

bradscholars

CFD as a tool to optimize aeration tank design and operation

Item Type	Article
Authors	Karpinska, A.M.;Bridgeman, John
Citation	Karpinska AM and Bridgeman J (2018) CFD as a tool to optimize aeration tank design and operation. Journal of Environmental Engineering 144(2).
DOI	https://doi.org/10.1061/(ASCE)EE.1943-7870.0001307
Rights	©2017 American Society of Civil Engineers. Reproduced in accordance with the publisher's self-archiving policy. This material may be downloaded for personal use only. Any other use requires prior permission of the American Society of Civil Engineers. This material may be found at https://ascelibrary.org/doi/pdf/10.1061/%28ASCE%29EE.1943-7870.0001307
Download date	2025-05-28 03:38:43
Link to Item	http://hdl.handle.net/10454/15323



The University of Bradford Institutional Repository

<http://bradscholars.brad.ac.uk>

This work is made available online in accordance with publisher policies. Please refer to the repository record for this item and our Policy Document available from the repository home page for further information.

To see the final version of this work please visit the publisher's website. Access to the published online version may require a subscription.

Link to publisher's version: <https://ascelibrary.org/doi/pdf/10.1061/%28ASCE%29EE.1943-7870.0001307>

Citation: Karpinska AM and Bridgeman J (2018) CFD as a tool to optimize aeration tank design and operation. *Journal of Environmental Engineering* 144(2).

Copyright statement: ©2017 American Society of Civil Engineers. Reproduced in accordance with the publisher's self-archiving policy. This material may be downloaded for personal use only. Any other use requires prior permission of the American Society of Civil Engineers. This material may be found at <https://ascelibrary.org/doi/pdf/10.1061/%28ASCE%29EE.1943-7870.0001307>

CFD as a Tool to Optimise Aeration Tank Design and Operation

Anna M. Karpinska, PhD¹ and John Bridgeman, PhD²

¹ Research Fellow, Department of Civil Engineering, School of Engineering, University of Birmingham, Birmingham, B15 2TT, United Kingdom. Email: annamkportela@gmail.com

² Professor of Environmental Engineering, Department of Civil Engineering, School of Engineering, University of Birmingham, Birmingham, B15 2TT, United Kingdom.

ABSTRACT

In a novel development on previous computational fluid dynamics (CFD) studies, the work reported here employed an Eulerian two-fluid model with the shear stress transport (SST) $k - \omega$ turbulence closure model and bubble interaction models to simulate aeration tank performance at full scale and to identify process performance issues resulting from design parameters and operating conditions. The current operating scenario was found to produce a fully developed spiral flow. Reduction of the air flow rates to the average and minimum design values led to a deterioration of the mixing conditions and formation of extended unaerated fluid regions. The influence of bubble-induced mixing on the reactor performance was further assessed via simulations of the residence time distribution (RTD) of the fluid. Internal flow recirculation ensured long contact times between the phases; however, hindered axial mixing and the presence of dead zones were also identified. Finally, two optimization schemes based on modified design and operating scenarios were evaluated. The adjustment of the air flow distribution between the control zones led to improved mixing and a 20 % improvement to the mass transfer coefficient. Upgrading the diffuser grid was found to be an expensive and ineffective solution, leading to worsening of the mixing conditions and yielding the lowest mass transfer coefficient compared to the other optimization schemes studied.

26 INTRODUCTION

27 The activated sludge (AS) process is a well documented standard for many municipal
28 wastewater treatment plants (WWTPs) worldwide. Regardless of the site-specific process
29 configuration, AS systems rely on a steady energy supply for operation of air compressors
30 and recycling pumps (Karpinska Portela 2013). Aeration is the most energy-intensive unit
31 process at municipal WWTPs and accounts for the largest fraction of the total net electricity
32 expenditure (45-85 %) (Reardon 1995; WEF 2009). The importance of the linkage between
33 water and energy has been recognized globally in the context of water shortages, increasing
34 energy and material costs, climate change and food availability. To address this, the historical
35 high energy use of aeration systems and relatively low standard oxygen transfer efficiencies
36 of aeration devices must now be addressed via implementation of cost-effective energy
37 management measures and engineering practices.

38 However, design and operation of AS systems is still largely based on empiricism, general
39 guidelines and operator experience, often with little regard for the influence of site-specific
40 tank hydraulics, type, number and distribution of aerators and mixers, energy input or the
41 influence of mixing on efficient distribution of the dissolved and suspended components in
42 the AS bioreactor (Karpinska and Bridgeman 2016; Samstag and Wicklein 2012). Numerical
43 modelling of WWTPs has been recognized as a powerful tool, providing detailed knowledge
44 of the unit processes, as well as reactor behaviour in response to varying input conditions.
45 Over the last two decades the fast growth in computational power and commercialization of
46 advanced software suites for the solution and visualization of complex flows has contributed
47 to the successful spread of computational fluid dynamics (CFD) in wastewater engineering
48 (Karpinska and Bridgeman 2016).

49 A key advantage of CFD-aided modelling of aeration tanks over the traditional and relatively
50 well-established Activated Sludge Models (ASM) is its capacity to predict the actual flow

51 field in multiphase non-ideal reactor systems, accounting for local scale phenomena,
52 interfacial mass transfer and chemical reactions. A few workers have attempted to couple
53 hydrodynamics with biokinetics to simulate the combined physical-chemical-biological
54 processes within different AS system configurations, e.g. a full-scale oxidation ditch aerated
55 with diffusers (Glover et al. 2006) and a lab-scale channel reactor aerated with porous tube
56 (Le Moullec et al. 2010). While it was possible to predict simultaneously the hydrodynamics
57 and its impact on the biochemical conversion of organics and nutrients by AS biomass,
58 differences between concentration profiles obtained experimentally and those predicted by
59 the numerical model were identified and reported. These errors arose from excessive model
60 simplifications, use of a coarse grid necessitated by RAM/CPU constraints, and the need for
61 simulation runs in realistic time frames. Consequently, the coupled CFD-ASM simulation of
62 AS tanks remains a challenge, due to the complexity of the models involved and the solution
63 accuracy which demands a high level of mesh refinement resulting in significant
64 computational requirements and long run times (Karpinska and Bridgeman 2016). Therefore,
65 common practice is to simplify the modelling approach in a computationally efficient
66 manner, to simulate individual components of the AS system separately, and to couple the
67 results afterwards (Pereira et al. 2012). The literature offers several examples of the use CFD
68 to study aeration process in different AS systems, e.g. to acquire an insight into the mutual
69 interaction between the phases and the global and local mass transfer coefficients (Cockx et
70 al. 2001; Fayolle et al. 2007), to assess the impact of the diffuser arrangement on mixing
71 patterns and nitrification (Gresch et al. 2011) and to identify operating scenarios that promote
72 the formation of anoxic zones reducing energy expenditure on aeration (Yang et al. 2011).

73 To date, no agreed protocol for robust CFD modelling of aeration tanks has been defined.
74 Nonetheless, the modelling procedure exploiting the most computationally inexpensive
75 modelling scenario, based on the Reynolds-Averaged Navier-Stokes (RANS) equations

76 closed by the standard $k - \varepsilon$ model, a neutral density Eulerian model, and constant bubble
77 size assumption has become widely accepted by the wastewater modelling community as a
78 standard approach (Karpinska and Bridgeman 2016; Samstag et al. 2016). However, the
79 pitfalls of that modelling scheme have been reflected in overestimated values of the
80 volumetric mass transfer coefficient $k_L a$ (Fayolle et al. 2007; Le Moullec et al. 2010).
81 Nonetheless, the proposed method to rectify this error focused exclusively on determination
82 of the actual bubble sizes either experimentally or through implementation of add-on
83 statistical models. This underestimated the influence of the dispersed model on predicted
84 values of turbulent kinetic energy dissipation rate ε , involved in computation of the mass
85 transfer coefficient, $k_L a$, and hence the simulations of dissolved oxygen (DO) and organics
86 and nutrients transformations in the AS process (Karpinska and Bridgeman 2017).

87 Unlike most previous CFD models of aeration systems, the work reported here used the SST
88 $k - \omega$ turbulence model (Menter 1994) to account for the turbulent interactions between the
89 gas and liquid phases to analyse the performance of a full-scale conventional plug flow AS
90 tank aerated and mixed by means of fine pore diffusers. Moreover, the dynamic changes in
91 bubble sizes due breakage and coalescence were simulated using the Hibiki-Ishii model
92 (Hibiki and Ishii 2000) embedded into the transport equation for interfacial area
93 concentration (IAC). The selection of this modelling approach, developed previously for the
94 lab-scale aeration tanks (Karpinska and Bridgeman 2017) was justified by its reliability in
95 prediction of the turbulent interactions between the phases and resulting oxygen transfer,
96 outperforming the standard $k - \varepsilon$ model. The impact of the design and operating parameters
97 on the flow field induced by the aeration system and the resulting gas holdup were assessed
98 to detect and quantify the shortcomings of each operating scenario. Simulations of the RTD
99 of the fluid in the AS tank were performed to determine the influence of the current operating
100 conditions on the macromixing and reactor performance and to quantify site-specific process

101 limitations. Finally, two optimization scenarios based on the modification of either operating
102 parameters or diffuser density were evaluated taking into consideration mixing and oxygen
103 mass transfer in the tank.

104 **METHODS**

105 **Full-scale Aeration Tank**

106 WWTP 'A', located in the Midlands region of the UK serves a population equivalent of
107 450000 and treats an average 120000 m³ of wastewater each day. Biological treatment
108 consists of three AS modules, each having four identical, rectangular plug flow tanks aerated
109 by means of fine pore diffusers. The single AS tank has an active volume of approximately
110 5000 m³ and consists of anoxic and aerated compartments separated by a baffle (Fig. 1a). The
111 anoxic zone constitutes 11 % of the total tank volume. The average influent flow rate into the
112 single tank is 10800 m³ d⁻¹ (max. 20000 m³ d⁻¹), and the Return Activated Sludge (RAS) flow
113 rate is 6750 m³ d⁻¹ (max. 12500 m³ d⁻¹). The tank is equipped with 1920 dome diffusers fixed
114 over the tank bottom in a full-floor coverage configuration (Fig. 1b). The aeration system is
115 divided into two control zones, Z1 and Z2 (Fig. 1c), with differing diffuser density and
116 operating air flow rates. The airflow distribution between Z1 and Z2 is 60 and 40 %,
117 respectively. The process design parameters characterizing aeration system are listed in Table
118 1. For convenience, the parameters enabled in optimization studies are also included in the
119 table. Currently, the AS tanks are operated at the average influent and maximum design air
120 flow rate. The target DO concentration in both zones is 2.0 mg L⁻¹.

121 **Numerical Studies - CFD**

122 *3D geometry and mesh*

123 The three-dimensional (3D) geometry of the aeration tank was designed using ANSYS 17.0
124 Design Modeler pre-processor. The work presented here considered only the aeration tank

125 compartment, hence the anoxic zone was not included in the computational domain. The grid
126 was generated using sweep and patch conforming methods and the face sizing function was
127 used to refine the mesh in the diffuser regions (Supplementary Information, Fig. S1). Three
128 meshes, comprising 1.2 to 3.8 million hexa- and tetrahedral cells were produced initially
129 (Table 2).

