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Hydrodynamic Characterization of Physicochemical Process in Stirred Tanks and Agglomeration Reactors

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Abstract

A short review of the state of the art in experimental and computational fluid dynamics (CFD) characterization of micro-hydrodynamics and physicochemical processes in stirred tanks and agglomeration reactors is presented. Results of experimental and computational studies focusing on classical mixing tanks as well as other innovative reactors with various industrial applications are briefly reviewed. The hydrodynamic characterization techniques as well as the influence of the fluid dynamics on the efficiency of the physicochemical processes have been highlighted including some of the limitations of the reported modeling approach and solution strategy. Finally, the need for specialized CFD codes tailored to the specific needs of fluid-particle reactor design and optimization is advocated to advance research in this field.

Keywords: physicochemical, hydrodynamics, wet agglomeration, stirred tanks, CFD

1. Introduction

Hydrodynamic and physicochemical interactions play an important role in many industrial unit processes and hence its importance in many engineering applications of fluid flow. Fluid flow investigations in a wide range of process conditions as well as complex biological, physical and chemical processes have been the subject of many scientific publications over the past two decades. Several studies on bench, pilot and industrial scales have been conducted on a wide variety of hydrodynamic conditions and different reactor geometric designs. In many of these studies, the aim is to provide an insight into the fluid flow and process dynamics in terms of the spatial and temporal evolution within the flow device, and in some cases, performance testing of newly designed flow units and processing techniques with potential applications on

industrial scale. Regardless of the focus of these studies, it is quite apparent that valuable information can be obtained from the basic study of fluid flow dynamics in process units especially from design and optimization perspective.

A quick survey of the studies in this field shows that many innovative process reactors have been successfully tested on different scales for a wide variety of technical applications ranging from fine particle separation and water purification to cell culture preparation [1–6]. Experimental data, which are collected in these studies for numerical validation purposes, are often used to characterize the hydrodynamic behaviour as well as to quantify the fluid parameters of interest such as the flow velocity profile, vorticity, turbulent kinetic energy and its rate of dissipation, turbulent intensity, and so on. While there is a large body of scientific literature focusing on the hydrodynamics and physicochemical processes in stirred tank reactors, the aim of the present communication is to briefly summarize developments in this field especially in the application of the knowledge of the fluid dynamics to fluid-particle reactor design, development and optimization.

2. Design and formulation of mixing tank problems

2.1. Design parameters and process optimization

In fluid engineering problems, research has shown that it is possible to optimize all influencing process parameters in an evolutionary manner right from the conceptual design to the final performance testing phase. This will entail the integration of the fluid flow investigation with the process reactor conceptual design and system optimization [1]. Nowadays, this multistage process design and optimization work flow shown in **Figure 1** can be fully automated through the use of computational platform. In formulating and developing a numerical solution strategy to a particular physical problem involving fluid-particle interactions, a sound theoretical

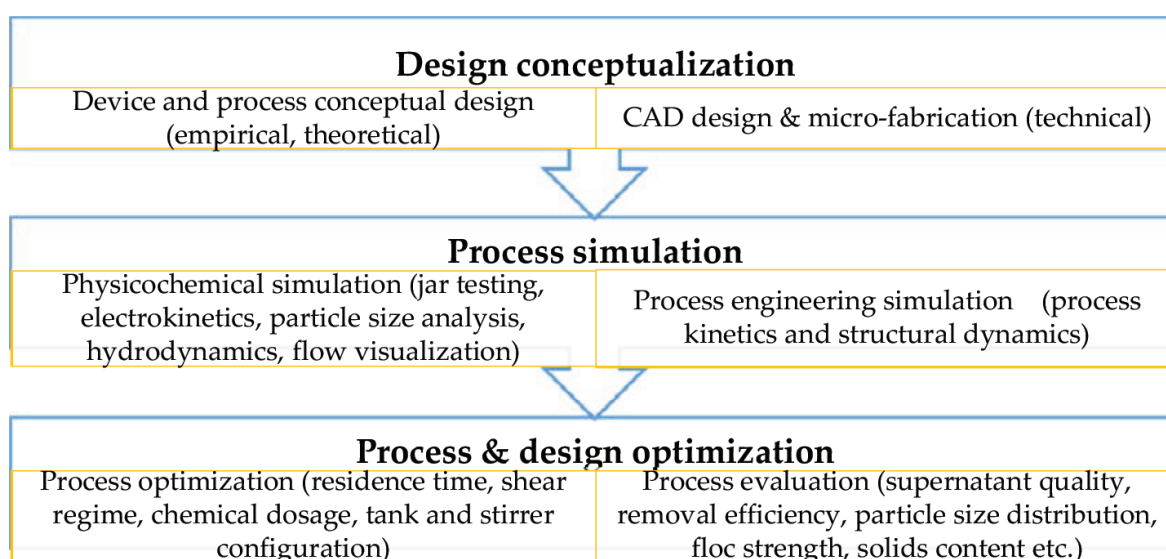


Figure 1. Reactor design and process optimization parameters in mixing tank applications.

understanding and analysis of the problem is often required. This will assist in the selection of appropriate experimental data collection methods and mathematical models that sufficiently encapsulate the physics of the problem. A number of numerical approaches and solution strategies discussed in the subsequent sections have been developed for a multitude of fluid flow scenarios. Therefore, it is important to evaluate each circumstance individually and form an opinion regarding which model would provide the best fit for a particular fluid engineering problem. It has been suggested that the robustness of any mathematical model is a function of the numerical code being used and the flow scenario being modeled [7].

2.2. Fluid dynamics and governing equations

The interactions of different phases in fluid flow occur on different scales of the fluid motion as depicted in **Figure 2**. Fluid dynamics is primarily focused on the macroscopic phenomena of the fluid flow in which the fluid is treated as a continuum. For instance, a fluid element is composed of many molecules, and the fluid dynamics represent the behaviour of the numerous molecules within the system. This concept with certain assumptions forms the basis of the derivation of fluid conservation equations of mass and momentum also known as the Navier-Stokes equation using a fluid control volume [8, 9]. The general form of the governing equations of mass and momentum conservation in any fluid flow system can be written as follows (Eqs. (1) and (2)):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\vec{\tau}) + \rho \vec{g} + \vec{F} \quad (2)$$

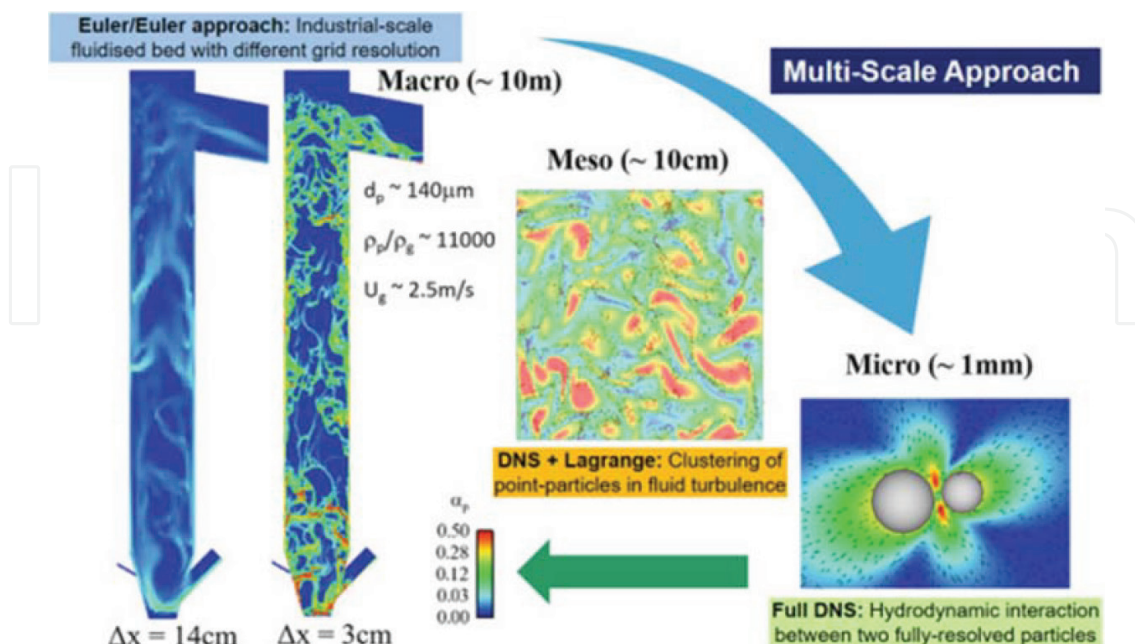


Figure 2. Multiscale modeling approach to fluid-particle interactions (reproduced from [14] with permissions © 2017 Springer).

where ρ is the density, p is the static pressure, \vec{v} is the velocity component, S_m is the source term that represent the mass added to the continuous phase from the disperse phase or any user define source, $\vec{\tau}$ represents the stress tensor due to viscous stress, $\rho\vec{g}$ is the gravitational force and \vec{F} represent the exerted body forces [10–13].

