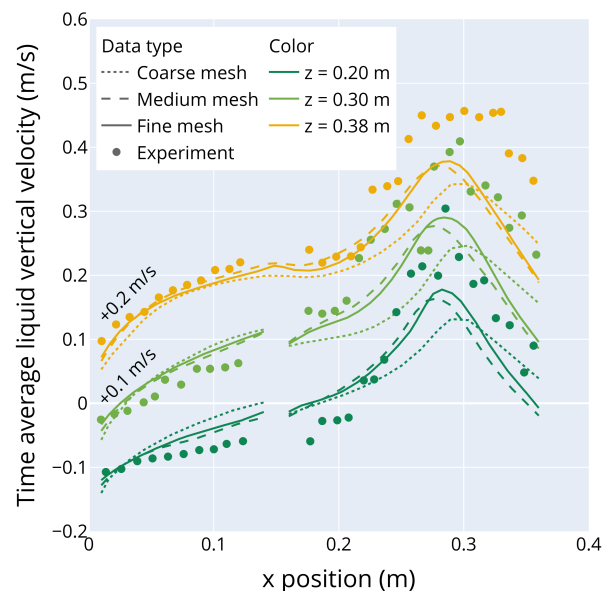


Fig. 5. Mesh convergence for the fluid flow validation case. Bubble diameter - 3 mm. Profile averaging time 200 seconds

Figure 9 presents a visualization of the flow while Figure 10 presents both experimental and numerical results for the three tested bubble diameters. As one can see, the agreement is reasonable, with 3-mm bubbles being the closest to the experimental observations. The downcomer velocity profiles are overall well predicted, with trends well captured, but absolute value deviations for the two lowest profiles. The riser velocity profiles show a good qualitative agreement, but absolute values are off target most of the time. While not

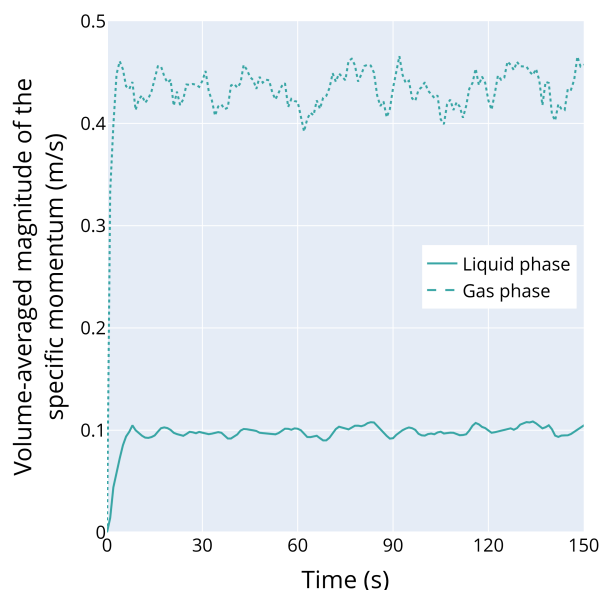


Fig. 6. Liquid and gas phase volume-averaged magnitude of momentum the fluid flow validation case. Bubble diameter - 3 mm

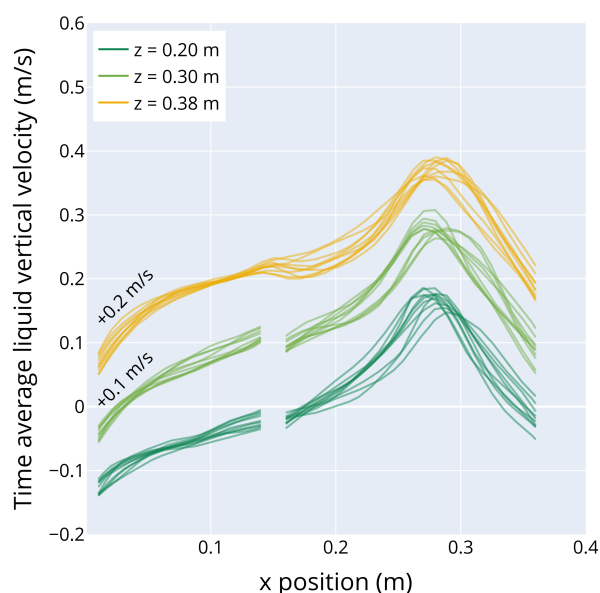


Fig. 7. Extraction of velocity profiles (20-second time averaging) for fluid flow validation case. Bubble diameter - 3 mm.

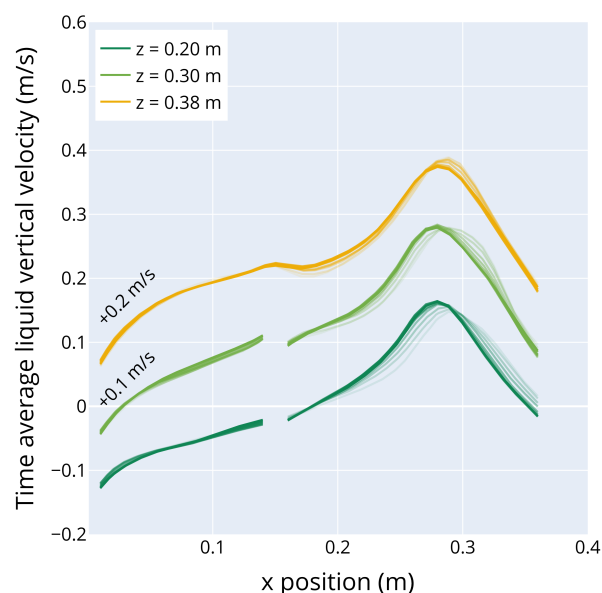


Fig. 8. Extraction of velocity profiles for fluid flow validation case. Bubble diameter - 3 mm. Time averaging increases from 20 to 200 seconds as line opacity increases

ruling out possible misdescription of the physical phenomena at play, the quality of the experimental data is to be considered. Indeed, some information is missing (*e.g.*, bubble diameter, sparger porosity, and pore size), and the reliability of measurements can also be challenged to some extent. Regarding the measurements performed by the authors, they hint that the averaging window they chose (60 seconds) might have been too short. Indeed, as the bubble plume oscillates, a longer averaging time might have been needed to obtain a sufficiently converged value of the local velocity. This argument is supported by the sharp drop in velocity (-0.15 m/s) for 2 points around $x = 0.27$ m, for the $z = 0.30$ m line, or the surge in velocity ($+0.10$ m/s) for one data point ($x = 0.28$ m) for the $z = 0.20$ m line. Indeed, the plume might have shifted away from the laser spot when they carried out the measurements at these locations. This argument is further supported by the tracking of the numerical plume that suggests that a 60-second averaging might indeed be too short (Fig. 11), while the plume centroid can move over a 8-cm span. To deliver converged results, the numerical profiles presented here were averaged for 200 seconds. Despite the aforementioned discrepancies, all in all, this partial validation allows to consider that the workflow delivers adequate results for the task at hand.