130 The Grid Convergence Index (GCI) approach (Roache 1998) was employed in grid
131 refinement studies as a recommended uncertainty estimator method. The outcomes of the
132 GCI calculations and the grid independence studies are provided in Supplementary
133 Information (Table S1 and Figs. S2-S3, respectively). The results indicated that mesh 2,
134 having 2.2 million elements, was appropriate for the subsequent modelling work.

135 *Modelling approach*

136 Simulations of the hydrodynamics, mass transfer and macromixing in the lab-scale aeration
137 tank were performed using ANSYS 17.0 Fluent CFD software. Each simulation was run in
138 parallel on the University of Birmingham BlueBEAR Linux HPC Cluster using dual-
139 processor 8-core (16 cores/node) 64-bit 2.2 GHz Intel Sandy Bridge E5-2660 worker node
140 with 32 GB of RAM.

141 *Hydrodynamics*

142 The multiphase flow in AS tank was simulated with an Eulerian two-fluid model derived
143 from unsteady RANS (URANS) equations and the two-equation SST $k - \omega$ turbulence
144 model, following Karpinska and Bridgeman (2017). The governing equations representing
145 conservation of mass and momentum for each phase, described comprehensively in
146 Karpinska and Bridgeman (2016) and the bubbly flow models, can be found in
147 Supplementary Information.

148 *Mass transfer*

149 The aeration process was reproduced numerically via a species mass transfer model. Oxygen
 150 was treated as an active scalar and the effects of its gradients across the domain were coupled
 151 to the momentum equation. Two scalars representing transport of concentration in the
 152 primary and secondary phase can be written in general form following Talvy et al. (2007):

$$\frac{\partial \alpha_{ph} c_{ph}}{\partial t} + \vec{\nabla}(\alpha_{ph} c_{ph} \vec{v}_{ph}) = -\vec{\nabla}(\alpha_{ph} (\vec{J}_{ph} + \overline{c'_{ph} v'_{ph}})) + \overline{c_{ph} \dot{m}_{ph}} + \overline{L_{ph}} \quad (1)$$

153 where α_{ph} is volume fraction of liquid/gas phase, c_{ph} is local instantaneous scalar
 154 concentration in phase, t denotes time, \vec{J}_{ph} is the flux due to molecular diffusion, the term
 155 $\overline{c'_{ph} v'_{ph}}$ denotes turbulent diffusion of the concentration, $\overline{c_{ph} \dot{m}_{ph}}$ represents the transport of
 156 concentration c_{ph} by mass transfer and L_{ph} is interfacial transfer of concentration between
 157 the phases.

158 The interfacial oxygen mass transfer occurring between air bubbles and liquid phase can be
 159 written as (Talvy et al. 2007):

$$\overline{L_{ph}} = \overline{L_L} = k_L a (C_L^* - C_L) \quad (2)$$

160 where L_L is interfacial mass transfer between air bubble and liquid, k_L is the local mass
 161 transfer coefficient, a is the interfacial area, C_L^* is oxygen saturation concentration, C_L is
 162 actual oxygen concentration and the term $(C_L^* - C_L)$ is the driving force causing oxygen
 163 transfer.

164 The local mass transfer coefficient k_L is obtained from the Higbie penetration theory (Higbie
 165 1935):

$$k_L = 2 \sqrt{\frac{D_L v_r}{\pi d_b}} \quad (3)$$

166 where D_L is molecular diffusion coefficient of oxygen in water at 20°C, v_r is relative velocity
 167 between the phases and d_b is bubble diameter.

168 The interfacial area a is calculated as (Fayolle et al. 2007):

$$a = \frac{6}{d_b} \frac{\alpha_G}{1 - \alpha_G} \quad (4)$$

169 where α_G denotes volume fraction of air phase.

170 In the work reported here, the global volumetric mass transfer coefficient $k_L a$ was
 171 implemented via a User Defined Function (UDF) routine written in C language. Successively,
 172 the α factor, being a factor applied to the mass transfer coefficient to account for substrate
 173 and nutrient loading variations within the reactor, was used to modify (i.e. reduce) the CFD-
 174 derived $k_L a$ in standard conditions ($= k_L a_{20}$) in order to account for the effects of shrinking
 175 gas-liquid interface surface area due to surfactant accumulation on the bubble and mean cell
 176 residence time. Considering a plug flow AS system characterized by varying substrate
 177 loading along the tank, the recommended values of $0.3 < \alpha < 0.8$ (WPCF-ASCE 1988) were
 178 applied to represent oxygen transfer rates in process conditions ($\alpha k_L a_{20}$) in both control
 179 zones.

180 *Macromixing*

181 The overall mixing in the aeration tank was studied numerically through the simulation of a
 182 pulse tracer experiment. The RTD of the fluid (Danckwerts 1953) was computed from the
 183 time history of a tracer concentration recorded at the outlet of the aeration tank. The transport
 184 of the nonreactive tracer injected into the fluid entering the tank at the inlet was modelled
 185 using a passive scalar approach, based on prediction of the local mass fraction of tracer
 186 species, Y_{tr} . Assuming no tracer production in the system, its transport due to convection and
 187 diffusion can be written in the general form as (Glover et al. 2000):

$$\frac{\partial}{\partial t} (\rho_L Y_{tr}) + \nabla (\rho_L \vec{v}_L Y_{tr}) = -\nabla \vec{J}_{tr} + S_{tr} \quad (5)$$

188 where ρ_L denotes density of the liquid, \vec{v}_L is velocity of the liquid phase, \vec{J}_{tr} is diffusive mass
189 flux of tracer; and S_{tr} is the source term which injects tracer into the domain by addition any
190 user-defined sources.

191 The RTDs of the fluid expressed as normalized exit age distribution function $E(t)$ is defined
192 as (Fogler 1999; Levenspiel 1999):

$$E(t) = \frac{Q_e C(t)}{M} \quad (6)$$

193 where Q_e is the effluent flow rate, M is the quantity of the introduced tracer and $C(t)$ denotes
194 concentration-time series recorded in the outflow from the tank.

195 The observed mean residence time τ is (Levenspiel 1999):

$$\tau = \frac{\int_0^{\infty} tC dt}{\int_0^{\infty} C dt} \cong \frac{\sum_i t_i C_i \Delta t_i}{\sum_i C_i \Delta t_i} = \frac{V}{Q_e} \quad (7)$$

196 where V denotes the reactor volume.

197 Additional modelling details can be found in Supplementary Information.

198 ***Model setup, boundary and operating conditions***

199 The properties of the primary and secondary phases are summarized in Table 3. The
200 modelling of hydrodynamics and mass transfer in the aeration tank was achieved by setting
201 water and air as a working fluid. A parallel modelling scenario based on the passive scalar
202 approach was run, in which the continuous phase was defined as a mixture of water and AS.
203 RTD simulations considered a tracer having physical properties equal to those of water. The
204 boundary and operating conditions were summarized in Table 4.

205 Convergence criteria for the solutions were set at 10^{-6} . For the sake of stability of
206 convergence of the SST $k - \omega$ model, the first 10^5 iterations were run with an initial time
207 step size (Δt) of 0.001 s. With stable residual monitors, Δt was gradually increased to 0.1 s.

208 All the hydrodynamic simulations considered a flow time equivalent to 24 h (≈ 2.5 times
209 greater than the designed hydraulic retention time, $\tau = 9.6$ h). The RTD simulations
210 considered a flow time of 50 h.

211 **Experimental Studies**

212 *Measurement of the liquid-phase velocity*

213 The 3D velocity of the mixed liquor was measured using an acoustic Doppler velocimeter
214 (ADV) (Nortek AS, model Vectrino Plus), operating at acoustic frequency of 10 MHz,
215 sampling rate of 200 Hz and with 7 mm vertical extent of the sampling volume. The
216 measurements were performed from a platform located above Z2 and at a distance (L) of 30.0
217 m from the outflow weir. Location of the measurement points was dictated by access and
218 power restrictions. The velocity was measured in 10 points distributed across the lane at two
219 depths (y), 0.3 and 0.7 m below the surface. The ADV sensor was attached to a custom-made
220 aluminium structure fixed to the handrail to render it immobile. During measurements, a total
221 of 40000 velocity data points were collected at each measurement location. In order to
222 remove invalid data noise (related to the presence of the dispersed air bubbles moving with
223 different velocities than the liquid phase and, to a lesser extent, due to Doppler signal aliasing
224 (Mori et al. 2007)), the output ADV velocity time-series were processed by Velocity Signal
225 Analyser (VSA) software (Jesson et al. 2015) using a correlation and signal-to-noise-ratio
226 (SNR) pre-filter, Modified Phase-Space Thresholding (PST) despiking filter and linear
227 interpolation method of spike replacement. The ADV data-cleaning procedure is discussed in
228 detail in Karpinska and Bridgeman (2017).

229 *Mixed liquor analysis*

230 Composition of the mixed liquor in the AS tank was evaluated from the results of
231 measurements of DO and Mixed Liquor Suspended Solids (MLSS) and the analyses of the

232 Biochemical Oxygen Demand (BOD), ammonia nitrogen ($\text{NH}_4\text{-N}$), and nitrates ($\text{NO}_3\text{-N}$)
233 concentrations in samples taken from ten points distributed along the aeration tank. Access
234 limitations meant that location of the measurement points was restricted to 0.4 m from the
235 external wall. MLSS concentrations were measured in 36 points within the same vertical
236 cross-section over Z2 as the liquid velocity. MLSS and DO concentrations were measured
237 directly with optical sensors (Hach HQ40 IntelliCal LDO101 Field Luminescent DO probe
238 and Partech 740 Monitor) fixed to a submerged telescopic support. In order to determine
239 longitudinal concentration profiles, DO and MLSS concentrations were measured at each
240 sampling point at three depths: *viz.* 0.1 m below the fluid surface; at mid-depth (2.60 m); and
241 just above the diffusers, at 5.0 m. BOD and nutrients were determined indirectly from
242 analyses of the mixed liquor samples pumped carefully from the same three depths from the
243 sampling points. 50 mL aliquots were transferred to labelled plastic containers and
244 transported to the laboratory for immediate colorimetric assays using a Hach DR/890
245 Portable Colorimeter and Hach Test'N Tube Vial kits: AmVer™ Salicylate Method and
246 NitraVer™ X Chromotropic Acid Method. BOD was determined in accordance with
247 Luminescence Measurement of DO in Water and Wastewater using Hach HQ40 IntelliCal
248 BOD LDO.

249 **RESULTS AND DISCUSSION**

250 **Concentration Patterns in a Full-scale AS Tank**

251 Preliminary experiments were performed to gain an insight into the site-specific aeration
252 process performance. Fig. 2 illustrates the DO, BOD and nutrients concentration profiles
253 along the full-scale AS tank. Relatively minor DO concentration gradients were observed
254 over the depth in the majority of the measurement points in Fig. 2a. These are likely to be an
255 effect of the rising bubbles from the diffusers promoting vertical mixing. DO levels measured
256 from the anoxic tank along the first 50 m were low ($0.3 - 1.0 \text{ mg L}^{-1}$). Thereafter, DO

257 concentrations rose in an approximately linear manner for 50 m to a maximum DO
258 concentration of 3.1 mg L^{-1} , whereupon they decreased, again linearly, to 1.1 mg L^{-1} at the
259 outlet. At the same time, the readings from the WWTP's online LDO analysers (Hach Lange
260 sc100) for sensors located in the middle of the lane at depth of 1.0 m were: 0.35 mg L^{-1} in Z1;
261 and 3.08 mg L^{-1} in Z2, compared to the set-point values of 2.0 mg L^{-1} . During several visits to
262 the WWTP, the same trend of non-equal DO concentrations in both zones was observed.