2.3. Modeling approach and solution strategies

In modeling complex single and multiphase flows in mixing tanks and process reactors, there exist two common numerical solution strategies, namely Eulerian-Eulerian and Eulerian-Lagrangian modeling approach, depending on the scale of the fluid flow as shown schematically in **Figure 3**. In the former, the fluid domain is treated as an interpenetrating continuum, while in the latter, the discrete or distinct particles of the dispersed phase are tracked in the Lagrangian reference frame. In addition to the flow field, information on the particle population such as the mean size, mass or volume fraction, and number density can be obtained using either of the two approaches [10]. Several variants of these two classes exist such as the Eulerian granular model based on the kinetic theory of granular flow (KTGF), disperse phase model (DPM), discrete element model (DEM) and the macroscopic particle model (MPM). In the case of Eulerian-Eulerian approach, the species distribution of the discrete phase may be accounted for using the population balance model (PBM), while the Eulerian-Lagrangian models can directly compute the particle size distribution while taking into account different collision and interaction mechanisms using DEM [15–18].

2.3.1. Treatment of flow domain and turbulent flow conditions

Turbulence modeling forms an integral part of the numerical analysis of complex fluid flows since most engineering fluid flows entail certain form of instability. Several closure models

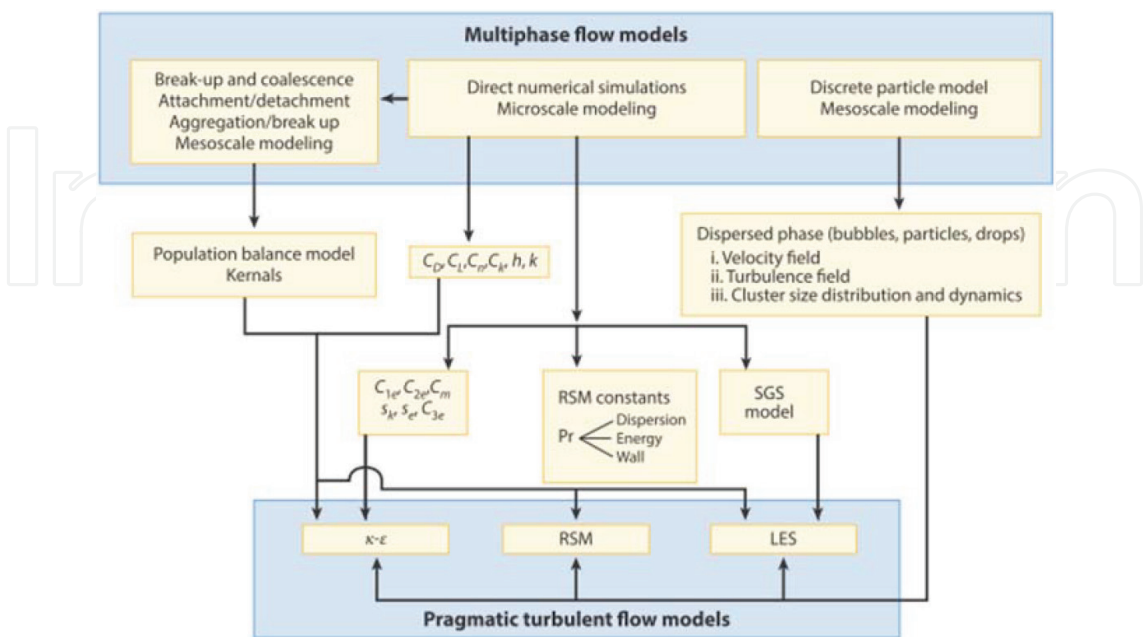


Figure 3. Parametric relationships between different modeling strategies (reproduced from [19] with permissions © 2015 Annual Reviews).

have been developed for resolving turbulence parameters in steady-state Reynolds Averaged Navier-Stokes (RANS) equations. The two equation eddy viscosity models such as $k-\epsilon$ and $k-\omega$ have been found to perform reasonably well in the modeling of rotating flows in process reactors with the only drawback being the assumption of local isotropic turbulence. The underlying theoretical assumptions underpinning the use of these models can be found in the following reference texts [12, 13]. Since the reactors encountered in most of the practical physicochemical processes contain moving or rotating parts, it is therefore necessary to take this into consideration in the preparation of the computational grid. The most common strategy for steady-state calculations include the single reference frame (SRF), multiple reference frame (MRF) or frozen rotor approach, mixing plane model (MPM) and snapshot approach, while the sliding or dynamic mesh is frequently used in transient calculations of fluid flow. For detailed information on the practical applications of the above-mentioned methods, readers are referred to the following reference texts [20, 21].

2.3.2. Model coupling for multiphase flow problems

Modeling complex physicochemical processes involving fluid flow sometimes necessitates the integration of the existing mathematical models in order to appropriately describe the physics of the problem. This can be achieved through the use of specially developed or customized in-house numerical codes or a modification of the existing ones with several software package vendors offering a platform for software improvement through the use of Application Programming Interface API or Application Customization Toolkit ACT. Such flexibility allows engineers and researchers to extend the capability and versatility of the existing numerical codes. Many software vendors go a step further in this respect by actively encouraging the development of scalable apps that extend the capability of their core software; an excellent example is the mixing tank template released by ANSYS Inc. for the automation of mixing tank simulation process. However, there exist several other flexible options for numerical code development using the open source platform, and the readers are advised to consider available options for their specific problem.

3. Experimental analysis of physicochemical processes

Several analytical and instrumental techniques have been developed for the study of complex hydrodynamic-mediated processes found in particle-laden flow—flocculation, wet agglomeration, sedimentation, floatation, fluidization and crystallization that often occur in a wide range of process conditions. These techniques shown in **Figure 4** are used either in the quantification of the hydrodynamics of the carrier and dispersed phase, or in the determination of the spatial and temporal evolution of the discrete phase properties such as the change in the particle size and distribution. In the case of the hydrodynamic interactions of the carrier and dispersed phase, a number of laser-based fluid flow techniques such as particle image velocimetry (PIV), particle tracking velocimetry (PTV), laser Doppler anaemometry (LDA), laser Doppler velocimetry (LDV), and more recently, radioactive tracking techniques such as positron emission particle tracking (PEPT) and computer-aided radioactive particle tracking (CARPT) have gained wider acceptance in the scientific community and in industry due to

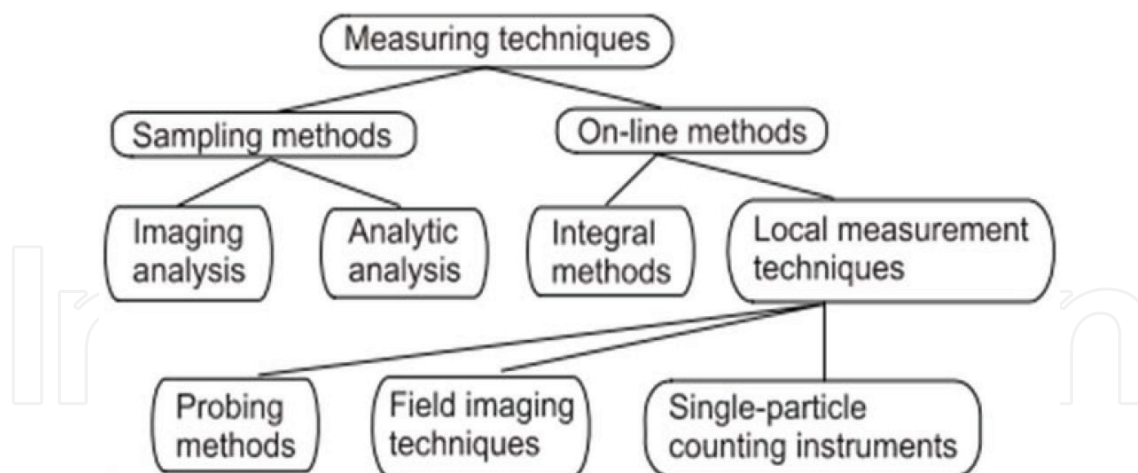


Figure 4. Experimental measurement techniques for multiphase particulate flow (reproduced from [18] with permissions © 2012 CRC Press).

their ease of use and non-intrusive nature [20–22]. These techniques provide valuable insight into the salient macroscale fluid flow characteristics such as the instantaneous and time-averaged hydrodynamic behaviour of the continuous phase, as well as the influence of the dispersed phase on the fluid flow. This is achieved by coupling the flow field measurements with the particulate phase properties and motion [21]. The experimental data set is subsequently used in the validation of numerical simulation results [18, 23].