2. Oxygen saturation

To determine whether it was possible to operate at 0.1 Vessel Volume per Minute (VVM) aeration without inducing oxygen inhibition, an assessment of the resulting dissolved oxygen level was carried out. The overall derivation process is based on a mass balance at the system level, followed by considerations on mass transfer within the liquid. First of all, the oxygen production can be evaluated using the culture growth rate (Eq. 9), then assuming steady state is reached, the equilibrium oxygen concentration in the liquid is governed by Eq.

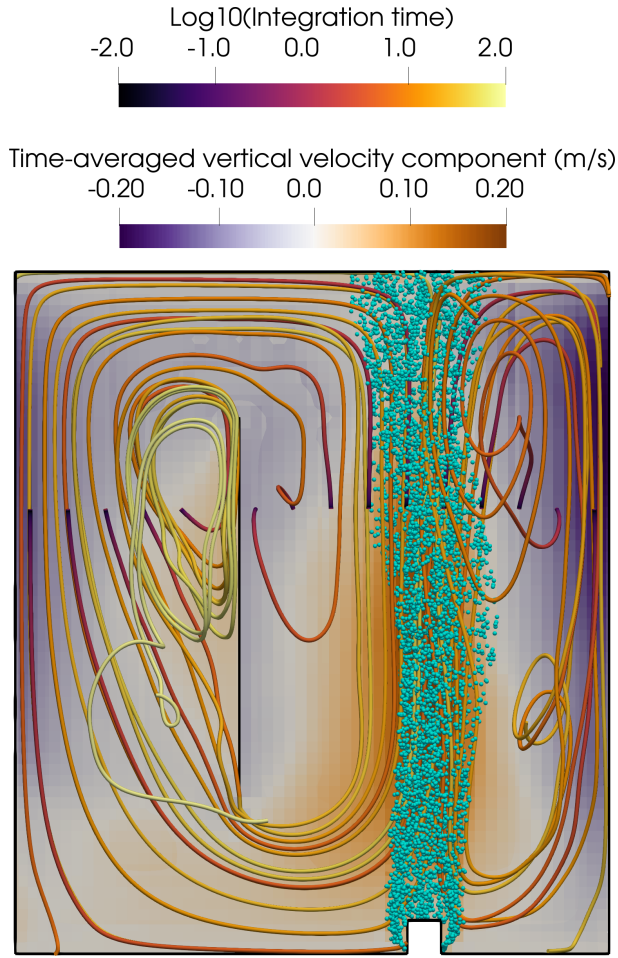


Fig. 9. Visualization of the flow. Bubble diameter - 3 mm. Velocity averaging time 200 seconds. Maximum streamline length - 2 m

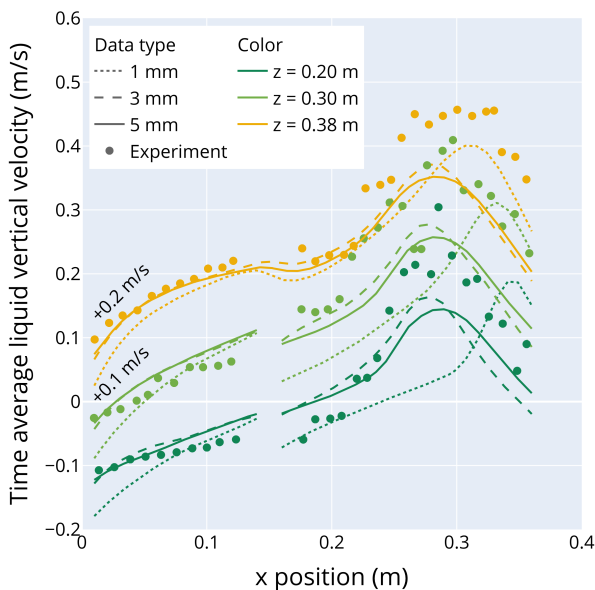


Fig. 10. Extraction of velocity profiles for fluid flow validation case. Profile averaging time 200 seconds

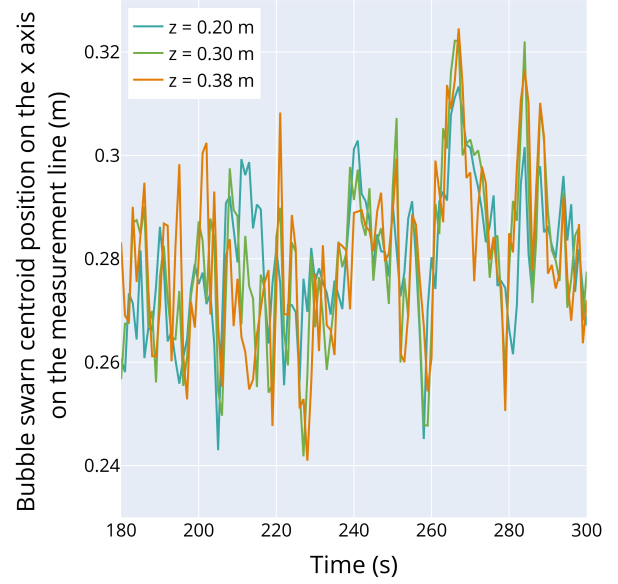


Fig. 11. Plume centroid position on the x axis within the measurement windows described by the authors. Bubble diameter - 3 mm

10. Yet, the interface concentration is not easy to assess, but can be replaced by the more conservative outlet oxygen concentration (Eq. 11) obtained from the same assessment. This calculation requires evaluating the k_l and a parameters. In this case, it was done using data from the simulation (bubble sliding velocity, number of bubbles present at once in the domain) and Winnikow's correlation (Eq. 12) (3). While some uncertainty prevents blindly trusting the obtained dissolved oxygen value (123% of saturation, for air at 25 °C), it remains far below the level dangerous for *Chlorella vulgaris* (about 250% of saturation (4)) and can therefore allow to conclude that 0.1 VVM is enough to prevent harmful oxygen build up in the photobioreactor. Details of the symbol's meaning and parameter values are available in Table 1.

$$P_{O_2} = C\mu Y_{O_2/X} \quad (9)$$

$$[O_2]_{eq} = H[O_2]_{interface} + \frac{P_{O_2}}{k_l a} \simeq H[O_2]_{out} + \frac{P_{O_2}}{k_l a} \quad (10)$$

$$[O_2]_{out} = [O_2]_{in} + \frac{P_{O_2} V}{Q} \quad (11)$$

$$Sh = \frac{2\sqrt{ReSc}}{\pi} \left(1 - \frac{2.89}{\sqrt{Re}}\right)^{1/2} \quad (12)$$

3. Flow numerical convergence & transient state

Several parameters have to be taken into account to ensure the numerical convergence of the case. The main ones are: the mesh refinement, the Courant number used to integrate the system, the thickness of the domain, and its height. In ad-

dition to ensuring numerical convergence, it is also important to ensure that results are produced once the flow within the photobioreactor has entered the pseudo-steady state. Indeed, the time required to set the fluid in motion is anticipated to be short compared to the intended operation, spanning over several hours, at least. These different parameters are discussed hereinafter over four metrics: liquid and gas phase volume-averaged norm of momentum - a proxy of the fluid flows intensities -, the liquid volume-averaged norm of vorticity - a proxy of the vortices intensities -, and the shear rate at the wall - a proxy of the faithfulness of the flow near the walls -. Overall, a domain featuring a 3 mm width and 4 convection cells on top of each other, meshed with 40 divisions over the depth of a convection cell, and operated at a Courant number of 0.5 was deemed adequate. The time for the flow to establish was then around 60 seconds.

