

# CFD numerical simulation of particle suspension and hydromechanical stress in various designs of multi-stage bioleaching reactors

Jonathan Chéron, Céline Loubière, Stéphane Delaunay, Anne-Gwenaelle Guezennec, Eric Olmos

# ▶ To cite this version:

Jonathan Chéron, Céline Loubière, Stéphane Delaunay, Anne-Gwenaelle Guezennec, Eric Olmos. CFD numerical simulation of particle suspension and hydromechanical stress in various designs of multistage bioleaching reactors. Hydrometallurgy, 2020, 197, pp.105490. 10.1016/j.hydromet.2020.105490 . hal-02968771

# HAL Id: hal-02968771 https://hal.science/hal-02968771v1

Submitted on 17 Oct 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



- 1 CFD numerical simulation of particle suspension and hydromechanical stress in various designs of
- 2 multi-stage bioleaching reactors
- 3 Jonathan CHERON<sup>a</sup>, Céline LOUBIERE<sup>b</sup>, Stéphane DELAUNAY<sup>a</sup>, Anne-Gwénaëlle GUEZENNEC<sup>b</sup>, Eric
- 4 OLMOSa,\*

8 9

10 11

12

13

14

15

16

17

18

19

20

21

22

23

24

25

26

27 28

29 30

31

32

33

34

35

36

37

38

39

40

41

42

43

44

45

46

47

48

- <sup>a</sup> Laboratoire Réactions et Génie des Procédés, Université de Lorraine, CNRS, LRGP, 54000 Nancy,
   France
  - <sup>b</sup> Bureau de Recherches Géologiques et Minières, BRGM, 45100 Orléans, France
  - \*Corresponding author: eric.olmos@univ-lorraine.fr (E. Olmos).

Abstract: The performance of bioleaching stirred tank reactors (STR) is related to the homogeneity of biomass, substrates and dissolved gases. This work was focused on the characterization of the impeller design on bioreactor hydrodynamics and, more specifically on power, mixing efficiency and particle stress. Few studies addressed the issue of the impact of the impeller design on these, especially for multi-stage bioreactors which are the most commonly used at the industrial scale. To fill this lack, a two-stage solid-liquid computational fluid dynamics (CFD) model was simulated on more than 50 conditions to assess power consumption, dissipated power, suspension quality and particle stress. A dual impeller configuration was chosen using Rushton turbines, R600, Hydrofoil, Elephant Ear and HTPG impellers. Grinded pyrite-rich materials (average particles size: 80 µm) were considered as the solid phase at 3 different solid concentrations (10, 18 and 26 % w/w). Considering the impeller power number  $(N_p)$ , the configuration with an axial impeller consumed less energy than a radial impeller in concordance with literature data. The results show that the impeller design had few to no effect on mixing efficiency considering a given power dissipation per unit volume. Independently on the impeller used, unique relationships were found between particle stress and mixing efficiency. This study gives new insights for reactor design and scaling of bioleaching stirred tank reactor and more specifically on the reduction of shear stress for the attached bacterial communities.

## 1. Introduction

In the last decades, bioleaching has been successfully implemented at the industrial scale and used, either in the form of dump or heap treatments, or by using large-scale stirred tank reactors (STR) (Clark et al., 2006; Brierley and Brierley, 2013). Dump or heap treatments were widely used for low-grade copper-based sulphides because of the low cost of implementation and maintenance of these processes. On the other hand, bioleaching STR have proven to be more efficient to extract metals from low-grade or refractory ores but are limited to precious metals because of their significant cost of implementation (Rawlings and Johnson, 2007). Nonetheless, bioleaching is evolving towards the exploitation of 'unconventional' resources caused by the declining trend in mean ore grades (Mudd et al., 2013; Frenzel et al., 2017). These resources are represented with unusual features such as very low-grades, complex mineralogy, or high sulphur content. If heap bioleaching has been the main process option for their treatment until now, it is not always suitable. The main reasons that precludes heap application are the composition of the materials to be treated (presence of carbonate causing heap clogging, or high concentrations of sulphides that lead to uncontrolled and excessive temperature increase in the heap) and the lack of sufficient space, especially in densely populated areas like in Europe. In such cases, bioleaching STR might be a technical alternative but is mostly too expensive except in very few cases when the metal value is high enough (e.g. such as in Uganda for the cobalt recovery in flotation tailings (Morin and d'Hugues, 2007) or in Finland for the valorization of nickel from talc mining residues (Wakeman et al., 2011; Neale et al., 2017)). The expansion of STR bioleaching requires thus further technical optimization to reach an economic viability.

As in any chemical engineering process, the management of bioleaching bioreactors is aimed at optimizing the reacting conditions to accelerate the oxidation processes of the sulphides and to maximize the solubilization or liberation efficiency of valuable metals. This optimization of the reacting conditions is closely related to the homogeneity of biomass, substrates and dissolved gases throughout the reactor. This is especially important considering that the interactions between the microorganisms and sulphides (microbial attachment and biofilm formation) are considered key parameters to improve bioleaching (Brierley and Brierley, 2013). To this end, improving mixing efficiency would result in a better mass transfer of the components in the system (Petersen, 2010; Buffo et al., 2016). Furthermore, significant power consumption of the process comes from mechanical mixing, which is directly related to the solid content (through sufficient agitation rate ensuring suspension and gasliquid mass transfer efficiency) and its physical properties (Bujalski et al., 1999; Jafari et al., 2012). Bioleaching in STR involves substantial power consumption, which results in high operating costs that limit, until now, the use of this technology to the treatment of high added-value resources (mainly refractory gold ores). Besides these commodities, the expansion of bioleaching to 'unconventional' primary resources with lower value, such as low-grade ores or base metal ores and tailings, requires adapting the STR process to the characteristics of these resources in order to limit investment and operating costs while maintaining high extraction efficiency (Bouquet and Morin, 2006; Morin and d'Hugues, 2007) as these resources present a wide range of shape, size and physical properties.

Solid-liquid stirred tanks were widely studied in the literature to define standard designs in order to optimize their efficiency through a better solid distribution (Montante et al., 2012; Tamburini et al., 2014). The power consumption per unit of volume P/V is generally considered as one of the best criterion for the scale-up of these vessels (Rushton, 1950; Chapple et al., 2002) as it could be related to mass transfer capacities or mixing times (Bouaifi and Roustan, 2001; Zhang et al., 2017). Dimensional analysis indicates that its value is provided by dimensionless models relating the power number  $N_p$  to the Reynolds number Re, the impeller power number  $N_p$  being represented by the following equation:

$$N_p = \frac{P}{\rho_1 N^3 D^5} = f \left( Re = \frac{\rho_1 N D^2}{\mu} \right) \tag{1}$$

with P the power required for the impeller rotation,  $\rho_l$  the fluid density, N the agitation rate,  $\mu$  the liquid viscosity and D the impeller diameter. It is a well-known result that, in baffled vessels, the power number is independent of the Reynolds number in the turbulent regime ( $Re > 10^4$ ) and reaches a constant value that only depends on bioreactor design (Rushton, 1950). It is also important to emphasize that the required power P (which is related to the electric power consumption) should be preferentially minimized to limit the OPEX of the bioleaching process.

Nevertheless, this parameter is not sufficient to describe the suspension quality, defined by the spatial distribution of the particles within the flow. To describe the suspension quality, the just-suspended agitation rate  $N_{\rm js}$ , defined as the minimal agitation rate ensuring the suspension of all solid particles, has often been used as a good compromise between optimal mass transfer and minimal power consumption (Zwietering, 1958; Brucato et al., 2010; Tamburini et al., 2012, 2011). However, this criterion fails to describe the solid suspension quality (Harrison et al., 2012). Mak (1992) used the standard deviation of the local solid concentration as a way to characterize the solid distribution but the experimental set-up complexity makes difficult the use of this method to screen a high number of bioreactor designs. Furthermore, the solid distribution within the liquid phase should be related to the local values of turbulent dissipation rates (Kumaresan and Joshi, 2006) which strongly depend on both the vessel and the impeller design (Houcine et al., 2000). However, while an increase of power dissipation is expected to sensibly improve the mixing efficiency of the bioreactor from a physical point of view, the hydromechanical stress generated by the agitation may also weaken the microbial adhesion or even lower the process performances. This is particularly detrimental for bioleaching

processes due to the major importance of microbial attachment and biofilm formation (Rodríguez et al., 2003; Guezennec et al., 2017). This was observed with Acidithiobacillus ferrooxidans cultures in shaking flasks (Xia et al., 2008). Similar observations were made in STR during thermophilic cultures of Sulfolobus sp. (d'Hugues et al., 2002; Sissing and Harrison, 2003). Moreover, it was shown by Wang et al. (2014) that, for moderately thermophiles cultures, the proportion of attached cells is higher than of planktonic cells. Also, altering the capacity of the cell to attach on the mineral surface leads to a decrease of bioleaching efficiency (d'Hugues et al., 2008). Considering the effect of solid loading, it was demonstrated by Witne and Phillips (2001) that the increase of solid concentration in continuous STR induced an increase of the leaching rate until a point where it had a negative effect, which could be caused by the attrition of cells. Similar results were observed by Raja (2005) in shaking bottles where a decrease in specific oxygen consumption rate and cell viability was observed at increasing quartzite concentrations. In the same way, Nemati and Harrison (2000) observed that if a partial suspension of the pulp was obtained for a concentration of 18 % w/v (corresponding to 16 % w/w with the hypothesis of  $\rho_{\rm s}$  = 2610 kg m<sup>-3</sup>), the rate of iron solubilization was reduced. However, achieving complete particle suspension led to an apparent cell damage, as shown by a reduced cell count. More generally, it must be underlined that solid concentration has not the same influence on mesophilic and moderately thermophilic bacteria (such as Leptosirillum and Acidithiobacillus sp.), and extremely thermophilic archaea (such as Acidianus, Metallosphaera, and Sulfolobus sp.). As reviewed by Brierley and Brierley (2013), STR bioleaching with archaea, which have no rigid cell wall, necessitates a somewhat lower solid concentration than 12.5 % in reactor opposed to the common 20 % in plants processing sulfidicgold concentrates with mesophilic and moderately thermophilic bacteria, due to their difference of shear sensitivity.