The dominant and widely used macroscale experimental fluid flow characterization techniques are the laser velocimetry and radioactive particle tracking techniques such as the PIV or PTV, LDV or LDA with the PIV reported to be a more efficient technique [24]. These on-line methods facilitate the determination of the properties of multiphase particle-laden flow especially at low concentration. These local methods are quite superior to other similar techniques such as optical fiber probing and light scattering due to their non-intrusive nature with little or no interference on the flow while providing time series and time-averaged fluid flow characteristics with a high spatial resolution [18]. The workings of typical field imaging technique such as PIV consist of the tracer particles, laser source for flow illumination and high capacity cameras—complementary metal-oxide semiconductor (CMOS) or charge-coupled device (CCD) for the fluid flow image recording. The captured images are thereafter post-processed and correlated to obtain the hydrodynamic parameters of interest. **Table 1** provides a list of recent publications on the experimental analysis of physicochemical processes in stirred tanks. These studies demonstrated the importance of robust and reliable experimental data for complex fluid flow analysis and numerical model validation. Recent advances in experimental techniques have led to the emergence of radioactive particle tracing measurement techniques which aim to improve the ease of data collection, data accuracy and reliability.

In order to correlate the hydrodynamic and process conditions with the suspension or dispersion properties especially the change in the species concentration—spatial and temporal evolution of the particle size distribution, a number of laboratory measurement techniques are widely adopted [25]. The choice will depend to a large extent on the concentration and size distribution of the disperse phase and the nature of the flow. Regardless of the chosen analytical approach, such a correlation will facilitate an assessment of the treatment process

Reactor configuration	Stirrer configuration	Experimental technique	Technical application	Tracer particles
Cylindrical tank	Rotating disc	2D PIV	Mixing/agglomeration	Silver-coated and hollow glass spheres [1]
Cylindrical tank	Hydrofoil impellers	PEPT	Mixing	Radioactive particles [26]
Cylindrical tank	Rushton turbine	PIV	Mixing	Polymeric and glass particles [27]
Cylindrical tank	Hollow blade semi-elliptic disc turbine	TRPIV, PIV	Mixing	Neutrally buoyant glass beads [24]
Cylindrical tank	Pitched-blade turbine impeller	FPIV	Mixing	Soda-lime glass beads [28]
Cylindrical tank	Rushton turbine	CARPT	Mixing	Radioactive particles [29]
Cylindrical tank	Rushton turbine	LDA	Mixing	Hollow glass spheres [30]
Cylindrical tank	Kenics static mixer	PEPT	Mixing	Radioactive particles [31]
Cylindrical tank	Pitched-blade turbine	PEPT	Mixing	Radioactive particles [32]
Cylindrical tank	Pitched-blade turbine	PIV	Mixing	Silica glass spheres [23]
Square tank	Hydro foil impeller	PIV, image analysis	Mixing/agglomeration	In situ agglomerated flocs [33]
Cylindrical tank	Six-blade Rushton turbine	3V3	Mixing	Opt image polycrystalline particles [34]
Cylindrical tank	Rushton turbine, pitched-blade turbine	PEPT	Mixing	Monosized silica gel particles [35]
Cylindrical tank	Six-blade Rushton turbine	PEPT, LDA	Mixing	Ion-exchange resin particles [36]
Cylindrical tank	Rotor-stator mixer	PIV	Mixing	Polyamide particles [37]

Table 1. Selected studies on the experimental analysis of physical and chemical processes in stirred tanks.

and the reactor performance under a particular process condition. For instance, the conventional physicochemical simulation tests such as the cylinder, Imhoff cone and jar tests can be combined with parametric analytical techniques such as the Buchner-funnel or pressure filtration test, capillary suction time (CST) test, electrokinetic charge analysis using colloidal titrations (i.e. zeta and streaming potential), laser light scattering or laser diffraction, microscopy, image analysis, photometric dispersion analysis (PDA), fiber optic sensor and HNMR spectroscopy. These techniques have been successfully employed to characterize the physicochemical process in bench, pilot and full-scale studies [38–41]. A careful consideration of the limitations of each of these approaches will ensure proper selection of an appropriate method.

In most of the physicochemical processes involving particulate flow either as a colloidal dispersion or granular suspension, the species attributes — mean size, particle concentration and distribution and fractal properties of the resulting agglomerates — are the primary parameters of interest [21]. In this case, an appropriate physicochemical simulation such as a jar or cylinder test is often followed by a parametric analysis to characterize the process performance as a function of species attributes. Several other parameters may be of interest depending on the type of reactor and the required solid-liquid separation method. Such parameters may include aggregate mean size, shape and distribution, aggregate volume concentration, aggregate strength, sludge volume index, silting index, residual supernatant turbidity, absorbance or optical density, electrical conductivity, viscosity, zeta or streaming potential, specific resistance to filtration, capillary suction time, and so on [38, 39]. In the case of chemical optimization, a parametric dose-response curve will give reasonably accurate information on the required chemical dose for a particular process condition [42–45]. **Table 2** and **Figure 5** show a typical correlation of the agglomerate test properties with the process condition—shear rate. However, regardless of the choice of parametric test, an examination of the supernatant, sediment, filtrate and residue will yield some valuable information on the reactor performance under specific process conditions. Such assessment is carried out either by direct *in situ* measurements such as in particle counting, *ex situ* analysis in which the samples are extracted for measurements or by other indirect parametric indicators. A detailed discussion on the practical applications of different dispersed phase measurement techniques is available elsewhere [40, 41].

Considering the wide range of options available to select from, optimizing a given physicochemical condition for a particular process reactor under laboratory conditions is a daunting task. Therefore, in optimizing the design and process parameters for a particular reactor, a statistical correlation of these parameters from a data set is often required, depending on the available time and complexity of the problem, to obtain accurate information on the optimum design and process conditions. A number of statistical methods such as the design of experiment and response surface methodology can be applied to a large set of experimental data to obtain the desired optimization points. This will facilitate an understanding of the influence of different process conditions on the reactor performance which will assist in the selection of optimized operating conditions.

Test parameters	Agitation speed	
	145 rpm	165 rpm
Mean agglomerate diameter, mm	3.8330	3.9182
Mean agglomerate compressive strength, Nm m ⁻²	0.4298	0.4351
Mean strain rate, s ⁻¹	0.3639	0.4088
Mean maximum compressive force, N	4.9476	5.2303

Table 2. Agglomerate characteristics test properties as a function of the reactor agitation speed in a wet agglomeration process.