263 Oxygen transfer rates in the AS tank are governed by the local hydrodynamics; hence the
264 variations in DO concentration are a function of the hydrodynamic time-scales (in seconds).
265 For this reason, thorough analysis of the specific DO patterns in Fig. 2a requires assessment
266 of the overall mixing phenomena, accounting for the site-specific process conditions, such as
267 diffusers age and performance and wastewater temperature. At the same time, BOD and
268 nutrients concentrations are governed by biokinetic time-scales (sludge age) measured in
269 days. Hence, the concentration profiles shown in Figs.2 b-d mirror the longer-term effects of
270 the adopted aeration scenario rather than response to the actual oxygenation rates.

271 Accordingly, while there is no clear pattern in vertical distribution of the concentrations, the
272 biokinetic-related parameters shown all correlate with each other as expected.

273 Similar to DO, the MLSS distribution within the tank is closely related to the local
274 hydrodynamics. The longitudinal evolution of the MLSS profile is shown in Figure 3a. The
275 solids content along the length of the tank ranged from 3160 to 3420 mg L^{-1} . MLSS sensor
276 readings at three depths within the same sampling point differed by less than 5 %. Fig. 3b
277 shows the transverse MLSS profile through Z2. The MLSS concentration measured in 36
278 points was found to vary from 3280 to 3360 mg L^{-1} (a difference of 2.4 %), indicating
279 approximately homogenous distribution of the solids in the section analysed. The
280 approximately uniform solids content (Figs. 3a-b), and the lack of evident settling zones

281 associated with locally increased MLSS values, are a result of the favorable mixing
282 conditions achieved at the given operating air flow rate.

283 **Validation of the CFD Model**

284 Preliminary numerical studies considered two different simulation schemes for prediction of
285 the flow field in the aeration tank. The results of the simulations performed for water-air and
286 water-air-sludge scenarios subject to the same operating air and influent flow rates (Q_a and
287 Q_L) yielded similar velocity contour maps and distribution of the velocity vectors
288 (Supplementary Information, Fig. S4) and hence the less computationally expensive neutral
289 density simulations were found to be suitable to represent liquid flow patterns within the AS
290 tank.

291 To validate the CFD model used in prediction of the air-induced mixing of the liquid phase,
292 despiked ADV data points representing average velocity magnitude were plotted against CFD
293 results corresponding to the measurement points across zone Z2 (Fig. 4). The figures
294 illustrating raw and despiked velocity-time series and the resulting velocity magnitude are
295 provided as Supplementary Information (Figs. S5-S7). The CFD simulations were performed
296 considering actual operating conditions in the AS tank, *viz.* the average influent flow rate
297 ($Q_L = 0.1 \text{ m}^3 \text{ s}^{-1}$) and the maximum air flow rate ($Q_a = 1.1 \text{ m}^3 \text{ s}^{-1}$). The average liquid velocity
298 magnitude in the analysed cross-section measured at depths of 0.3 and 0.7 m varied from 0.12
299 to 0.22 m s^{-1} and from 0.15 to 0.18 m s^{-1} , respectively. When comparing the numerical and
300 experimental results shown in Fig. 4 it is evident that the CFD model reproduced the values
301 of the local velocities at measurement points located at $L = 0.4, 1.9$ and 3.3 m ($y = 0.3 \text{ m}$)
302 and $L = 0.4, 3.3$ and 6.3 m ($y = 0.7 \text{ m}$), respectively with good accuracy. The liquid
303 velocities at $L = 6.3 \text{ m}$ ($y = 0.3 \text{ m}$) and 1.9 m ($y = 0.7 \text{ m}$), although slightly overestimated
304 by the numerical model, were still in good agreement with the experimental data. However,
305 at $L = 4.8 \text{ m}$ from the internal wall, the CFD model overestimated the velocities at both

306 depths. One reason for the difference between the measurement and simulation results may
307 be that the SST $k - \omega$ model is based on the Bussinesq isotropic eddy viscosity assumption,
308 which may lead to inaccurate prediction of the flows driven by anisotropy of the normal
309 Reynolds stresses and secondary shear stresses, and flows characterized by large extra strains
310 (Bridgeman et al. 2008). Alternatively, the discrepancy may be a result of poor aerator
311 performance, likely due to the device ageing, fouling and scaling. While CFD simulations did
312 account for the uniform flow distribution to each diffuser and non-uniform inlet bubble sizes
313 to approximate changes in diffuser porosity over time, the possibility of faulty performance
314 of partially or entirely clogged diffusers below the ADV sensor was not considered.
315 Nonetheless, good agreement between the numerical and experimental data in 8 of 10
316 measurement points provides confidence that the CFD model was able to predict the
317 hydrodynamics of the full-scale aeration tank.

318 **Impact of the Operating Conditions on the Hydrodynamics in AS Tank**

319 Figs. 5 and 6 show the liquid and air velocity magnitude and air holdup in the aeration tank
320 for different operating conditions. In Fig. 5, the vector and contour maps on the left side
321 represent vertical cross-sections through zones Z1 and Z2 at $L = 30.0$ m, while the contour
322 maps on the right side (with flow direction indicated by an arrow), relate to the horizontal
323 cross-section through the mid-depth ($y = 2.6$ m).

324 Gas holdup is a key hydrodynamic parameter governing distribution of the interfacial surface
325 area between the air and liquid phases. Thus, for the given diffused air system, selection of
326 the optimal operating conditions yielding higher air holdups is essential to achieve oxygen
327 transfer rates required by the AS process. Fig. 6 shows that the spatial distribution of the gas
328 holdup in the analysed sections follows the pattern observed in air velocity profiles. Slightly
329 higher air velocities and volume fractions observed in zone Z1 result from the more dense
330 arrangement of the diffusers in comparison with zone Z2. Flow regions characterized by the

331 highest air velocities are usually associated with either presence of larger bubbles, including
332 those generated in coalescence-inducing turbulent flow conditions, or with the co-current
333 flow of both phases. Low-air velocity regions are associated with counter-current movement
334 of swarms of minute bubbles having larger interfacial surface areas, a proportion of which
335 may have been generated due to impact with turbulent eddies.

336 Figs. 5a-6a show the CFD results obtained for the actual operating conditions at the WWTP.
337 The current aeration scenario results in fully developed spiral flow, characterized by liquid
338 loop circulation with limited mixing in the axial direction. The smallest fluid velocities occur
339 in the centre of the rotating cells and in the bend of the tank, as seen in the horizontal velocity
340 profile (Fig. 5a). The decrease in air holdup observed in Z2 (Fig. 6a) is likely to be due to the
341 larger intervals between the diffuser rows (Fig. 1c). This operating scenario resulted in some
342 aeration of the central portion of the tank, as shown by the higher values of air volume
343 fractions (up to 0.6 %), whereas adjacent to the lateral walls and above the tank bottom, the
344 air holdup decreases to zero, possibly linked to the occurrence of the locally lower DO
345 concentrations.

346 Similar spiral flow patterns were observed for the average operating air flow rate of $0.7 \text{ m}^3 \text{ s}^{-1}$
347 (Fig. 5c); however, a decrease of the liquid velocities and smoothed flow patterns in the
348 horizontal section through the tank were also observed. Furthermore, a significant decrease in
349 values of the gas holdup in the tank to around 0.3 % was also observed (Fig. 6c), giving rise
350 to lower oxygenation capacities imposed by this operating mode.

351 Doubling the influent flow rate to the maximum design value Q_L of $0.2 \text{ m}^3 \text{ s}^{-1}$ resulted in the
352 formation of two circulating counter-current flow loops observed in the section through Z1
353 (Fig. 5b). This flow pattern was observed to destabilize over the length of the reactor,
354 resulting in re-occurrence of the single rotating cell in Z2. The influence of the air velocity
355 shown in Fig. 6b on the liquid flow field is also evident. At the same time, the increase of the

356 liquid velocities yielded an improved distribution of the gas holdup in Z2 compared to the
357 current operating scenario (Fig. 6a).
358 The lowest air flow rate of $0.5 \text{ m}^3 \text{ s}^{-1}$ yielded the poorest air mixing scenario in terms of
359 increased percentage of the tank regions where fluid velocity was found to drop below 0.1 m
360 s^{-1} (Fig. 5d), giving rise to possible sludge settling. The change of the $Q_L : Q_a$ ratio led to
361 formation of two counter-current rotating cells along the whole tank. Nonetheless, this
362 operating air flow rate was insufficient to aerate the tank contents sufficiently (Fig. 6d),
363 yielding the lowest air holdup of around 0.1 %.
364 Considering the results of the simulations performed for all aeration process design
365 parameters, the choice of the current operating scenario for the average Q_L ensuring highest
366 air holdups is justified. Therefore, the subsequent studies reported below focus on further
367 characterization of the mixing patterns within the tank induced by the diffusers operated at
368 maximum air flow rate.

369 **Residence Time Distribution**

370 The RTD of the fluid in the AS tank was calculated to evaluate the impact of the flow
371 patterns induced by the site-specific aeration system on the macromixing and the reactor
372 performance. Evolution of the $E(t)$ curve shown in Fig. 7 corresponds to the typical output
373 curve of n -CSTRs (Continuous Stirred Tank Reactors) in series. The observed mean
374 residence time τ (vertical dashed line) was 8.3 h, 14 % shorter than the design value of 9.6 h.
375 The analysis of the area below the $E(t)$ curve showed that by time $t = \tau$, 60% of the injected
376 tracer had exited the AS tank, whilst its complete removal from the system took place after
377 40 h ($=4.8 \tau$). It is believed, that the prolonged contact time between the phases (indicated by
378 $t > \tau$) is likely to have been caused by the internal recirculating eddies in the vertical
379 direction, usually associated with flow patterns of the rising bubbles and the spiral flow (Fig.
380 5a). On the other hand, a characteristic shallow tail in the $E(t)$ curve (Fig. 7) indicates the

381 presence of stagnant fluid regions, and consequently, reduction of the active volume of the
382 tank available for biochemical processes. This outcome is also consistent with the
383 conclusions drawn from the analysis of the liquid phase velocities in Fig. 5a. Retention of the
384 remainder of the tracer in dead volumes and its hindered transport in the axial direction is
385 manifested through its delayed washout from the system, yielding a long RTD tail. Thus, it is
386 clear that the spiral flow contributes to the extension of the mixing time, whereas hindered
387 longitudinal mixing and occurrence of the stagnant fluid regions may have an adverse effect
388 on the oxygen transfer and biochemical conversion reaction rates, and therefore on the
389 efficiency of the treatment processes, and on nitrification in particular.

390 **Improvements to Mixing Patterns in the AS Tank**

391 Two scenarios for improving mixing, and hence process performance, in the aeration tank
392 were considered; *viz.* (i) alteration of the operating parameters, and (ii) modification of the
393 diffuser grid through addition of one unit to each row (Fig. S7), whilst maintaining original
394 operating influent and air flow rates (Table 1).

