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3 Euler-Lagrange Computational Fluid Dynamics 4 Simulation of a Full-Scale Unconfined Anaerobic 5 Digester for Wastewater Sludge Treatment

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10

11 **Abstract**

12

13 For the first time, an Euler-Lagrange model for Computational Fluid Dynamics (CFD)
14 is used to model a full-scale gas-mixed anaerobic digester. The design and operation
15 parameters of a digester from a wastewater treatment works are modelled, and mixing
16 is assessed through a novel, multi-faceted approach consisting of the simultaneous
17 analysis of *(i)* velocity, shear rate and viscosity flow patterns, *(ii)* domain characteri-
18 zation following the average shear rate value, and *(iii)* concentration of a non-diffusive
19 scalar tracer. The influence of sludge's non-Newtonian behaviour on flow patterns and
20 its consequential impact on mixing quality were discussed for the first time. Recom-
21 mendations to enhance mixing effectiveness are given: *(i)* a lower gas mixing input
22 power can be used in the digester modelled within this work without a significant
23 change in mixing quality, and *(ii)* biogas injection should be periodically switched
24 between different nozzle series placed at different distances from the centre.

25 **Keywords:** wastewater, sludge, CFD, Euler-Lagrangian, non-Newtonian fluid, turbu-
26 lence, energy.

27 **1 Introduction**

28 This paper considers the Computational Fluid Dynamics (CFD) modelling of a full-
29 scale gas-mixed anaerobic digester. The purpose of this work was to develop recom-
30 mendations to minimize the input mixing power without compromising, and indeed
31 enhancing, biogas yield for the scenario considered. This was done by progressively
32 lowering the mixing input power while analyzing the resulting flow patterns. This
33 work is based on Dapelo et al. [1], but the current article also includes: *(i)* a sys-
34 tematic assessment of the model mesh-independence through the Grid Convergence
35 Index (GCI) as proposed by [2]; *(ii)* a more complete analysis of the flow patterns

36 by comparison of velocity and viscosity plots; (iii) additional simulations to track the
37 distribution of a non-diffusive scalar field to be used as a virtual tracer and to repro-
38 duce the Herschel-Bulkley rheology; (iv) an analysis of the presence of low-viscosity
39 corridors in the digester, and their detrimental effect on mixing; (v) an assessment of a
40 mitigation strategy consisting of abruptly switching biogas injection between two noz-
41 zle series at regular intervals; and (vi) an alternative approach to calculate the value of
42 minimum power per unit volume necessary for a satisfactory level of mixing computed
43 in the original conference paper is presented here.

44 Wastewater treatment is an energy-intensive operation. Energy use at wastewater
45 treatment works (WwTWs) which come under the auspices of the Urban Wastewater
46 Treatment Directive (UWwTD) and for which EU Member States returned data ex-
47 ceeds 23,800 GWh per annum[3]. Energy consumption has increased significantly in
48 the last two decades, and further increases of 60% are forecast in the next 10-15 years,
49 primarily due to tightened regulation of effluent discharges from WwTWs (e.g. Water
50 Framework Directive, WFD) [4]. WFD impacts will not be truly appreciated for many
51 years, but the UK water industry forecasts a GBP 100M energy cost increase from im-
52 plementation of more stringent treatment standards [5]. However, predictions show
53 that by 2030 the world will have to produce 50% more food and energy and provide
54 30% more water [6], while mitigating and adapting to climate change, threatening to
55 create a “perfect storm” of global events. Therefore, we must address the explicit link
56 between wastewater and energy.

57 Renewable energy resources development is an integral part of several EU Gov-
58 ernments’ environmental strategies. Mesophilic anaerobic digestion (MAD) is the
59 most widespread technology for sludge treatment, the by-product of wastewater treat-
60 ment, in which sludge is mixed with anaerobic bacteria to break down biodegradable
61 material and produce a methane-rich biogas. The current drive to maximise energy
62 recovery means biogas is increasingly harnessed via combined heat and power tech-
63 nology. So, we need to optimise MAD reactor (digester) and mixing performance to
64 maximize energy recovery.

65 In order to predict confidently optimum digester mixing, we need to determine to
66 what extent biogas output is influenced by flow patterns in a digester; flow patterns
67 which are determined by physical parameters of the digesters, inflow mode, sludge
68 rheology and, crucially, mixing regimes. Yet research is lacking in this area. Tradi-
69 tional approaches to digester design are firmly rooted in empiricism and rule of thumb
70 rather than science, and design standards focus only on treated sludge quality, not
71 quality and gas yield/energy consumption.

72 Although the importance of thorough mixing has been recognized, recent stud-
73 ies [7, 8, 9, 10, 11], have questioned traditional approaches. A consistent body of
74 literature[15, 16, 17, 18, 14, 12, 13, 19, 20] has shown that computational fluid dy-
75 namics (CFD) offers significant potential for understanding flow patterns of the non-
76 Newtonian sewage sludge within digesters. However, there are clear limitations with
77 the work undertaken to date; for example, while much work has been done to under-
78 stand mechanical mixing, gas mixing remains poorly studied. Although it is recognized

79 that mechanical mixing is the most efficient mode of mixing [21, 14], gas mixing is not
80 prone to problems specific to mechanical mixing such as wear and expensive maintenance
81 due to the presence of moving elements (e.g., impellers, shafts, ball bearings)
82 inside the digester. Hence, there is a clear industrial interest in investigating gas mixing.
83 Despite this, only [15, 14, 22, 23] have proposed robust multiphase models. [16]
84 adopted a simplified approach by considering *de facto* a single-phase model and re-
85 producing the effect of the bubbles through appropriate boundary conditions, but such
86 approach is valid only for the specific case of the draft-tube digester they considered.

87 [15, 14, 22] used the Euler-Euler model for their simulations. It is well-known that
88 the Euler-Euler model can handle very complex fluids, but needs a relevant quantity of
89 empirical information to close the momentum equations, and for this reason [24] recom-
90 mends it only when other models are not available. A novel Euler-Lagrangian CFD
91 model introduced in [25] to simulate the gas mixing of sludge for anaerobic digestion
92 is described in which fluid motion is driven by momentum transfer from the bubbles
93 to the liquid. The bubbles rise in columns via buoyancy and transfer momentum to
94 the surrounding sludge. This momentum transfer takes place due to the push force
95 that the bubbles exert to the surrounding liquid, and the riptide effect arising from the
96 low-pressure region created by the motion of the bubbles. This model successfully
97 described a laboratory-scale setup with a much reduced amount of empirical informa-
98 tion when compared to the Euler-Euler model. Validations were performed through
99 Particle Image Velocimetry [25] and Positron Emission Particle Tracking [26] tech-
100 niques.

101 Sludge is opaque, corrosive and biochemically hazardous: this makes experiments
102 difficult to perform and therefore makes the use of CFD more valuable, but for the
103 same reason it makes also the process of validation more difficult. The only experiments—
104 and, consequently, validations—reported in the literature on full-scale anaerobic di-
105 gesters consist of the introduction of a tracer fluid at the inlet and its detection at
106 the outlet [17, 18]. They are costly experiments and only give a “black box” rep-
107 resentation of the flow through the digester. Other approaches consist of comparing
108 dimensionless groups calculated from specifications such as the power absorbed by
109 the impeller [27, 28, 29]. [19, 20] reported the validation performed by [17], but did
110 not perform any of their own. An alternative approach consists of providing a vali-
111 dation for a CFD model through laboratory-scale experiments, and then, applying the
112 validated model to a set of full-scale scenarios. This approach has the advantage of
113 informing modelling strategies involved in the full-scale simulations, such as bubble
114 injection methods, boundary conditions or multiphase momentum transfers, and was
115 followed in the work presented here.

116 Within this work, the model of [25] was applied to examine the mixing regime of
117 a full-scale anaerobic digester. In gas-mixed digesters, biogas is taken from the top
118 and pumped into the sludge at the base through a series of nozzles. The outcome of
119 the simulations was analysed through a novel multi-faceted approach. First, velocity,
120 shear rate and apparent viscosity flow patterns were considered, with the latter being
121 examined for the first time. Then, the computational domain was divided into high,

122 medium, low and very low shear rate zones and each zone's relative occupancy was
123 reported, similar to how [12] considered the velocity magnitude. Finally, the concen-
124 tration of a non-diffusive scalar tracer was studied. The flow patterns analysis reported
125 for the first time the effect of non-Newtonian rheology on mixing; in particular, the
126 issue of low-viscosity corridors was identified as a possible condition for detrimental,
127 short-circuited mixing. The assessment of the shear rate relative occupancies showed
128 that mixing is not significantly altered if mixing input power is lowered to a minimum
129 acceptable level. The study of the tracer concentration made it possible to assess a
130 mitigation strategy for the low-viscosity corridors. In practice, it was suggested to ar-
131 range a second series of concentric nozzles at a different radius from the tank centre,
132 and to switch biogas injection between the original and the new series at regular time
133 intervals.

134 **2 CFD modelling**

135 Sludge is a complex material, which displays a broad range of multiphase and rhe-
136 ological phenomena. In order to successfully model sludge within CFD work, it is
137 necessary to introduce a series of assumptions and simplifications, depending on the
138 type of sludge and the aims of the CFD study.

139 **2.1 Multiphase Dynamics**

140 Sludge is a mixture of water, biogas, flocculant and sedimenting debris, both organic
141 and inert. The dimensions of the debris varies from molecules to sand and grit of ap-
142 proximately one millimetre. The dimension of the debris can increase to centimetres,
143 if silage or food waste are added as in the case of agricultural digesters. In addition,
144 gas mixing introduces an additional (gaseous) phase.

145 Given the level of complexity, some simplifying assumptions are necessary for
146 modelling. Firstly, no information on scum or other floating matter is available from
147 the industrial digesters used for the full-scale modelling work presented in this article,
148 and therefore flocculation was ignored for the sake of simplicity. Sedimentation in the
149 digesters is known to take place over a timeframe of years, while the retention times
150 do not exceed one month. The problem of sedimentation within anaerobic digesters is
151 important, complex and deserving of dedicated study. However, the focus of the work
152 presented in this article is biogas yield optimization; hence, it is reasonable to ignore
153 sedimentation. Finally, as wastewater is screened prior to primary sedimentation, it is
154 reasonable to assume that larger debris is removed, and only fragments of the order
155 of one millimetre are present in sewage sludge. As the computational mesh size was
156 expected to be much larger and the trajectories of the single debris were of no interest
157 in the analysis, it was natural to consider sludge as a single phase. The biogas bubbles
158 constituted an obvious exception, as it was their motion that generated the sludge flow
159 patterns.