3 1. Mesh refinement

The numerical domain is made of several square-section convection cells stacked on top of each other. Therefore, the unit length of interest was taken as the depth (or height) of a given cell. As the mesh is generated automatically using *snappy-HexMesh*, a few comments are worth drawing. First of all, the refinement referred here corresponds to the background mesh. The intersections between the background mesh and the geometry are refined twice (with six guard cells (5)). Then, the mesh is extruded to ensure it only features one cell on its thickness, allowing for a 2D resolution of the case. Finally, no boundary layer was added as the refinement in the vicinity of the wall already provided refined boundary cells. Figure 12 displays the three indicators for the tested background mesh refinements (10, 20, 30, 40, and 50 divisions over the depth of a convection cell). The tests were carried out with a Courant number of 0.5, a width of 3 mm, and 4 convection cells. As one can see, calculations with 10 to 30 divisions cannot be deemed converged. 40 and 50 divisions yielded identical results, except for vorticity, while being close by. This observation is supported by the calculation of the extrapolated error (following the guidelines of Celik *et al.* (6)), and the Grid Convergence Index (a.k.a. GCI (7)),

which are 1.04% and 1.31%, respectively when 40 divisions are used (reduced to 0.88 and 1.11% when 50 divisions are used, leading to 26% increase in the number of cells). Therefore, the 40-division case was deemed accurate enough in addition to offering a good compromise between accuracy and computational time.

3 2. Courant number

Five Courant numbers were tested to try to identify any unexpected behavior (0.25, 0.375, 0.5, 0.625, and 0.75). Indeed, while the Courant number manages the timestep based on the interplay between the liquid velocity and the mesh elements, it does not account directly for the Lagrangian particle motion. This is not a problem with the numerical microalgae, because they act as tracers of the flow. Still, it may be for the bubbles, even though they have their own sub-stepping procedure (splitting each time step into four). The tests were carried out with 40 divisions over the depth of a convection cell, a width of 3 mm, and 4 convection cells. Figure 13 reports the four indicators for the five tested Courant numbers. The differences between the runs appear subtle and may not clearly justify the choice of one versus the other. Still, overall, Courant numbers of 0.625 and 0.75 seem to detach marginally from the three others. Based on these observations, and because it aligns with conventional CFD practices, a Courant number of 0.5 was retained for the study.

3 3. Domain thickness

While the computations were carried out in 2D, it is worth noting the pseudo-thickness of the domain matters. Indeed, the aeration of the photobioreactor is based on its volume (aeration in Vessel Volume per Minute - VVM). Therefore, the number of bubbles entering the domain per unit of time is a function of the total volume, hence the pseudo-thickness. In an asymptotic case where the thickness would be infinitely small, then no bubble would enter the reactor. In a less dire case, the bubbling frequency would simply not be representative of the stable operation of the photobioreactor. Consequently, five thicknesses, ranging from 1 to 5 mm, were tested. The runs were carried out with 40 divisions over the

Symbol	Property	Value	Unit
P_{O_2}	Oxygen productivity	5.02	$g_{O_2}/L/day$
C	Cell concentration	1.14	g/L
$Y_{O_2/X}$	Biomass oxygen yield	2	$g_{O_2}/g_{Biomass}$
μ	Growth rate	2.2	1/day
k_l	Mass transfer coefficient	$5.10 \cdot 10^{-4}$	m/s
a	Specific surface area	229	m^2/m^3
H	Henry constant oxygen in water	$3.2 \cdot 10^{-2}$	-
V	Culture volume	10	L
Q	Gas flow rate	0.1	VVM
Re	Reynolds number of a bubble	277	-
Sc	Schmidt number of oxygen in water	441	-
Sh	Sherwood number of a bubble	358	-
$[O_2]_{eq}$	Equilibrium oxygen concentration	9.98	mg/L

Table 1. Dissolved oxygen calculation symbol's meaning and parameter values

depth of a convection cell, a Courant number of 0.5, and 4 convection cells. Figure 14 presents the results of this analysis. A 1-mm thickness tends to produce a lower liquid volume-averaged norm of vorticity and shear rate at the wall. From 2 mm on, the results appear as converged with respect to this parameter. As its computational cost is marginal, a thickness of 3 mm was chosen for the rest of the runs.

3.4. Domain height

Once the mesh resolution, the temporal integration, and the domain thickness have been determined, comes its height. Indeed, the first convection cell features the gas inlet, which may perturb the system and not be representative of the whole photobioreactor. Therefore, domains on increasing height were tested to identify from which height the system can be deemed large enough to minimize the perturbation. Five heights were tested: 2, 4, 6, 8, and 10 convection cells (as odd would not allow for a perfectly identical pattern). The runs were carried out with 40 divisions over the depth of a convection cell, a Courant number of 0.5, and a thickness of 3 mm. Figure 15 presents the results of this exploration, with the abscissa scaled by the number of units (a large unit naturally requiring more time to be set in motion). The only indicator showing a major deviation between the systems is the liquid phase volume-averaged norm of momentum for the 2-cell configuration, which seems to require an extensive time to reach the same value as the others. It was therefore ruled out. Consequently, the 4-convection cell geometry was adopted as it reaches the same liquid phase volume-averaged norm of momentum within a reasonable amount of time.

3.5. Transient state duration

With the mesh selected, the next important point is to assess the duration of the transient evolution of the system before it enters a pseudo (or fluctuating) steady state. Indeed, photobioreactor operation time scales can be foreseen to be of the order of several hours. Consequently, as the CFD simulation will not span over this entire duration, due to computational power constraints, the initial transient phase has to be evaluated and discarded. Figure 16 presents the four indicators used for mesh quality assessment over a longer duration (180 vs. 30 seconds) as well as the slopes of the associated curves (over 5 seconds, see Section 4). All the indicators seem to stabilize relatively quickly (less than 30 seconds), except liquid volume-averaged specific momentum, which required 40 to 50 seconds to stabilize. Using the slope to ascertain the delineation of the transient duration, it can be concluded that the liquid volume-averaged specific momentum is indeed the longest to reach a slope oscillating around zero (in about 60 seconds). Therefore, it can be concluded that the system requires 60 seconds to enter the targeted pseudo-steady state.