395 The power required for blower operation was estimated using the adiabatic compression
396 equation (Mueller et al. 2002; Tchobanoglous et al. 2003):

$$P = \frac{wRT}{29.7 \cdot 0.283 \cdot e_B \cdot e_M} \left[\left(\frac{p_{out}}{p_{in}} \right)^{0.283} - 1 \right] \quad (8)$$

397 where P is the power requirement for each blower, w is air mass flow rate, R is universal gas
398 constant for air ($R= 8.314 \text{ kJ kmol}^{-1}\text{K}^{-1}$), T is the design inlet temperature, p_{in} and p_{out} are
399 absolute pressures at the inlet assumed atmospheric and outlet assumed 2.0 atm (following
400 Quasim (1999)) of compressor, e_B and e_M are blower and motor efficiencies.

401 Assuming typical values of e_B and e_M (70 % and 92 %) the compressor power demand (Eq.
402 8) was found to be 130 kW.

403 For scenario (i), the flow distribution in the control zones Z1 and Z2 was adjusted from 60 %
404 and 40 % to 75 % and 25 % in an attempt to destabilize the spiral flow and to improve
405 aeration (higher air holdup) in zone Z1. The reduction of the air flow rate in zone Z2 aimed to
406 ensure more uniform distribution of the air bubbles within the tank volume, as observed in
407 the contour map of gas holdup in Fig. 6c.

408 The results of the CFD analyses were compared with the original design and operating
409 scheme, as shown in Fig. 8. Liquid and air velocities and gas holdup values are summarized
410 in Table 5. The operational changes resulted in an increase of the liquid velocity in the centre
411 of Z1 (Fig. 8b), reducing stagnant regions adjacent to the lateral walls and in the centre of the
412 rotating cell (Fig. 8a). However, the features of the fluid circulation loops found in the
413 original design were still preserved, especially in Z2. The average liquid velocity of 0.25 m s^{-1}
414 in cross-section Z1 was lower than in the case of the original scenario (Table 5), in contrast
415 to the horizontal section, where the new scheme yielded slightly higher fluid velocities of
416 0.23 m s^{-1} . As expected, the induced gas holdup was more uniformly distributed within both
417 zones and yielded significantly higher values up to 0.6 % in section through Z1 in
418 comparison with the original operating scheme, but distinctly lower in Z2 (0.2 %).

419 In line with expectations, the air flow split between the larger number of diffusers led to a
420 reduction of the air velocities in the control zones in comparison with the original design
421 (Fig. 8c). Diffused air is the main driving force inducing fluid motion in the tank, and
422 therefore the modified layout resulted in a 50 % decrease of the average axial liquid
423 velocities to 0.11 m s^{-1} (Table 5). The lack of spiral flow loops observed in the original
424 scenario and less intense vertical mixing manifested by lower fluid velocities were also seen
425 in the vertical section through the tank (Fig. 8c). Such flow conditions promoted longer
426 contact times between the phases providing the most homogenous aeration in both control

427 zones in comparison with other operation scenarios investigated. The air holdup of 0.5 % in
428 Z1 (Table 5) was also higher than the one resulting from the original diffusers arrangement.

429 **Oxygen Transfer in the AS Tank**

430 The oxygen transfer rate in aeration tanks is governed by several hydrodynamic parameters,
431 *viz.* bubble size, velocity and turbulence in the liquid phase and resulting gas holdup
432 (Karpinska and Bridgeman 2017). Accordingly, higher values of liquid velocities, ε and air
433 holdup were observed for all operating and design scenarios in zone Z1, resulting in distinctly
434 higher global mass transfer coefficients than in zone Z2, as seen when comparing data
435 summarized in Table 5. The maximum value of $k_L a_{20}$ of 224 d^{-1} in Z1 was reported for the
436 scheme based on an adjustment to the air flow distribution. The air holdup in Z2 was the
437 lowest, yielding a value of $k_L a_{20}$ nearly three-times lower than the original scenario. The
438 operating scheme with an increased number of diffusers was found to yield relatively high air
439 holdups in both zones, but distinctly lower liquid velocities and hence, ε (Table 5). For this
440 reason, the resulting oxygen transfer rate coefficients were lower than the ones obtained with
441 the original design scenario. After the simulated aeration time of 15 mins, a constant
442 equilibrium DO concentration was achieved for all three operating scenarios, which was in
443 the range of $10.1\text{-}10.3 \text{ mg L}^{-1}$ in both control zones (Table 5). Due to the different global
444 values of $k_L a_{20}$ in control zones, the equilibrium DO concentration in Z1 was achieved in a
445 much shorter time than in Z2 (3.7 mins for the original design, 2.2 mins for modified
446 operating scenario and 5.2 mins for modified design). Similar observations were identified
447 for the operating scenario with adjusted distribution of the air flow between the control zones.
448 In this case, improvement of the horizontal mixing and the highest mass transfer rates
449 resulted in markedly faster and uniform oxygenation of zone Z1, whereas the decrease of
450 $k_L a_{20}$ in Z2 contributed to a longer aeration time being required to achieve saturation DO
451 concentration. At the same time, modification of the diffuser density resulted in lower

452 oxygenation rates, requiring longer contact times to achieve DO equilibrium levels, but
453 characterized by a more homogenous evolution of the DO profile across the AS tank. The DO
454 profiles along and across the tank are provided in Supplementary Information (Figs. S8a-c)

455 **Discussion**

456 Analysis of the CFD results shows that adjustment of the air flow rate distribution between
457 the control zones resulted in the highest oxygen transfer rate in zone Z1, which is subject to
458 the highest (influent) BOD and ammonia loadings. Since the oxygen uptake by biomass
459 decreases over the length of the plug flow tank, further reduction of the oxygen transfer rates
460 in zone Z2 resulting from the imposed scenario should not affect overall aerobic process
461 efficiencies. However, this assumption requires further investigation through e.g.
462 experimental assessment of the oxygen transfer and biochemical reaction rates. At the same
463 time, the scenario based on the increase of diffuser density results in moderate oxygenation
464 rates in Z1, but a doubling of oxygen transfer rates in Z2 compared to the original design.
465 Nonetheless, this setup requires capital costs associated with the diffuser grid upgrade.
466 The recommended α values for plug flow tanks were used to reduce the global $k_L a_{20}$, in
467 order to represent mass transfer coefficient values in control zones Z1 and Z2 having
468 different oxygen uptake rates due to non-uniform substrate and nutrient loading along the
469 tank. Assuming that the DO profile observed in Fig. 2a was representative of the simulated
470 original operating scenario (over-aeration of the zone Z2) and comparing the data listed in
471 Table 5, modification of the diffuser layout and consequential lowering of $\alpha k_L a_{20}$ in Z1 from
472 56 to 48 d^{-1} can be seen to result in insufficient aeration performance to satisfy biodegradation
473 and nitrification oxygen requirements. In this context, modification of the process parameters
474 is the only viable among the analysed scenarios, to ensure the high oxygen transfer conditions
475 necessary to boost biochemical conversion reactions rates. In this case, the $\alpha k_L a_{20}$ in Z1 was
476 the highest (67 d^{-1}), exceeding the value obtained for the original design by almost 20 %.

477 CONCLUSIONS

478 The research presented in this paper evaluated and then improved performance of a full-scale
479 plug flow aeration tank through CFD simulations of hydrodynamics, macromixing and mass
480 transfer. The following key conclusions have been drawn:

- 481 • A validated CFD approach based on the SST $k - \omega$ turbulence closure model and the
482 IAC model was used to assess the hydrodynamics of a full-scale AS tank. The results
483 were used to identify and localize adverse phenomena resulting from the imposed
484 operating conditions. The maximum operating air flow rate resulted in formation of
485 spiral flow conditions. Increasing the influent flow to the maximum design value
486 improved mixing and aeration of the fluid volume. The results obtained with average
487 and minimum design air flow rates gave rise to the formation of extended unaerated
488 fluid volumes associated with the stagnant fluid regions, possible sludge settling and
489 limited distribution of the bubble plume.
- 490 • Macromixing data were used to assess the impact of air-driven mixing on reactor
491 behaviour and quantification of the site-specific process limitations. Internal
492 recirculation of the flow, linked to rising bubbles promoted extended contact times
493 between the phases, ensuring efficient oxygenation of the fluid. However, hindered
494 axial mixing and the presence of the dead zones reducing the active volume of the AS
495 tank are suspected to have a significant impact on the oxygen transfer and the reaction
496 yield, and thus the treatment process performance.
- 497 • Considering the optimization scenarios investigated, adjustment of the air flow
498 distribution between the control zones led to improved mixing and reduction of the
499 dead volumes, and furthermore yielded the highest $\alpha k_L a_{20}$ of 67 d^{-1} in Z1
500 outperforming the original design scenario by 20 %. The more capital intensive
501 optimization scenario related to upgrade of the diffuser grid provided a more uniform

502 aeration pattern. However, the resultant significant decrease of the fluid velocities
503 gave rise to the lowest $\alpha k_L a_{20}$ of 48 d^{-1} compared with the other scenarios. In this
504 context, modification of the process parameters would appear to be the only feasible
505 solution to ensure high oxygen transfer rates in the influent zone which is subject to
506 highest BOD and ammonia loadings.

- 507 • The CFD analysis presented in this work, validated using hydrodynamic-,
508 macromixing- and mass transfer data, demonstrates the technique's use for prediction
509 of reactor behaviour and process performance at varying operating conditions, as well
510 as troubleshooting and optimization, and provides a blueprint for future workers in the
511 field.
- 512 • The follow-up study will focus on improved experimental characterization of the
513 reactor performance, expanded through the determination of the oxygen uptake- and
514 biochemical reaction rates and the RTDs.

515 **ACKNOWLEDGEMENTS**

516 The research work of Dr. Anna M. Karpinska Portela was funded by the College of
517 Engineering and Physical Sciences, University of Birmingham, UK.

518 **NOMENCLATURE**

519 *The following symbols are used in this paper:*

520 a = interfacial area;

521 C = concentration;

522 C_L = bulk liquid phase oxygen concentration;

523 C_L^* = oxygen saturation concentration in a liquid phase;

524 c_{ph} = local instantaneous scalar concentration in phase;

525 c'_{ph} = local instantaneous concentration in phase;

- 526 D_h = hydraulic diameter;
- 527 D_L = liquid molecular diffusivity;
- 528 d_b = bubble diameter;
- 529 I = turbulence intensity;
- 530 \vec{J}_{ph} = flux due to molecular diffusion;
- 531 \vec{J}_{tr} = flux of tracer due to molecular diffusion;
- 532 k = turbulent kinetic energy;
- 533 k_L = local mass transfer coefficient;
- 534 $k_L a$ = volumetric mass transfer coefficient;
- 535 $k_L a_{20}$ = clean water volumetric mass transfer coefficient at 20°C;
- 536 L = distance;
- 537 L_L = interfacial mass transfer;
- 538 L_{ph} = interfacial mass transfer between the phases;
- 539 M = quantity of tracer;
- 540 m_{ph} = local instantaneous interfacial mass transfer;
- 541 P = power;
- 542 p = pressure;
- 543 p_{in} = inlet blower pressure;
- 544 p_{out} = outlet blower pressure;
- 545 Q_a = air flow rate;
- 546 Q_e = effluent flow rate;
- 547 Q_L = influent flow rate;
- 548 S_{tr} = source term representing rate of creation of tracer from and any user-defined sources;

- 549 T = temperature;
- 550 t = time;
- 551 V = volume;
- 552 \vec{v}_{dr} = drift velocity;
- 553 \vec{v}_G = velocity of gas phase;
- 554 \vec{v}_i = interfacial velocity;
- 555 \vec{v}_L = velocity of liquid phase;
- 556 $v_{L,hor}$ = velocity of liquid phase in a horizontal section through the tank;
- 557 v'_{ph} = local instantaneous velocity;
- 558 \vec{v}_{ph} = phasic velocity;
- 559 v_r = relative velocity;
- 560 w = air mass flow rate;
- 561 Y_{tr} = mass fraction of the tracer;
- 562 y = depth;
- 563 α = factor applied to the mass transfer coefficient to account for substrate and nutrient
564 loading variations within the reactor, (i.e. ratio of process- to clean- water $k_L a$);
- 565 α_G = volume fraction of gas;
- 566 α_L = volume fraction of liquid;
- 567 α_{ph} = phasic volume fraction;
- 568 α_{tr} = volume fraction of tracer;
- 569 ε = turbulent kinetic energy dissipation rate;
- 570 μ_L = dynamic viscosity of the liquid phase;
- 571 ρ = density;
- 572 ρ_G = density of the gas phase;
- 573 ρ_L = density of the liquid phase;

574 τ = mean residence time; and
575 ω = specific turbulence dissipation.