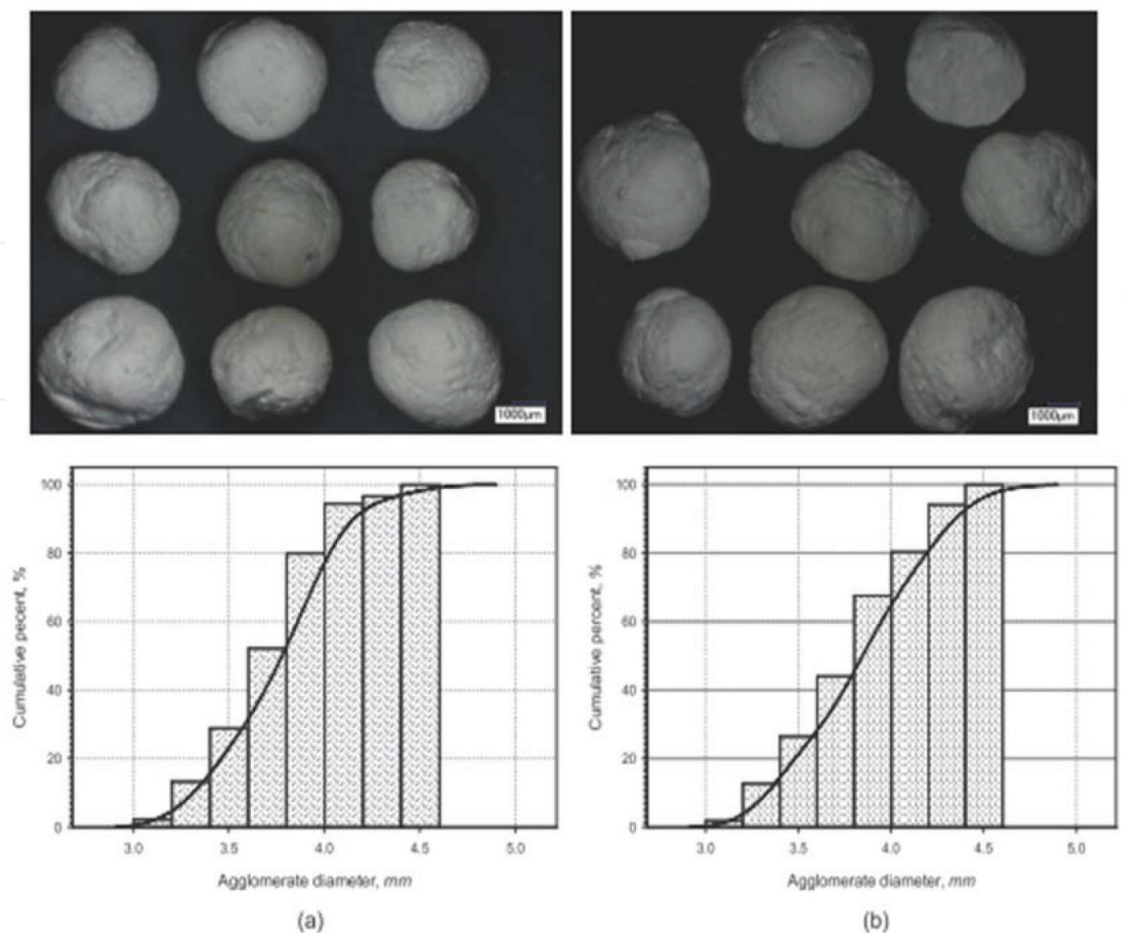


Figure 5. A parametric correlation of agglomerate properties with the process condition—shear rate (a) 145 rpm and (b) 165 rpm.

4. Modeling physicochemical processes in stirred tank reactor

The use of computational fluid dynamics (CFD) as a research tool to investigate complex fluid-particle interactions has been growing in popularity both in academia and in the industry [46]. CFD provides a powerful alternative and a more robust platform for engineers in the design of equipment and processes involving fluid flow and heat transfer when compared to the classical experimental approach. Nowadays, numerical simulations complement the experimental and analytical techniques and are increasingly being performed in many fluid engineering applications ranging from chemical and mineral processing to civil and environmental process engineering [46]. However, it is worth pointing out that the continual development of reliable empirical, mathematical and computational models relies on a robust and detailed experimental data.

Tables 3 and 4 provide a list of recent experimentally validated numerical studies focusing on the physicochemical analysis of fluid-particle reactors. The former is focused on the analysis of the mixing phenomena in stirred tanks while the latter deals with the technical application of mixing

for several industrial processes. The modeling approach in most of these studies is applicable to mixing tanks and process reactors of various geometric designs. Joshi et al. [47, 48] provide a comprehensive review of CFD applications in a single phase mixing tank hydrodynamic analysis focusing on axial and radial flow impellers in a multitude of flow scenarios. Their two-part study, which is one of the most detailed and comprehensive reviews in this field, summarizes developments in mixing tank modeling by bringing together the results of scientific investigations spanning several decades. Similar reviews focusing on turbulent multiphase flows and multiphase

Reactor configuration	Fluid agitator/ application	Experimental validation method	Numerical code/ modeling approach	Turbulence models
Cylindrical tank	Grid disc impeller	LDA	CFX/MRF	k- ϵ [53]
Cylindrical tank	Grid disc impeller, solid disc, propeller	LDA	CFX/MRF	k- ϵ [52]
Cylindrical tank	Rushton turbine, flotation impeller	2D PIV	Fluent/MRF	k- ϵ [54]
Cylindrical tank	Rushton disc impeller	LDA	Fluent/snapshot	k- ϵ [55]
Cylindrical tank	Rushton turbine	LDA	Fluent/MRF	k- ϵ , DES [56]
Cylindrical tank	Foil impeller, Rushton turbine	Image analysis	PHOENICS/MRF	k- ϵ [57]
Cylindrical Tank	Pitched-blade turbine	PEPT	CFX/MRF	k- ϵ [58]
Cylindrical tank	Rushton turbine	LDV	Fluent/MRF	k- ϵ [59, 60]
Cylindrical tank	Rushton turbine	PLIF	Fluent/MRF	k- ϵ [61]
Square tank	Rushton turbine	Power consumption measurements	Fluent/MRF	RSM [62]
Cylindrical tank	Pitched-blade turbine	2D PIV	Fluent/sliding mesh	k- ϵ [63]
Cylindrical tank	Rushton turbine	CARPT	Fluent/MRF	k- ϵ [64]
Cylindrical tank	Rushton turbine	Solids concentration measurements	CFX/MRF	k- ϵ [65]
Cylindrical tank	Pfaudler retreat curve impeller	2D PIV, laser granulometry, nephelometry	Fluent/sliding mesh	k- ϵ [66]
Square tank	Rotating cylinder	LDA	Fluent/MRF	k- ϵ [67]
Cylindrical tank	Rushton turbine, pitched blade turbine	RPT, LDA	Fluent/MRF	k- ϵ [68]
Cylindrical tank	Rushton turbine	LDV	Fluent/MRF	k- ϵ , LES [69]
Cylindrical tank	Flat blade turbine, pitched blade turbine, Rushton turbine	LDV	Fluent/MRF	k- ϵ [70]
Cylindrical tank	Rushton turbine	LDV	Fluent/MRF	RSM [71]
Cylindrical tank	Rushton turbine, disc turbine, elliptical blade disc turbine	SPIV	Fluent/sliding mesh	k- ϵ , LES [72]

Reactor configuration	Fluid agitator/ application	Experimental validation method	Numerical code/ modeling approach	Turbulence models
Cylindrical tank	Rushton turbine	2D PIV, LDA	Fluent/sliding mesh	DES [73]
Cylindrical tank	Double Rushton turbine	LDA	CFX/MRF	k- ϵ [74]
Cylindrical tank	Rushton turbine	Mixing time, power consumption, solids concentration measurements	CFX/MRF/sliding grid	k- ϵ [75]
Cylindrical tank	Rushton turbine	Particle size analysis, conductometry	Fluent/MRF	k- ϵ [76]
Cylindrical tank	Pitched-blade turbine, double disc impeller	PIV, critical impeller speed measurements	Fluent/MRF	k- ϵ [77]
Cylindrical tank	Rushton turbine	LDV	Fluent/MRF	k- ϵ [78]
Cylindrical tank	Pitched-blade turbine	PEPT	Fluent/MRF	k- ω , k- ϵ , RSM [79]
Cylindrical tank	Rigid, rigid-flexible and punched rigid-flexible impeller	Solids concentration measurements	Fluent/MRF	k- ϵ [80]
Cylindrical tank	Flat blade impeller, angle pitch impeller	DPIV	Fluent/MRF	k- ϵ [81]
Cylindrical tank	Rotor-stator mixer	PIV	Fluent/MRF/sliding mesh	k- ϵ , k- ω [82]
Cylindrical tank	Rotor-stator mixer	LDA	Fluent/sliding mesh	k- ϵ [83]

Table 3. Selected studies on CFD characterization of single phase and multiphase flows in classical stirred tank reactors.

reactor modelling, and which provide a more comprehensive discussion on the subject matter are available elsewhere [19, 49–51].