3.6. Conjugate Heat Transfer case

Moving from pure fluid flow to a Conjugate Heat Transfer configuration adds another level of complexity to the case, *i.e.*, accounting for heat transport. Therefore, a dedicated mesh convergence study was carried out. First, the sys-

tem was run without a heat source for 60 seconds, so that it entered the hydrodynamic pseudo-steady state. Then, a grossly overpowered heat source was activated. It was distributed following the light absorption pattern (introduced in the manuscript body) and amounted to 20 times maximum sunlight, *i.e.*, $40\,000\ \mu\text{molPhotonPAR}/\text{m}^2/\text{s}$. While surely not relevant from a biological perspective, this configuration was intended as a stress test for the numerical implementation. Following the same approach as for the hydrodynamic mesh convergence, five levels of refinement were tested (starting at 20 divisions per convection cell, as 10 led to a simulation crash), while the rest of the numerical parameters were set as a Courant number of 0.5, a width of 3 mm, and 4 convection cells. Figure 17 presents the results of the simulation in terms of mixing cup average temperature (*i.e.*, accounting for the specific heat and density of each part of the domain), spatial average temperature, and standard deviation. While less accurate, the last two indicators allow for gauging the temperature homogeneity. First of all, both average temperatures are close, suggesting that despite having different meanings, they can be used interchangeably as indicators. Second, the mesh refinement has no effect on them. This is a token of the quality of the implementation, as they are driven by an energy balance at the system level. Hence, they should not be sensitive to the mesh. Finally, the standard deviation shows sensitivity to the number of divisions used across a convection cell. Refining the mesh led to an initial rise of the standard deviation value (from 20 to 40 divisions per convection), before entering an oscillatory convergence state (40 to 60 divisions per convection). Consequently, a mesh with 40 divisions per convection can be deemed adequate to simulate the Conjugate Heat Transfer configuration of the system.

4. Lagrangian Coherent Structure

As microalgae are used to track illumination histories, it is important to ensure that the Lagrangian particles remain distributed homogeneously so that they explore the system in a manner faithfully representing their real-life counterparts. Upon designing the numerical workflow, spatial segregation of the numerical microalgae was observed over time (Fig. 20). Neither grid refinement (both space and time) nor Lagrangian integration improvement avoided the appearance of the phenomenon. Consequently, the potential existence of Lagrangian Coherent Structures was investigated (8). To do so, a dedicated OpenFOAM library - *lcs4Foam* (9) - was employed for both backward (attracting) and forward (repelling) tracking of the Lagrangian Coherent Structures. Figure 21 presents the structures observed over time for an integration time of 2.66 seconds. This integration time was chosen as it corresponds to the system characteristic time, as the perimeter of a convection cell is 20 cm and the liquid characteristic velocity is about 0.075 m/s (Fig. 16). As one can see, the detected structures match the segregation patterns observed for the particle (Fig. 20).

While insightful, these observations are qualitative. In order to elaborate a more quantitative assessment of the parti-

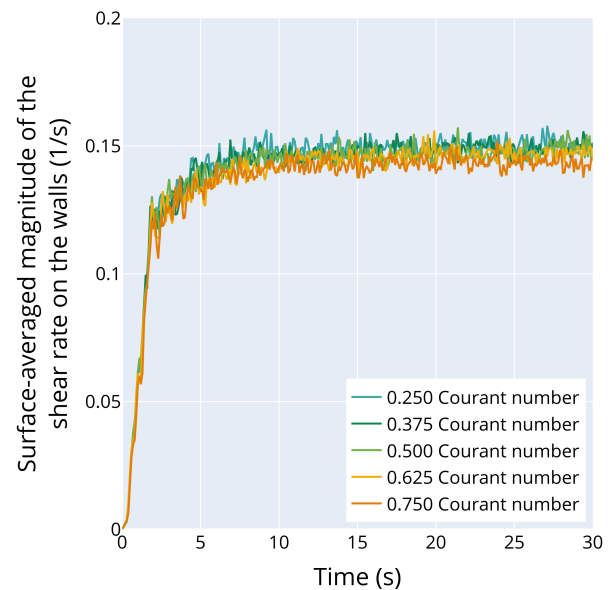
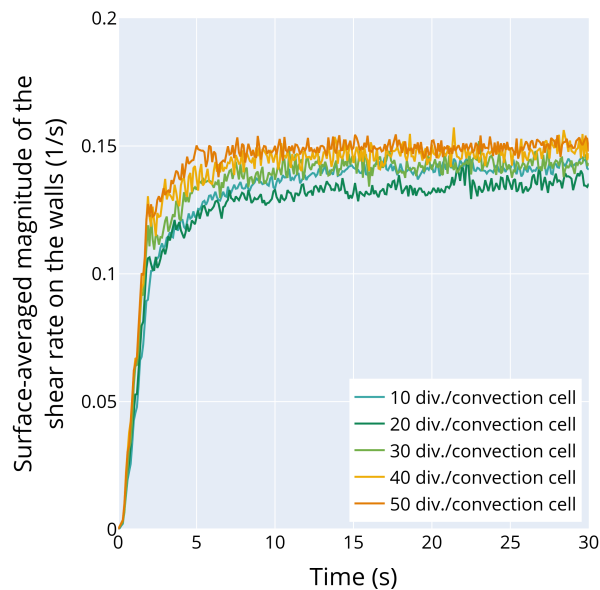
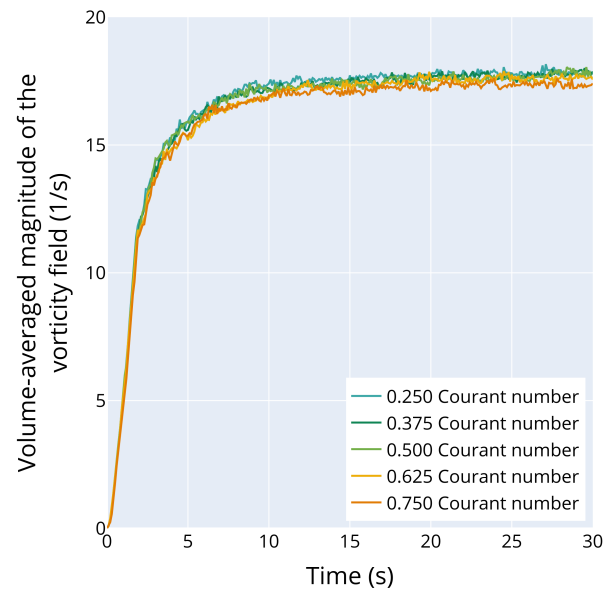
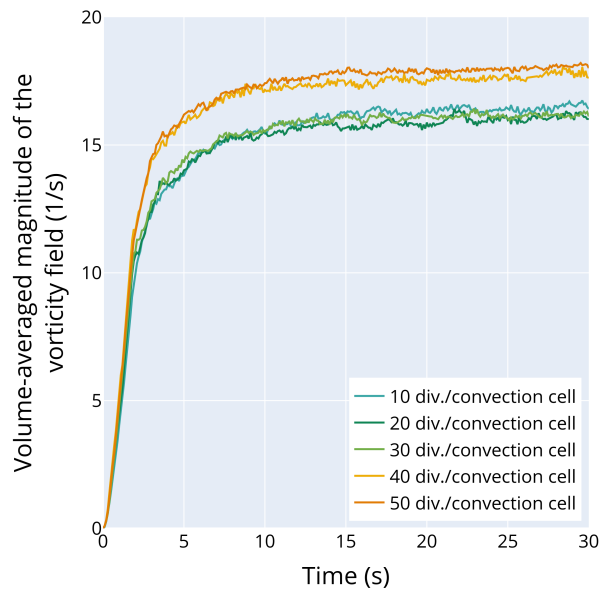
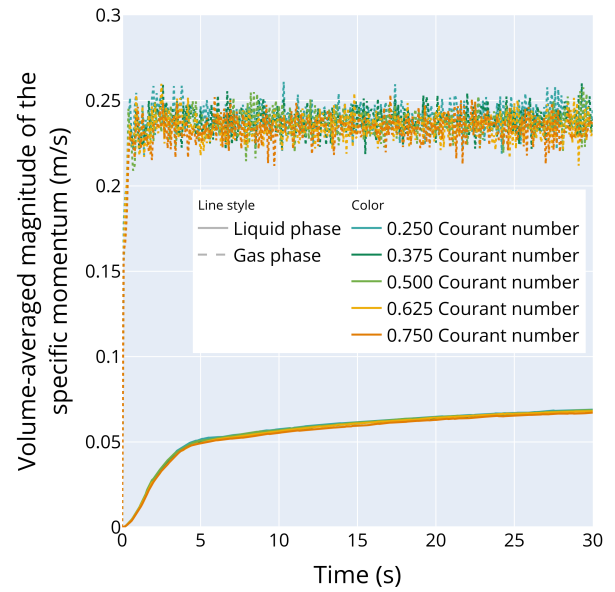
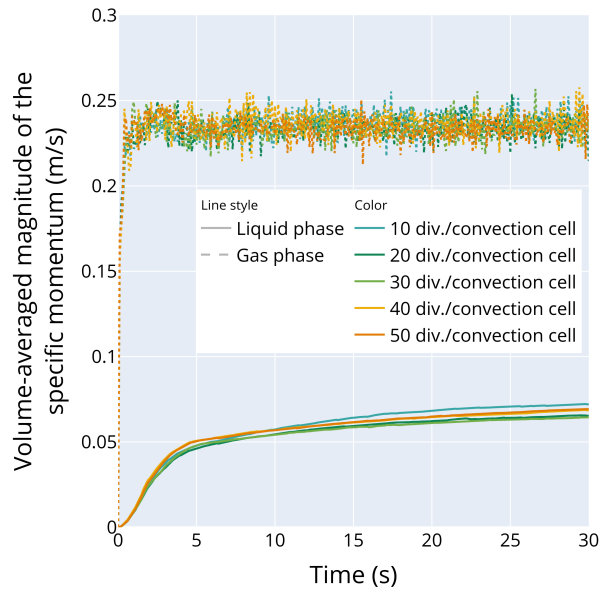