576 **SUPPLEMENTAL DATA**

577 The GCI calculations, governing equations related to hydrodynamics and IAC model, Table
578 S1 and Figs. S1-S9 are available online in the ASCE Library (ascelibrary.org)

579 **REFERENCES**

- 580 Bokil, S. D., and Bewtra, J. K. (1972). "Influence of mechanical blending on aerobic
581 digestion of waste activated sludge." *Proc., 6th Int. Association on Water Pollution*
582 *Research and Control (IAWPRC) Jerusalem*, 421-438.
- 583 Bridgeman, J., Jefferson, B., and Parsons, S. (2008). "Assessing floc strength using CFD to
584 improve organics removal." *Chem. Eng. Res. Des.*, 86(8), 941-950.
- 585 Cockx, A., Do-Quang, Z., Audic, J. M., Liné, A., and Roustan, M. (2001). "Global and local
586 mass transfer coefficients in waste water treatment process by computational fluid
587 dynamics." *Chem. Eng. Process.*, 40(2), 187-194.
- 588 Danckwerts, P. V. (1953). "Continuous flow systems. Distribution of residence times." *Chem.*
589 *Eng. Sci.*, 2(1), 1-13.
- 590 Fayolle, Y., Cockx, A., Gillot, S., Roustan, M., and Héduit, A. (2007). "Oxygen transfer
591 prediction in aeration tanks using CFD." *Chem. Eng. Sci.*, 62(24), 7163-7171.
- 592 Fogler, H. S. (1999). *Elements of chemical reaction engineering*, Prentice-Hall International,
593 London.
- 594 Glover, G. C., Generalis, S. C., and Thomas, N. H. (2000). "CFD and bubble column
595 reactors: simulation and experiment." *Chem. Pap. - Chem. Zvesti*, 54(6A), 361-369.
- 596 Glover, G. C., Printemps, C., Essemiani, K., and Meinhold, J. (2006). "Modelling of
597 wastewater treatment plants - how far shall we go with sophisticated modelling
598 tools?" *Water Sci. Technol.*, 53(3), 79-89.

599 Gresch, M., Armbruster, M., Braun, D., and Gujer, W. (2011). "Effects of aeration patterns
600 on the flow field in wastewater aeration tanks." *Wat. Res.*, 45(2), 810-818.

601 Hibiki, T., and Ishii, M. (2000). "One-group interfacial area transport of bubbly flows in
602 vertical round tubes." *Int. J. Heat Mass Tran.*, 43(15), 2711-2726.

603 Higbie, R. (1935). "The Rate of Absorption of a Pure Gas into a Still Liquid during Short
604 Periods of Exposure." *Trans. AIChE*, 31, 365-389.

605 Jesson, M. A., Bridgeman, J., and Sterling, M. (2015). "Novel software developments for the
606 automated post-processing of high volumes of velocity time-series." *Adv. Eng. Softw.*,
607 89, 36-42.

608 Karpinska, A. M., and Bridgeman, J. (2016). "CFD-aided modelling of activated sludge
609 systems – A critical review." *Wat. Res.*, 88, 861-879.

610 Karpinska, A. M., and Bridgeman, J. (2017). "Towards a robust CFD model for aeration
611 tanks for sewage treatment – a lab-scale study." *Eng. Appl. Comp. Fluid* 11(1), 371-
612 395.

613 Karpinska Portela, A. M. (2013). "New Design Tools for Activated Sludge Process." PhD
614 thesis, Faculdade de Engenharia, Universidade do Porto, Portugal.

615 Larsen, P. (1977). "On the Hydraulics of Rectangular Settling Basins, Experimental and
616 Theoretical Studies. Report No. 1001." Department of Water Resources Engineering.
617 Lund Institute of Technology, University of Lund, Sweden.

618 Le Moullec, Y., Gentric, C., Potier, O., and Leclerc, J. P. (2010). "CFD simulation of the
619 hydrodynamics and reactions in an activated sludge channel reactor of wastewater
620 treatment." *Chem. Eng. Sci.*, 65(1), 492-498.

621 Levenspiel, O. (1999). *Chemical Reaction Engineering*, Wiley & Sons, New York, NY.

622 Menter, F. R. (1994). "Two-equation eddy-viscosity turbulence models for engineering
623 applications." *AIAA J.*, 32(8), 1598-1605.

624 Mori, N., Suzuki, T., and Kakuno, S. (2007). "Noise of Acoustic Doppler Velocimeter Data
625 in Bubbly Flows." *J. Eng. Mech.-ASCE*, 133(1), 122-125.

626 Mueller, J. A., Boyle, W. C., and Pöpel, H. J. (2002). *Aeration: principles and practice*, CRC
627 Press, Boca Raton, FL.

628 Pereira, J. P., Karpinska, A., Gomes, P. J., Martins, A. A., Dias, M. M., Lopes, J. C. B., and
629 Santos, R. J. (2012). "Activated Sludge Models Coupled to CFD Simulations." *Single
630 and Two-Phase Flows in Chemical and Biomedical Engineering*, R. Dias, R. Lima, A.
631 A. Martins, and T. M. Mata, eds., Bentham Science Publishers Ltd., 153-173.

632 Quasim, S. R. (1999). *Wastewater Treatment Plants: Planning, Design and Operation* CRC
633 Press LLC, Boca Raton, FL.

634 Reardon, D. J. (1995). "Turning down the power." *Civil Eng.*, 65(8), 54-56.

635 Roache, P. J. (1998). "Verification of Codes and Calculations." *AIAA Journal*, 36(5), 696-
636 702.

637 Samstag, R. W., Ducoste, J. J., Griborio, A., Nopens, I., Batstone, D. J., Wicks, J. D.,
638 Saunders, S., Wicklein, E. A., Kenny, G., and Laurent, J. (2016). "CFD for
639 wastewater treatment: an overview." *Wat. Sci. Technol.*, 74(3), 549-579.

640 Samstag, R. W., and Wicklein, E. (2012). "Application of CFD to Activated Sludge Mixing
641 Analysis. CFD Workshop- Presentation." *3rd IWA/WEF Wastewater Treatment
642 Modelling Seminar-WWTmod2012* Mont-Sainte-Anne, QC.

643 Talvy, S., Cockx, A., and Line, A. (2007). "Modeling of oxygen mass transfer in a gas-liquid
644 airlift reactor." *AICHE* 53(2), 316-326.

645 Tchobanoglous, G., Burton, F. L., Stensel, H. D., and Eddy, M. (2003). "Wastewater
646 engineering: Treatment and reuse." *McGraw-Hill Series in Civil and Environmental
647 Engineering*, McGraw-Hill New York, NY.

648 WEF (2009). "Energy Conservation in Water and Wastewater Treatment Facilities." *Water*
649 *Environment Federation Manual of Practice No. 32*, McGraw-Hill, New York, NY.

650 Joint Task Force of the Water Pollution Control Federation and the American Society of Civil
651 Engineers (WPCF-ASCE) (1988). "Aeration: A Wastewater Treatment Process."
652 *WPCF- Manual of Practice No. FD-13. ASCE- Manuals and Reports on Engineering*
653 *Practice No.68*, Water Pollution Control Federation, Alexandria, VA.

654 Yang, Y., Yang, J., Zuo, J., Li, Y., He, S., Yang, X., and Zhang, K. (2011). "Study on two
655 operating conditions of a full-scale oxidation ditch for optimization of energy
656 consumption and effluent quality by using CFD model." *Wat. Res.*, 45(11), 3439-
657 3452.

658

659

660

661

662

663

664

665

666

667

668

669 **Table 1.** Aeration process design parameters.

	Air requirements (m³ h⁻¹)			
	AS plant	Single tank	Z1	Z2
Max. (1)	45819	3818	2279	1539
Average	31431	2619	1563	1056
Min.	20040	1670	997	673
Max. (2)	45819	3818	2864	955
Max. (3)	45819	3818	2279	1539

670 Note: 1 - actual operating parameters; 2 - optimization studies: airflow distribution between
671 Z1 and Z2: 75 and 25%; 3 - optimization studies: total number of diffusers in Z1 and Z2:
672 2166.

673

674

675

676

677

678 **Table 2.** Characteristic features of several selected meshes.

Mesh No.	Min. cell size (m)	Max. face size (m)	No. of elements	Max. cell skewness	Notes
1	0.01	0.25	3846947	0.77	Converged solution (RAM/CPU expensive)
2	0.01	0.30	2223660	0.76	Converged
3	0.01	0.35	1266172	0.75	solution

679

680

681

682

683

684

685

686

687

688

689

690

691

692 **Table 3.** Physical properties of the phases enabled in CFD simulations of the aeration tank.

Phase	Components	Physical properties
Continuous	Water, tracer	$\rho_L = 998.2 \text{ kg m}^{-3}$ $\mu_L = 0.001 \text{ Pa s}$
	Activated sludge	$\rho_L = 1450 \text{ kg m}^{-3}$ (Larsen 1977) $\mu_L = 0.008 \text{ Pa s}$ (Bokil and Bewtra 1972) Mass fraction – corresponds to the concentration* of 3.3 g L^{-1}
Dispersed	Air	$\rho_G = 1.225 \text{ kg m}^{-3}$ $d_b = 0.5 \div 3.0 \text{ mm}$ Mass fraction of oxygen: 0.23

693 Note: μ_L is dynamic viscosity of the fluid; *- average MLSS concentration measured in AS
694 tank.

695

696

697

698

699

700

701

702

703 **Table 4.** Boundary and operating conditions set in CFD simulations of the aeration tank.

Place	Boundary Condition	Parameters/ Operating Conditions
Inlet pipe	Velocity inlet	v_L - corresponds to maximal and average operating flow rates $I = 5\%$ $D_h = 1.2\text{ m}$ $\alpha_G = 0$ $\alpha_{tr} = 0$ or $\alpha_{tr} = 1$ (tracer injection time)
Outflow weir	Pressure outlet	I (backflow) = 5% D_h (backflow) = 0.4 m α_G (backflow) = 0
Diffusers	Velocity Inlet	v_G - corresponds to design and operating air flow rates in Z1 and Z2 (Table 1) $I = 5\%$ $D_h = 0.16\text{ m}$ $\alpha_G = 1$
Fluid surface	Degassing	$p = 101325\text{ Pa}$
Side walls, bottom	No-slip wall	-
Fluid zone	-	$T = 293\text{ K}$ $\rho = 1.225\text{ kg m}^3$

704 Note: I - turbulence intensity; D_h - hydraulic diameter; p , T and ρ - operating pressure,

705 temperature and density; α_{tr} - volume fraction of tracer.