2.2 Continuous Phase

Considering the foregoing discussion, it can be seen that the components of sludge (apart from the gas bubbles) can be approximated as a single, continuum phase. Given the predominance of water in the relative volume ratios, sludge was modelled as an incompressible, constant-density fluid obeying the Navier-Stokes equations.

2.3 Rheology of sewage sludge

Sludge is a complex material. Sludge characteristics depend on total solid content (TS) and temperature [30], and its rheology displays a broad variety of complex phenomena such as pseudoplasticity, viscoelasticity, shear banding and thixotropy [31]. Although a number of authors adopted the radical simplification of modelling sludge as a Newtonian fluid [15, 16, 17], pseudoplasticity has been reported to affect the flow patterns [32]. A simple, successful approach in anaerobic digestion CFD modelling has consisted of considering only the pseudoplastic behaviour while neglecting all the remaining layers of complexity [14, 29, 12] This means that the (apparent) viscosity, instead of being constant, depends on the shear rate magnitude $|\dot{\gamma}|$ following a power-law relationship:

$$\mu = K |\dot{\gamma}|^{n-1} , \quad (1)$$

where K is the consistency coefficient (Pa s^n) and n is the power law index. “Pseudoplastic” means $n < 1$. All the authors cited above used the experimental data of [33]. More recently, the Herschel-Bulkley model has been adopted [19, 20]. The Herschel-Bulkley is a power-law model, in which flow occurs only if the shear stress exceeds a critical value τ_0 :

$$\mu = \tau_0 |\dot{\gamma}|^{-1} + K |\dot{\gamma}|^{n-1} . \quad (2)$$

The authors cited above used the experimental data of [34] and, more recently, of [35] for digested sludge.

In the work presented here, the power-law model (Equation 1) was adopted following the data of [33] for TS values of 2.5, 5.4 and 7.5%. These values cover a wide range of sludge types used in industrial digesters—and in fact have already been investigated in previous literature [14, 29, 12]—and are similar to the conditions of the laboratory-scale validation of the present model [25]. In addition, the Herschel-Bulkley model (Equation 2) was also adopted following the data of [35] for 1.85% TS, and a Newtonian model was considered for comparison. Table 1 presents the details of these models. To avoid a singularity at $|\dot{\gamma}| = 0$, the numerical solvers adopt a Newtonian model continuously when the shear rate drops below a user-defined threshold. For the work reported in this article, this threshold was set to 0.001 s^{-1} . When appropriate, the curves reported in Table 1 were extrapolated beyond the experimentally-measured range. As in mesophilic conditions the temperature is kept constant at $35 \text{ }^\circ\text{C}$, the temperature dependence can be dropped. As discussed in [25], the values of density for the TS range considered vary from $1,000.36$ to $1,001.73 \text{ kg m}^{-3}$ [30], which differ for

	TS (%)	τ_0 (Pa)	K (Pa s ^{<i>n</i>})	n (–)	$ \dot{\gamma} $ range (s ^{–1})
Power-law [33]	2.5	0	0.042	0.710	226–702
	5.4	0	0.192	0.562	50—702
	7.5	0	0.525	0.533	11—399
Herschel-Bulkley [35]	1.85	0.092	0.169	0.308	0.01–30
Newtonian	–	0	12	1	–

Table 1: Rheological properties of sludge. “ $|\dot{\gamma}|$ range” refers to the limits of the shear range interval in which the experimental measurements were performed

197 less than 1% from water density at 35 degrees (994 kg m^{–3}), and therefore density
198 was approximated to 1,000 kg m^{–3} in all cases for simplicity.

199 2.4 Multiphase model

200 The Euler-Lagrange model for gas-mixing in anaerobic digestion developed and val-
201 idated with lab-scale data in [25, 26] was adopted for the work presented within this
202 article.

203 Mixing is driven by diffusion, turbulent diffusion and advection [36]. While the
204 first is related to the biochemical properties of sludge, the latter two pertain to phys-
205 ical modes of mixing, and hence the discussion focusses on them. In an unconfined,
206 gas-mixed digester, turbulent diffusion occurs due to the swift motion of the rising
207 bubbles, and is confined to the immediate proximity of the bubbles. However, in a
208 full-scale plant, the bubbles are arranged in vertical plumes the diameter of which is
209 small compared with the digester size, and therefore such a mechanism becomes negli-
210 gible. Hence, advection was considered as the main mixing mechanism. Thus, the aim
211 of the multiphase model is to reproduce the flow patterns away from the bubble plume,
212 without necessarily resolving the bubble motion in detail on the basis that, in a full-
213 scale plant, turbulent diffusion around the bubble plume is negligible, and therefore
214 the details of the liquid phase motion near the bubbles are not of interest [25]. For this
215 reason, the following approximations were made: (i) spherical bubbles, (ii) pointwise
216 bubbles, and (iii) no bubble-bubble interaction. In parallel with these assumptions,
217 a two-way coupling was defined such that sludge exchanges momentum with single
218 parcels (biogas bubbles), and the force acting on the single bubbles is broken down
219 into buoyancy, drag and lift forces. Bubble drag and lift forces were reproduced with
220 the models developed by Dewsbury et al. [37] and Tomiyama et al. [38] respectively.
221 As explained in [25], the drag force depended on the particle Reynolds number, which
222 in turn was computed from the sum of the eddy and apparent viscosity.

223 Nominal bubble diameter is requested by the model as an input to compute the
224 force acting on each bubble. However, there are no data in the literature about the

225 dimension of the bubbles inside a digester—this is unsurprising, as the problem of
226 measuring bubble size inside an industrial digester presents the same afore-mentioned
227 challenges of determining full-scale digester flow patterns experimentally. In addition,
228 bubbles are expected to expand when rising. Under these circumstances, the approach
229 followed in this work was to run multiple series of simulations, each with a fixed bub-
230 ble size. In this way, albeit the outcome of a single run may depend on the particular
231 choice of a given bubble size, common trends can be identified and used to give pre-
232 dictions that hold for all the different choices of bubble size. For the work presented
233 within this article, the values of $d = 2, 6$ and 10 cm were chosen.

234 **2.5 Meshing**

235 In this article, a CFD simulation consisting of a series of transient PISO runs is de-
236 scribed. The modelled digester comprises a cylindrical digester with an inclined base
237 (Figure 1) (i.e., a cylinder over an inverted cone) with twelve nozzles placed along a
circle at the bottom of the tank. Details of the digester are reported in Table 2.

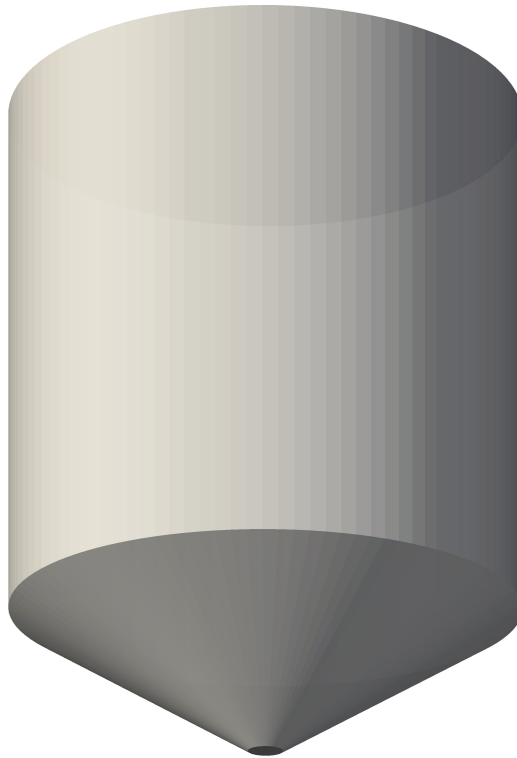


Figure 1: Computational domain

238
239 The model domain consists of a wedge comprising an angle of $\pi/6$ radians. A
240 single nozzle lies on the symmetry plane of the wedge. Four grids were generated—
241 the details are reported in Table 3. As an example, Figure 2 shows side elevation, plain

242 view and two details of Grid 2.

243 The computational work was undertaken using the BlueBEAR high performance
 244 computing facility at the University of Birmingham. Each simulation was run in paral-
 245 lel on three dual-processor 8-core 64-bit 2.2 GHz Intel Sandy Bridge E5-2660 worker
 246 nodes with 32 GB of memory, for a total of 48 nodes. OpenFOAM 2.3.0 was used to
 247 run the computational work.

248 In [25] the Reynolds stress Launder-Gibson model [39] was successfully employed

External diameter	D_{ext}	14.63 m
Diameter at the bottom of the frustum	D_{int}	1.09 m
Cylinder height	h	14 m
Frustum height	h_0	3.94 m
Distance of the nozzle from the axis	R_{noz}	1.75 m
Distance of the nozzle from the bottom	h_{noz}	0.3 m
Maximum gas flow rate per nozzle	Q_{max}	$4.717 \cdot 10^{-3} \text{ m}^3 \text{ s}^{-1}$

Table 2: Details of the digester geometry (courtesy of Peter Vale and Severn Trent Water Inc.)