94 95

96 97

98

99

100

101

102

103

104

105

106107

108

109

110

111

112

113

114

115

116

117

118119

120

121122

123124

125

126

127

128

129

130

131

To understand the previous results, it is important to consider that, in bioleaching reactors, hydromechanical stresses may impact the process performance following three phenomena: (i) direct shear of the liquid phase on the microorganisms in suspension (Fig. 1a), (ii) shear stress on particles that potentially hold adhered microorganisms or biofilms (Fig. 1b), and (iii) particle-particle frictions and collisions (Fig. 1c). The occurrence of direct shear is still debated. It is generally assumed, but not completely demonstrated, that hydrodynamics has no impact on planktonic microorganisms if, locally, the Kolmogorov length scale  $l_K = (v^3/\varepsilon)^{0.25}$  is higher than the microorganism diameter (Nienow, 2006). In this equation,  $\varepsilon$  (W kg<sup>-1</sup>) is the power dissipation per unit of mass (or turbulent dissipation rate) and  $\nu$  is the kinematic viscosity (m<sup>2</sup> s<sup>-1</sup>). Considering microorganisms of the micrometer scale, the maximal power dissipation necessary to induce direct cell damage would be  $\varepsilon \sim 10^6$  W kg<sup>-1</sup>, which is unlikely to be reached in standard stirred tank bioreactors. In comparison, the value of power dissipation that would induce hydrodynamic stress on particle with a diameter in the range 10-100 µm would be  $\varepsilon \sim 0.01\text{-}100 \text{ W kg}^{-1}$ , which is more likely to be observed with usual mixing conditions. Lastly, particle-particle frictions frequency and intensity depend on the local volume fraction of particles and the relative velocity between particles, and consequently on the design of the bioreactor, the agitation rate and the mean particle concentration.

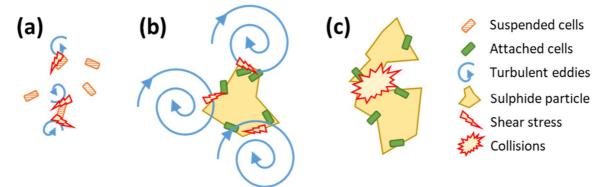


Fig. 1: Description of the hydromechanical stress applied on microorganisms due to: (a) direct shear of the liquid; (b) shear stress on particles; (c) particle-particle frictions and collisions.

From a physical point of view, a quantitative description of the bioreactor hydrodynamics relies on a better knowledge of the coupling between bioreactor design, operating conditions, solid distribution within the bioreactor and particle stress. Computational Fluid Dynamics (CFD) can be used as an efficient approach to locally represent or calculate the hydrodynamics parameters of these processes. Among others, the local solid concentration, the liquid mean and fluctuating velocities and the impeller torque are representative parameters (Wadnerkar et al., 2012; Zheng et al., 2018b). In a gas-mixed leaching tank, Song et al. (2015) used a gas-liquid Euler-Euler approach to enhance the design of the reactor in terms of bubble diameter or draft tube diameter. In the study of Gradov et al. (2017), the rheology of the slurry was modelled using a power law while a gas-liquid Euler-Euler approach was used to determine the volumetric distribution of the gas-liquid mass transfer coefficient within the bioreactor. Three-phase flow was simulated in a vessel equipped with an HEDT impeller by Zheng et al. (2018a) ; the authors showed that a gas-liquid-solid Euler-Euler combined with a  $k-\varepsilon$ turbulence model was able to predict the mechanical power dissipation with an error lower than 15 %. Recently, Loubière et al. (2019) developed strategies to determine optimal bioreactor configurations for the culture of mesenchymal stem cells in stirred tank vessels, on spherical microcarriers by using a coupled CFD-genetic algorithm approach. The optimization criterion was a minimization of power dissipation encountered by the particles, at the particle just-suspended state.

Despite the referenced studies, the identification of the impact of impeller geometry choice on bioleaching reactor hydrodynamics remains incomplete, especially in multi-stage bioreactors, which are the most commonly used at the industrial scale. Moreover, no studies put into evidence the coupling between power dissipation, solid homogeneity and occurrence of particle stress. The present work was focused on the comparison of the effects of the impellers design on the hydrodynamics of a two-stage solid-liquid bioleaching reactor. For this, more than 50 CFD simulations based on a liquid-solid granular Euler-Euler model were carried-out with six radial and axial impeller designs. The performance of each impeller was quantified through the power number  $N_p$  and compared with literature data. Furthermore, the standard deviation of the solid concentration distribution was calculated to determine the respective efficiency of the impellers on solid scattering. The spatial distribution of hydromechanical stress on particles was determined for each bioreactor configuration and for three solid concentrations of 10, 18 and 26 % w/w.

# 2. Material and Methods

2. 1. Model description

- 168 In this work, a steady-state Eulerian-Eulerian multiphase approach was used to simulate the solid-
- 169 liquid flow, where the continuous and dispersed phases are considered as interpenetrating continua.
- Both phases are identified by their own volume fraction and are related as:

$$\alpha_{\rm S} + \alpha_{\rm I} = 1 \tag{2}$$

- where  $\alpha_s$  and  $\alpha_l$  are the volume fractions of the solid and liquid phases respectively. The continuity
- 172 equation for each phase can be written as:

$$\nabla \cdot (\alpha_1 \rho_1 \mathbf{u}_1) = -\nabla (\gamma_s \nabla \alpha_s) \tag{3}$$

$$\nabla \cdot (\alpha_{s} \rho_{s} \mathbf{u}_{s}) = \mathbf{F}_{TD} = \nabla (\gamma_{s} \nabla \alpha_{s}) \tag{4}$$

- where  $\rho$  and  $\mathbf{u}$  are the density and velocity of each phase, and  $\mathbf{F}_{TD}$  is related to the turbulent dispersion
- 174 force. This turbulent dispersion force takes into account the dispersion due to turbulent velocity
- 175 fluctuations and was modelled using the diffusion-in-VOF model. The diffusion coefficient  $\gamma_s$  is related
- to the turbulent viscosity  $\mu_{t,l}$  by  $\gamma_s = (\mu_{t,l}/0.75)$ . The momentum conservation equation for each
- 177 phase is:

$$\nabla \cdot (\alpha_{l} \rho_{l} \mathbf{u}_{l}) = -\alpha_{l} \nabla p + \alpha_{l} \rho_{l} \mathbf{g} + \nabla \cdot \overline{\mathbf{\tau}}_{l} + \mathbf{F}_{D,ls}$$
(5)

$$\nabla \cdot (\alpha_{s} \rho_{s} \mathbf{u}_{s} \mathbf{u}_{s}) = -\alpha_{s} \nabla p - \nabla p_{s} + \alpha_{s} \rho_{s} \mathbf{g} + \nabla \cdot \overline{\mathbf{\tau}}_{s} - \mathbf{F}_{D.ls}$$

$$\tag{6}$$

- where p is the pressure field shared by the two phases,  $p_s$  is the solid pressure,  $\mathbf{g}$  the gravitational
- acceleration,  $\bar{\bar{\tau}}$  the phase stress strain tensor and  $F_{D,ls}$  the interphase momentum transfer.
- 180 Interphase forces that are generally expected in a multiphase liquid-solid flow include: turbulent
- dispersion, drag, virtual mass, Basset and lift forces. Previous studies have shown that solid-liquid flows
- in STR are correctly represented using only turbulent dispersion and drag forces with a low effect of
- other forces on simulation results (Ljungqvist and Rasmuson, 2001; Khopkar et al., 2006; Qi et al.,
- 184 2013). The turbulent dispersion force  $\mathbf{F}_{\mathrm{TD}}$  should be modelled when the size of turbulent eddies is
- larger than the particle size (Kasat et al., 2008; Wadnerkar et al., 2012) which is a priori expected in
- standard bioreactors. Furthermore, the virtual mass, Basset and lift forces may be neglected as they
- have a much lower magnitude than the drag forces. (Tatterson, 1991; Tamburini et al., 2014; Raja
- 188 Ehsan Shah et al., 2015).
- The drag force  $F_{D,ls}$  between liquid and solid phases was calculated by the following equation:

$$\mathbf{F}_{\mathrm{D,ls}} = K_{\mathrm{ls}}(\mathbf{u}_{\mathrm{s}} - \mathbf{u}_{\mathrm{l}}) \tag{7}$$

- with  $K_{\rm ls}$  the interphase exchange coefficient between liquid and solid phases respectively, determined
- 191 by

$$K_{\rm ls} = C_{\rm D,ls} \frac{3}{4} \rho_{\rm l} \frac{\alpha_{\rm s} \alpha_{\rm l}}{d_{\rm p}} |\mathbf{u}_{\rm s} - \mathbf{u}_{\rm l}| \tag{8}$$

The drag coefficient  $C_{\rm D,ls}$  is given by the Schiller and Naumann model (Schiller, 1933):

$$C_{\text{D,ls}} = \begin{cases} 24(1 + 0.15Re_{\text{p}}^{0.687})/Re_{\text{p}} & Re_{\text{p}} < 1000\\ 0.44 & Re_{\text{p}} \ge 1000 \end{cases}$$
(9)

193 with  $Re_p$  the particle Reynolds number:

$$Re_{\rm p} = d_{\rm p}(\mathbf{u}_{\rm s} - \mathbf{u}_{\rm l})/v_{\rm l} \tag{10}$$

- 194 The dispersed  $k \varepsilon$  model was chosen as it is recommended for multiphase flows considering a
- continuous and a dispersed phases with a density ratio between phases equal or higher to 2.5 (s.n.