Fig. 12. Screened parameter values for mesh refinement. Top - Momentum. Middle - Vorticity. Bottom - Shear rate at the walls

Fig. 13. Screened parameter values for Courant number. Top - Momentum. Middle - Vorticity. Bottom - Shear rate at the walls

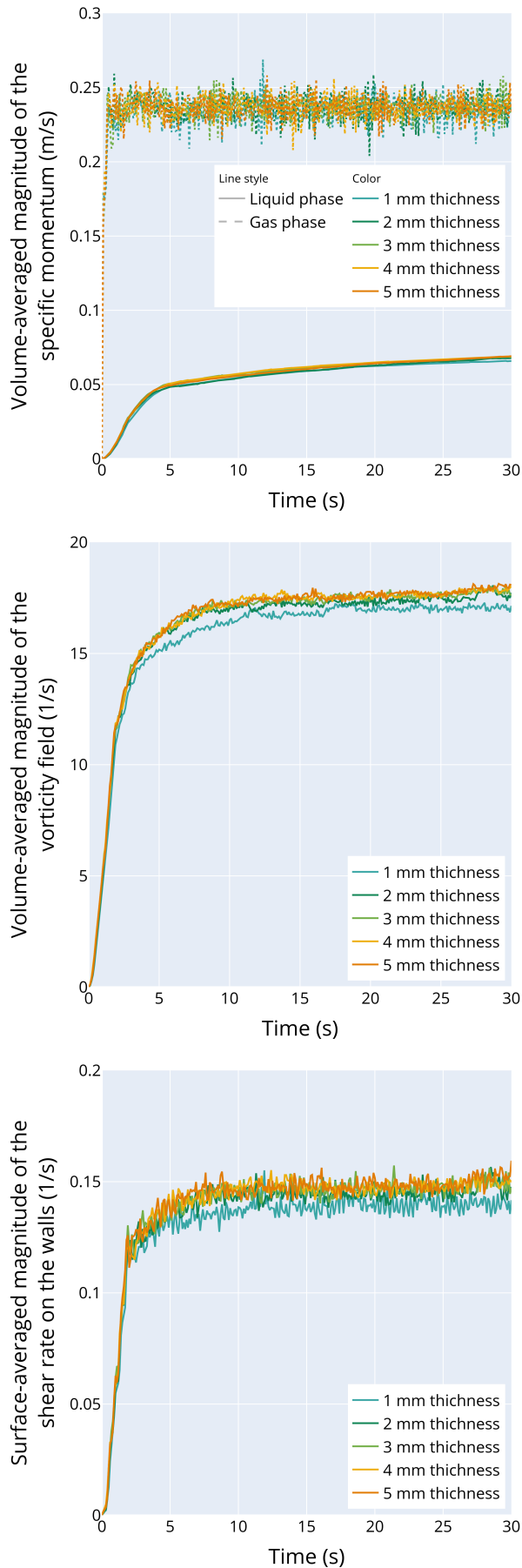


Fig. 14. Screened parameter values for domain thickness. Top - Momentum. Middle - Vorticity. Bottom - Shear rate at the walls