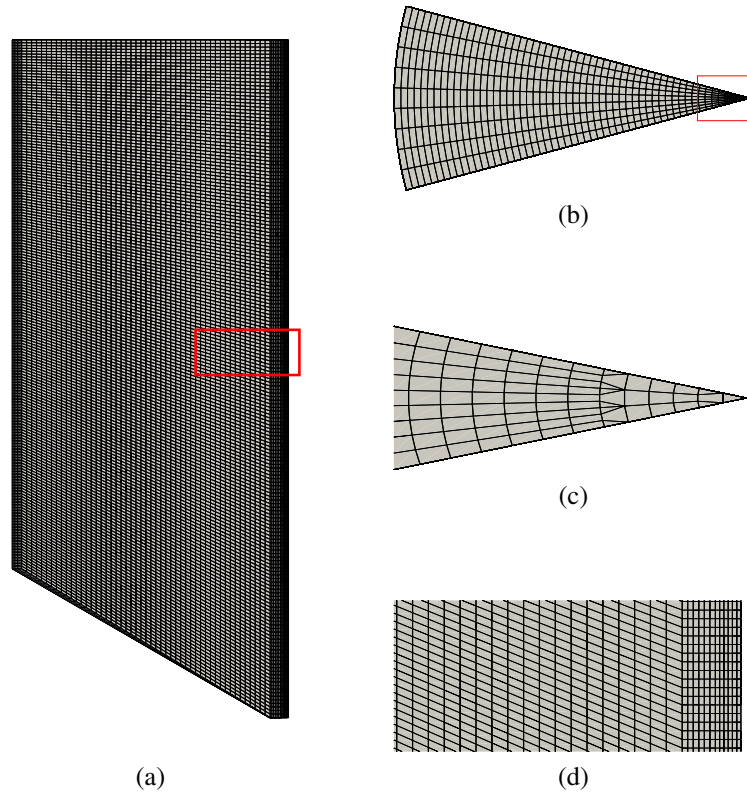


Figure 2: Grid example. Side elevation (a) and plain view (b), wedge apex (c) and side detail (d). The areas occupied by (c) and (d) are identified in (b) and (a) respectively

Id.	Number of cells	Max skewness	Max aspect ratio	Non-ortho max	Non-ortho avg	Volume min (m ³)	Volume max (m ³)	Vol wedge (m ³)
1	394,400	1.123	13.24	30.03	14.00	1.500e-5	1.011e-3	215.8
2	98,420	1.064	9.974	30.00	13.66	3.158e-5	4.241e-3	215.8
3	36,720	1.112	10.53	30.03	13.78	3.333e-5	1.116e-2	215.3
4	18,760	1.304	13.54	30.01	13.84	4.286e-5	2.144e-2	215.3

Table 3: Details of the grids

249 to reproduce the turbulent motion of the liquid around the bubbles and therefore the
250 same model was employed in the study reported here. The timestep was defined dy-
251 namically with an algorithm aimed at keeping the maximum Courant number just
252 below a specified value of 0.2, in the same way as in [25]. For a given cell i of lin-
253 ear magnitude L_i where the fluid velocity is $|\mathbf{u}_i|$, given the timestep Δt , the Courant
254 number is defined as:

$$\text{Co}_i = \frac{|\mathbf{u}_i| \Delta t}{L_i} . \quad (3)$$

255 The maximum Courant number, Co , is the maximum value of Co_i over i . Following
256 [25], after a small initial value of 10^{-5} s, the timestep was corrected to keep the
257 maximum Courant number near but less than the limit of 0.2. At each timestep, the
258 solution was considered as converged when the residual for the pressure fell below
259 10^{-7} , and all the other quantities below 10^{-6} .

260 The initial condition for the fields simulated within the numerical work presented
261 here consists of a system configuration in which the bubble plume is fully developed.
262 In [25] this condition was obtained by performing a series of preliminary, first-order
263 (transient) runs in which the bubble column developed from a state in which there were
264 neither bubbles nor liquid phase motion. In the work described here, preliminary runs
265 were performed for a computational time of 60 s. Then the last timestep was used as
266 initial condition for a series of main (second-order) runs while the previous timesteps
267 were discarded. The second-order runs were performed for an additional 240 s, for an
268 overall computational time of 300 s. As in [25], binary files were collected for every
269 integer-second timestep of the main runs.

270 The boundary conditions are reported in Table 4. The values of C_μ , κ and E for the
271 wall functions were set to 0.09, 0.41 and 9.8 respectively. The initial conditions for
272 the preliminary runs were: $4.95 \cdot 10^{-4} \text{ m}^2 \text{ s}^{-3}$ for the ε field, zero for p , u and R_{ij} . The
273 differencing schemes used were: linear for interpolations, limited central differencing
274 for the Gradient operator, linear for the Laplacian, Van Leer for all the other spatial
275 operators, first-order Eulerian scheme for the time derivative in the preliminary runs
276 and second-order backward for the main runs.

277 The computational runtime remained below 20 hours per run, and the timestep was
278 observed to be between 0.0013 and 0.14 seconds.

279 2.6 Mesh size dependency analysis

280 In an Euler-Lagrangian model, the parcels (in our case, single bubbles) are approx-
 281 imated to be pointwise, and therefore the mesh size should be much larger than the
 282 parcel diameter in order to respect this approximation [40]. In [41, 42] it was shown
 283 that this requirement can be relaxed to the point of having a mesh volume comparable
 284 with parcel volume under certain conditions (number of parcels below $\sim 10^3$), but
 285 nevertheless care must be taken in order to avoid resolving the hydrodynamics of the
 286 fluid around the bubble when the mesh cell size is similar to the bubble diameter and,
 287 hence, mesh-dependant results when the mesh size becomes smaller than the parcel
 288 size [25]. This is possible, as the bubble volumes are $4 \cdot 10^{-6}$, 10^{-4} and $5 \cdot 10^{-4}$ m³
 289 for diameters of 2, 6 and 10 cm respectively, which means that bubble sizes are be-
 290 tween 0.3 and 40 times the smallest cell size in Grid 1, and between 0.004 and 4 times
 291 the largest cell in Grid 1. A grid independence test is always appropriate in research
 292 involving CFD simulations in order to identify a mesh that is refined enough to secure
 293 mesh-independent results. In addition, with the specific model adopted in this work,
 294 it was shown in [25] that such a test is necessary to exclude meshes that are too fine
 295 compared to the bubble size.

296 For the reasons cited above, the Grid Convergence Index (GCI) proposed by [2] was
 297 performed and a series of mesh independence tests was run. Two tests were performed
 298 for each run series, one involving Grids 1, 2 and 3, and another one involving Grids
 299 2, 3 and 4. The tests were performed over all the values for TS and d and $q = 1$,
 300 the latter being justified by the fact that the number of bubbles in the computational
 301 domain is greater for higher flow rates. All the details of the mesh independence test
 302 are similar to the procedure detailed in [25]; the only difference being that the volume
 303 proportion of the shear rate interval $\langle \dot{\gamma} \rangle \in [0, 0.1]$ s⁻¹ was considered in place of the
 304 average shear rate. This was because the proportions of different shear rate intervals
 305 were used in the discussion to assess mixing quality, as will be shown in Section 3.3.

Top	p	Pressure	Constant zero
	\mathbf{u}	Velocity	Slip
	ε	Turb. dissipation	Slip
	R_{ij}	Reynolds stress	Slip
Wall/bottom	p	Pressure	Adjusted such that the velocity flux is zero
	\mathbf{u}	Velocity	Constant zero
	ε	Turb. dissipation	Standard wall function
	R_{ij}	Reynolds stress	Standard wall function
Front/back	All		Cyclic

Table 4: Boundary conditions [25]

3 Discussion

A series of runs was performed for values of gas flow rate corresponding to fractions of Q_{\max} viz. $q \equiv Q/Q_{\max} = 0.1, 0.2, 0.3, 0.5, 0.7$ and 1.0 .

3.1 Assessment of the mesh dependence

The results of the GCI study are reported in Table 5. For each run, two tests were performed, one involving Grids 1, 2 and 3, and one involving Grids 2, 3 and 4. The grids of a given test were considered to be in the asymptotic range of convergence when the asymptotic convergence indicator differed from the value of 1 by less than 25%. In such cases, the value of the indicator is shown in Table 5. The test was performed for all values of TS and d to assess the effect of these variables on grid convergence.

For almost all the combinations of TS and d values, either all the grids were in the asymptotic range of convergence (both Asymp.1 and Asymp.2 are evidenced), or Grids 1, 2 and 3 were in the asymptotic range of convergence but not Grids 2, 3 and 4 (Asymp.1 is evidenced but not Asymp.2), or the converse (Asymp.2 is evidenced but not Asymp.1). In the second case, Grid 4 was too coarse to be within the mesh-independence range; in the third case, the cells composing Grid 1 were as small as, or smaller than, the individual bubbles and the simulation results became mesh-dependent. In all the cases, Grid 2 was within the asymptotic range of convergence. For this reason, Grid 2 was used for further simulations.

3.2 Flow patterns

Figures 3, 4 and 5 show the velocity field at the last timestep (300 s)). The inlet position is marked with a white triangle. All values of TS (%), bubble diameter (d), and air flow rate ($q = 1, 0.5, 0.2$) are shown. It can be observed that the general structure of the flow patterns is the same for all runs. The rise of the bubbles forms a column of fast rising liquid phase above the nozzle. Once it reaches the surface, the liquid phase is displaced horizontally towards the exterior, and then forms a large vortex that occupies most of the remaining part of the domain. The centre of the vortex is located approximately at the centre of the upper part of the domain. Once inside the vortex, the liquid phase slowly descends along the external boundary of the domain, follows the slope of the bottom of the tank and finally approaches the zone around the nozzle. Advection throughout the whole digester is the driving mixing mechanism, as discussed in Section 2.4.