Ansys, 2019). This is often validated in bioleaching as most substrates are sulphidic materials of density higher than 2.5. In our case, water was chosen as the liquid phase ( $\rho_l$  = 1000 kg m<sup>-3</sup>,  $\mu_l$  = 0.001 Pa s) and particles with the characteristics of grinded pyrite-rich materials ( $\rho_s$  = 2610 kg m<sup>-3</sup>,  $d_p$  = 80 µm, pyrite fraction = 51 %) were considered for the solid phase. In this approach, turbulence is fully-modelled for the continuous phase and the turbulence of the dispersed phase is possibly taken into account through additional interaction terms. The  $k-\varepsilon$  model provides the transport equations of the turbulent kinetic energy k and its dissipation rate  $\varepsilon$ :

$$\nabla \cdot (\alpha_{l} \rho_{l} \mathbf{u}_{l} k_{l}) = \nabla \cdot \left( \alpha_{l} \left( \mu_{l} + \frac{\mu_{t,l}}{\delta_{\nu}} \right) \nabla k_{l} \right) + \alpha_{l} G_{k,l} - \alpha_{l} \rho_{l} \varepsilon_{l}$$
(11)

$$\nabla \cdot (\alpha_{l} \rho_{l} \mathbf{u}_{l} \varepsilon_{l}) = \nabla \cdot \left( \alpha_{l} \left( \mu_{l} + \frac{\mu_{t,l}}{\delta_{\varepsilon}} \right) \nabla \varepsilon_{l} \right) + \alpha_{l} \frac{\varepsilon_{l}}{k_{l}} \left( C_{\varepsilon 1} G_{k,l} - C_{\varepsilon 2} \rho_{l} \varepsilon_{l} \right)$$
(12)

203  $\mu_{t,l}$  is the turbulent viscosity of the continuous liquid phase:

$$\mu_{\rm t,l} = \rho_{\rm l} C_{\rm \mu} \frac{k_{\rm l}^2}{\varepsilon_{\rm l}} \tag{13}$$

- $G_{k,l}$  is the term of production of turbulent kinetic energy and the constants are defined as follow:
- 205  $C_{\mu} = 0.09, C_{\varepsilon 1} = 1.44, C_{\varepsilon 2} = 1.92, \delta_k = 1 \text{ and } \delta_{\varepsilon} = 1.$
- 206 Lastly, no additional interaction terms were taken into account for turbulence as preliminary
- simulations showed no impact of these terms on simulation results (data not shown).
- 208 The particle-particle interactions were modelled by the kinetic theory of granular flows, which is an
- 209 extension of the model for molecular motion in a dense gas phase. It aims at determining the solid
- 210 pressure  $p_s$  which represents the normal forces due to particle interactions. From the kinetic theory,
- 211 Jenkins and Savage (1983) proposed that this solid pressure is the sum of a kinetic energy term and of
- one term that includes the particle-particle collisions:

$$p_{\rm S} = \alpha_{\rm S} \rho_{\rm S} \theta_{\rm S} + 2\rho_{\rm S} (1 + e_{\rm SS}) \alpha_{\rm S}^2 r_0 \theta_{\rm S} \tag{14}$$

The coefficient of restitution of particle collision  $e_{ss}$  is set to 0.9. The granular temperature  $\theta_s$  is a measure of the kinetic energy due to the fluctuating velocities  $u'_s$  of the particles:

measure of the kinetic energy due to the fluctuating velocities 
$$u_{\mathrm{s}}'$$
 of the particles:

$$\theta_{\rm S} = \frac{1}{3}u_{\rm S}^{\prime 2} \tag{15}$$

- 215 Neglecting the convective and diffusive transports, the transport of the granular temperature within
- 216 the bioreactor is provided by Ding and Gidaspow (1990):

$$\left(-p_{\rm s}\bar{\bar{I}} + \bar{\bar{\tau}}_{\rm s}\right): \nabla \mathbf{u}_{\rm s} - \gamma_{\theta_{\rm s}} + \Phi_{\rm ls} \tag{16}$$

- 217 First-term of the left-hand side represents the generation of fluctuating energy due to the solid
- 218 pressure and viscous force; the second term is the dissipation of the fluctuating energy and the last
- 219 term is the exchange of fluctuating energy between liquid and solid phases respectively. The transfer
- of fluctuating energy is given by:

$$\Phi_{\rm ls} = -3K_{\rm ls}\theta_{\rm s} \tag{17}$$

The collisional dissipation of energy  $\gamma_{\theta_{\rm S}}$  is provided by:

$$\gamma_{\theta_{\rm S}} = \frac{12(1 - e_{\rm SS}^2)r_0}{d_{\rm D}\pi^{0.5}} \rho_{\rm S} \alpha_{\rm S}^2 \theta_{\rm S}^{3/2} \tag{18}$$

- The radial distribution function  $r_0$  is a correction factor that modifies the probability of collisions
- between particles when the solid granular phase becomes dense:

$$r_0 = \frac{a + d_p}{a} \tag{19}$$

with a the distance between the particles. In our case, this distribution is determined by:

$$r_0 = \left[1 - \left(\frac{\alpha_{\rm s}}{\alpha_{\rm s,max}}\right)^{1/3}\right]^{-1} \tag{20}$$

- with  $\alpha_{s,max}$  = 82 % w/w (corresponding to 63 % v/v), the particle packing limit.
- The solid shear stress tensor  $\bar{\overline{\tau}}_S$  arises from particle momentum exchange due to translations and
- 227 collisions and depends on the solid viscosity:

$$\bar{\bar{\tau}}_{s} = \mu_{s} \nabla \mathbf{u}_{s} = (\mu_{s,col} + \mu_{s,kin}) \nabla \mathbf{u}_{s}$$
(21)

The collisional contribution to the shear viscosity is given by:

$$\mu_{\rm s,col} = \frac{4}{5} \alpha_{\rm s} \rho_{\rm s} d_{\rm p} r_0 (1 + e_{\rm ss}) \left(\frac{\theta_{\rm s}}{\pi}\right)^{1/2}$$
 (22)

229 And the kinetic viscosity by:

$$\mu_{\rm s,kin} = \frac{10\rho_{\rm s}d_{\rm s}\sqrt{\theta_{\rm s}\pi}}{96\alpha_{\rm s}(1+e_{\rm ss})r_0} \left[1 + \frac{4}{5}r_0\alpha_{\rm s}(1+e_{\rm ss})\right]^2 \tag{23}$$

2. 2. Simulation setup

- The geometry setup for the simulation of the lab-scale bioreactor is shown on Fig. 2; this bioreactor is routinely used for bioleaching experiments. The tank was a cylindrical vessel of diameter T=0.12 m and liquid height H=0.187 m. The tank was equipped with four conical baffles of width equal to T/10,
- 235 placed symmetrically.

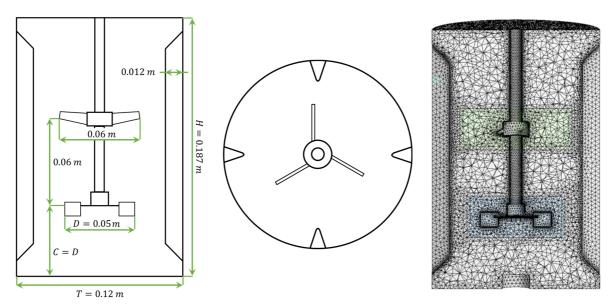


Fig. 2: Planar view (left), cross-section (middle) and mesh (right) of the two-stage stirred tank reactor.

A dual impeller configuration was chosen using various bottom impeller designs but a fixed design for the top impeller (Fig. 3). Considering the height on tank diameter ratio, the choice of a multi-stage design is recommended to provide sufficient liquid mixing near the surface. As the focus was put on particles suspension and stress, and to limit the number of configurations simulated, only the bottom impeller design was modified. The bottom impellers had a fixed diameter D = 0.05 m with an off-bottom clearance C = D. The top impeller, a three-blade hydrofoil (A310), was positioned at a spacing S = 0.06 m above the bottom impeller and had a diameter equal to 0.06 m.

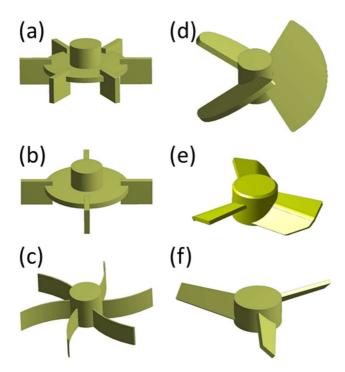


Fig. 3: Impellers used in simulations. (a) 6-bladed Rushton turbine (RT6B); (b) 4-bladed Rushton turbine (RT4B); (c) R600 spiral backswept impeller (R600); (d) Elephant-Ear impeller operating in down-pumping mode (EEd); (e) HTPG impeller operating in down-pumping mode (HTPGd); (f) Lightnin A310 impeller operating in up-pumping mode (A310).

Each impeller configuration was simulated at 6 different agitation rates (N=200,300,400,500,600 and 700 rpm), ensuring fully turbulent conditions for each case ( $10^4 < Re < 5 \times 10^4$ ). Moreover, the impact of the solid concentration on solid-liquid suspension was also determined by fixing three different solid concentrations: 10, 18 and 26 % w/w. A non-uniform mesh structure was created to divide the geometry setup using the Fluent Meshing tool and was composed of 400,000 tetrahedral elements. Refinements were done along the wall and in the impellers regions. Mesh independence was preliminary verified by comparing velocity vectors fields and volume-averaged power dissipation.