706

707

708 **Table 5.** Hydrodynamic and oxygen transfer parameters obtained from the CFD simulations of the aeration tank for different operating
 709 scenarios.

Operating scenario	$v_{L,hor}$	v_L		v_a		α_G		ε		$k_L a_{20}$		$\alpha k_L a_{20}$		DO*	
		m s ⁻¹				%		×10 ⁻³ m ² s ⁻³		d ⁻¹		d ⁻¹		mg L ⁻¹	
	Tank	Z1	Z2	Z1	Z2	Z1	Z2	Z1	Z2	Z1	Z2	Z1	Z2	Z1	Z2
1	0.22	0.27	0.24	0.30	0.33	0.43	0.34	1.62	1.00	186	130	56	104	10.05	10.28
2	0.23	0.25	0.24	0.30	0.31	0.56	0.16	1.20	0.36	224	46	67	37	10.09	10.24
3	0.11	0.17	0.08	0.25	0.21	0.49	0.31	0.58	0.34	161	90	48	72	10.06	10.28

710 Note: 1 - original diffuser layout & operating scenario; 2 - original diffuser layout & modified operating scenario; 3 - modified diffuser layout &
 711 original operating scenario, * - equilibrium concentration reached at the oxygenation time of 15 min.

712

713

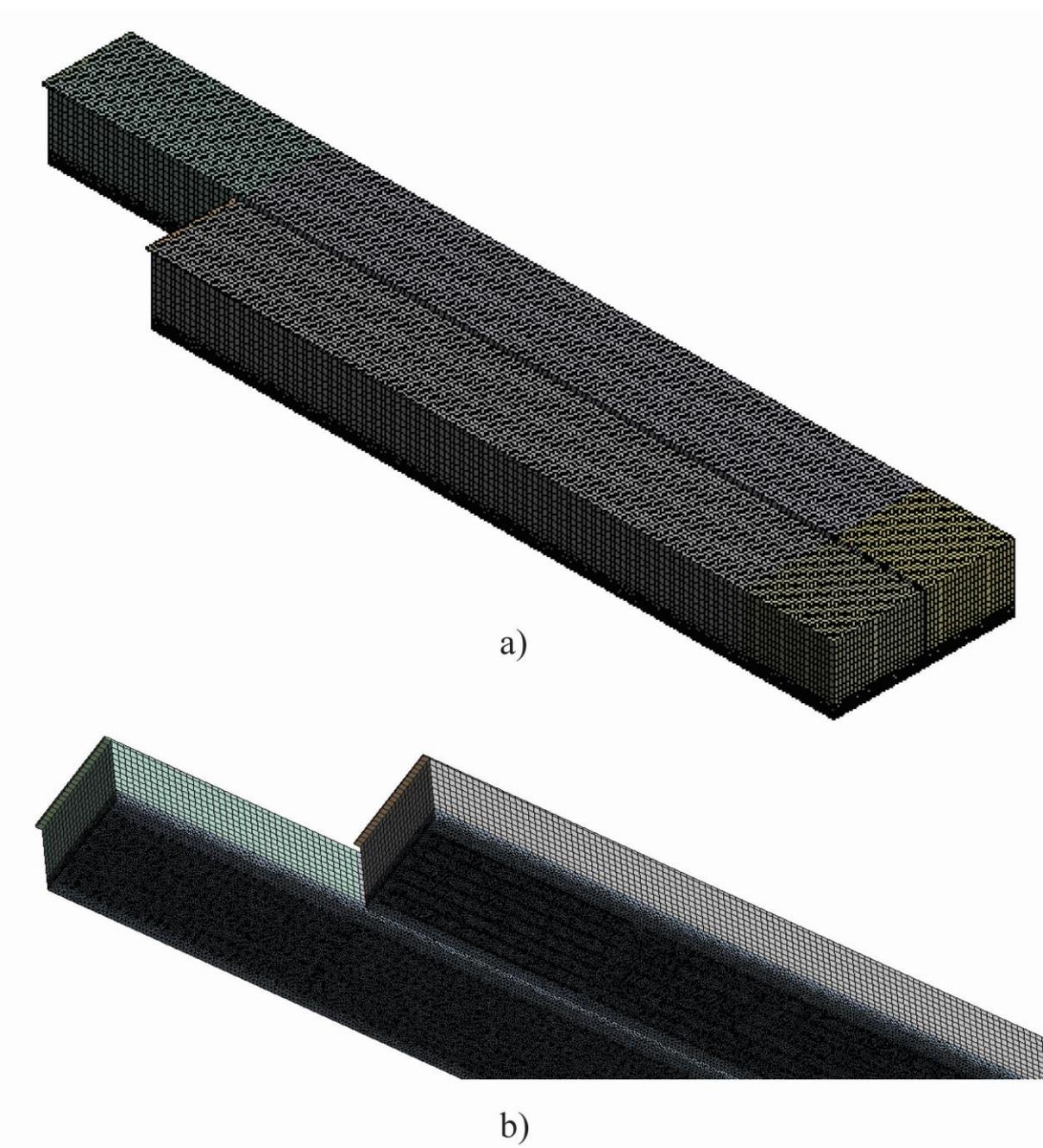


Fig. S1. Computational mesh a) iso-view; b) detail – mesh refinement in the diffuser region (bottom).

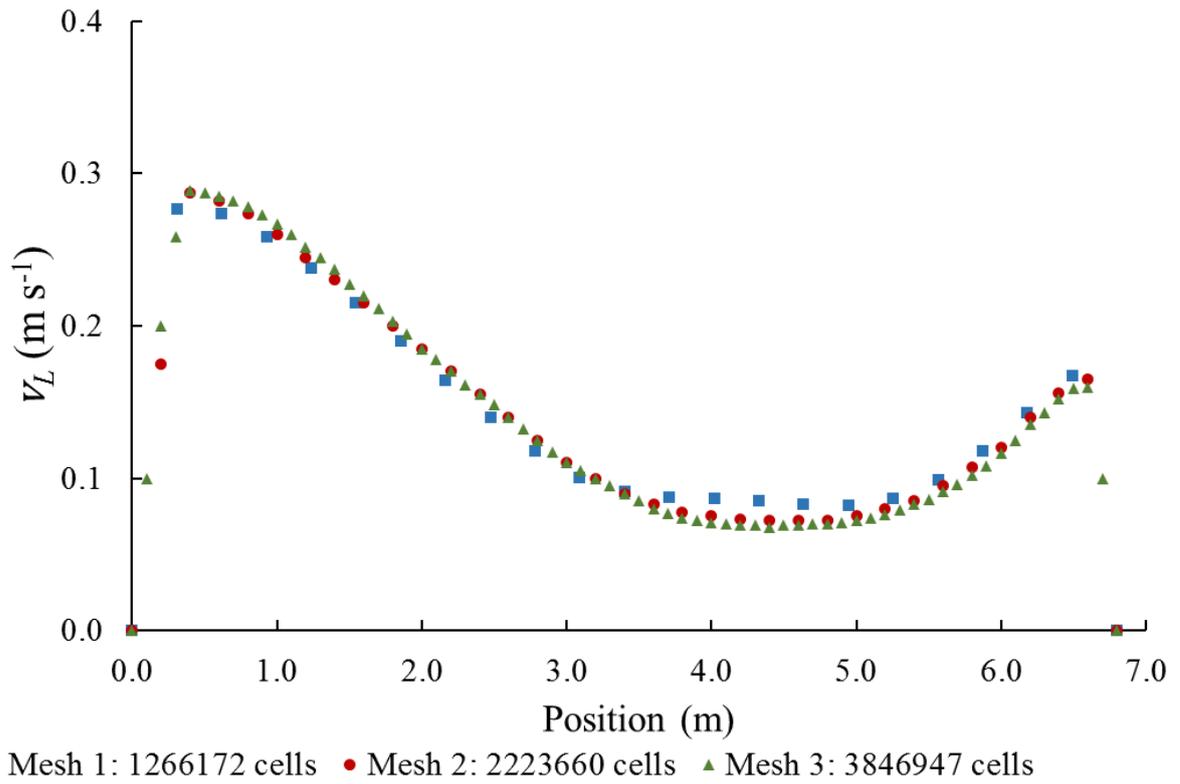


Fig. S2. Average liquid phase velocity on a transversal line across the aeration tank (Z_1 , $L=30$ m, $H=4.9$ m) obtained with different mesh sizes.

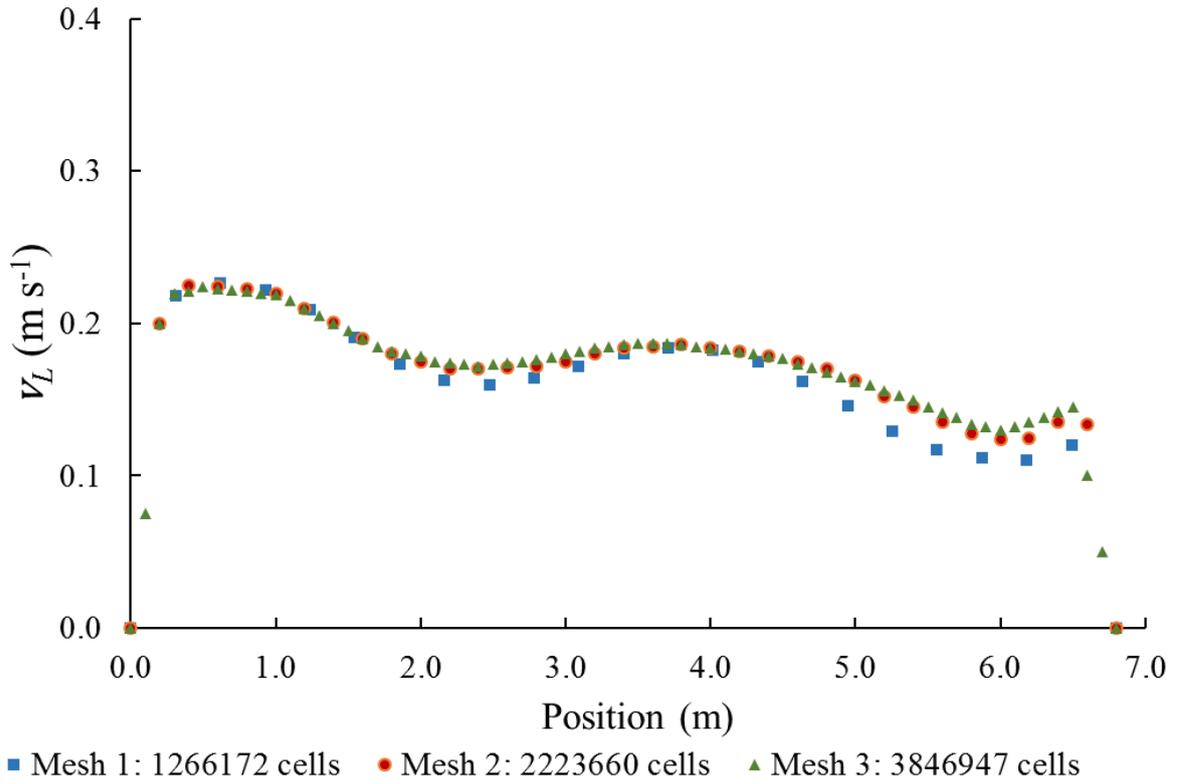


Fig. S3. Average liquid phase velocity on a transversal line across the aeration tank (Z1, L= 30 m, H= 4.5 m) obtained with different mesh sizes.