Beyond this general description, effects arising as a result of the gas flow rate, the rheology (as a function of TS) and the bubble size can be observed. Specifically, the velocity magnitude increases and the vortex becomes more and more developed as gas flow rate, q rises; in particular, the vortex does not reach the lower part of the domain for small values of q . The vortex becomes less compact and the velocity patterns are

Table 5: GCI analysis

	2.5% TS		5.4% TS		7.5% TS	
	$d = 2 \text{ cm}$	$d = 6 \text{ cm}$	$d = 2 \text{ cm}$	$d = 6 \text{ cm}$	$d = 2 \text{ cm}$	$d = 6 \text{ cm}$
		$d = 10 \text{ cm}$		$d = 10 \text{ cm}$		$d = 10 \text{ cm}$
SpVol ₄	0.53	0.5	0.6	0.530	0.6	0.5719
SpVol ₃	0.57	0.6	0.47	0.57990	0.6	0.625100
SpVol ₂	0.544	0.5	0.51	0.5780	0.5	0.62540
SpVol ₁	0.5469	0.7	0.6	0.702	0.6	0.5624
p_2	1.463	0.710	3.787	14.32	1.220	24.31
p_1	6.343	0.790	1.237	7.060	—	0.594
GCI2 ₄₃	0.18	1.3	0.2	0.005	0.3	5e-4
GCI2 ₃₂	0.08	0.8	0.04	4e-5	0.3	1.6e-7
GCI1 ₃₂	0.007	0.7	0.19	5e-4	—	2e-5
GCI1 ₂₁	3e-4	0.6	0.3	0.009	—	0.0018
Asymp.2	1.40	1.24	1.50	1.06	0.59	1.37
Asymp.1	1.16	0.86	0.39	0.0020	—	0.88
						1.00
						1.5e-4
						0.92
						1.06

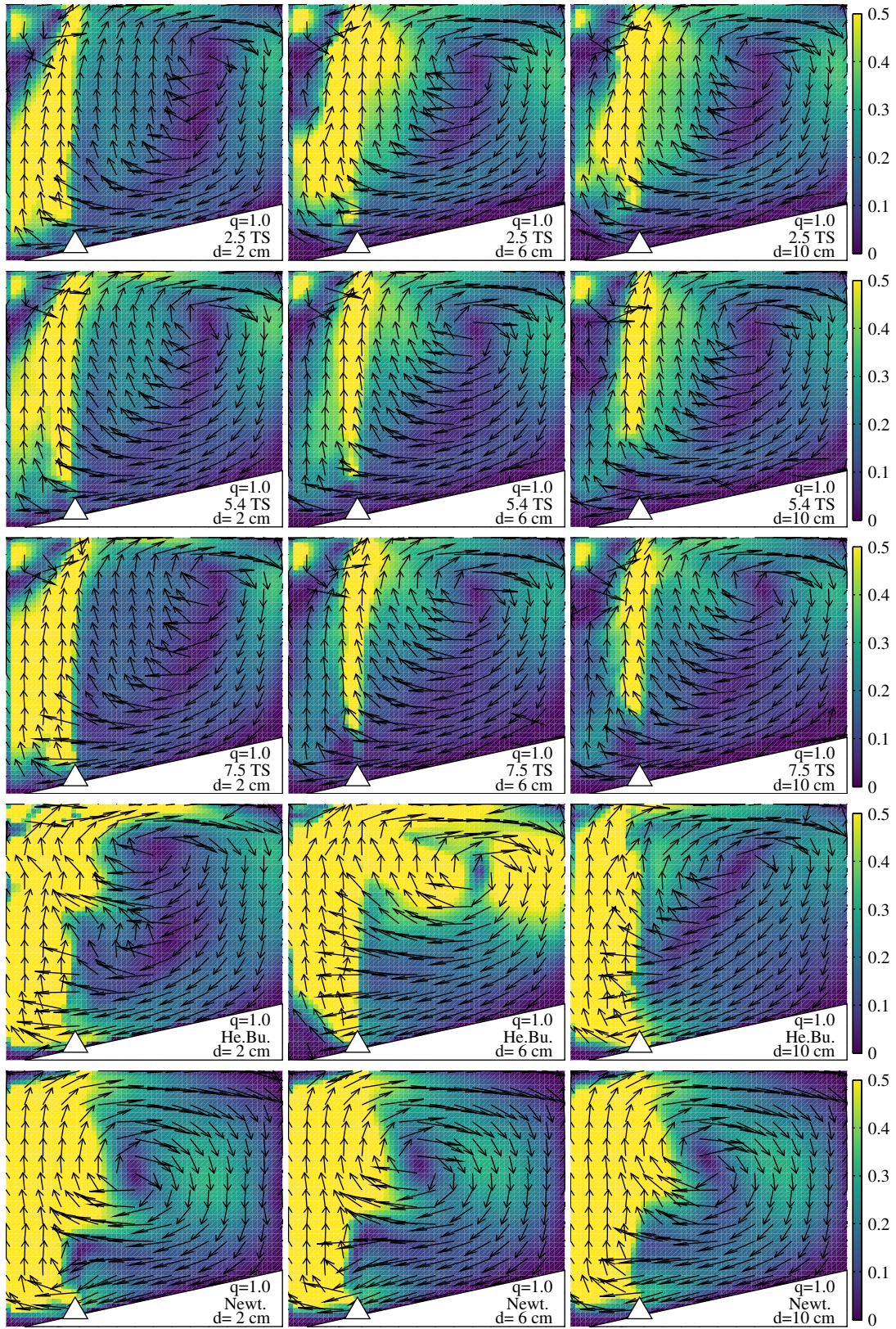


Figure 3: Flow patterns for $q = 1.0$ with $|\mathbf{u}| \in (0, 0.5) \text{ m s}^{-1}$

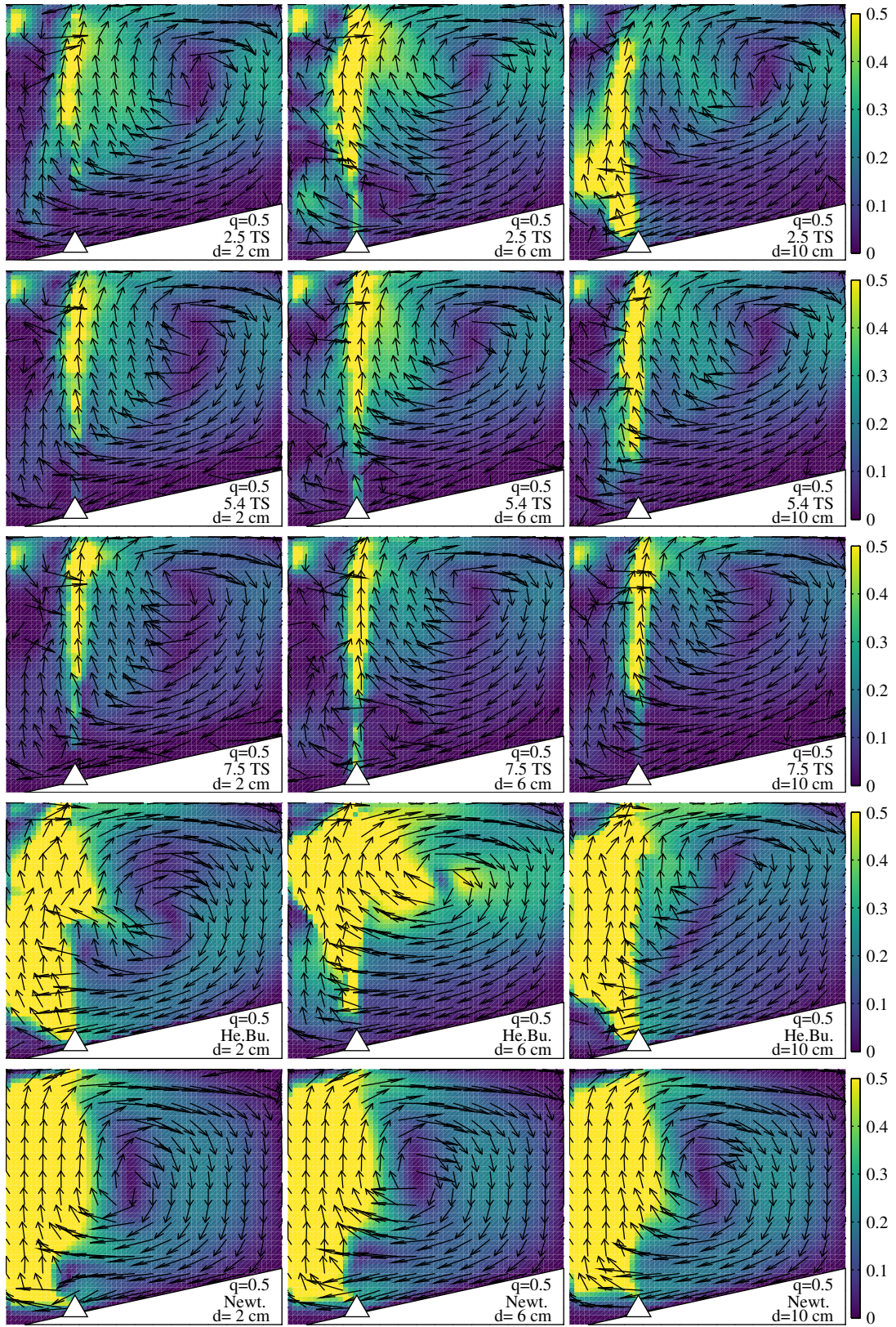


Figure 4: Flow patterns for $q = 0.5$ with $|\mathbf{u}| \in (0, 0.5) \text{ m s}^{-1}$