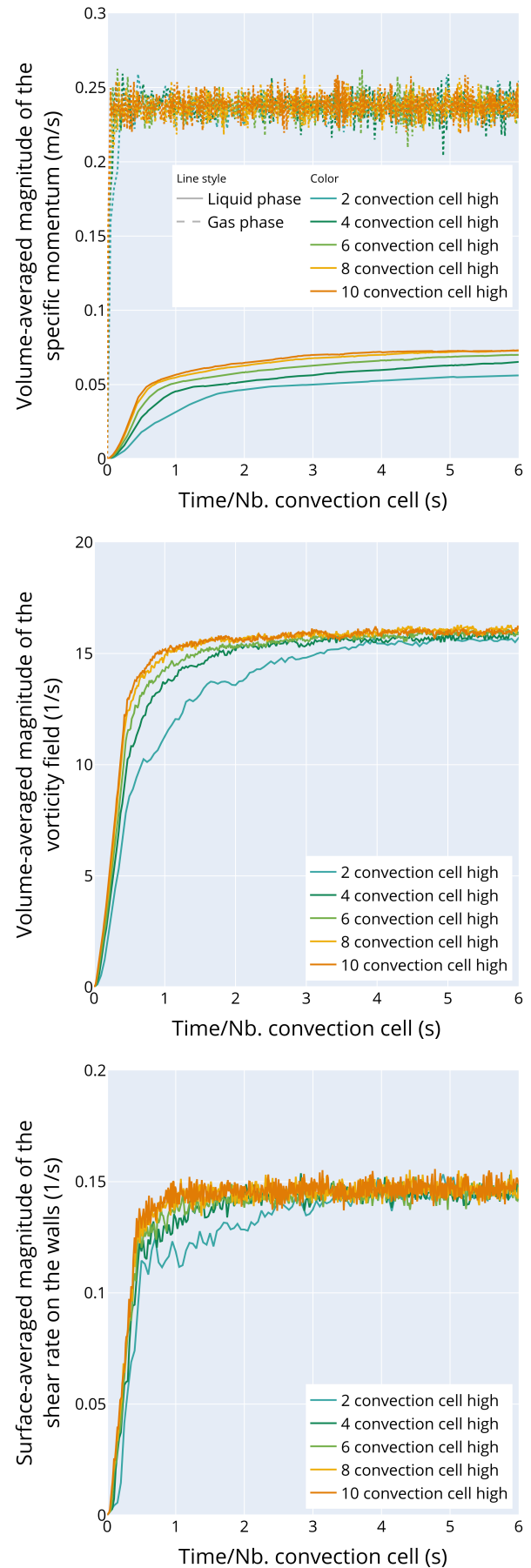


Fig. 15. Screened parameter values for domain height. Top - Momentum. Middle - Vorticity. Bottom - Shear rate at the walls

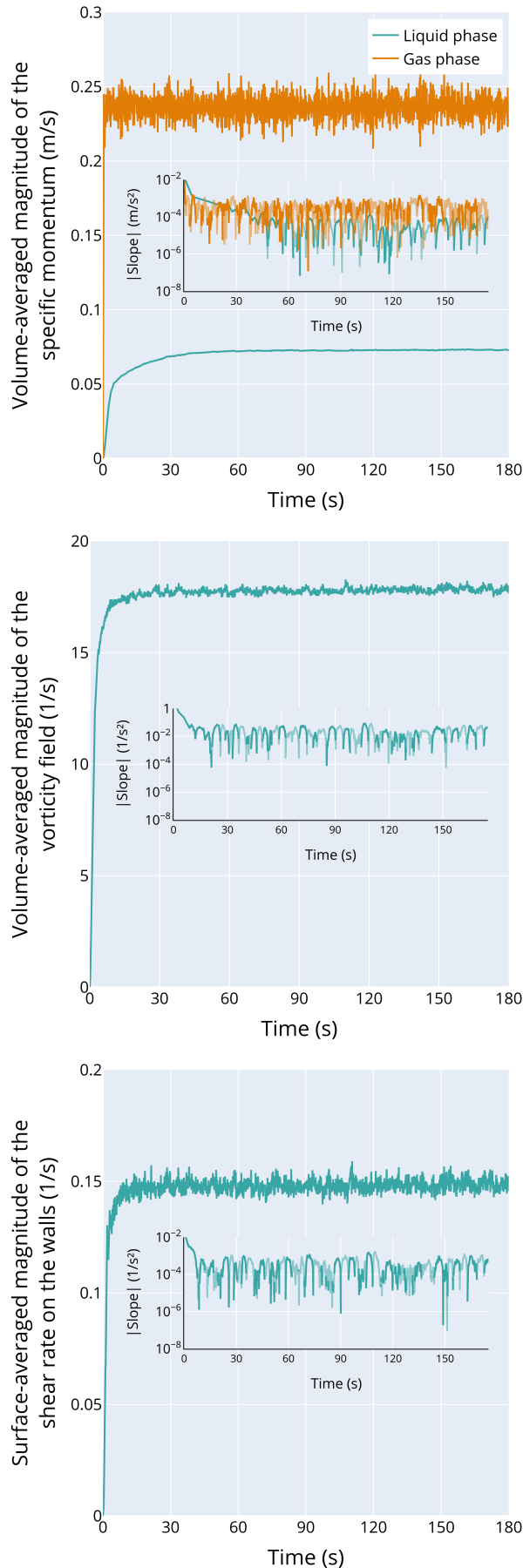


Fig. 16. Screened parameter values over time for the retained mesh configurations. Inset - slope of the curve over 5 seconds forward. Light color - negative slope value. Dark color - positive slope value. Top - Momentum. Middle - Vorticity. Bottom - Shear rate at the walls

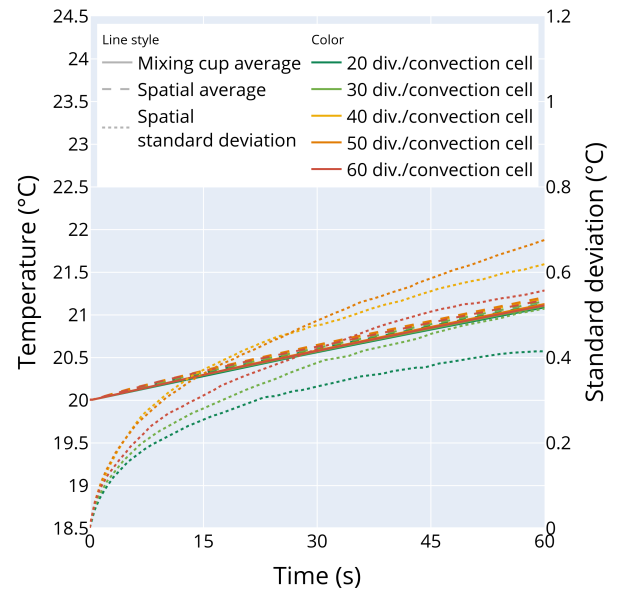


Fig. 17. Screened parameter values for mesh refinement in the Conjugate Heat Transfer configuration

cle swarm dispersion, the local particle density was tracked over time in the bottommost convection cell. The convection cell was divided into a 20×20 grid (uniform in both directions). For each timestep, the number of numerical microalgae within each subgrid cell was counted and divided by the initial number. This procedure allows for monitoring how heterogeneously distributed the numerical microalgae become over time. As reporting 400 local histories in a graph seems impossible, the features of the distribution were drawn instead (Fig. 18). As one can see, the distribution widens relatively quickly. 2.66 seconds of integration allow the quartiles to be roughly within a 0.9 - 1.1 range, while the 5th and 95th percentiles have already passed a 0.75 - 1.25 range. Also, over time, the median of the population decreases, hinting towards numerical microalgae leaving the convection cell (confirmed by the total count within the cell). This explains why, in Figure 20, the upper convection cells appear less affected than the lower ones. This is a visualization artifact coming from the fact that some tracers enter their domains.

This bears very practical consequences: numerical microalgae can be considered faithfully describing what their real-life counterparts live for only about 5 seconds (twice the system characteristic times suggested upper limit for particle tracking (8), already leading to a 0.8 - 1.2 quartile range). Afterward, reseeded will be mandatory to ensure reliable results. This also explains why the time window of 5 seconds was chosen for the stability analysis.