Regardless of the specific focus of each study, most of the studies differ only in terms of stirrer-vessel configurations, experimental validation methods and the choice of modeling approach. In terms of the stirrer-vessel configuration, there is a wide variety of flow inducers available for fluid flow investigation, each with different power demands and flow patterns. In addition to well-established impeller designs employed in most of the studies—Rushton turbine, pitched-blade turbine, propeller, and so on, a few innovative designs have been used with good results [52]. The turbulence models of choice in most of the investigations are the two equation eddy viscosity models such as k- ϵ and k- ω , and RSM models which are quite efficient in handling rotating flows in stirred tanks and multiphase reactors. The dominant modeling approaches for rotating flow problems are the MRF and sliding mesh. The former is suitable for steady-state problems while the latter is employed for transient calculations. Despite the technical limitations of some of the experimental flow measurement techniques, reasonable agreement was obtained in most of the studies between the experimental data and numerical simulation. In a few of the studies, the model predictions were not quite robust enough when compared to the experimental data set partly due to the complexity of the flow scenario being modeled.

Reactor configuration	Fluid agitator/application	Experimental validation method	Numerical code/modeling approach	Turbulence models
Cylindrical flocculator	Paddle mixer/flocculation	LDA, 2D PIV	CFX/MRF	k- ϵ , RSM [84]
Rectangular flocculator	Axial impeller/water purification	2D PIV	Fluent/MRF	k- ϵ [85]
Cylindrical sedimentation tank	Axial impeller/water purification	Laser diffraction	CFX/MRF	k- ϵ [86]
Cylindrical Jar testing device	Paddle stirrer/flocculation	LDA	Fluent/MRF	k- ϵ , k- ω , RSM [7, 87, 88]
Cylindrical flocculation reactor	Rushton turbine/bio-flocculation	LDV	Fluent/MRF	k- ϵ [89]
Cylindrical stirred tank	Pitched turbine blade/silica particle deagglomeration	Laser diffraction/PIDS	Fluent/MRF	k- ϵ [90]
Cylindrical stirred bioreactor	Marine impeller/cell cultivation	Tracer and dynamic method	Fluent/MRF	k- ϵ [91]
Cylindrical tank	R1342-type impeller/flocculation	Image analysis	Fluent/MRF	k- ϵ [92]
Cylindrical tank	Rushton impeller/cell culture	Optical sensor	CFX/MRF	k- ϵ [93]
Cylindrical bioreactor	Rushton, scaba and paddle impellers/cell culture	Optical density	Fluent/MRF	k- ϵ [94]
Cylindrical tank	Turbine, anchor and oblique impellers/autoclave	Tracer injection	Fluent/MRF	k- ϵ [95]
Cylindrical bioreactor	Marine impeller/recombinant protein synthesis	PIV	Fluent/MRF	k- ϵ [91, 96]
Cylindrical tube reactor	Impeller/bacterial inactivation	2D PIV	CFX/MRF	RSM [2]
Cylindrical bioreactor	Rushton turbine/anaerobic digestion	Gas chromatography	Fluent/MRF	k- ϵ [97]
Cylindrical tank	Turbine impeller/polymerization	Droplet size measurements	Fluent/MRF	k- ϵ [98]
Cylindrical tank	Rushton impeller/cell cultivation	Dynamic method	Fluent/MRF	k- ϵ [99]
Cylindrical tank	Rushton turbine/cell inactivation	PIV	Fluent/MRF	k- ϵ [100]
Cylindrical tank	Rushton turbine and propellers/cell culture	Dynamic method	Fluent/MRF	RSM [101]
Cylindrical crystallizer	Rushton impeller/precipitation	X-ray/laser diffraction	Fluent/MRF	k- ϵ [102]
Cylindrical Photobioreactor	Rotating cylinder/algal culture	Optical density	Fluent/SRF	k- ω [103, 104]

Table 4. Selected studies on CFD characterization of hydrodynamics and physicochemical processes in field-assisted process reactors.

5. Conclusions and future perspectives

A review of recent advances in the experimental analysis and numerical modeling of physicochemical processes in stirred tanks and agglomeration reactors have been presented. This review briefly summarizes important findings and major contributions from numerous publications in this field. This short review of the developments in this field clearly shows that significant progress has been made over the past decade in the understanding of complex physicochemical phenomena that are vital for many industrial and environmental processes, especially from experimental and theoretical perspective. However, there is still a gap in knowledge especially in the suitability of the existing mathematical models to accurately predict the reactor performance in a wide range of existing and emerging processes. This clearly calls for a numerical code programming and development to form an integral part of the engineering training and curriculum in future. The successful design, development and optimization of agglomeration units depend on the robustness of the experimental data, mathematical models and simulation tools. This short review is by no means an exhaustive one, and readers are advised to consult other multitudes of scientific publications on the subject matter. In conclusion, numerical modeling along with robust experimental data will continue to be highly indispensable well into the foreseeable future.

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References

- [1] Oyegbile B, Hoff M, Adonadaga M, Oyegbile B. Experimental analysis of the hydrodynamics, flow pattern and wet agglomeration in rotor-stator vortex separators. *Journal of Environmental Chemical Engineering*. 2017;5:2115-2127. DOI: 10.1016/j.jece.2017.04.016

- [2] Thomas SF, Rooks P, Rudin F, Cagney N, Balabani S, Atkinson S, et al. Swirl flow bioreactor containing dendritic copper-containing alginate beads: A potential rapid method for the eradication of *Escherichia coli* from waste water streams. *Journal of Water Process Engineering*. 2015;**5**:6-14. DOI: 10.1016/j.jwpe.2014.10.010
- [3] Sievers M, Stoll SM, Schroeder C, Niedermeiser M, Onyeche TI. Sludge dewatering and aggregate formation effects through Taylor vortex assisted flocculation. *Separation Science and Technology*. 2008;**43**:1595-1609. DOI: 10.1080/01496390801973888
- [4] Wang X, Jin P, Yuan H, Wang E, Tambo N. Pilot study of a fluidized-pellet-bed technique for simultaneous solid/liquid separation and sludge thickening in a sewage treatment plant. *Water Science and Technology*. 2004;**49**:81-88
- [5] Dionysiou DD, Balasubramanian G, Suidan (M) MT, Khodadoust AP, Baudin I, Laine J-M. Rotating disk photocatalytic reactor: Development, characterization, and evaluation for the destruction of organic pollutants in water. *Water Research*. 2000;**34**:2927-2940. DOI: 10.1016/S0043-1354(00)00022-1
- [6] Loraine G, Chahine G, Hsiao C-T, Choi J-K, Aley P. Disinfection of gram-negative and gram-positive bacteria using DynaJets® hydrodynamic cavitating jets. *Ultrasonics Sonochemistry*. 2012;**19**:710-717. DOI: 10.1016/j.ultsonch.2011.10.011
- [7] Bridgeman J, Jefferson B, Parsons SA. Computational fluid dynamics modelling of flocculation in water treatment: A review. *Engineering Applications of Computational Fluid Mechanics*. 2009;**3**:220-241. DOI: 10.1080/19942060.2009.11015267
- [8] Krüger T, Kusumaatmaja H, Kuzmin A, Shardt O, Silva G, Viggen EM. *The Lattice Boltzmann Method: Principles and Practice*. Basel: Springer; 2017
- [9] Jahanshaloo L, Pouryazdanpanah E, Sidik NAC. A review on the application of the lattice Boltzmann method for turbulent flow simulation. *Numerical Heat Transfer, Part A: Applications*. 2013;**64**:938-953. DOI: 10.1080/10407782.2013.807690
- [10] Lian G, Moore S, Heeney L. Population balance and computational fluid dynamics modelling of ice crystallisation in a scraped surface freezer. *Chemical Engineering Science*. 2006;**61**:7819-7826. DOI: 10.1016/j.ces.2006.08.075
- [11] Das S, Bai H, Wu C, Kao J-H, Barney B, Kidd M, et al. Improving the performance of industrial clarifiers using three-dimensional computational fluid dynamics. *Engineering Applications of Computational Fluid Mechanics*. 2016;**10**:130-144. DOI: 10.1080/19942060.2015.1121518
- [12] ANSYS, Inc. *ANSYS Fluent Theory Guide 18.2* 2017
- [13] ANSYS, Inc. *ANSYS Fluent User's Guide 18.2* 2017
- [14] Sommerfeld M. Numerical methods for dispersed multiphase flows. In: Bodnár T, Galdi GP, Nečasová Š, editors. *Part. Flows*. Heidelberg: Springer; 2017. pp. 327-396
- [15] Jeldres RI, Fawell PD, Florio BJ. Population balance modelling to describe the particle aggregation process: A review. *Powder Technology*. 2017;**326**:190-207. DOI: 10.1016/j.powtec.2017.12.033