## 2. 3. Power consumption

To obtain the power number  $N_p$  defined in eq. (1), the power consumption P was calculated by the following equation:

$$P = 2\pi N C_{\rm w} \tag{24}$$

with N the agitation rate and  $C_w$  the impeller torque, which was determined by the numerical simulations. Mechanical energy balance within the bioreactor imposes that the power consumption P should be of the same order of magnitude as the dissipated power  $P_{\rm diss}$  determined by the turbulence model:

$$P_{\rm diss} = \rho_{\rm l} \langle \varepsilon \rangle V_{\rm l} \tag{25}$$

## 2. 4. Solid dispersion

Solid dispersion is a key process parameter in solid-liquid bioreactors as it strongly impacts the mass transfer to the particles but also the microenvironment of substrates around the particles. One way to determine the suspension quality is to use the Zwietering correlation which models the just-suspended

agitation rate of the particles  $N_{\rm js}$  in the bioreactor (based on the Zwietering criterion that considers the particles as they do not remain settled more than 2 seconds near the vessel bottom at the just-suspended state). It is generally assumed that the bioreactor and impeller geometries have an impact on  $N_{\rm js}$  but also on the operating conditions of the process:

$$N_{\rm js} \propto \nu_{\rm l}^{0.1} \left[ \frac{g(\rho_{\rm s} - \rho_{\rm l})}{\rho_{\rm l}} \right]^{0.45} \cdot X^{0.13} d_{\rm p}^{0.2} D^{-0.85}$$
 (26)

Thus, for a given bioreactor configuration and operating conditions, the scaling law  $N_{\rm js} \propto X^{0.13}$  should be obtained. Despite the interest of determining this criterion, it is insufficient if the distribution of particle concentrations or stresses are also looked for. One way to improve the description of the particles suspension behaviour is to determine the suspension quality  $H_{\rm s}$  which can be calculated as the volume-averaged difference between the local and the mean concentration of solid particles (Mak, 1992; Khopkar et al., 2006; Murthy et al., 2007; Hosseini et al., 2010). This parameter is determined using the local fraction of each elements of the mesh:

$$H_{\rm s} = 1 - \sqrt{\frac{1}{V_{\rm tot}} \cdot \iiint_{V_{\rm tot}} (\alpha_{\rm s} - \langle \alpha_{\rm s} \rangle)^2 dV}$$
 (27)

where  $\alpha_s$  denotes the local volume fraction of the solid phase and  $\langle \alpha_s \rangle$  represents the volumeaveraged value of particle concentration in the vessel. This value of  $H_s$  had to be adjusted to take into account the packing limit of the particles given by the maximal local solid concentration of 82 % w/w:

$$H_{\text{s,adj}} = \frac{H_{\text{s}} - H_{\text{s,min}}}{H_{\text{s max}} - H_{\text{s min}}} \tag{28}$$

where 0.75 <  $H_{\rm s,min}$  < 0.85 and  $H_{\rm s,max}=1$  are respectively the minimal and maximal values of  $H_{\rm s}$  for  $\alpha_{\rm s}=\alpha_{\rm s,max}=0.82$  and  $\alpha_{\rm s}=\alpha_{\rm s,min}=\langle\alpha_{\rm s}\rangle$ . The value of  $H_{\rm s,min}$  is dependent on the volume-averaged concentration of particles considered in the calculations.

### 2. 5. Solution method

The commercial software ANSYS Fluent 2019R3 was used for the numerical simulation of the multiphase flow. The conservation equations presented in Eq. (2-23) were applied in all meshes and were solved using the steady-state Eulerian method. The impellers rotation was modelled using the multiple reference frame approach. The rotating domain was positioned at  $r_{\rm bottom} = 0.035$  m, 0.036 m  $\leq z_{\rm bottom} \leq 0.066$  m and  $r_{\rm top} = 0.040$  m, 0.096 m  $\leq z_{\rm top} \leq 0.126$  m, respectively for the bottom and the top impellers. The pressure-velocity based solver using the SIMPLE algorithm was used to solve the set of conservation equations. Discretization of the mass, momentum and volume fraction equations was carried-out using the second-order upwind scheme while pressure was spatially discretized using the PRESTO! scheme (s.n. Ansys, 2019). Convergence of the simulations was admitted when transport equations residuals were less than  $10^{-3}$  and when the local solid volume fraction reached a steady state at three locations of the vessel (r = 0.025 m and z = 0.025, 0.090 and 0.160 m).

#### 3. Results and discussion

3.1. Liquid flow patterns

Firstly, to validate the accuracy of the CFD model, the flow patterns were qualitatively compared with data from the literature. The dimensionless liquid velocity profiles shown in Fig. 4 present the flow patterns induced by the dual-impellers bioreactor. The top A310 showed the predicted pattern of a mixed flow, presenting a one-loop flow pattern as it operates in up-pumping mode, which was also shown by Vrábel et al. (2000) on a multiple impellers configuration. The proximity of the liquid surface promoted the formation of two supplementary liquid loops. For the bottom impeller, various flow patterns were observed depending on the impeller used: the radial impellers (RT4B, RT6B and R600) generated a two-loop pattern with a radial ejection of the liquid towards the reactor wall while the down-flow axial impellers (HTPGd and EEd) showed a single-loop flow pattern. These results agreed with the experimental results of previous studies as similar flow patterns were shown for radial impellers by Zhang et al. (2017) and for down-flow axial impellers by Bouaifi and Roustan (2001). As expected, the choice of the tip speed  $u_{\rm tip} = \pi ND$  as a representative design parameter is highly questionable, as shown by the variability of the flow pattern from one configuration to another (Nienow, 2006).

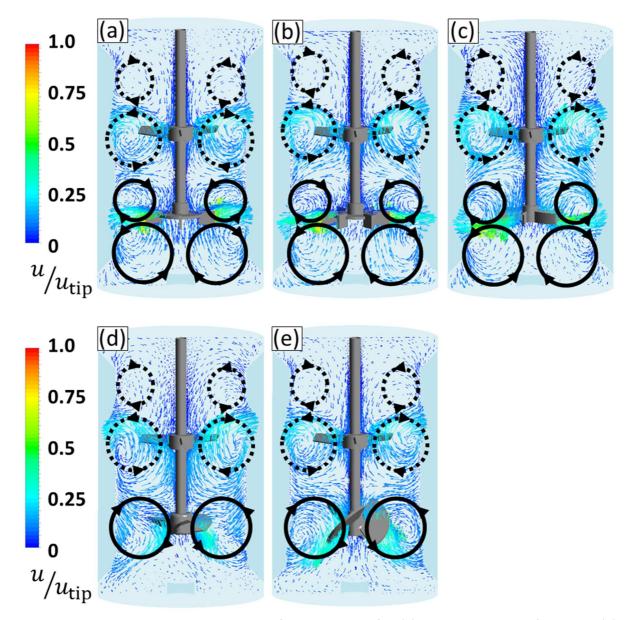


Fig. 4: Normalized liquid velocity vectors profiles at 500 rpm for: (a) the RT4B-A310 configuration; (b)

the RT6B-A310 configuration; (c) the R600-A310 configuration; (d) the HTPGd-A310 configuration; (e) the EEd-A310 configuration. The tip speed was given by  $u_{\rm tip}=\pi ND$ .

## 3.2. Power consumption

The power numbers of each impeller were calculated using eq. (1) for each agitation rates and solid concentrations and the mean value obtained and standard deviation were compared with data from literature, as shown in Table 1.

Table 1. Mean value and standard deviation of the calculated impeller power numbers for each impeller configuration used and comparison with data from literature (referenced  $N_p$ ).

Impeller	Calculated $N_p$	Referenced $N_p$	Literature reference
RT4B	$3.1 \pm 0.1$	4.0	Roustan (2005)
RT6B	$4.0 \pm 0.1$	4.0 - 6.0	Chapple et al. (2002)
R600	$3.6 \pm 0.3$	4.2	Roustan (2005)
HTPGd	0.73 ± 0.07	0.67	Roustan (2005)
EEd	$1.9 \pm 0.1$	1.7 - 2.1	Zhu et al. (2009); Loubière et al. (2019)
A310	0.76 ± 0.05	0.3 - 0.5	Kumaresan and Joshi (2006)

The results showed that for fully turbulent conditions, the variation of agitation rates induced few variations of the power numbers compared to the expected values, as classically expected in turbulent regime (Rushton, 1950; Furukawa et al., 2012). Moreover, the predicted values of  $N_p$ , calculated for each impeller in the two-stage configurations, are similar to those reported for single-impeller configurations meaning that the total power consumption is approximately equal to the additive power consumption of both impellers. This can be explained by the fact that, with enough spacing between the impellers (S/D > 1), the respective dissipated power of the impellers in a two-stage reactor is similar to those obtained in a single-stage reactor (Hudcova et al., 1989; You et al., 2014). Lastly, the power consumption of the upper A310 impeller was independent of the bottom impeller design (data not shown), which confirmed that both impellers were not interacting with each other. The CFD simulations also showed that the power dissipation calculated by the turbulence model was, on average over all configurations, equal to 58 % of the power consumption determined by the torque of the impeller. This result is in accordance with most CFD simulations carried-out with the  $k-\varepsilon$  turbulence model (Ochieng and Onyango, 2008).

As shown by Loubière et al. (2019) for various designs of impellers, the particle just-suspended state is clearly related to the total power consumption per unit of volume  $P_{\rm tot}/V$ , which considers the power demand of both impellers. Thus, the values of this parameter were evaluated for the different impeller configurations in order to determine the best configuration in term of particle suspension, at a given agitation rate (Fig. 5). The results showed that, independently of the agitation rate, the configurations with a bottom axial impeller (HTPGd and EEd) consumed less energy than the configurations with a bottom radial impeller (RT4B, RT6B and R600). This agreed with the relative power numbers given in Table 1 and with the experimental results reported by Bouaifi and Roustan (2001) and Wang et al. (2010).

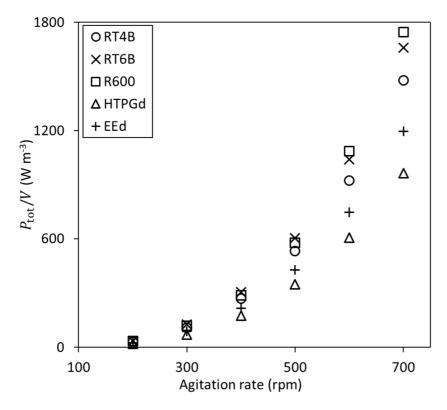


Fig. 5: Variation of the total power consumption per unit volume  $P_{\rm tot}/V$  with the agitation rate, for each impeller configuration. Particle concentration was 10 % w/w.