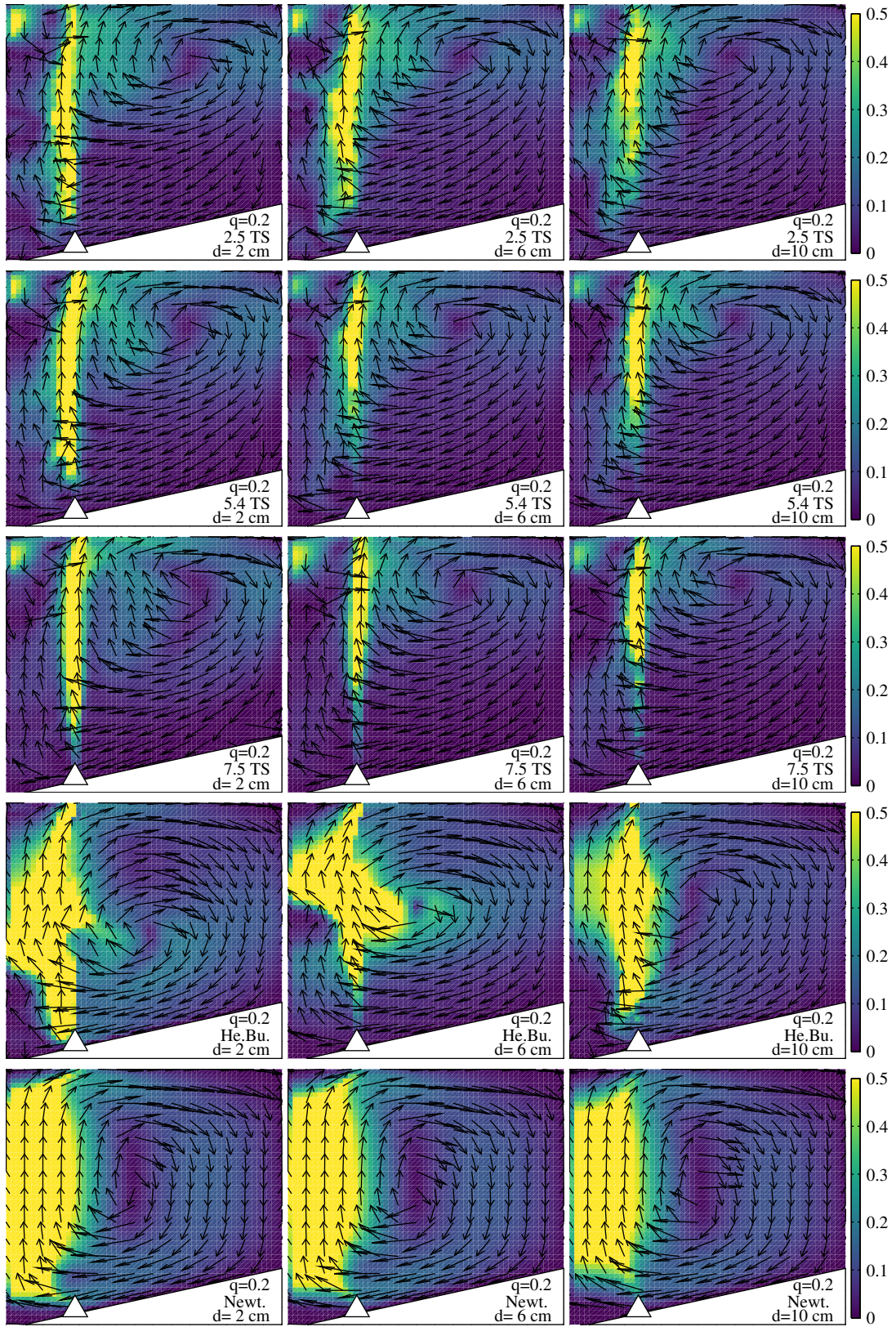


Figure 5: Flow patterns for $q = 0.2$ with $|\mathbf{u}| \in (0, 0.5) \text{ m s}^{-1}$

344 more dispersed as TS rises—on the other side, an increase of gas flow rate brings to
345 the creation of more bubbles, and hence momentum transfer is increased and the main
346 vortex is developed more widely. Finally, the shape of the vortex changes slightly;
347 i.e., the vortex is more extended when d is small.

348 An analysis of viscosity under different flow regimes was undertaken. Figures 6,
349 7 and 8 depict the viscosity field at the last timestep for all the values of TS and
350 d ($q = 1, 0.5$ and 0.2). It can be seen that the viscosity drops along the vertical
351 column and, more interestingly, along the descending branch of the vortex. This is
352 due to the fact that sludge is a pseudoplastic fluid, and its viscosity decreases when
353 shear rate increases. As a consequence of this, flow patterns in which the viscosity
354 is considerably lower than in the surroundings arise inside the domain. Such patterns
355 can be observed in Figure 6 as the rising column and the vortex descending branch.

356 The low-viscosity domains offer less resistance against incoming liquid, when
357 compared to surrounding high-viscosity zones. Hence, it is reasonable to expect that
358 circulation will be enhanced within the low-viscosity areas and, conversely, will be in-
359 hibited in the surrounding high-viscosity zones. This is expected to have a detrimental
360 effect in the uniform distribution of nutrients throughout the digester, and therefore is
361 not desirable.

362 **3.3 Average shear rate**

363 Following the seminal work presented in [43], average shear rate has become a funda-
364 mental process characteristic to classify mixing in vessels in the water industry [12].
365 Despite the fact that the representation of complex flow patterns with one number is
366 something of a simplification, [44], the concept of average velocity gradient is still
367 useful in environmental engineering design [45].

368 [12] reported an analysis of an impeller-stirred lab-scale digester with different TS
369 values and rotational regimes. In that work, high, medium and low-velocity zones
370 were identified, and additionally, the average shear rate was computed. The conclu-
371 sions of [12] can be summarized as: (i) an increase of TS raises the volume of low-
372 mixed zones, but does not have significant effects on the volume of the high-mixed
373 zones; (ii) a change of the impeller angular velocity scarcely affects the average shear
374 rate in the bulk of the domain; (iii) in all cases considered, the average shear rate was
375 well below (up to an order of magnitude) of the suggested value of $50\text{--}80\text{ s}^{-1}$ [45]
376 for optimum mixing, and yet biogas production was achieved.

377 The considerations above show that, for an impeller-stirred lab-scale digester such
378 as the one reported in [12], mixing power input of an anaerobic digester can be lowered
379 without affecting the average shear rate significantly. It is hypothesised here that these
380 conclusions can be extended to a gas-mixed, full-scale digester. In order to verify this
381 statement, the average shear rate $\langle \dot{\gamma} \rangle$ was plotted against q for different TS and bubble
382 diameters and the results are shown in Figure 9. It can be seen that the behaviour of
383 average shear rate depends on both TS and bubble size. For instance, for a bubble
384 diameter of 2 cm $\langle \dot{\gamma} \rangle$ grows proportionally to q , but the rate of increase slows slightly

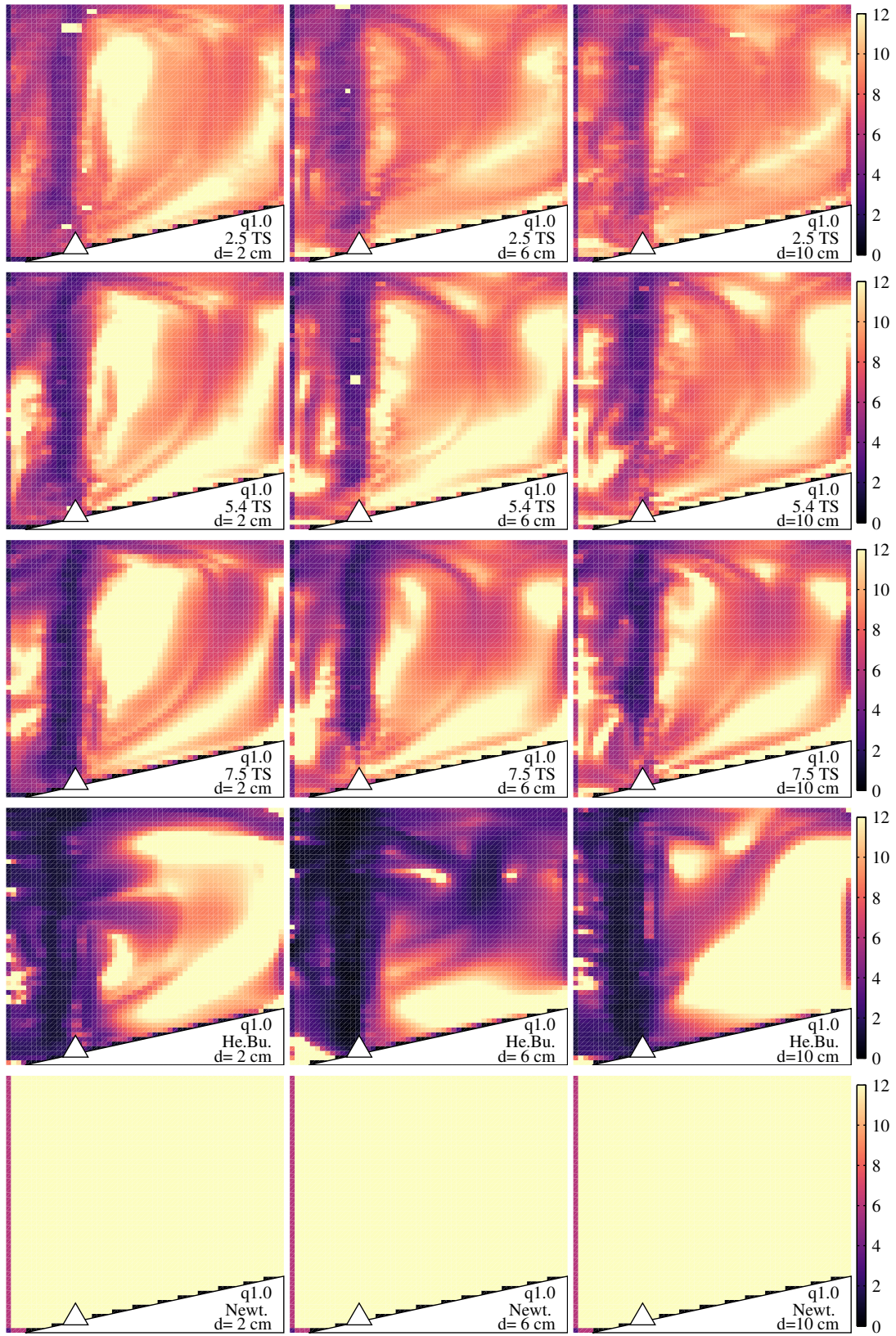


Figure 6: Apparent viscosity for $q = 1.0$ with $\mu \in (0, 0.1)$ Pa s for the 2.5 TS runs, $(0, 0.6)$ Pa s for the 5.4 TS runs, $(0, 2.0)$ Pa s for the 7.5 TS runs