Liquid velocity

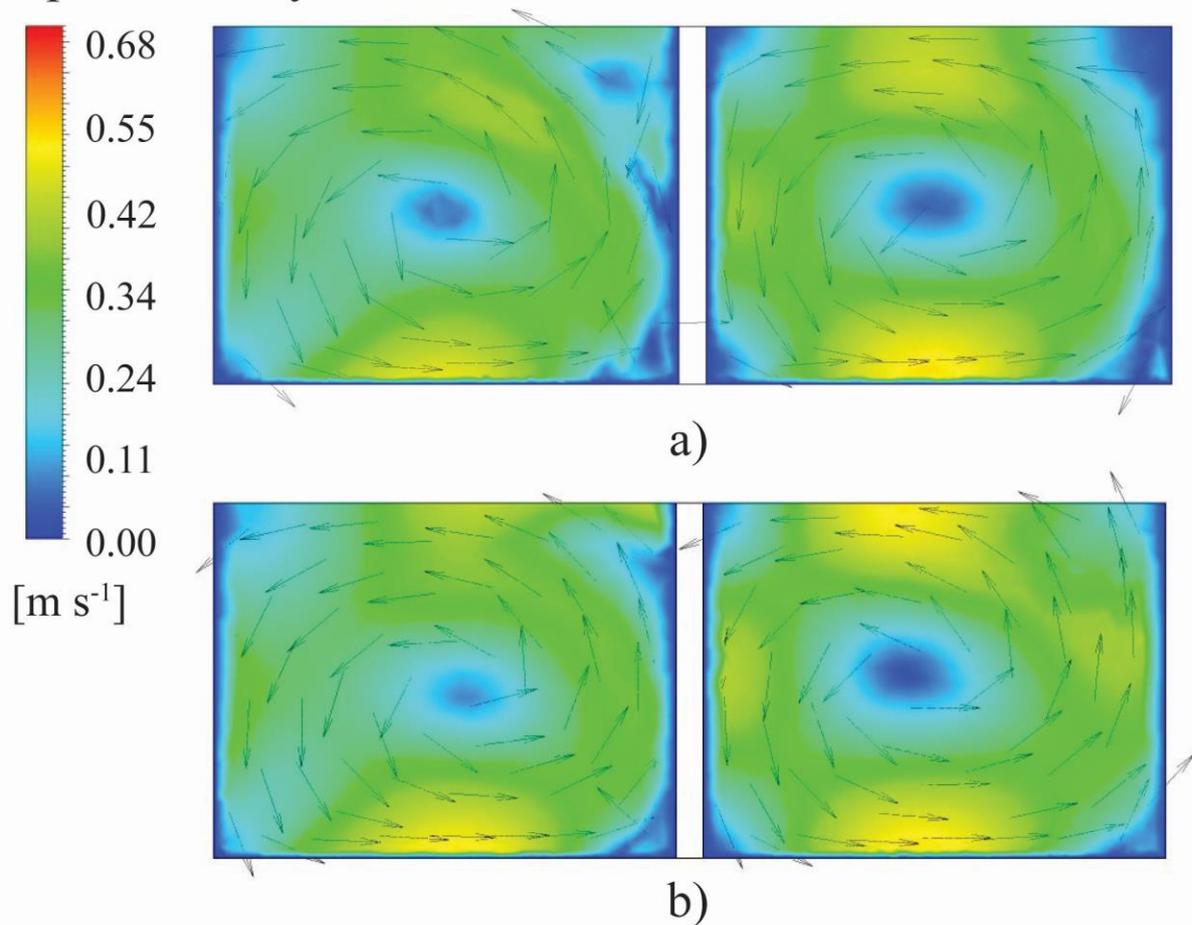


Fig. S4. Contour and vector maps of the velocity magnitude obtained for $Q_L = 0.1 \text{ m}^3 \text{ s}^{-1}$, $Q_a = 1.1 \text{ m}^3 \text{ s}^{-1}$ with a) neutral density approach, and b) accounting for the presence of sludge ($L = 30 \text{ m}$).

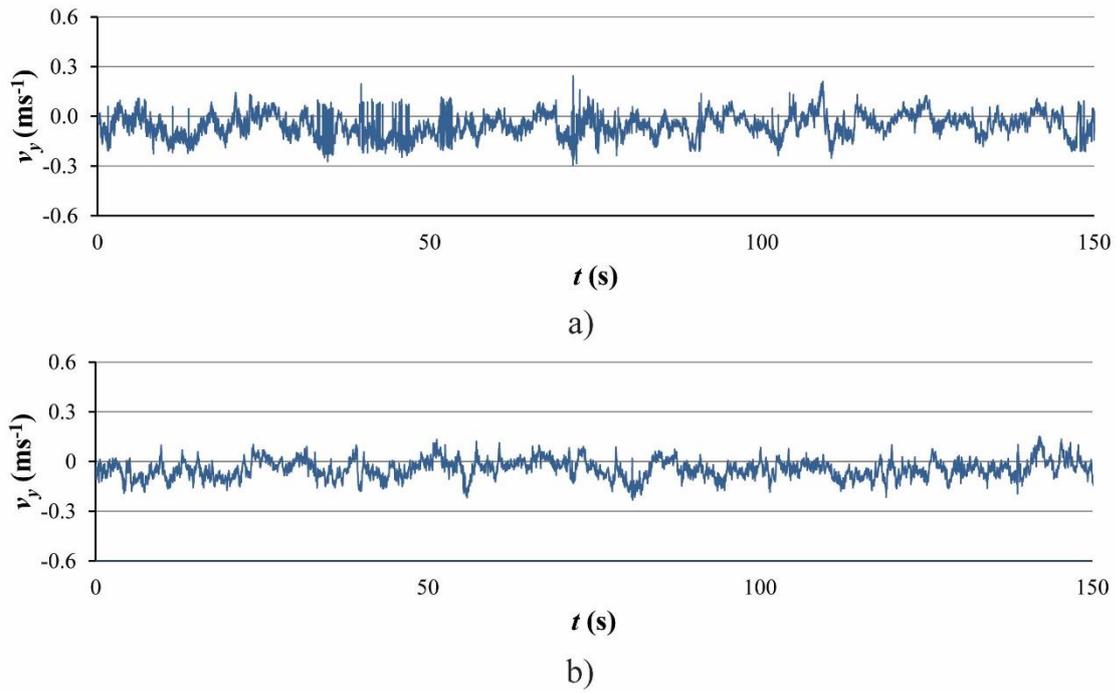


Fig. S5. ADV time-series obtained in the measurements of the vertical component of the water velocity in the full-scale AS tank: a) raw data-set; b) clean data-set after despiking procedure.

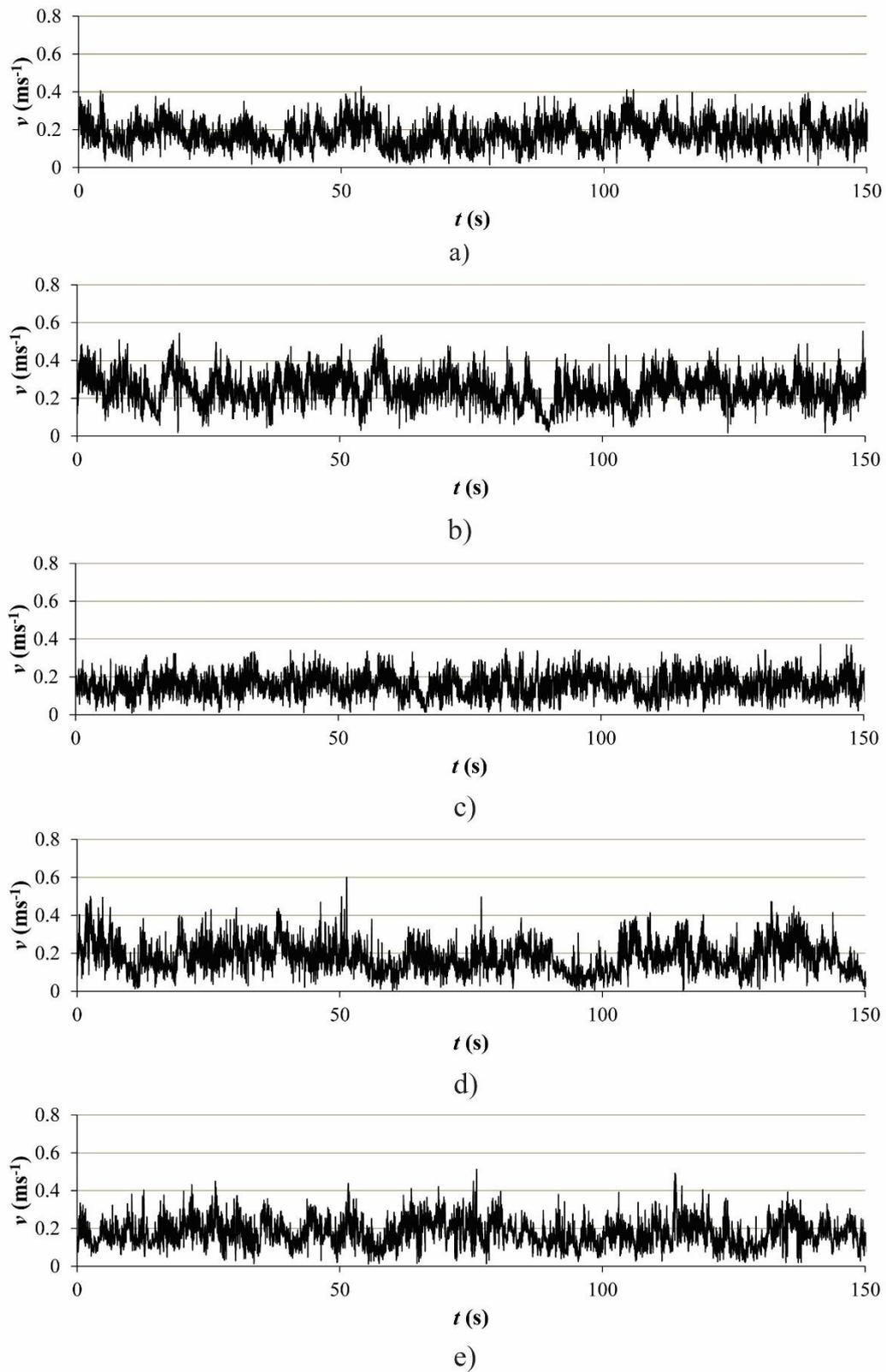


Fig. S6. The filtered ADV time-series obtained in the measurements of the water velocity in the full-scale aeration tank at the submergence of 0.3 m and at the distance of: a) 0.4 m; b) 1.85 m; c) 3.30 m; d) 4.80 m; e) 6.25 m from the external wall.