5. Light/Dark numerical convergence

With the numerical microalgae trajectories ascertained, the question of the amount of light/dark cycle to be collected to obtain a converged representation of the experienced patterns could be tackled. The first step was to identify the cycles themselves among the collected light histories. As ex-

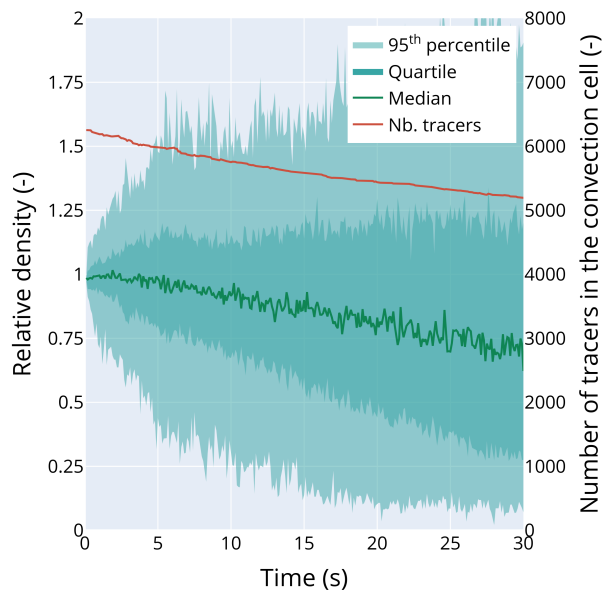


Fig. 18. Features of the distribution of the local density in the bottommost convection cell (20×20 grid, yielding a 400-history population) and total numerical microalgae count over time

plained in the manuscript body, the level to determine the dark phase of the cycle was taken as the saturation illumination (at $100 \mu\text{molPhotonPAR}/\text{m}^2/\text{s}$ for *Chlorella vulgaris* (10, 11)). Then, each cycle can be described using two parameters: its frequency and its duty cycle. Frequency was extracted as the inverse of the total cycle duration (light & dark phase), while the duty cycle was extracted as the ratio of the light phase duration over the total cycle duration.

To ensure a sufficient number of cycles were agglomerated, an increasingly large number of cycles were used to draw the parameter distributions and the distribution properties (median and inter-quartile distance are used as the frequency distribution is obviously not Gaussian). Figure 19 presents the distributions and the related indicators for populations made of 3 000 to 15 000 cycles. As one can see, qualitatively, from 9 000 cycles and on, it is difficult to differentiate the distributions. Using the indicators (median and inter-quartile distance), 12 000 cycles or more can be deemed sufficient. Yet, in order to be on the safe side, 15 000 light cycles were used to produce the results presented in the manuscript body.

References

- Phillip P. Brown and Desmond F. Lawler. Sphere Drag and Settling Velocity Revisited. *Journal of Environmental Engineering*, 129(3):222–231, March 2003. .
- Akio Tomiyama, Isao Kataoka, Iztok Zun, and Tadashi Sakaguchi. Drag Coefficients of Single Bubbles under Normal and Micro Gravity Conditions. *JSME International Journal Series B*, 41(2):472–479, 1998. .
- S. Winnikow. Letter to the editors. *Chemical Engineering Science*, 22(3):477, March 1967. ISSN 0009-2509. .
- Barry J. Shelp and David T. Canvin. Photorespiration and Oxygen Inhibition of Photosynthesis in *Chlorella pyrenoidosa*. *Plant Physiology*, 65(5):780–784, May 1980. ISSN 0032-0889. .
- John G. Baker and James R. van Meter. Reducing reflections from mesh refinement interfaces in numerical relativity. *Physical Review D*, 72(10):104010, November 2005. .
- Ishmail B. Celik, Urmila Ghia, Patrick J. Roache, and Christopher J. Freitas. Procedure for estimation and reporting of uncertainty due to discretization in CFD applications. *Journal of fluids Engineering-Transactions of the ASME*, 130(7), 2008. ISBN: 0098-2202.

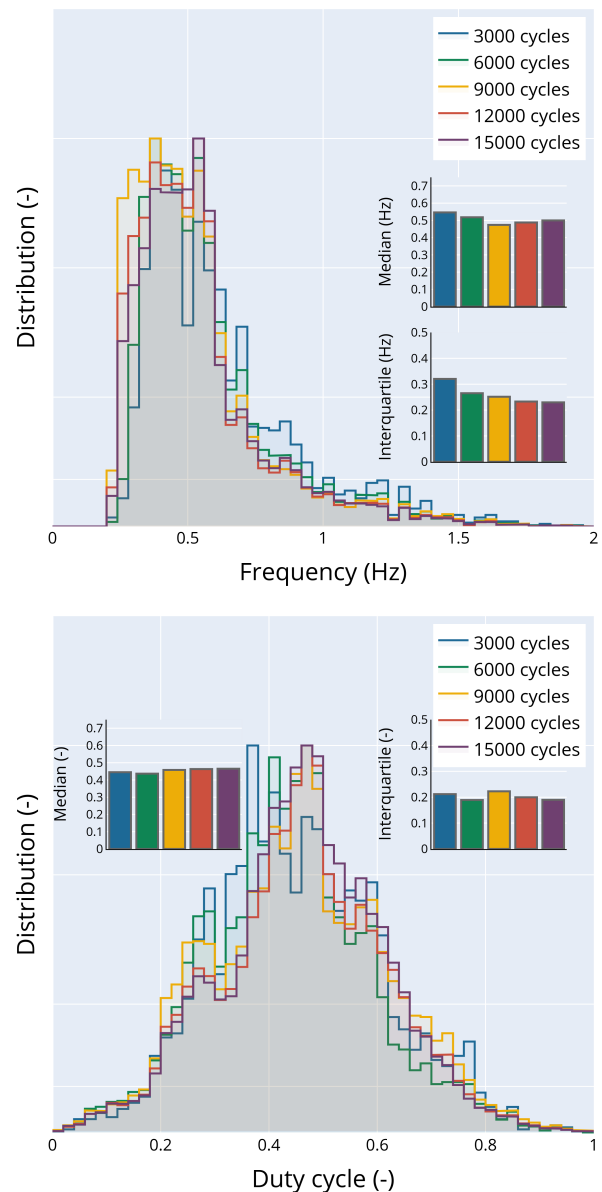


Fig. 19. Convergence of the distributions of the cycle properties (Top - Frequency. Bottom - Duty cycle), as a function of the number of cycle considered

7. P. J. Roache. Perspective: A Method for Uniform Reporting of Grid Refinement Studies. *Journal of Fluids Engineering*, 116(3):405–413, September 1994. ISSN 0098-2202. .
8. G. Haller. Lagrangian coherent structures from approximate velocity data. *Physics of Fluids*, 14(6):1851–1861, June 2002. ISSN 1070-6631. .
9. Constantin Habes, Alexandra von Kameke, Mohammed Elwardi Fadeli, and Holger Marschall. lcs4Foam – An OpenFOAM Function Object to Compute Lagrangian Coherent Structures. *OpenFOAM® Journal*, 4:118–131, November 2024. ISSN 2753-8168. .
10. Jörg Degen, Andrea Uebele, Axel Retze, Ulrike Schmid-Staiger, and Walter Trösch. A novel airlift photobioreactor with baffles for improved light utilization through the flashing light effect. *Journal of Biotechnology*, 92(2):89–94, December 2001. ISSN 0168-1656. .
11. Wendie Levasseur, Patrick Perré, and Victor Pozzobon. *Chlorella vulgaris* acclimated cultivation under flashing light: An in-depth investigation under iso-actinic conditions. *Algal Research*, 70:102976, March 2023. ISSN 2211-9264. .