- [16] Hellesto A, Ghaffari M, Balakin B. A parametric study of cohesive particle agglomeration in a shear flow—Numerical simulations by the discrete element method. *Journal of Dispersion Science and Technology*. 2016;**38**:611-620. DOI: 10.1080/01932691.2016.1185015
- [17] Schellander D. *CFD Simulations of Particle Laden Flow: Particle Transport and Separation*. Hamburg: Anchor Academic Publishing; 2014
- [18] Crowe CT, Schwarzkopf JD, Sommerfeld M, Tsuji Y. *Multiphase Flows with Droplets and Particles*. 2nd ed. Boca Raton, FL: CRC Press; 2011
- [19] Joshi JB, Nandakumar K. Computational modeling of multiphase reactors. *Annual Review of Chemical and Biomolecular Engineering*. 2015;**6**:347-378. DOI: 10.1146/annurev-chembioeng-061114-123229
- [20] Johnson RW, editor. *Handbook of Fluid Dynamics*. 2nd ed. Boca Raton, FL: CRC Press; 2016
- [21] Michaelides E, Crowe CT, Schwarzkopf JD, editors. *Multiphase Flow Handbook*. 2nd ed. Boca Raton, FL: CRC Press; 2016
- [22] Mavros P. Flow visualization in stirred vessels: A review of experimental techniques. *Chemical Engineering Research and Design*. 2001;**79**:113-127. DOI: 10.1205/02638760151095926
- [23] Li G, Gao Z, Li Z, Wang J, Derksen JJ. Particle-Resolved PIV experiments of solid-liquid mixing in a turbulent stirred tank. *AIChE Journal*. 2018;**64**:389-402. DOI: 10.1002/aic.15924
- [24] Liu X, Bao Y, Li Z, Gao Z. Analysis of turbulence structure in the stirred tank with a deep hollow blade disc turbine by time-resolved PIV. *Chinese Journal of Chemical Engineering*. 2010;**18**:588-599. DOI: 10.1016/S1004-9541(10)60262-5
- [25] Hasan BO. Breakage of drops and bubbles in a stirred tank: A review of experimental studies. *Chinese Journal of Chemical Engineering*. 2017;**25**:698-711. DOI: 10.1016/j.cjche.2017.03.008
- [26] Fangary YS, Barigou M, Seville JPK, Parker DJ. A Lagrangian study of solids suspension in a stirred vessel by positron emission particle tracking PEPT. *Chemical Engineering and Technology*. 2002;**25**:521-528. DOI: 10.1002/1521-4125(200205)25:5<521::AID-CEAT521>3.0.CO;2-C
- [27] Montante G, Paglianti A, Magelli F. Analysis of dilute solid-liquid suspensions in turbulent stirred tanks. *Chemical Engineering Research and Design*. 2012;**90**:1448-1456. DOI: 10.1016/j.cherd.2012.01.009
- [28] Unadkat H, Rielly CD, Hargrave GK, Nagy ZK. Application of fluorescent PIV and digital image analysis to measure turbulence properties of solid-liquid stirred suspensions. *Chemical Engineering Research and Design*. 2009;**87**:573-586. DOI: 10.1016/j.cherd.2008.11.011
- [29] Rammohan A, Kemoun A, Al-Dahhan M, Dudukovic M. Characterization of single phase flows in stirred tanks via computer automated radioactive particle tracking (CARPT). *Chemical Engineering Research and Design*. 2001;**79**:831-844. DOI: 10.1205/02638760152721343

- [30] Komrakova AE, Liu Z, Machado MB, Kresta SM. Development of a zone flow model for the confined impeller stirred tank (CIST) based on mean velocity and turbulence measurements. *Chemical Engineering Research and Design*. 2017;**125**:511-522. DOI: 10.1016/j.cherd.2017.07.025
- [31] Rafiee M, Simmons MJH, Ingram A, Stitt HE. Development of positron emission particle tracking for studying laminar mixing in Kenics static mixer. *Chemical Engineering Research and Design*. 2013;**91**:2106-2113. DOI: 10.1016/j.cherd.2013.05.022
- [32] Guida A, Nienow AW, Barigou M. PEPT measurements of solid-liquid flow field and spatial phase distribution in concentrated monodisperse stirred suspensions. *Chemical Engineering Science*. 2010;**65**:1905-1914. DOI: 10.1016/j.ces.2009.11.005
- [33] Kilander J, Blomström S, Rasmuson A. Spatial and temporal evolution of floc size distribution in a stirred square tank investigated using PIV and image analysis. *Chemical Engineering Science*. 2006;**61**:7651-7667. DOI: 10.1016/j.ces.2006.09.001
- [34] Sharp KV, Hill D, Troolin D, Walters G, Lai W. Volumetric three-component velocimetry measurements of the turbulent flow around a Rushton turbine. *Experiments in Fluids*. 2009;**48**:167-183. DOI: 10.1007/s00348-009-0711-9
- [35] Fishwick R, Winterbottom M, Parker D, Fan X, Stitt H. The use of positron emission particle tracking in the study of multiphase stirred tank reactor hydrodynamics. *Canadian Journal of Chemical Engineering*. 2005;**83**:97-103. DOI: 10.1002/cjce.5450830117
- [36] Chiti F, Bakalis S, Bujalski W, Barigou M, Eaglesham A, Nienow AW. Using positron emission particle tracking (PEPT) to study the turbulent flow in a baffled vessel agitated by a Rushton turbine: Improving data treatment and validation. *Chemical Engineering Research and Design*. 2011;**89**:1947-1960. DOI: 10.1016/j.cherd.2011.01.015
- [37] Mortensen HH, Innings F, Håkansson A. The effect of stator design on flowrate and velocity fields in a rotor-stator mixer – An experimental investigation. *Chemical Engineering Research and Design*. 2017;**121**:245-254. DOI: 10.1016/j.cherd.2017.03.016
- [38] Bache DH, Gregory R. *Flocs in Water Treatment*. London: IWA Publishing; 2007
- [39] Bratby J. *Coagulation and Flocculation in Water and Wastewater Treatment*. 3rd ed. London: IWA Publishing; 2016
- [40] Gregory J. Flocculation Measurement Techniques. In: Tadros T, editor. *Encycl. Colloid Interface Sci*. Heidelberg: Springer; 2013. pp. 492-52
- [41] Gregory J. Monitoring particle aggregation processes. *Advances in Colloid and Interface Science*. 2009;**147-148**:109-123. DOI: 10.1016/j.cis.2008.09.003
- [42] Bache DH, Zhao YQ. Optimising polymer use in alum sludge conditioning: An ad hoc test. *Journal of Water Supply: Research and Technology – AQUA*. 2001;**50**:29-38
- [43] Oyegbile B, Ay P, Narra S. Optimization of physicochemical process for pre-treatment of fine suspension by flocculation prior to dewatering. *Desalination and Water Treatment*. 2016;**57**:2726-2736. DOI: 10.1080/19443994.2015.1043591