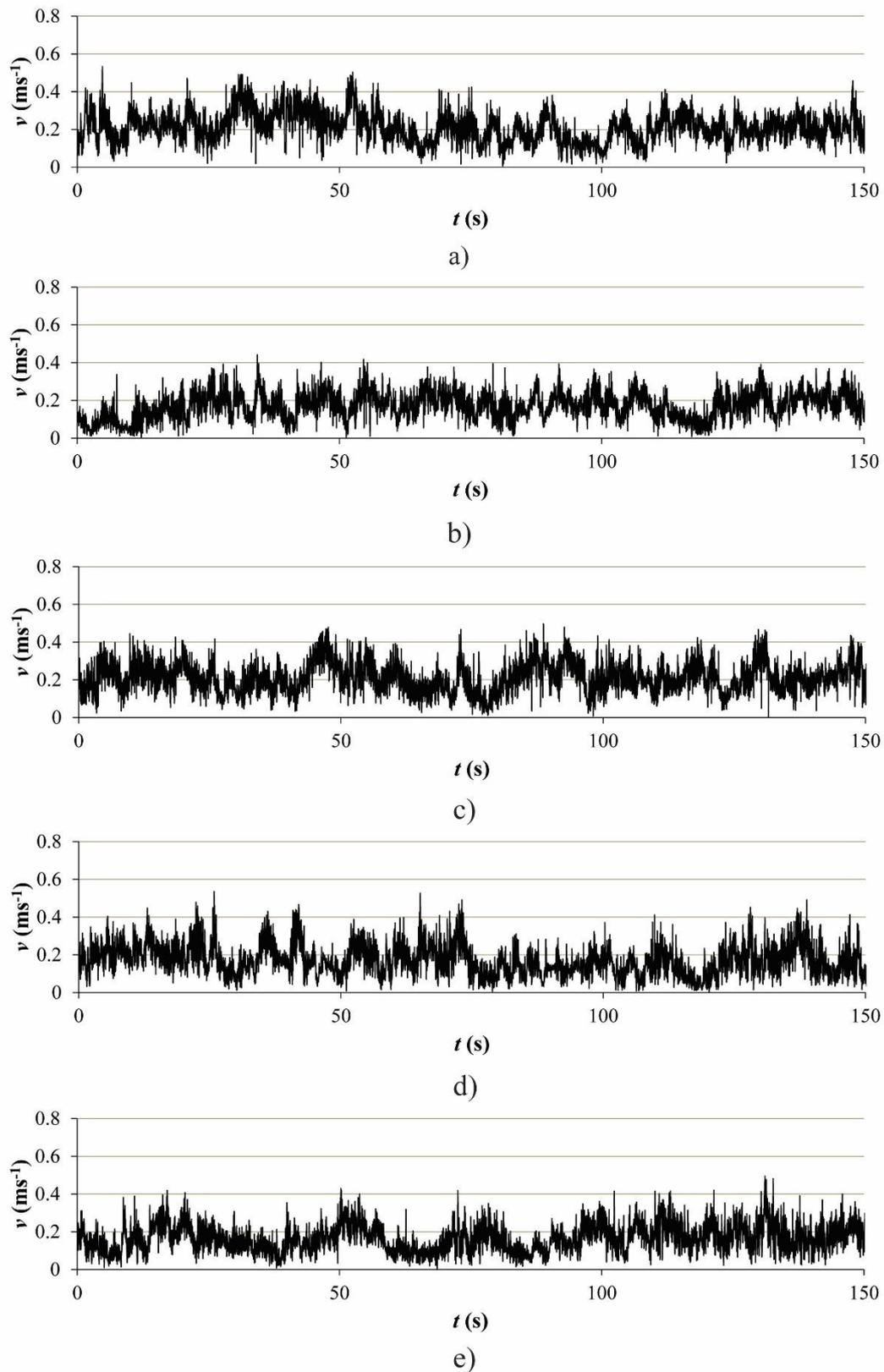
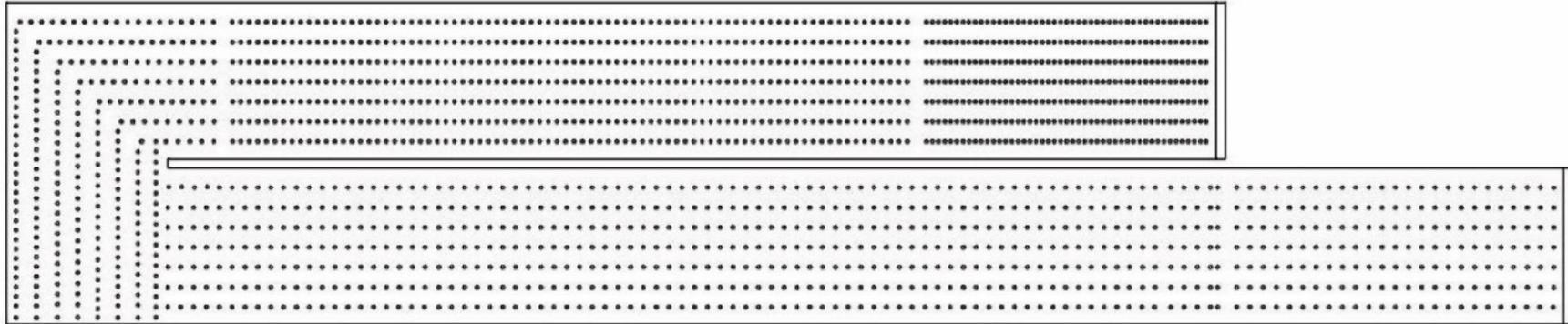
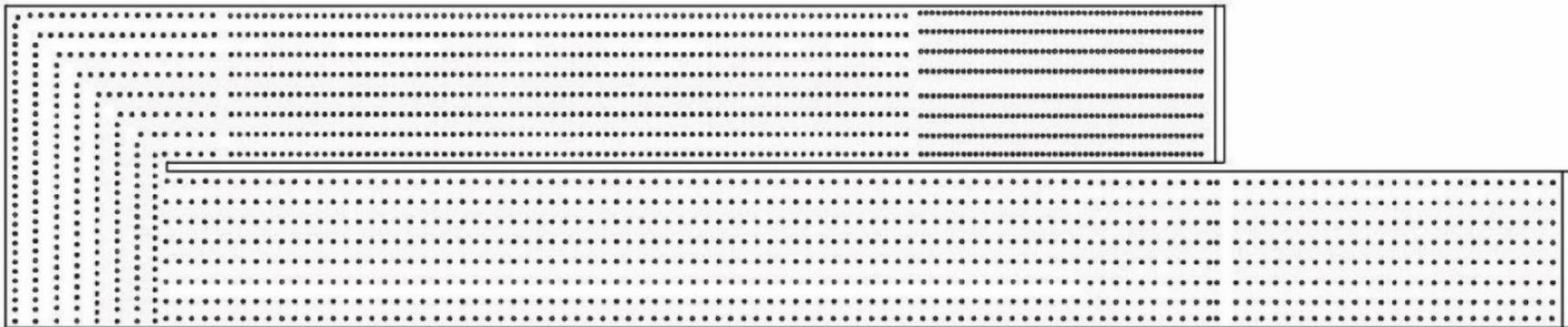


Fig. S7. The filtered ADV time-series obtained in the measurements of the water velocity in the full-scale aeration tank at the submergence of 0.7 m and the distance of: a) 0.4 m; b) 1.85 m; c) 3.30 m; d) 4.80 m; e) 6.25 m from the external wall.



a)



b)

Fig. S8. Diffuser grid a) original layout; b) modified layout (one diffuser added to each row).

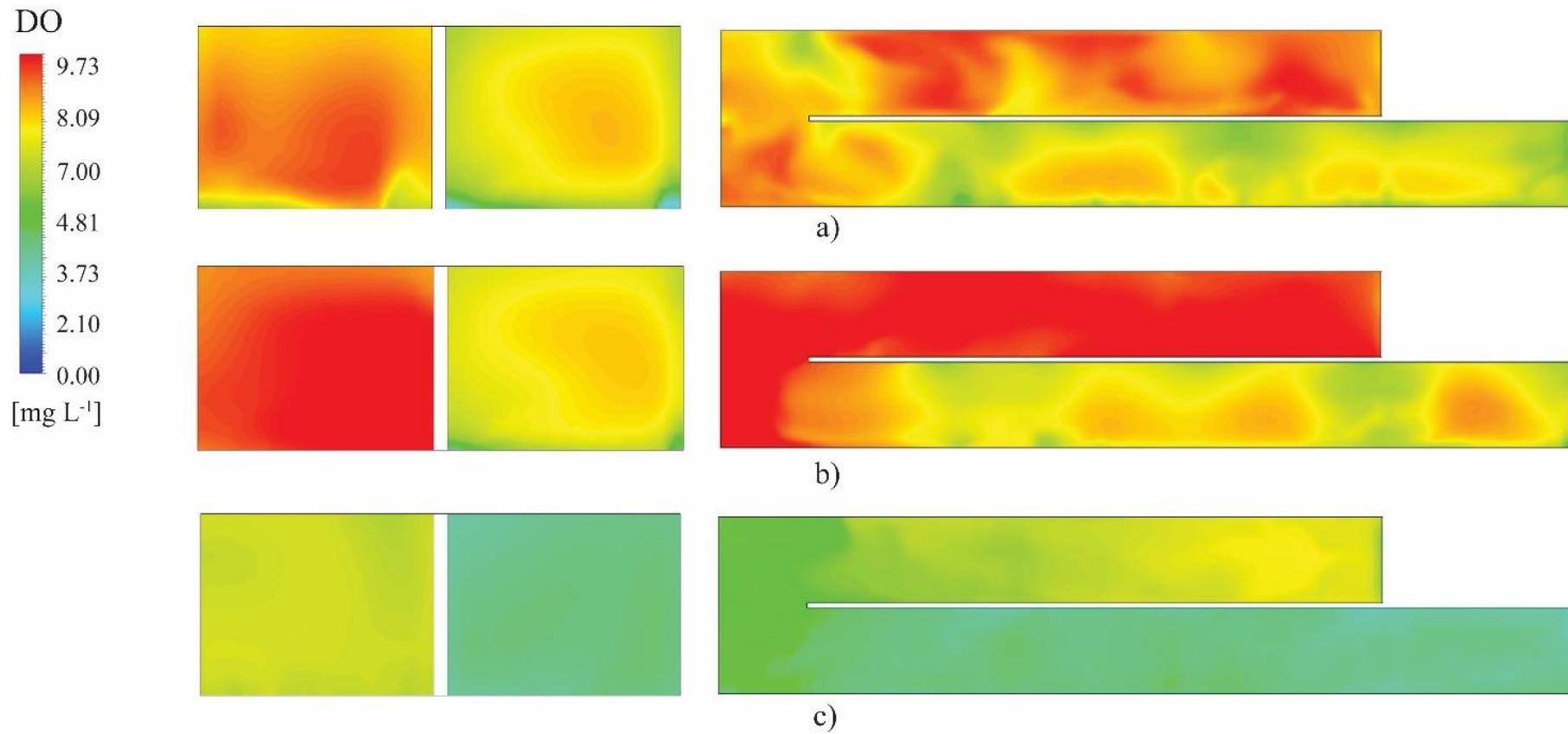


Fig. S9. Evolution of the DO concentration in the AS tank after aeration time of 2 mins for a) original diffuser layout & operating scenario; b) original diffuser layout & modified operating scenario; c) modified diffuser layout & original operating scenario.