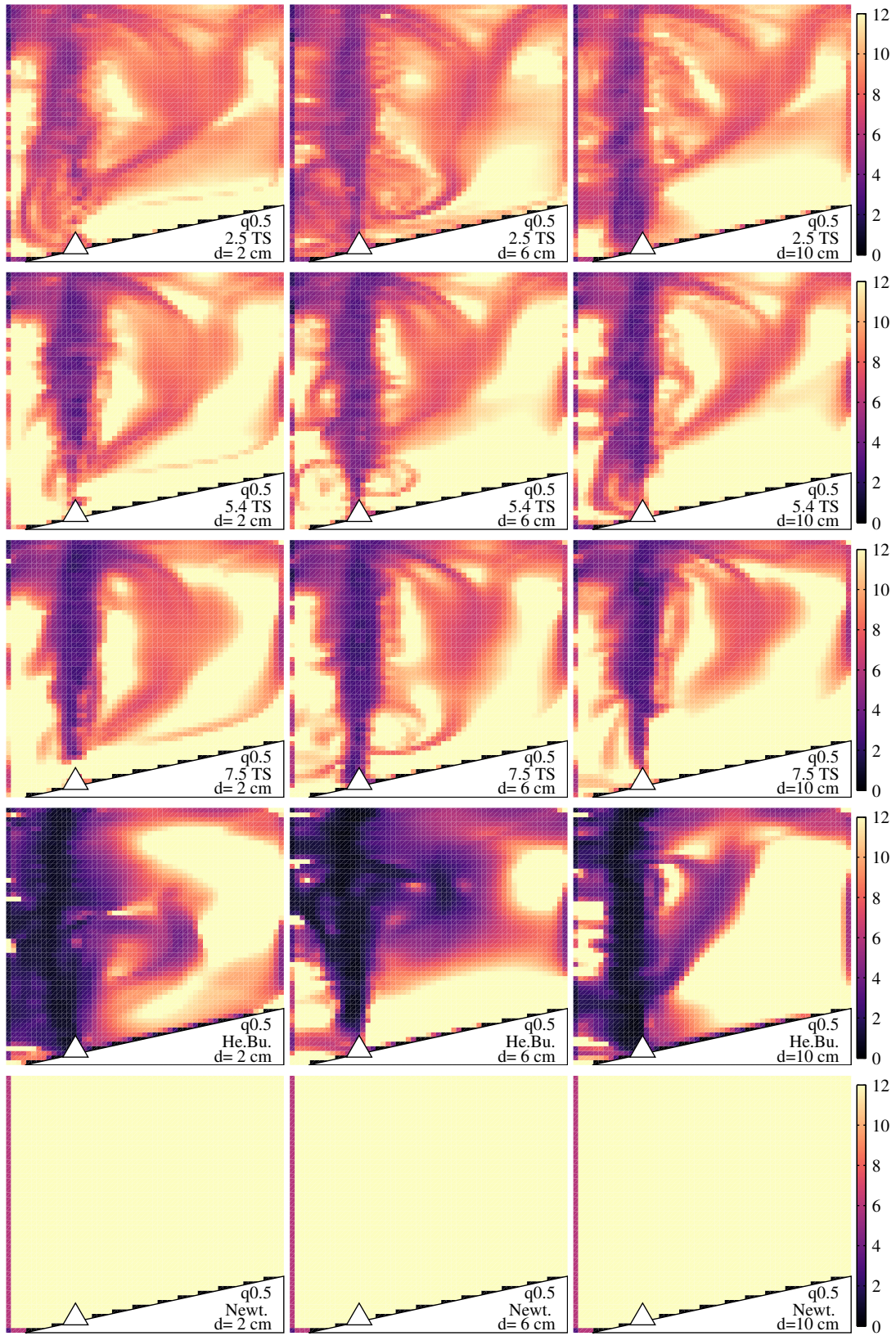


Figure 7: Apparent viscosity for $q = 0.5$ with $\mu \in (0, 0.1)$ Pa s for the 2.5 TS runs, $(0, 0.6)$ Pa s for the 5.4 TS runs, $(0, 2.0)$ Pa s for the 7.5 TS runs

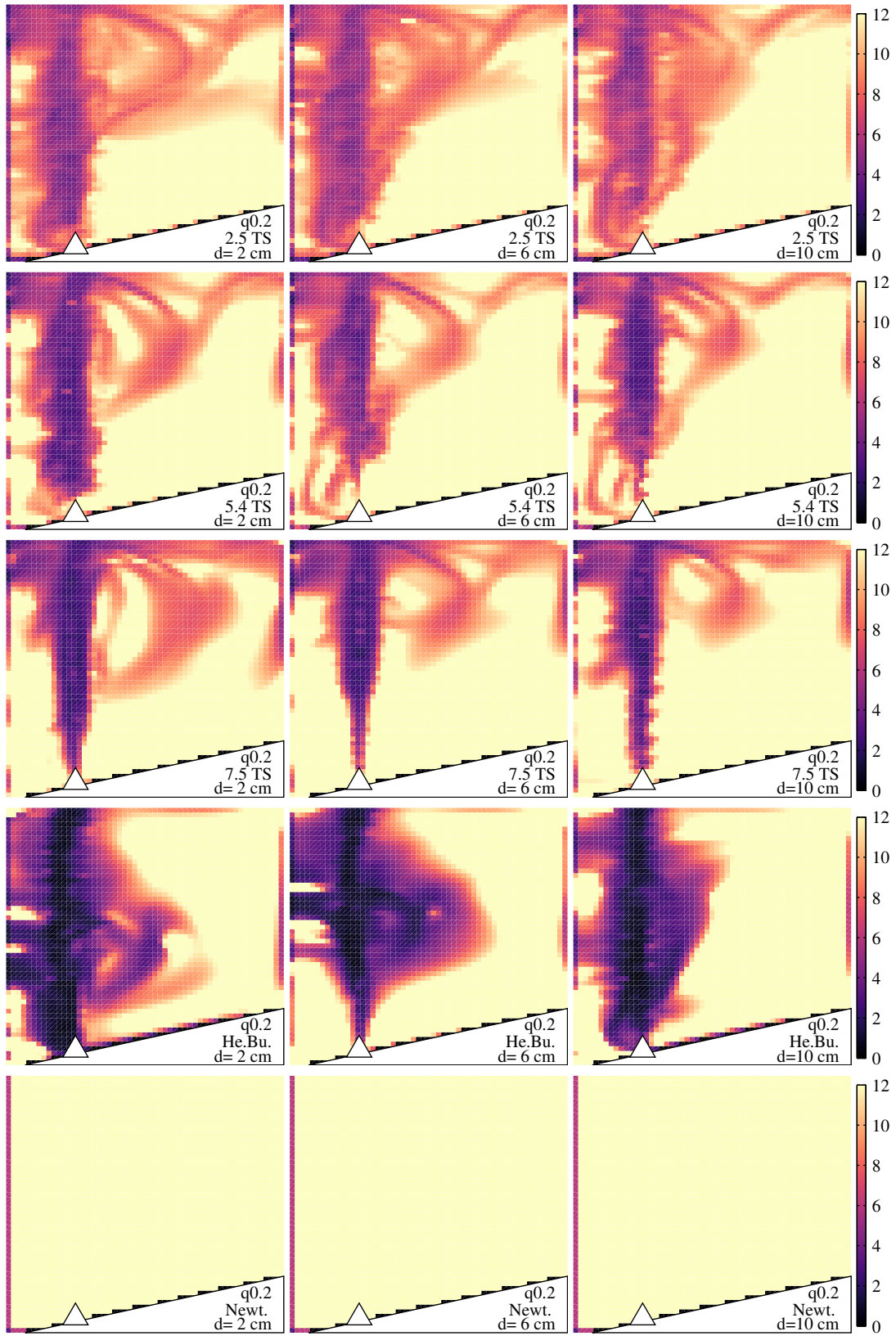


Figure 8: Apparent viscosity for $q = 0.2$ with $\mu \in (0, 0.1)$ Pa s for the 2.5 TS runs, $(0, 0.6)$ Pa s for the 5.4 TS runs, $(0, 2.0)$ Pa s for the 7.5 TS runs

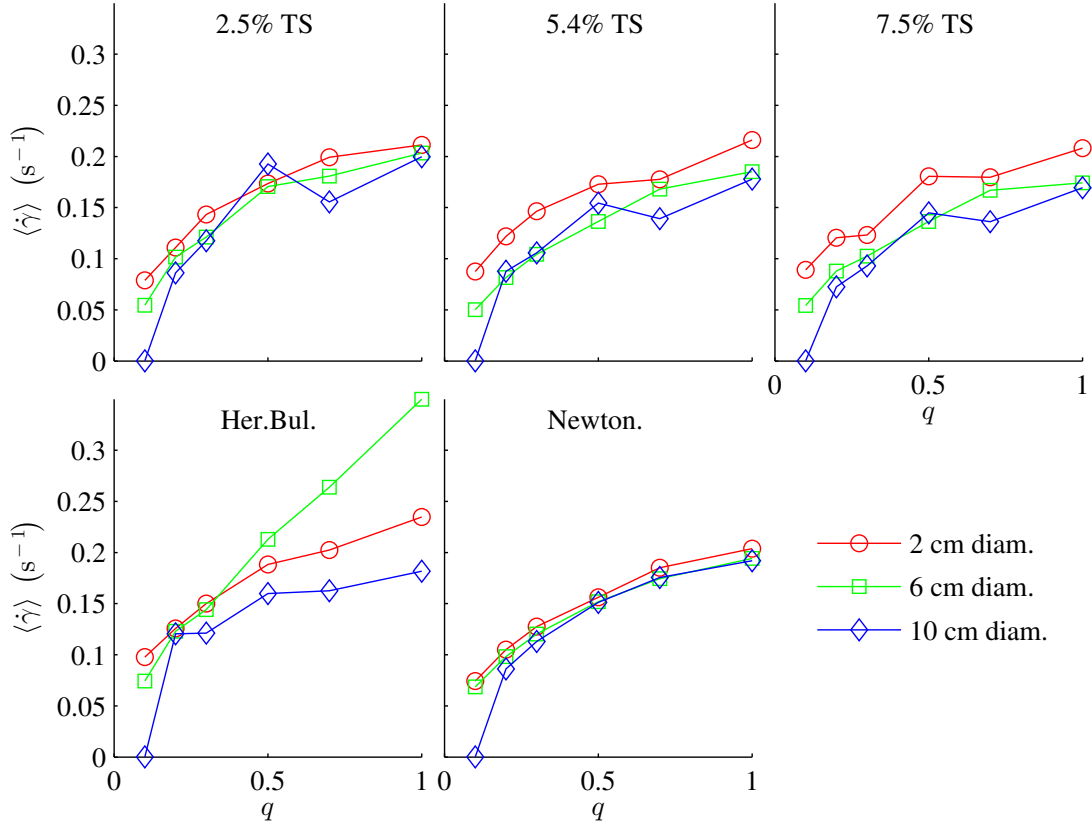


Figure 9: Average shear rate against the power input for different values of TS and d

385 for $q \geq 0.25$ and, more pronouncedly, for $q \geq 0.7$. This behaviour is reproduced by
 386 the 6 cm and 10 cm bubble size runs, with the difference that the decrease happens
 387 for values of q between 0.5 and 0.7, but not for 7.5% TS, where the decrease is not
 388 achieved. Apart from these differences, however, the relevant points that Figure 9
 389 shows are: (i) the trend generally shows a similar growth for all the TS and bubble
 390 diameters, with a slower growth at $q \geq 0.7$, with similar values of $\langle \dot{\gamma} \rangle$ for all the runs;
 391 (ii) in all the cases and, relevantly, in the case $q = 1$ which is known to correspond to
 392 real, well-working digesters, the average shear rate is lower than the values suggested
 393 by widely-accepted literature [45] for optimum mixing, proving that such a criterion
 394 should not be applied to the case of gas mixing in full-scale anaerobic digestion.