## 3.3. Particle mixing degree

To determine the particle mixing degree, the values of  $H_{\rm s,adj}$  were calculated for each configuration and operating condition of the bioreactor (Fig. 6). The values obtained showed a logarithmic increase with the agitation rate, with values ranging from 35 to 95 %. All configurations showed the same shape of particle mixing profile but with non-negligible relative differences, especially at low agitation rates. These differences were up to 40 % at 200 rpm between HTPGd and RT6B impellers but less than 10 % at 500 rpm and below. Independently of the agitation rate, both the RT6B and the EEd were the best to scatter particles throughout the tank at a given agitation rate. On the other hand, the HTPGd was the less efficient impeller in term of solid homogenization, with the lowest  $H_{\rm s,adj}$  for all the simulated agitation rates. This was emphasized by the discrepancies observed on the particle distribution, as shown by Fig. 7 (a-b) for 400 rpm. While for the RT6B impeller, the just-suspended state was clearly observed, the suspension of particles was still partial in the case of the HTPGd impeller, as indicated by the occurrence of settled particles ( $\alpha_{\rm s,max}=0.82$  w/w) near the vessel bottom. Moreover, the radial impellers clearly showed a higher efficiency at bringing the particles upward (Fig. 7a), making the particle bed evolves to a cone shape at high agitation rate while the axial impellers promoted a pseudo-planar shape of particle bed.

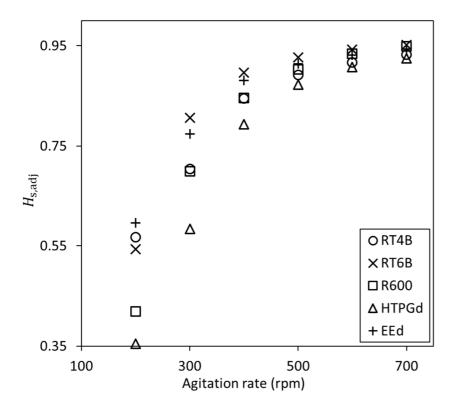


Fig. 6: Suspension quality  $H_{
m s,adj}$  for each impeller configuration. Particle concentration was 10 % w/w.

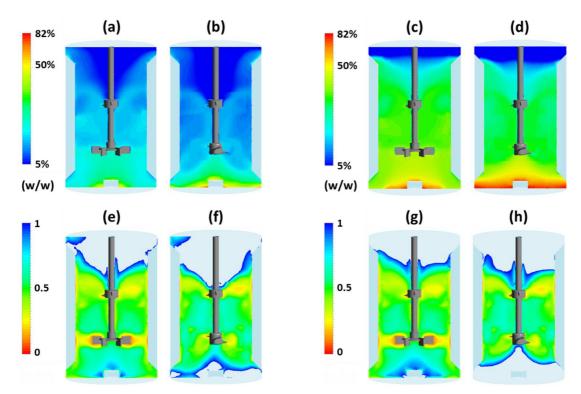


Fig. 7: Simulated particles distribution at N = 400 rpm for: (a) RT6B-A310 configuration with 10 % w/w solid; (b) HTPGd-A310 configuration with 10 % w/w solid; (c) RT6B-A310 configuration with 26 % w/w solid; (d) HTPGd-A310 configuration with 26 % w/w solid. Comparison of the particle size with the Kolmogorov length scale ( $l_K/d_p$ ) for: (e) RT6B-A310 configuration with 10 % w/w solid; (f) HTPGd-A310 configuration with 10 % w/w solid; (g) RT6B-A310 configuration with 26 % w/w solid; (h) HTPGd-A310 configuration with 26 % w/w solid.

375

376

377

378

379380

381 382

383 384

385

386

387

388

389 390

391

392393

394

395

396

397

398 399 Aiming at determining a robust design criterion, the suspension quality  $H_{\mathrm{s,adj}}$  variation with the total power dissipation per unit volume was also determined (Fig. 8a). This variation could be divided into two zones. For power dissipation per unit of volume less than 600 W m<sup>-3</sup> approximately, the parameter  $H_{\rm s,adi}$  rapidly increased till a value of  $H_{\rm s,adi} \simeq 0.90$ ; regarding the particles distribution obtained for this range of power dissipation, only partial suspension was determined. For  $P_{\rm tot}/V$  higher than 600 W m<sup>-3</sup>, the value of  $H_{s,adj}$  slowly increased till 0.95 approximately, indicating a progressive particle homogenization beyond the just-suspended state. Thus, a substantial increase of mechanical energy consumption is required to achieve a minor enhancement of the particle homogenization. Moreover, it was also shown that total homogeneity ( $H_{s,adj} = 1.0$ ) is not achievable as all the data tend to stagnate below  $H_{\rm s.adi}$  = 0.95. This could be explained by the fact that, even for high power dissipations per unit of volume, a small region near the free surface remained free or poorly concentrated in particles, as demonstrated by Delafosse et al. (2018). Lastly, it is interesting to note that, for a given power dissipation per unit of volume, the variations of  $H_{s,adi}$  were approximately independent of the bioreactor designs, meaning that power dissipation per unit of volume could be used not only as scaling parameter for particles just-suspended state determination but also to predict the quality of particles homogenization. Previous experiments by Magelli et al. (1991) have shown similar results in a singlestage vessel and pointed that it could be a basis for design optimization. Based on these results, it could be advised to promote the use an impeller which can achieve a high power dissipation per unit volume, even at the lowest agitation rate. This could indeed allow to get particle suspension at lower values of agitation rate and tip speed, which should limit the mechanical problems expected at high tip speeds.

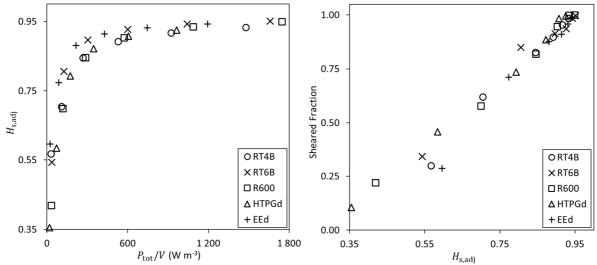


Fig. 8: Solid distribution  $H_{\rm s,adj}$  as a function of power dissipation per unit volume  $P_{\rm tot}/V$  (left); Suspension quality  $H_{\rm s,adj}$  as a function of the sheared fraction (right). Particle concentration was 10 % w/w.

#### 3.4. Particle stress

As discussed in the introductive part, it is generally assumed that only the turbulent eddies of the same order of length or lower than the particle size are potentially detrimental to the particles and thus the microbial adhesion and biofilm formation. Henzler (2000) stated that turbulent eddies of the same size of the particles are the most likely to damage the particles. In this case, namely some turbulent eddies are lower than the particle diameter, particles are transported in the inertial subrange of turbulence and are subjected to turbulent stresses. To quantify the relationships between particle stress and hydrodynamics, Thomas (1964) provided the expression of particle stress as related to the local mean square fluctuating liquid velocities  $\overline{u_1'}$ .

$$\sigma_{\rm p} = \rho_{\rm l} \overline{u_{\rm l}^{\prime 2}} = 0.7 \rho_{\rm l} (\varepsilon d_{\rm p})^{2/3} \propto \varepsilon^{2/3} \tag{29}$$

In isotropic and homogeneous turbulence, the local mean square fluctuating liquid velocities depends on the local turbulent dissipation rate  $\varepsilon$  and on particle diameter  $d_{\rm p}$ . If  $d_{\rm p} < l_{\rm K}$ , the particles are transported in the viscous subrange of the turbulence and are mainly subjected to viscous stresses given by:

$$\sigma_{\rm p} = \mu G = \mu \sqrt{\frac{\varepsilon}{\nu_{\rm l}}} \propto \varepsilon^{1/2}$$
 (30)

with G (s<sup>-1</sup>) the local velocity gradient.

From the preceding results, it appears clear that the determination of hydromechanical stresses acting on particles when suspended in the mixing tank should be determined locally and considering the relative ratio of the particle size on the Kolmogorov length scale. Thus, it was proposed here to assert the hydromechanical stress by calculating the sheared fraction SF (eq. 31), representing the percentage of particles volume under sheared conditions, namely in areas showing Kolmogorov scales lower than the particle diameter ( $l_K < d_p$ ).

$$SF = \frac{1}{V_{\rm S}} \cdot \iiint_{V_{\rm S}(l_K < d_{\rm p})} dV_{\rm S} = \frac{1}{V_{\rm S}} \cdot \iiint_{V_{\rm S}(l_K < d_{\rm p})} \alpha_{\rm S} \cdot dV \tag{31}$$

The variation of the sheared fraction SF with the suspension quality  $H_{\rm s,adj}$  was reported in Fig. 8. As one could expect, the stress on particles was growing higher as the suspension quality increased. You et al. (2020) obtained similar results using bioleaching continuous STR and reported that it was clearly linked to the mechanical forces acting on microbial productivity through the damaging mechanisms explained in this work. The variation of SF also showed that all the impeller designs presented the same linear evolution of SF, meaning that all the configurations would generate a similar particle stress for a given suspension quality. This could be partially explained by the previous results that put into evidence the relation between particle homogenization and total power demand. It is also interesting to note that, reaching a quasi-consistent homogenization of the particles implied that almost all the particles would encounter potentially damaging turbulent eddies that could promote biofilm detachment. When particles were not homogeneously distributed in the bioreactor, it is also important to consider the spatial distribution of the Kolmogorov length scales  $l_K$ , as it differed from one impeller to another, as shown in Fig. 7e and Fig. 7f. In conclusion, despite each bioreactor configuration generated different turbulent dissipation fields, the physical link between flow velocity, turbulent dissipation and particle concentrations led to unique relationships between sheared fraction of particles and suspension quality, whatever the impeller used. This also potentially questions the existence of 'shearing' or 'non-shearing' impellers when the degree of homogenization is considered as comparison parameter.