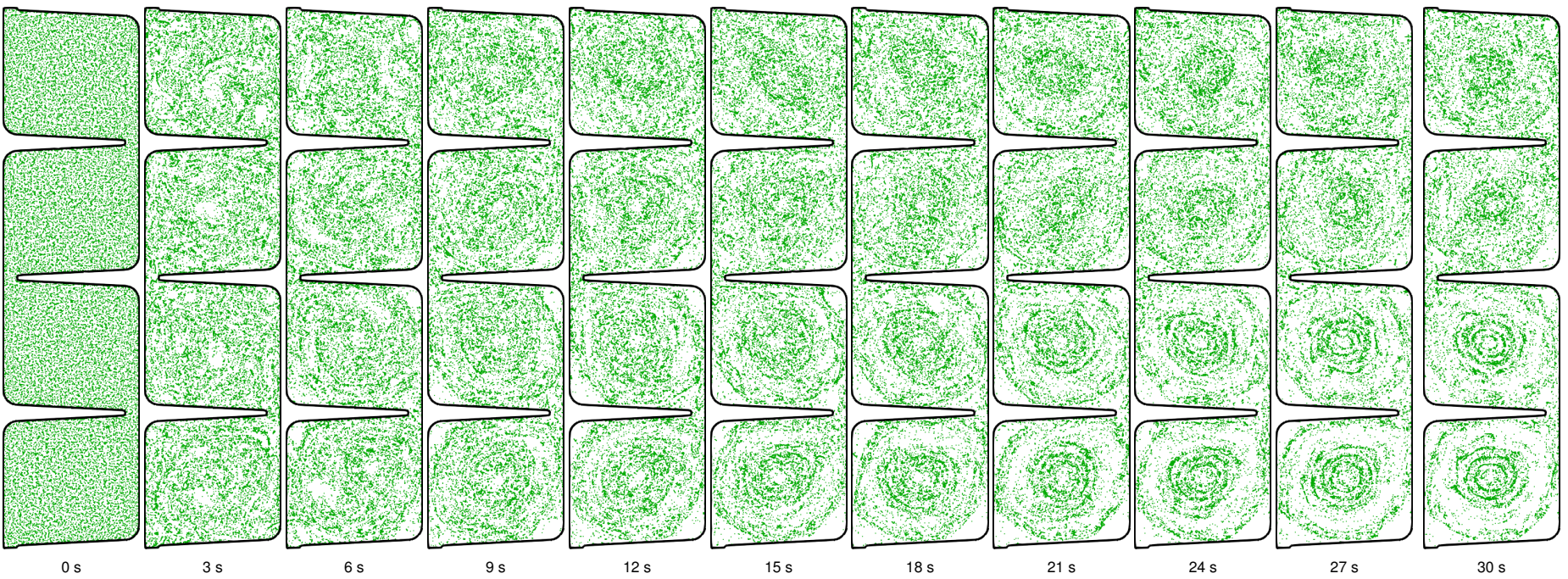


Fig. 20. 25 000 positions (green dots) over 30 seconds. Air inlet - bottom left. Air outlet - top left

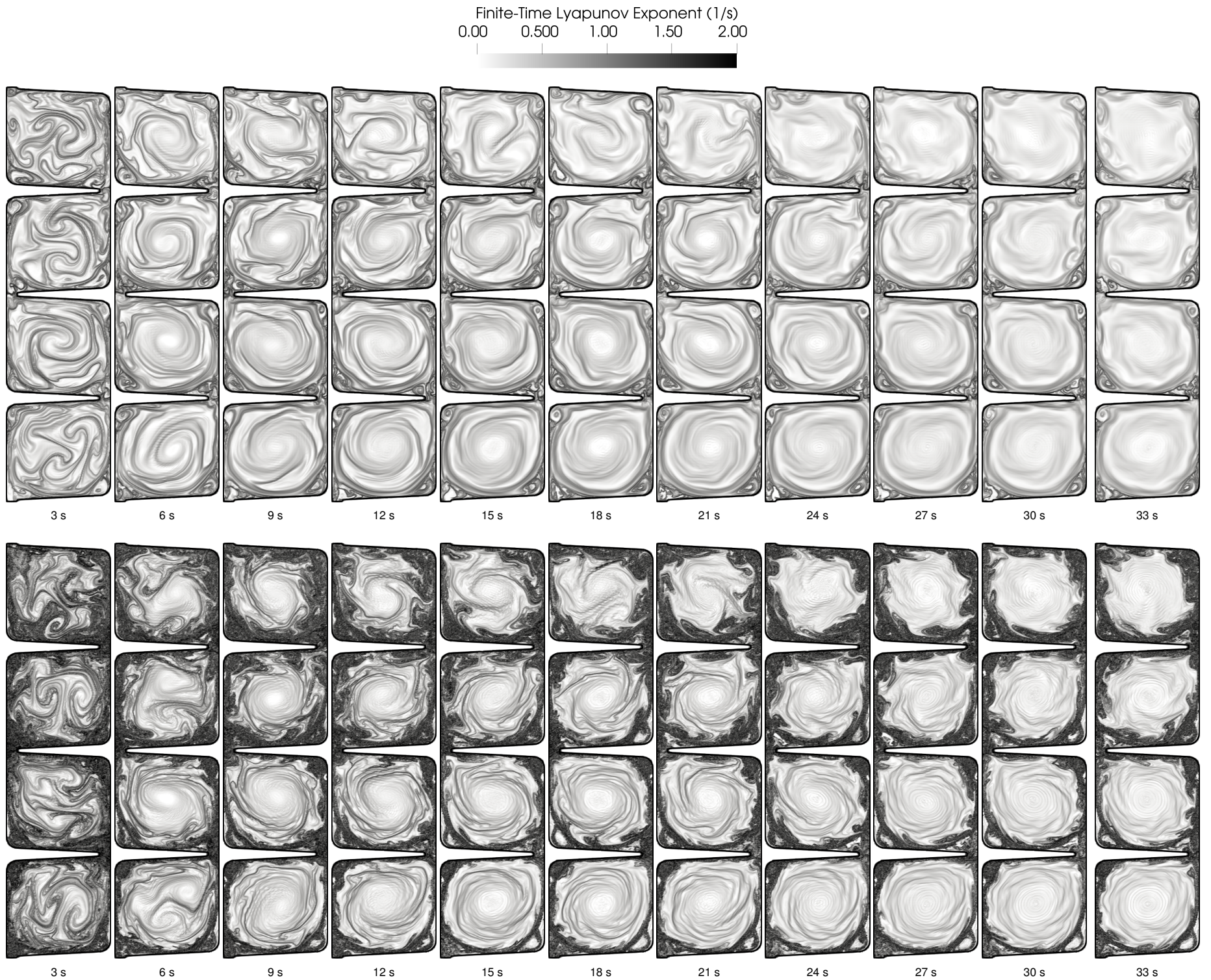


Fig. 21. Lagrangian Coherent Structures integrated over 2.66 seconds. Top - Backward integration (attracting structures). Bottom - Forward integration (repelling structures)