395 An analysis was also undertaken on the proportions of different shear rate intervals.
 396 Four shear rate intervals were defined: $\langle \dot{\gamma} \rangle < 0.01 \text{ s}^{-1}$ (very low), $0.01 \leq \langle \dot{\gamma} \rangle < 0.1 \text{ s}^{-1}$
 397 (low), $0.1 \leq \langle \dot{\gamma} \rangle < 1 \text{ s}^{-1}$ (medium), $\langle \dot{\gamma} \rangle > 1 \text{ s}^{-1}$ (high). The results are shown in Fig-
 398 ure 10. The magnitude and behaviour of the shear rate relative volumes are similar for
 399 all the TS irrespective of bubble diameter. In particular: (i) the relative vessel volume
 400 with very low shear rate is initially high (approximately 0.5), then drops quickly to
 401 assume low values at $q = 0.3$ — 0.7 ; (ii) low shear rate relative volume is roughly con-
 402 stant with a value of approximately 0.5; (iii) the medium shear rate relative volume

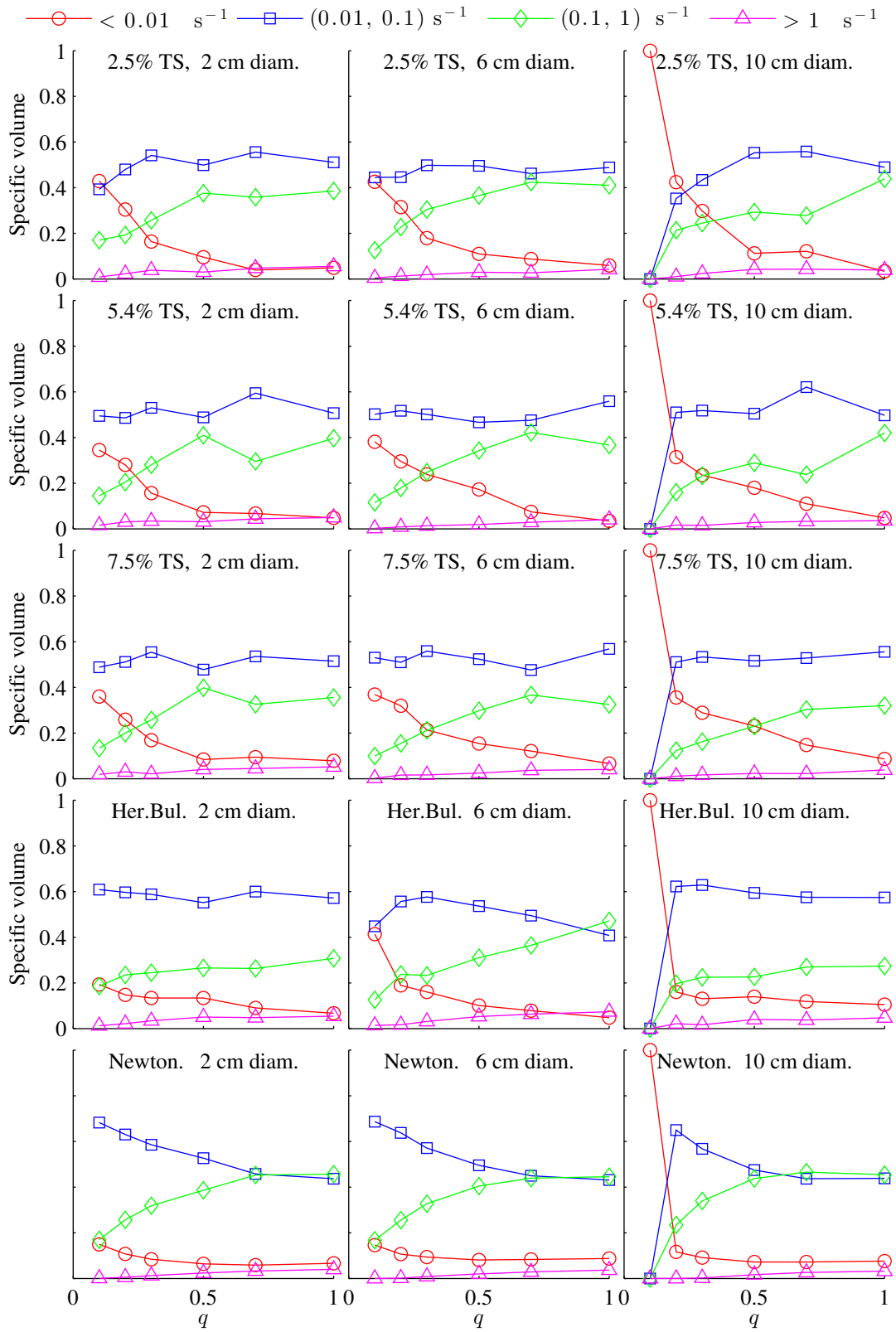


Figure 10: Specific volume of the shear rate intervals against flow rate for different values of TS and d

403 shows a growing trend up to $q = 0.5$ — 0.7 and then is approximately constant; (iv) the
 404 high shear rate relative volume is always negligible, but increases proportionally with
 405 q ; (v) most of the volume is occupied by very low shear rate up to $q \simeq 0.2$; very low,
 406 low and average shear rates equally occupy the domain for q from 0.2 to 0.5 — 0.7 ; and
 407 for q greater than 0.5 — 0.7 most of the volume is equally occupied by low and average
 408 shear rates.

409 As the high shear rate relative volume is negligible, the effectiveness of mixing is
 410 expected to depend on the mutual balance of very low, low and average shear rate
 411 relative volume, rather than on an absolute criterion such as the one proposed by [45].
 412 In particular, good quality mixing can be defined as when the average shear relative
 413 volume is high compared to the relative occupancies of the other shear rate intervals,
 414 and, similarly, very low shear relative volume is low. Considering the results shown
 415 in Figure 10, this condition can be considered to be verified for $q \geq 0.5$.

416 The power input for a single nozzle is [14]:

$$E = P_1 Q \ln(P_2/P_1) , \quad (4)$$

417 where Q is the volumetric flow rate, P_1 is the absolute pressure at the surface (that
 418 is, the atmospheric pressure), and P_2 is the absolute pressure at the nozzle (that is,
 419 $P_2 = P_1 + \rho g H$ if the nozzle discharges at the same pressure of the surrounding fluid,
 420 as in the case presented here). Considering the value of Q_{\max} in Table 2, the value of
 421 the total power per volume unit corresponding to $q = 0.5$ is 1.079 W m^{-3} , which can
 422 be effectively approximated to 1 W m^{-3} . This value corresponds to half of the mixing
 423 power for $q = 1$ of 2.159 W m^{-3} , and is significantly lower than the input mixing
 424 power of 5 — 8 W m^{-3} recommended by US EPA for proper mixing [46]

425 **3.4 Switching nozzles**

426 An alternative way to improve mixing by amending the geometry of the digester—
 427 specifically, by arranging a second concentric series of nozzles at a different distance
 428 from the tank symmetry axis was modelled. Biogas injection was switched between
 429 the original and the new nozzles series, at constant time intervals. This strategy differs
 430 from, and is complementary to, what literature commonly defines as alternated mix-
 431 ing. “Alternated” mixing means that the mixing mechanism (which is in principle not
 432 limited to gas mixing) is activated only for given time intervals as opposed to continu-
 433 ous mixing, where mixing is always active. As such, the strategy of switching nozzles
 434 can be applied to continuous and alternated mixing. In order to avoid confusion, “al-
 435 ternated” here refers to the mode of mixing consisting of activating and de-activating
 436 the mixing mechanism at given time interval, while “switched” or “switching” refers
 437 to the mixing strategy consisting of changing biogas injection between two nozzle
 438 series.

439 The effectiveness of the switching nozzles strategy was tested by performing a
 440 series of simulations, with the additional nozzle series being placed at a distance
 441 $R'_{\text{noz}} = 5.49 \text{ m}$ from the tank axis. The value of $q = 0.5$ was chosen, in line with

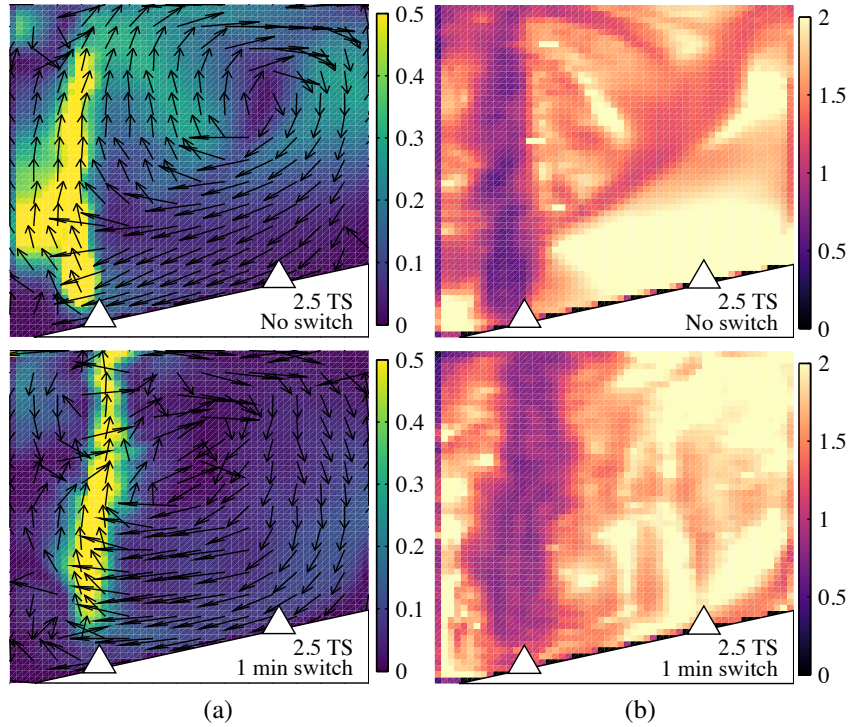


Figure 11: Comparison between original nozzle setup and one-minute switching for $q = 0.5$ and 2.5% TS. (a): Flow patterns with $|\mathbf{u}| \in (0, 0.5) \text{ m s}^{-1}$. (b): Viscosity with $\mu \in (0, 0.1) \text{ Pa s}$.