## 3.5. Impact of particle concentrations on bioreactor hydrodynamics

425

426

427

428

429

430

431

432

433 434

435

436

437

438

439

440

441

442

443

444

445

446

447

448

449450

451

452

453

454

455 456

457

458

459

460

461

462

463 464

465 466

467

Considering that an increase of solid concentrations could potentially simultaneously promote an increase in bioprocess productivity and detrimental physical phenomena, the impact of solid concentration (from 10 to 18 and 26 % w/w) on bioreactor hydrodynamics was determined. For these simulations, only the designs RT6B-A310 and HTPGd-A310 were considered. First, regarding the justsuspended state of the particles, the basic Zwietering's model predicts that the just-suspended agitation rate would be related to  $N_{\rm is} \propto X^{0.13}$ . The influence of X on  $N_{\rm is}$  was confirmed by the CFD simulations of the particles distributions generated by the RT6B and HTPGd configurations using solid concentrations of 10 and 26 % w/w as shown in Fig.7(a-d). Whereas no particle accumulation was observed for a particle loading of 10 % w/w at an agitation rate of 400 rpm for the RT6B impeller, settled particles were predicted by the simulations at the same agitation rate for a solid concentration of 26 % w/w, indicating that the agitation rate switched below  $N_{\rm is}$  (Fig.7a and Fig 7c). For the HTPGd impeller, the small accumulation observed for a solid concentration of 10 % was clearly magnified for a solid concentration of 26 % (Fig. 7b and Fig. 7d). Considering the Zwietering's model, for a constant power number expected in the turbulent regime, the total power demand at the just-suspended state would be  $P_{\rm js} \propto N_{\rm js}^3 \propto X^{0.4}$ . On the basis of this global scaling law, the power demand for a mean solid concentration of 26 % would be  $P_{is}^{26\%} \simeq 1.55 \cdot P_{is}^{10\%}$ .

The effect of the solid concentration on particle homogenization is shown in Fig. 9 for RT6B-A310 and HTPGd-A310 configurations. For both of them, the CFD simulation results confirmed that the increase in solid concentration led to a rise of power demand per unit volume to reach a given suspension quality. Moreover, it was also put into evidence that the asymptotic value of  $H_{\rm s,adj}$ , obtained for the highest  $P_{\rm tot}/V$  considered in this study, was progressively reduced as long as the solid concentration increased. For comparison, the power needed to achieve  $H_{\rm s,adj}=0.90$  with the RT6B was  $(P_{\rm tot}/V)_{26\%}\simeq 2\cdot (P_{\rm tot}/V)_{18\%}\simeq 6\cdot (P_{\rm tot}/V)_{10\%}$ . A similar trend was observed for the HTPGd with a smaller increase of power demand as the solid concentration rose, for  $H_{\rm s,adj}=0.87$ ,  $(P_{\rm tot}/V)_{26\%}\simeq 1.00$ 

 $1.7 \cdot (P_{\mathrm{tot}}/V)_{18\%} \simeq 3 \cdot (P_{\mathrm{tot}}/V)_{10\%}$ . Considering the sheared fraction SF, it was shown that, for a given  $H_{\mathrm{s,adj}}$ , a higher fraction of particles was transported in the inertial subrange at higher solid concentrations. However, for both configurations and the three solid concentrations, the parameter SF reached a value close to 1 for the highest degrees of homogenization  $H_{\mathrm{s,adj}}$  (Fig. 10). This could explained by the fact that, for the particles that were suspended, the local variations in solid concentration in the areas where  $d_{\mathrm{p}} > l_{K}$  were similar between 10 and 26 % w/w (Fig. 7 (e-h)). This was not true near the reactor bottom where settling was predicted for particle concentration of 26 % w/w and which explained the less efficient particle homogenization.

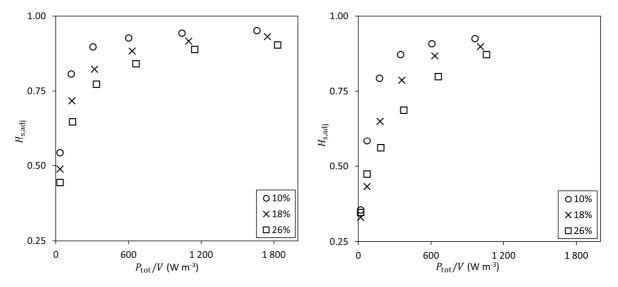


Fig. 9: Solid distribution  $H_{\rm s,adj}$  as a function of power consumption per unit volume  $P_{\rm tot}/V$  at different solid concentration for: (left) the RT6B-A310 configuration; (right) the HTPGd-A310 configuration.

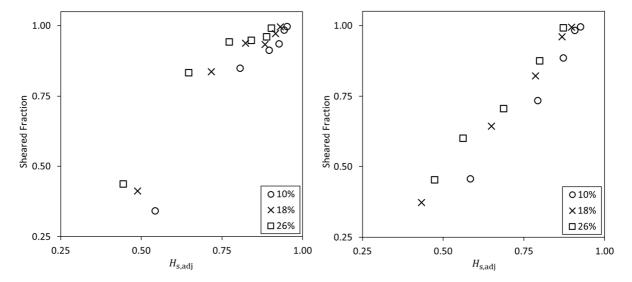


Fig. 10: Suspension quality  $H_{s,adj}$  as a function of the sheared fraction at different solid concentration for: (left) the RT6B-A310 configuration; (right) the HTPGd-A310 configuration.

## 4. Conclusion

The effect of the impeller design on the solid suspension was determined using 5 dual-impeller configurations and 3 solid concentrations. For this, the power consumption per unit of volume, the

mixing efficiency and the particle stress were characterized by 50 CFD numerical simulations and theoretical models of particle stress.

The results indicated that the power demand per unit volume could be used to predict the suspension quality as the variations of  $H_{s,adj}$  were independent of the bioreactor design for a given  $P_{tot}/V$ . However, due to higher power numbers, the impellers RT6B and EEd could achieve particle suspension at lower agitation rates. Furthermore, it was shown that increasing the solid loading let to a significant rise of the power consumption per unit volume to attain a given suspension quality. Lastly, the impact of each configuration on particle stress was assessed and the results showed that particle stress was independent of the reactor design at a given suspension quality. Consequently, it is difficult to advise a specific configuration and experimental conditions regarding particle stress when using the suspension quality as an optimisation criterion.

The choice of impeller design in a bioleaching STR is critical to ensure the best solid dispersion within the tank while maintaining a low power consumption and limiting the impact of shear stress on particles. For higher scales (pilot and industrial scales), the energy cost due to mixing represents a large part of OPEX expenses and impeller optimization should be closely considered. Nonetheless, further studies are still necessary to take into account the biological aspect of bioleaching and the impact of the design and the agitation on biomass.

#### Acknowledgments

The authors acknowledge the Institut Carnot ICEEL and the Institut Carnot BRGM for their financial support.

#### Nomenclature

#### **Variables**

486

487

488

489 490

491

492

493

494

495

496

497

498

499

500

501

502

503 504

505

506

а	distance between particles, m
С	impeller off bottom clearance, m
$C_{ m D}$	drag coefficient
$C_{\varepsilon 1},\ C_{\varepsilon 2}, C_{\mu}$	constants in turbulent equations
$C_w$	impeller torque, N m <sup>-1</sup>
D	impeller diameter, m
$d_{ m p}$	particle diameter, m
D	impeller diameter, m
$e_{ m ss}$	particle collision restitution coefficient
F	force per unit volume, N m <sup>-3</sup>
g	acceleration of gravity, m s <sup>-2</sup>
G	local velocity gradient, m s <sup>-1</sup>
$G_k$	turbulence production
Н	liquid height, m
$H_{S}$	suspension quality
k	turbulent kinetic energy, m <sup>2</sup> s <sup>-2</sup>
K	interphase exchange coefficient
$l_K$	Kolmogorov length scale, m
N	impeller speed, rpm
p	pressure, Pa
P	impeller power consumption, W
$r_0$	radial distribution function
S	spacing between both impellers, m
SF	sheared fraction
T	tank diameter, m
u	velocity, m s <sup>-1</sup>

Vworking volume, m<sup>3</sup>

particle concentration, w/w Χ

## **Greek Letters**

volume fraction diffusion coefficient γ

collisional dissipation of energy, m<sup>2</sup> s<sup>-2</sup>  $\gamma_{\theta_s}$ 