- [44] Al Momani FA, Örmeci B. Optimization of polymer dose based on residual polymer concentration in dewatering supernatant. *Water, Air, and Soil Pollution*. 2014;**225**:1-11. DOI: 10.1007/s11270-014-2154-z
- [45] Ramphal SR, Sibiya MS. Optimization of coagulation-flocculation parameters using a photometric dispersion analyser. *Drinking Water Engineering and Science*. 2014;**7**:73-82. DOI: 10.5194/dwes-7-73-2014
- [46] Tu J, Yeoh GH, Liu C. *Computational Fluid Dynamics: A Practical Approach*. Oxford: Butterworth-Heinemann; 2013
- [47] Joshi JB, Nere NK, Rane CV, Murthy BN, Mathpati CS, Patwardhan AW, et al. CFD simulation of stirred tanks: Comparison of turbulence models. Part I: Radial flow impellers. *Canadian Journal of Chemical Engineering*. 2011;**89**:23-82. DOI: 10.1002/cjce.20446
- [48] Joshi JB, Nere NK, Rane CV, Murthy BN, Mathpati CS, Patwardhan AW, et al. CFD simulation of stirred tanks: Comparison of turbulence models (part II: Axial flow impellers, multiple impellers and multiphase dispersions). *Canadian Journal of Chemical Engineering*. 2011;**89**:754-816. DOI: 10.1002/cjce.20465
- [49] Balachandar S, Eaton JK. Turbulent dispersed multiphase flow. *Annual Review of Fluid Mechanics*. 2009;**42**:111-133. DOI: 10.1146/annurev.fluid.010908.165243
- [50] Tinoco H, Lindqvist H, Frid W. Numerical simulation of industrial flows. In: Angermann L, editor. *Numer. Simul. – Ex. Appl. Comput. Fluid Dyn*. Rijeka: InTech; 2001
- [51] Pradip M. Computational fluid dynamics analysis of turbulent flow. In: Minin IV, Minin OV, editors. *Comput. Fluid Dyn. Technol. Appl*. Rijeka: InTech; 2011. pp. 255-92
- [52] Buwa V, Dewan A, Nassar AF, Durst F. Fluid dynamics and mixing of single-phase flow in a stirred vessel with a grid disc impeller: Experimental and numerical investigations. *Chemical Engineering Science*. 2006;**61**:2815-2822. DOI: 10.1016/j.ces.2005.10.066
- [53] Dewan A, Buwa V, Durst F. Performance optimizations of grid disc impellers for mixing of single-phase flows in a stirred vessel. *Chemical Engineering Research and Design*. 2006;**84**:691-702. DOI: 10.1205/cherd05044
- [54] Basavarajappa M, Draper T, Toth P, Ring TA, Miskovic S. Numerical and experimental investigation of single phase flow characteristics in stirred tanks using Rushton turbine and flotation impeller. *Minerals Engineering*. 2015;**83**:156-167. DOI: 10.1016/j.mineng.2015.08.018
- [55] Deshpande VR, Ranade VV. Simulation of flows in stirred vessels agitated by dual Rushton impellers using computational snapshot approach. *Chemical Engineering Communications*. 2003;**190**:236-253. DOI: 10.1080/00986440302144
- [56] Yang FL. Turbulent flow and mixing performance of a novel six-blade grid disc impeller. *Korean Journal of Chemical Engineering*. 2015;**32**:816-825. DOI: 10.1007/s11814-014-0255-4
- [57] Prat OP, Ducoste JJ. Simulation of flocculation in stirred vessels: Lagrangian versus Eulerian. *Chemical Engineering Research and Design*. 2007;**85**:207-219. DOI: 10.1205/cherd05001

- [58] Liu L, Barigou M. Numerical modelling of velocity field and phase distribution in dense Monodisperse solid–liquid suspensions under different regimes of agitation: CFD and PEPT experiments. *Chemical Engineering Science*. 2013;**101**:837-850. DOI: 10.1016/j.ces.2013.05.066
- [59] Karimi M, Akdogan G, Bradshaw SM. A computational fluid dynamics model for the flotation rate constant, part I: Model development. *Minerals Engineering*. 2014;**69**:214-222. DOI: 10.1016/j.mineng.2014.03.028
- [60] Karimi M, Akdogan G, Bradshaw SM. A CFD-kinetic model for the flotation rate constant, part II: Model validation. *Minerals Engineering*. 2014;**69**:205-213. DOI: 10.1016/j.mineng.2014.05.014
- [61] Coroneo M, Montante G, Paglianti A, Magelli F. CFD prediction of fluid flow and mixing in stirred tanks: Numerical issues about the RANS simulations. *Computers and Chemical Engineering*. 2011;**35**:1959-1968. DOI: 10.1016/j.compchemeng.2010.12.007
- [62] Chtourou W, Ammar M, Driss Z, Abid MS. CFD prediction of the turbulent flow generated in stirred square tank by a Rushton turbine. *Energy and Power Engineering*. 2014;**6**:95-110. DOI: 10.4236/epe.2014.65010
- [63] Ge C-Y, Wang J-J, Gu X-P, Feng L-F. CFD simulation and PIV measurement of the flow field generated by modified pitched blade turbine impellers. *Chemical Engineering Research and Design*. 2014;**92**:1027-1036. DOI: 10.1016/j.cherd.2013.08.024
- [64] Wadnerka D, Utika RP, Tade MO, Pareek VK. CFD simulation of solid–liquid stirred tanks. *Advanced Powder Technology*. 2012;**23**:445-453. DOI: 10.1016/j.appt.2012.03.007
- [65] Tamburini A, Cipollina A, Micale G, Brucato A, Ciofalo M. CFD simulations of dense solid–liquid suspensions in baffled stirred tanks: Prediction of suspension curves. *Chemical Engineering Journal*. 2011;**178**:324-341. DOI: 10.1016/j.cej.2011.10.016
- [66] Calvo S, Delafosse A, Collignon M-L, Crine M, Toye D. Experimental characterisation and modelling of homogeneous solid suspension in an industrial stirred tank. *Advances in Mechanical Engineering*. 2013;**5**:1-9. DOI: 10.1155/2013/329264
- [67] Escamilla-Ruiz IA, Sierra-Espinosa FZ, García JC, Valera-Medina A, Carrillo F. Experimental data and numerical predictions of a single-phase flow in a batch square stirred tank reactor with a rotating cylinder agitator. *Heat and Mass Transfer*. 2017;**53**:2933-2949. DOI: 10.1007/s00231-017-2030-7
- [68] Bashiri H, Alizadeh E, Bertrand F, Chaouki J. Investigation of turbulent fluid flows in stirred tanks using a non-intrusive particle tracking technique. *Chemical Engineering Science*. 2016;**140**:233-251. DOI: 10.1016/j.ces.2015.10.005
- [69] Zadghaffari R, Moghaddas JS, Revstedt J. Large-Eddy simulation of turbulent flow in a stirred tank driven by a Rushton turbine. *Computers and Fluids*. 2010;**39**:1183-1190. DOI: 10.1016/j.compfluid.2010.03.001
- [70] Ammar M, Chtourou W, Driss Z, Abid MS. Numerical investigation of turbulent flow generated in baffled stirred vessels equipped with three different turbines in one and two-stage system. *Energy*. 2011;**36**:5081-5093. DOI: 10.1016/j.energy.2011.06.002