442 the conclusions on minimum mixing power per volume unit outlined in Section 3.3.
 443 In Section 3.3 it was shown that the outcome of the simulations does not depend on
 444 bubble size; however, the computational expense is proportional to the number of bub-
 445 bles inside the system. For these reasons, $d = 10 \text{ cm}$ was chosen as the bubble size
 446 for all the simulations. During the simulations, biogas injection was switched every
 447 minute, for a total period of 5 minutes.

448 The results of the simulations are shown in Figure 11. The low-viscosity corridor
 449 corresponding to the descending vortex branch is absent under the switching-nozzles
 450 strategy. However, such rapid switching leads to a significant attenuation of the flow
 451 patterns; the velocity magnitude becoming substantially lower everywhere apart from
 452 the immediate vicinity of the bubble plume. This can be attributed to the fact that the
 453 system needs a non-zero time in order to develop flow patterns as the ones described
 454 in Section 3.2. The time interval of one minute is evidently too short for the system to
 455 develop significant flow patterns away from the bubble plume. It is not clear whether
 456 this situation corresponds to a better or worse level of mixing, and hence, a further
 457 investigations was undertaken.

458 A second analysis was performed by defining a non-diffusive tracer the concentra-

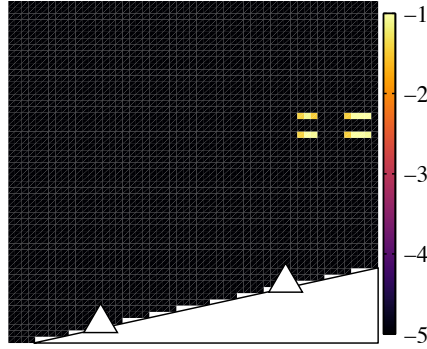


Figure 12: $\log_{10} \chi$ at the initial timestep. $\chi = 1$ inside the small squares, 0 elsewhere.

459 tion of which obeys the following equation:

$$\partial_t \chi + (\mathbf{u} \cdot \nabla) \chi = 0 . \quad (5)$$

460 At $t = 0$, a maximum tracer concentration was defined in four locations inside the
 461 domain, as shown in Figure 12.

462 Figure 13 shows the distribution of χ after 20 minutes, in the original (non-switched)
 463 nozzles configuration, and in setups where biogas injection was switched every minute
 464 and every five minutes respectively. In the original setup, the tracer spreads through
 465 an external ring following the vortex described in Figures 3, 4 and 5; under all the
 466 different rheologies, the stagnant zone at the centre (in black) is clearly evident.

467 In both the nozzle-switching configurations, the tracer becomes almost uniform
 468 throughout the domain, despite the above-mentioned attenuation of the velocity flow
 469 patters. The average value of χ evidently changes depending on rheology and switch-
 470 ing interval, and some minor differences in tracer distribution can be observed; how-
 471 ever, in all the cases, the stagnant zone at the centre of the domain vanishes completely.
 472 Such cancellation of the central dead zones is a critical benefit of the switching strat-
 473 egy, confirming the benefits to be derived from the introduction of the additional noz-
 474 zle series.

475 4 Conclusions

476 For the first time, an Euler-Lagrangian CFD model was used to model gas mixing in
 477 a full-scale anaerobic digester.

478 The traditional approach to assess mixing quality, based on evaluating the average
 479 shear rate, was shown to be inapplicable to the case of full-scale, gas-mixed digesters.
 480 As an alternative, two novel approaches, based on the analysis of shear rate relative
 481 intensity intervals, and the introduction of a passive, non-diffusive scalar tracer, were
 482 evaluated.

483 The formation of low viscosity flow patterns under certain mixing conditions was
 484 observed and their detrimental effect on mixing were discussed.

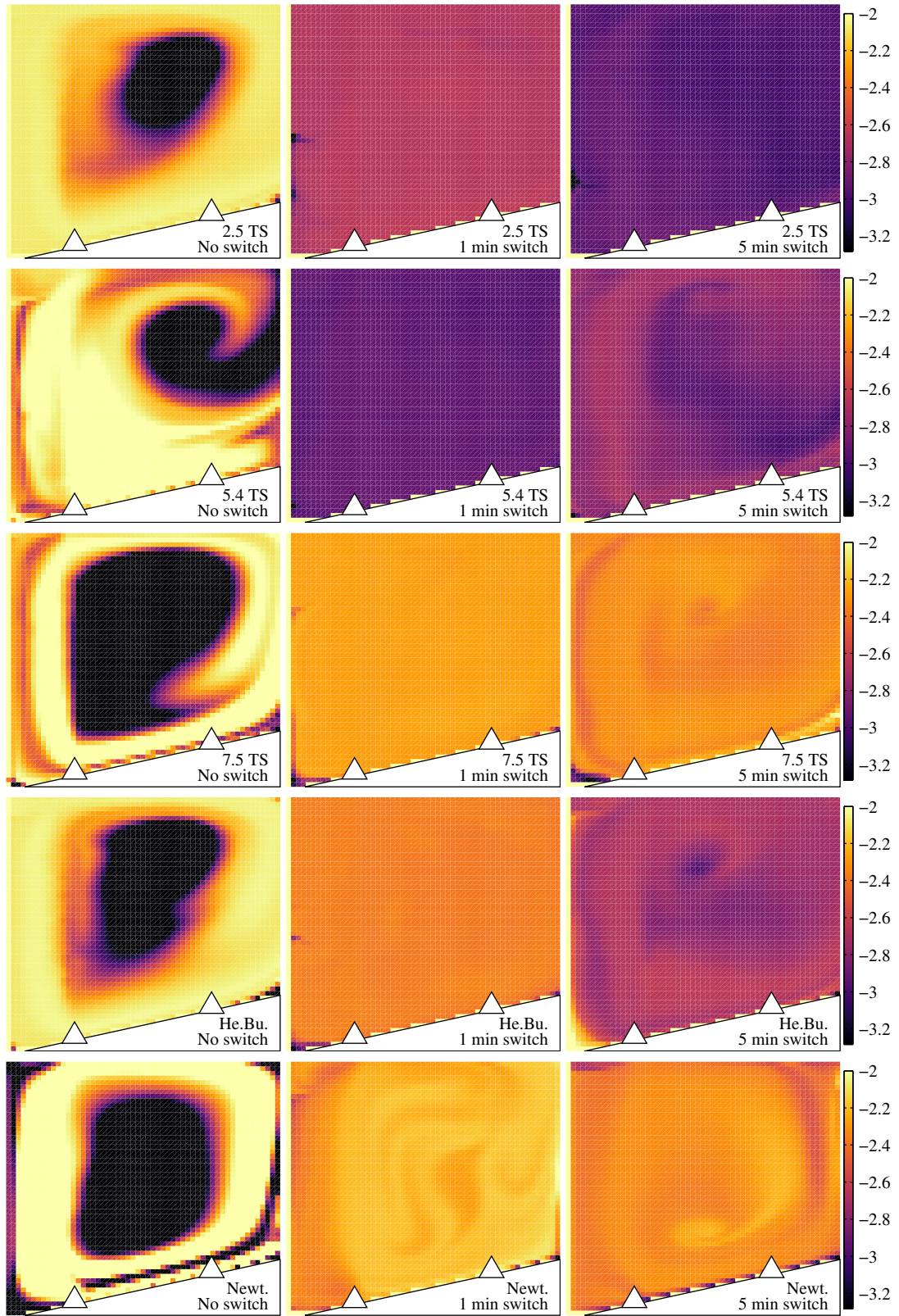


Figure 13: $\log_{10} \chi$ for $q = 0.5$ after 1,200 s.

485 A new strategy to improve mixing quality was introduced. Specifically, it consists
486 of arranging a second series of nozzles at a different distance from the tank symmetry
487 axis, and switching biogas injection between the original and the new series at regular
488 time intervals. This strategy was shown to be successful in removing the dead zones
489 at the centre of the tank, irrespective of the sludge rheology, when switching was
490 performed every minute or every five minutes.

491 Even without applying the above-mentioned strategy, the CFD results show that the
492 quality of mixing is not expected to drop significantly when the maximum gas flow
493 rate in the study presented here is halved. More generally, the power per unit volume
494 can be lowered down to approximately 1 W m^{-3} , thus saving half of the reference
495 input power for this study corresponding to $q = 1$, for the same expected biogas yield.
496 Further research aimed at implementing viscosity flow patterns mitigation strategies
497 is required to demonstrate that even higher input mixing power savings are achievable
498 without changes in the biogas yield.

499 The flow patterns depend on bubble size, and therefore further research aimed at
500 experimentally measuring bubble size in gas-mixed digesters is desirable. Neverthe-
501 less, the shear rate dependence over total solid and mixing input power show similar
502 trends for all the bubble sizes considered, and therefore the conclusions drawn hold
503 irrespective of the bubble size.

504 **Acknowledgments**

505 The details of the digester geometry were kindly provided by Peter Vale and Severn
506 Trent Water Ltd., whom the authors gratefully acknowledge.

507 The computational work reported in this paper was undertaken using the BlueBEAR
508 high performance computing facility at the University of Birmingham, UK. The au-
509 thors are grateful for the facility and support provided by the University.

510 The first author is funded via a University of Birmingham Postgraduate Teaching As-
511 sistantship award.

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