δ turbulent Prandtl number

turbulence eddy dissipation rate, m<sup>2</sup> s<sup>-3</sup> ε

granular temperature, m<sup>2</sup> s<sup>-2</sup>  $\theta_{\rm S}$ 

viscosity, Pas μ

kinematic viscosity, m<sup>2</sup> s<sup>-1</sup> ν

density, kg m<sup>-3</sup> ρ particle stress  $\sigma_{\mathrm{p}}$ 

stress strain tensor, Pa

transfer of fluctuating energy, m<sup>2</sup> s<sup>-2</sup>

## **Dimensionless number**

Power number  $N_p$ ReReynolds number

## Subscripts

adjusted adj col collisional D drag diss dissipated

js just-suspended state

kin kinetic 1 liquid phase

ls action between liquid and solid

maximal max p particle solid phase S t turbulence total

tot

TD turbulent dispersion

volume weight w

## **Abbreviations**

A310 Lightnin A310 impeller

CFD computational fluid dynamics EEd Elephant-Ear down impeller

HTPGd HTPG down impeller RT4B 4-bladed Rushton turbine RT6B 6-bladed Rushton turbine R600 R600 spiral backswept impeller

stirred tank reactor STR

- Bouaifi, M., Roustan, M., 2001. Power consumption, mixing time and homogenisation energy in dualimpeller agitated gas–liquid reactors. Chem. Eng. Process.: Process Intensif. 40, 87–95. https://doi.org/10.1016/S0255-2701(00)00128-8
- Bouquet, F., Morin, D., 2006. BROGIM®: A new three-phase mixing system testwork and scale-up.
  Hydrometall., 16th International Biohydrometallurgy Symposium 83, 97–105.
  https://doi.org/10.1016/j.hydromet.2006.03.040
- Brierley, C.L., Brierley, J.A., 2013. Progress in bioleaching: part B: applications of microbial processes
  by the minerals industries. Appl. Microbiol. Biotechnol. 97, 7543–7552.
  https://doi.org/10.1007/s00253-013-5095-3
- Brucato, A., Cipollina, A., Micale, G., Scargiali, F., Tamburini, A., 2010. Particle suspension in topcovered unbaffled tanks. Chem. Eng. Sci. 65, 3001–3008.
  https://doi.org/10.1016/j.ces.2010.01.026
- Buffo, M.M., Corrêa, L.J., Esperança, M.N., Cruz, A.J.G., Farinas, C.S., Badino, A.C., 2016. Influence of dual-impeller type and configuration on oxygen transfer, power consumption, and shear rate in a stirred tank bioreactor. Biochemical Engineering Journal 114, 130–139. https://doi.org/10.1016/j.bej.2016.07.003
  - Bujalski, W., Takenaka, K., Paoleni, S., Jahoda, M., Paglianti, A., Takahashi, K., Nienow, A.W., Etchells, A.W., 1999. Suspension and Liquid Homogenization in High Solids Concentration Stirred Chemical Reactors. Chemical Engineering Research and Design, Process and Product Development 77, 241–247. https://doi.org/10.1205/026387699526151
    - Chapple, D., Kresta, S.M., Wall, A., Afacan, A., 2002. The Effect of Impeller and Tank Geometry on Power Number for a Pitched Blade Turbine. Chem. Eng. Res. Des. 80, 364–372. https://doi.org/10.1205/026387602317446407
    - Clark, M.E., Batty, J.D., van Buuren, C.B., Dew, D.W., Eamon, M.A., 2006. Biotechnology in minerals processing: Technological breakthroughs creating value. Hydrometall., 16th International Biohydrometallurgy Symposium 83, 3–9. https://doi.org/10.1016/j.hydromet.2006.03.046
    - d'Hugues, P., Foucher, S., Gallé-Cavalloni, P., Morin, D., 2002. Continuous bioleaching of chalcopyrite using a novel extremely thermophilic mixed culture. International Journal of Mineral Processing 66, 107–119. https://doi.org/10.1016/S0301-7516(02)00004-2
    - d'Hugues, P., Joulian, C., Spolaore, P., Michel, C., Garrido, F., Morin, D., 2008. Continuous bioleaching of a pyrite concentrate in stirred reactors: Population dynamics and exopolysaccharide production vs. bioleaching performance. Hydrometallurgy, 17th International Biohydrometallurgy Symposium, IBS 2007, Frankfurt a.M., Germany, 2-5 September 2007 94, 34–41. https://doi.org/10.1016/j.hydromet.2008.05.045
    - Delafosse, A., Loubière, C., Calvo, S., Toye, D., Olmos, E., 2018. Solid-liquid suspension of microcarriers in stirred tank bioreactor Experimental and numerical analysis. Chem. Eng. Sci. 180, 52–63. https://doi.org/10.1016/j.ces.2018.01.001
  - Ding, J., Gidaspow, D., 1990. A bubbling fluidization model using kinetic theory of granular flow. AIChE J. 36, 523–538. https://doi.org/10.1002/aic.690360404
- Frenzel, M., Kullik, J., Reuter, M.A., Gutzmer, J., 2017. Raw material 'criticality'—sense or nonsense?
   J. Phys. D: Appl. Phys. 50, 123002. https://doi.org/10.1088/1361-6463/aa5b64
- Furukawa, H., Kato, Y., Inoue, Y., Kato, T., Tada, Y., Hashimoto, S., 2012. Correlation of Power Consumption for Several Kinds of Mixing Impellers. Int. J. Chem. Eng. 2012, 1–6. https://doi.org/10.1155/2012/106496
- Gradov, D.V., González, G., Vauhkonen, M., Laari, A., Koiranen, T., 2017. Experimental and Numerical
   Study of Multiphase Mixing Hydrodynamics in Batch Stirred Tank Applied to Ammoniacal
   Thiosulphate Leaching of Gold. J. Chem. Eng. Process Technol. 08.
   https://doi.org/10.4172/2157-7048.1000348
- Guezennec, A.-G., Joulian, C., Jacob, J., Archane, A., Ibarra, D., de Buyer, R., Bodénan, F., d'Hugues, P.,
   2017. Influence of dissolved oxygen on the bioleaching efficiency under oxygen enriched
   atmosphere. Miner. Eng., Biohydrometallurgy 106, 64–70.
- 561 https://doi.org/10.1016/j.mineng.2016.10.016

527

528

529

530

531

532

533

534

535

536

537

538

539

540

541

542

543

544

545

546

547

- Harrison, S.T.L., Stevenson, R., Cilliers, J.J., 2012. Assessing solids concentration homogeneity in
   Rushton-agitated slurry reactors using electrical resistance tomography (ERT). Chem. Eng.
   Sci. 71, 392–399. https://doi.org/10.1016/j.ces.2011.10.053
- Henzler, H.-J., 2000. Particle Stress in Bioreactors, in: Schügerl, K., Kretzmer, G., Henzler, H.J., Kieran,
   P.M., Kretzmer, G., MacLoughlin, P.E., Malone, D.M., Schumann, W., Shamlou, P.A., Yim, S.S.
   (Eds.), Influence of Stress on Cell Growth and Product Formation, Advances in Biochemical
   Engineering/Biotechnology. Springer, Berlin, Heidelberg, pp. 35–82.
   https://doi.org/10.1007/3-540-47865-5
- Hosseini, S., Patel, D., Ein-Mozaffari, F., Mehrvar, M., 2010. Study of Solid-Liquid Mixing in Agitated
   Tanks through Computational Fluid Dynamics Modeling. Ind. Eng. Chem. Res. 49, 4426–4435.
   https://doi.org/10.1021/ie901130z
  - Houcine, I., Plasari, E., David, R., 2000. Effects of the Stirred Tank's Design on Power Consumption and Mixing Time in Liquid Phase. Chem. Eng. Technol. 23, 605–613. https://doi.org/10.1002/1521-4125(200007)23:7<605::AID-CEAT605>3.0.CO;2-0

574

575

576

577

578

579

580

581 582

583

584 585

586

587

588

589

590

591

592

593

594

595

596

597

598

599

600

601

- Hudcova, V., Machon, V., Nienow, A.W., 1989. Gas-liquid dispersion with dual Rushton impellers. Biotechnol. Bioeng. 34, 617–628. https://doi.org/10.1002/bit.260340506
  - Jafari, R., Tanguy, P.A., Chaouki, J., 2012. Experimental investigation on solid dispersion, power consumption and scale-up in moderate to dense solid—liquid suspensions. Chemical Engineering Research and Design 90, 201–212. https://doi.org/10.1016/j.cherd.2011.07.009
  - Jenkins, J.T., Savage, S.B., 1983. A theory for the rapid flow of identical, smooth, nearly elastic, spherical particles. J. Fluid. Mech. 130, 187–202. https://doi.org/10.1017/S0022112083001044
- Kasat, G.R., Pandit, A.B., Ranade, V.V., 2008. CFD Simulation of Gas-Liquid Flows in a Reactor Stirred by Dual Rushton Turbines. Int. J. Chem. React. Eng. 6. https://doi.org/10.2202/1542-6580.1628
  - Khopkar, A.R., Kasat, G.R., Pandit, A.B., Ranade, V.V., 2006. Computational Fluid Dynamics Simulation of the Solid Suspension in a Stirred Slurry Reactor. Ind. Eng. Chem. Res. 45, 4416–4428. https://doi.org/10.1021/ie050941q
  - Kumaresan, T., Joshi, J.B., 2006. Effect of impeller design on the flow pattern and mixing in stirred tanks. Chem. Eng. J. 115, 173–193. https://doi.org/10.1016/j.cej.2005.10.002
- Ljungqvist, M., Rasmuson, A., 2001. Numerical Simulation of the Two-Phase Flow in an Axially Stirred Vessel. Chem. Eng. Res. Des., Fluid Flow 79, 533–546. https://doi.org/10.1205/02638760152424307
  - Loubière, C., Delafosse, A., Guedon, E., Toye, D., Chevalot, I., Olmos, E., 2019. Optimization of the Impeller Design for Mesenchymal Stem Cell Culture on Microcarriers in Bioreactors. Chem. Eng. Technol. 42, 1702–1708. https://doi.org/10.1002/ceat.201900105
  - Magelli, F., Fajner, D., Nocentini, M., Pasquali, G., Marisko, V., Ditl, P., 1991. Solids concentration distribution in slurry reactors stirred with multiple axial impellers. Chem. Eng. Process.: Process Intensif. 29, 27–32. https://doi.org/10.1016/0255-2701(91)87003-L
- Mak, A.T.-C., 1992. Solid-liquid mixing in mechanically agitated vessels (Doctoral). Doctoral thesis, University of London. University of London.
- Montante, G., Paglianti, A., Magelli, F., 2012. Analysis of dilute solid–liquid suspensions in turbulent stirred tanks. Chem. Eng. Res. Des. 90, 1448–1456. https://doi.org/10.1016/j.cherd.2012.01.009
- Morin, D.H.R., d'Hugues, P., 2007. Bioleaching of a Cobalt-Containing Pyrite in Stirred Reactors: a
   Case Study from Laboratory Scale to Industrial Application, in: Rawlings, D.E., Johnson, D.B.
   (Eds.), Biomining. Springer, Berlin, Heidelberg, pp. 35–55. https://doi.org/10.1007/978-3 540-34911-2 2
- Mudd, G.M., Weng, Z., Jowitt, S.M., 2013. A Detailed Assessment of Global Cu Resource Trends and Endowments. Econ. Geol. 108, 1163–1183. https://doi.org/10.2113/econgeo.108.5.1163
- Murthy, B.N., Ghadge, R.S., Joshi, J.B., 2007. CFD simulations of gas-liquid-solid stirred reactor:

  Prediction of critical impeller speed for solid suspension. Chemical Engineering Science, 8th

- International Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering 62, 7184– 7195. https://doi.org/10.1016/j.ces.2007.07.005
- Neale, J., Seppälä, J., Laukka, A., Aswegen, P., Barnett, S., Gericke, M., 2017. The MONDO Minerals
   Nickel Sulfide Bioleach Project: From Test Work to Early Plant Operation. Solid State Phenom.
   262, 28–32. https://doi.org/10.4028/www.scientific.net/SSP.262.28
- Nemati, M., Harrison, S.T.L., 2000. Effect of solid loading on thermophilic bioleaching of sulfide
   minerals. Journal of Chemical Technology & Biotechnology 75, 526–532.
   https://doi.org/10.1002/1097-4660(200007)75:7<526::AID-JCTB249>3.0.CO;2-4
- Nienow, A.W., 2006. Reactor Engineering in Large Scale Animal Cell Culture. Cytotechnol. 50, 9. https://doi.org/10.1007/s10616-006-9005-8
- Ochieng, A., Onyango, M.S., 2008. Homogenization energy in a stirred tank. Chem. Eng. Process.:
  Process Intensif. 47, 1853–1860. https://doi.org/10.1016/j.cep.2007.10.014
  - Petersen, J., 2010. Modelling of bioleach processes: Connection between science and engineering. Hydrometall., 18th International Biohydrometallurgy Symposium, IBS2009, Bariloche-Argentina, 13-17 September 2009 104, 404–409. https://doi.org/10.1016/j.hydromet.2010.02.023
- 630 Qi, N., Zhang, H., Zhang, K., Xu, G., Yang, Y., 2013. CFD simulation of particle suspension in a stirred tank. Particuology 11, 317–326. https://doi.org/10.1016/j.partic.2012.03.003
  - Raja Ehsan Shah, R.S.S., Sajjadi, B., Abdul Raman, A.A., Ibrahim, S., 2015. Solid-liquid mixing analysis in stirred vessels. Rev. Chem. Eng. 31. https://doi.org/10.1515/revce-2014-0028
  - Raja, S., 2005. The effect of particulate-induced hydrodynamic stress on the bioleaching of chalcopyrite by a Sulfolobus sp.
  - Rawlings, D.E., Johnson, D.B., 2007. The microbiology of biomining: development and optimization of mineral-oxidizing microbial consortia. Microbiol. 153, 315–324. https://doi.org/10.1099/mic.0.2006/001206-0
  - Rodríguez, Y., Ballester, A., Blázquez, M.L., González, F., Muñoz, J.A., 2003. Study of Bacterial Attachment During the Bioleaching of Pyrite, Chalcopyrite, and Sphalerite. Geomicrobiology Journal 20, 131–141. https://doi.org/10.1080/01490450303880
- 642 Roustan, M., 2005. Agitation. Mélange Caractéristiques des mobiles d'agitation. Tech. Ing.
- Rushton, J.H., 1950. Power Characteristics of Mixing Impellers Part 1. Chem. Eng. Prog. 46, 395–404.
- 644 Schiller, L., 1933. A Drag Coefficient Correlation. Zeit. Ver. Deutsch. Ing. 77, 318–320.
- Sissing, A., Harrison, S.T.L., 2003. Thermophilic mineral bioleaching performance: A compromise between maximizing mineral loading and maximizing microbial growth and activity. J. South. Afr. Inst. Min. Metall. 4.
- s.n. Ansys, 2019. Fluent Theory Guide 962.

627

628

629

632

633634

635

636 637

638

639

640

641

649

650

651

652

653

654

655

656

657

658

659

660

- Song, T., Jiang, K., Zhou, J., Wang, D., Xu, N., Feng, Y., 2015. CFD modelling of gas-liquid flow in an industrial scale gas-stirred leaching tank. Int. J. Miner. Process., Mineral processing in Australia and China 142, 63–72. https://doi.org/10.1016/j.minpro.2015.01.005
- Tamburini, A., Brucato, A., Cipollina, A., Micale, G., Ciofalo, M., 2012. CFD Predictions of Sufficient Suspension Conditions in Solid-Liquid Agitated Tanks. Int. J. Nonlinear Sci. Numer. Simul. 13. https://doi.org/10.1515/ijnsns-2012-0027
- Tamburini, A., Cipollina, A., Micale, G., Brucato, A., Ciofalo, M., 2014. Influence of drag and turbulence modelling on CFD predictions of solid liquid suspensions in stirred vessels. Chem. Eng. Res. Des. 92, 1045–1063. https://doi.org/10.1016/j.cherd.2013.10.020
- Tamburini, A., Cipollina, A., Micale, G., Brucato, A., Ciofalo, M., 2011. CFD simulations of dense solid–liquid suspensions in baffled stirred tanks: Prediction of suspension curves. Chem. Eng. J. 178, 324–341. https://doi.org/10.1016/j.cej.2011.10.016
- Tatterson, G.B., 1991. Fluid Mixing and Gas Dispersion in Agitated Tanks. McGraw-Hill.
- Thomas, D.G., 1964. Turbulent disruption of flocs in small particle size suspensions. AIChE J. 10, 517–523. https://doi.org/10.1002/aic.690100420
- Vrábel, P., van der Lans, R.G.J.M., Luyben, K.Ch.A.M., Boon, L., Nienow, A.W., 2000. Mixing in largescale vessels stirred with multiple radial or radial and axial up-pumping impellers: modelling

and measurements. Chem. Eng. Sci. 55, 5881–5896. https://doi.org/10.1016/S0009-2509(00)00175-5

- Wadnerkar, D., Utikar, R.P., Tade, M.O., Pareek, V.K., 2012. CFD simulation of solid–liquid stirred tanks. Adv. Powder Technol. 23, 445–453. https://doi.org/10.1016/j.apt.2012.03.007
  - Wakeman, K.D., Honkavirta, P., Puhakka, J.A., 2011. Bioleaching of flotation by-products of talc production permits the separation of nickel and cobalt from iron and arsenic. Process Biochem. 46, 1589–1598. https://doi.org/10.1016/j.procbio.2011.04.016
  - Wang, T., Yu, G., Yong, Y., Yang, C., Mao, Z.-S., 2010. Hydrodynamic Characteristics of Dual-Impeller Configurations in a Multiple-Phase Stirred Tank. Ind. Eng. Chem. Res. 49, 1001–1009. https://doi.org/10.1021/ie9006886
  - Wang, Y., Su, L., Zeng, W., Wan, L., Chen, Z., Zhang, L., Qiu, G., Chen, X., Zhou, H., 2014. Effect of pulp density on planktonic and attached community dynamics during bioleaching of chalcopyrite by a moderately thermophilic microbial culture under uncontrolled conditions. Miner. Eng. 61, 66–72. https://doi.org/10.1016/j.mineng.2014.03.012
  - Witne, J.Y., Phillips, C.V., 2001. Bioleaching of Ok Tedi copper concentrate in oxygen- and carbon dioxide-enriched air. Miner. Eng. 14, 25–48. https://doi.org/10.1016/S0892-6875(00)00158-8
  - Xia, L., Liu, X., Zeng, J., Yin, C., Gao, J., Liu, J., Qiu, G., 2008. Mechanism of enhanced bioleaching efficiency of Acidithiobacillus ferrooxidans after adaptation with chalcopyrite. Hydrometall. 92, 95–101. https://doi.org/10.1016/j.hydromet.2008.01.002
  - You, J., Solongo, S.K., Gomez-Flores, A., Choi, S., Zhao, H., Urík, M., Ilyas, S., Kim, H., 2020. Intensified bioleaching of chalcopyrite concentrate using adapted mesophilic culture in continuous stirred tank reactors. Bioresource Technology 307, 123181. https://doi.org/10.1016/j.biortech.2020.123181
  - You, S.T., Raman, A.A.A., Shah, R.S.S.R.E., Mohamad Nor, M.I., 2014. Multiple-impeller stirred vessel studies. Rev. Chem. Eng. 30. https://doi.org/10.1515/revce-2013-0028
  - Zhang, J., Gao, Z., Cai, Y., Cao, H., Cai, Z., Bao, Y., 2017. Power consumption and mass transfer in a gas-liquid-solid stirred tank reactor with various triple-impeller combinations. Chem. Eng. Sci., 13th International Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering 170, 464–475. https://doi.org/10.1016/j.ces.2017.02.002
  - Zheng, C., Guo, J., Wang, C., Chen, Y., Zheng, H., Yan, Z., Chen, Q., 2018a. Experimental study and simulation of a three-phase flow stirred bioreactor. Chin. J. Chem. Eng. https://doi.org/10.1016/j.cjche.2018.06.010
  - Zheng, C., Huang, Y., Guo, J., Cai, R., Zheng, H., Lin, C., Chen, Q., 2018b. Investigation of cleaner sulfide mineral oxidation technology: Simulation and evaluation of stirred bioreactors for gold-bioleaching process. J. Clean. Prod. 192, 364–375. https://doi.org/10.1016/j.jclepro.2018.04.172
  - Zhu, H., Nienow, A.W., Bujalski, W., Simmons, M.J.H., 2009. Mixing studies in a model aerated bioreactor equipped with an up- or a down-pumping 'Elephant Ear' agitator: Power, hold-up and aerated flow field measurements. Chem. Eng. Res. Des. 87, 307–317. https://doi.org/10.1016/j.cherd.2008.08.013
- Zwietering, Th.N., 1958. Suspending of solid particles in liquid by agitators. Chem. Eng. Sci. 8, 244–
   253. https://doi.org/10.1016/0009-2509(58)85031-9