- [71] Qi N, Wang H, Zhang K, Zhang H. Numerical simulation of fluid dynamics in the stirred tank by the SSG Reynolds stress model. *Frontiers of Chemical Engineering in China*. 2010;**4**:506-514. DOI: 10.1007/s11705-010-0508-7
- [72] Li Z, Song G, Bao Y, Gao Z. Stereo-PIV experiments and large Eddy simulations of flow fields in stirred tanks with Rushton and curved-blade turbines. *AICHE Journal*. 2013;**59**:3986-4003. DOI: 10.1002/aic.14117
- [73] Chara Z, Kysela B, Konfrst J, Fort I. Study of fluid flow in baffled vessels stirred by a Rushton standard impeller. *Applied Mathematics and Computation*. 2016;**272**:614-628. DOI: 10.1016/j.amc.2015.06.044
- [74] Wang H, Jia X, Wang X, Zhou Z, Wen J, Zhang J. CFD modeling of hydrodynamic characteristics of a gas-liquid two-phase stirred tank. *Applied Mathematical Modelling*. 2014;**38**:63-92. DOI: 10.1016/j.apm.2013.05.032
- [75] Tamburini A, Cipollina A, Micale G, Brucato A, Ciofalo M. Influence of drag and turbulence modelling on CFD predictions of solid liquid suspensions in stirred vessels. *Chemical Engineering Research and Design*. 2014;**92**:1045-1063. DOI: 10.1016/j.cherd.2013.10.020
- [76] Wang L, Zhang Y, Li X, Zhang Y. Experimental investigation and CFD simulation of liquid-solid-solid dispersion in a stirred reactor. *Chemical Engineering Science*. 2010;**65**:5559-5572. DOI: 10.1016/j.ces.2010.08.002
- [77] Murthy BN, Kasundra RB, Joshi JB. Hollow self-inducing impellers for gas-liquid-solid dispersion: Experimental and computational study. *Chemical Engineering Journal*. 2008;**141**:332-345. DOI: 10.1016/j.cej.2008.01.040
- [78] Deglon DA, Meyer CJ. CFD Modelling of stirred tanks: Numerical considerations. *Minerals Engineering*. 2006;**19**:1059-1068. DOI: 10.1016/j.mineng.2006.04.001
- [79] Wadnerkar D, Tade MO, Pareek VK, Utikar RP. CFD simulation of solid-liquid stirred tanks for low to dense solid loading systems. *Particuology*. 2016;**29**:16-33. DOI: 10.1016/j.partic.2016.01.012
- [80] Gu D, Liu Z, Xie Z, Li J, Tao C, Wang Y. Numerical simulation of solid-liquid suspension in a stirred tank with a dual punched rigid-flexible impeller. *Advanced Powder Technology*. 2017;**28**:2723-2734. DOI: 10.1016/j.appt.2017.07.025
- [81] Xinli W, Jie R, Xiangrui M. Simulation and Experiment Study of Flow Field and Dynamic Performance in Stirred Reactor, Hangzhou, China. 2007. pp. 1408-13. DOI: 10.1007/978-3-540-76694-0_265
- [82] Mortensen HH, Arlov D, Innings F, Håkansson A. A validation of commonly used CFD methods applied to rotor stator mixers using PIV measurements of fluid velocity and turbulence. *Chemical Engineering Science*. 2018;**177**:340-353. DOI: 10.1016/j.ces.2017.11.037
- [83] Utomo AT, Baker M, Pacek AW. Flow pattern, periodicity and energy dissipation in a batch rotor-stator mixer. *Chemical Engineering Research and Design*. 2008;**86**:1397-1409. DOI: 10.1016/j.cherd.2008.07.012
- [84] Korpijärvi J, Laine E, Ahlstedt H. Using CFD in the study of mixing in coagulation and flocculation. In: Hahn HH, Hoffmann E, Odegaard H, editors. *Chem. Water Wastewater Treat. VI*. Heidelberg: Springer; 2000. pp. 89-99

- [85] Essemiani K, De Traversay C. Optimisation of the flocculation process using computational fluid dynamics. In: Hahn H, Hoffman E, Odegaard H, editors. Chem. Water Wastewater Treat. VII. London: IWA Publishing; 2002. pp. 41-49
- [86] Samaras K, Zouboulis A, Karapantsios T, Kostoglou M. A CFD-based simulation study of a large scale flocculation tank for potable water treatment. Chemical Engineering Journal. 2010;**162**:208-216. DOI: 10.1016/j.cej.2010.05.032
- [87] Bridgeman J, Jefferson B, Parsons S. Assessing Floc strength using CFD to improve organics removal. Chemical Engineering Research and Design. 2008;**86**:941-950. DOI: 10.1016/j.cherd.2008.02.007
- [88] Bridgeman J, Jefferson B, Parsons SA. The Development and Use of CFD Models for Water Treatment Processes. St. Julians: Malta; 2007
- [89] Yang Z, Wu Z, Zeng G, Huang J, Xu H, Feng J, et al. Assessing the effect of flow fields on flocculation of kaolin suspension using microbial flocculant GA1. RSC Advances. 2014;**4**:40464-40473. DOI: 10.1039/C4RA04101A
- [90] Özcan-Taşkın GN, Padron GA, Kubicki D. Comparative performance of in-line rotor-stators for deagglomeration processes. Chemical Engineering Science. 2016;**156**:186-196. DOI: 10.1016/j.ces.2016.09.023
- [91] Kaiser SC, Eibl R, Eibl D. Engineering characteristics of a single-use stirred bioreactor at bench-scale the Mobius CellReady 3L bioreactor as a case study. Engineering in Life Sciences. 2011;**11**:359-368. DOI: 10.1002/elsc.201000171
- [92] He W, Xue L, Gorczyca B, Nan J, Shi Z. Experimental and CFD studies of floc growth dependence on baffle width in square stirred-tank reactors for flocculation. Separation and Purification Technology. 2018;**190**:228-242. DOI: 10.1016/j.seppur.2017.08.063
- [93] Zhang H, Zhang K, Fan S. CFD simulation coupled with population balance equations for aerated stirred bioreactors. Engineering in Life Sciences. 2009;**9**:421-430. DOI: 10.1002/elsc.200800074
- [94] Azargoshasb H, Mousavi SM, Jamialahmadi O, SAS MSB. Experiments and a three-phase computational fluid dynamics (CFD) simulation coupled with population balance equations of a stirred tank bioreactor for high cell density cultivation. Canadian Journal of Chemical Engineering. 2016;**94**:20-32. DOI: 10.1002/cjce.22352
- [95] Zheng H, Huang Z, Liao Z, Wang J, Yang Y, Wang Y. Computational fluid dynamics simulations and experimental validation of macromixing and flow characteristics in low-density polyethylene autoclave reactors. Industrial and Engineering Chemistry Research. 2014;**53**:14865-14875. DOI: 10.1021/ie502551c
- [96] Odeleye AOO, Marsh DTJ, Osborne MD, Lye GJ, Micheletti M. On the fluid dynamics of a laboratory scale single-use stirred bioreactor. Chemical Engineering Science. 2014;**111**:299-312. DOI: 10.1016/j.ces.2014.02.032

- [97] Azargoshasb H, Mousavi S, Amani T, Jafari A, Nosrati M. Three-phase CFD simulation coupled with population balance equations of anaerobic syntrophic acidogenesis and methanogenesis reactions in a continuous stirred bioreactor. *Journal of Industrial and Engineering Chemistry*. 2015;**27**:207-217. DOI: 10.1016/j.jiec.2014.12.037
- [98] Xie L, Liu Q, Luo Z-H. A multiscale CFD-PBM coupled model for the kinetics and liquid-liquid dispersion behavior in a suspension polymerization stirred tank. *Chemical Engineering Research and Design*. 2018;**130**:1-17. DOI: 10.1016/j.cherd.2017.11.045
- [99] Villiger TK, Neunstoecklin B, Karst D, Lucas E, Stettler M, Broly H, et al. Experimental and CFD physical characterization of animal cell bioreactors: From micro- to production scale. *Biochemical Engineering Journal*. 2017. DOI: 10.1016/j.bej.2017.12.004
- [100] Liu Y, Wang Z-J, Xia J, Haringa C, Liu Y, Chu J, et al. Application of Euler-Lagrange CFD for quantitative evaluating the effect of shear force on *Carthamus tinctorius* L. cell in a stirred tank bioreactor. *Biochemical Engineering Journal*. 2016;**114**:209-217. DOI: 10.1016/j.bej.2016.07.006
- [101] Sarkar J, Shekhawat LK, Loomba V, RAS. CFD of mixing of multi-phase flow in a bioreactor using population balance model. *Biotechnology Progress*. 2016;**32**:613-628. DOI: 10.1002/btpr.2242
- [102] Ojaniemi U, Puranen J, Manninen M, Gorshkova E, Louhi-Kultanen M. Hydrodynamics and kinetics in semi-batch stirred tank precipitation of L-glutamic acid based on pH shift with mineral acids. *Chemical Engineering Science*. 2017;**178**:167-172. DOI: 10.1016/j.ces.2017.12.029
- [103] Gao X, Kong B, Vigil RD. Comprehensive computational model for combining fluid hydrodynamics, light transport and biomass growth in a Taylor vortex algal photobioreactor: Lagrangian approach. *Bioresource Technology*. 2017;**224**:523-530. DOI: 10.1016/j.biortech.2016.10.080
- [104] Gao X, Kong B, Ramezani M, Olsen MG, Vigil RD. An adaptive model for gas-liquid mass transfer in a Taylor vortex reactor. *International Journal of Heat and Mass Transfer*. 2015;**91**:433-445. DOI: 10.1016/j.ijheatmasstransfer.2015.07.125

