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# Advances in Computational Fluid Dynamics modeling of anaerobic digestion process for renewable energy production: A review

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## ABSTRACT

Anaerobic digestion is a widely used process for organic waste treatment and biogas production. It is a complex process involving four main biochemical reactions, four microbial groups, and hydrodynamics phenomena. Research focuses on the development of numerical models based on mass transfer and biochemical reaction kinetics, adapted to a specific waste. However, parameters such as mass transfer, fluid rheology, and temperature strongly influence the physicochemical and biological reactions. These parameters are considered in computational fluid dynamic models. In this paper, we present a critical analysis of advances in computational fluid dynamic modeling of anaerobic digesters. This review addresses the work contributions, the technologies of bioreactors as well as the meshing approaches in order to model the mechanical mixing. A detailed analysis is also presented on the evaluation of the effects of waste rheology and total solid content on the flow. Specific studies on biofilm, high anaerobic digesters, multiphase studies, coupling of biochemical and computational fluid dynamic models, turbulence modeling are addressed in this review. In conclusion, computational fluid dynamic models provide a local description of the process and constitute a promising tool to design anaerobic digestion units and optimization the anaerobic digestion process (reduction of dead zone, fluid homogenization, etc.). Thermal modeling is mainly useful in cold countries or those experiencing significant temperature variations. Few studies concern the coupling of biochemical and computational fluid dynamic models, allowing to consider both the bio-physicochemical aspects and the flow field. Future research should focus on microbiological aspects, as well as the full integration of biochemical reactions in computational fluid dynamic models.

## 1. Introduction

The development of renewable and sustainable energies is growing as part of the sustainable development and the growing energy demand (Ourradi et al., 2022). Anaerobic digestion (AD) is a well-known solution to produce biogas from organic waste through five biochemical reactions: hydrolysis, acidogenesis, acetogenesis, homoacetogenesis, and methanogenesis (Di Maria et al., 2019). The biogas is mainly composed of methane and carbon dioxide, as well as traces of other gas such as dihydrogen, ammonia and hydrogen sulfide (Khalil et al., 2019; Sun et al., 2015). This process allows the biogas production from waste while respecting the natural carbon cycle. The main objective of the

process is to guarantee both the quality (high content in methane) and the volume of the biogas produced. AD was mainly employed in order to treat agricultural waste such as manure and green waste, or sewage sludge. Nowadays, many studies are carried out on the treatment of other type of waste including municipal solid waste, characterized by significant heterogeneity and high solids content (Sun et al., 2015; Lebon et al., 2020). The municipal organic waste are composed of cardboard, composite waste (such as milk packaging), putrescible matters, fine elements, household hazardous waste (such as pharmaceutical products), and papers (Lebon et al., 2020). The growth of the population will lead to the increase of municipal organic waste generation (El Gnaoui et al., 2022). Co-digestion (micro-algae, poultry slaughterhouse,

*Abbreviations:* AD, Anaerobic Digestion; ADM1, Anaerobic Digestion Model n°1; CFD, Computational Fluid Dynamics; HRT, Hydraulic Retention Time; KET, Kinetic Energy Transport; KTGF, Kinetic Theory of Granular Flow; LDA, Laser Doppler Anemometry; LES, Large Eddy Simulation; MRF, Multiple Reference Frame; RANS, Reynolds-averaged Navier-Stokes; RNG, Re-Normalization Group; RSM, Reynolds stress model; SGS, Sub grid-scale; SL, Smagorinsky-Lilly; SM, Sliding Mesh; SRT, Solid retention time; T, Temperature (°C); TS, Total Solid (% or g.L<sup>-1</sup>); UASB, Upflow anaerobic sludge blanket digestion; UI, Uniformity Index; WALE, Wall-Adapting Local Eddy-Viscosity.

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sludge, etc.) was also largely studied in order to improve the AD process (increase of the biogas production and the stability of the process) due to the synergistic effects of co-substrates (Solé-Bundó et al., 2019; Elalami et al., 2019; Latifi et al., 2019).

The AD process undergoes in a controlled environment, the anaerobic digesters. The monitoring of the process (measurements of total solid, volatile solid, volatile fatty acids (VFAs), pH, total alkalinity, temperature, biogas composition, feed flow rate, etc.) and the feeding substrate (carbon to nitrogen ratio, VFAs, protein content, etc.) allows to ensure a stable and efficient biogas production (Wu et al., 2019). However, more research is needed in order to reduce the amount of primary energy required for the operation and maintenance of the AD units (Di Maria et al., 2019). Due to the diversity of organic wastes and the growing interest for high-solid digestion, many research efforts have been focused on the development of increasingly complex numerical models. Therefore, numerical models were developed in the aim to understand the existing digesters but also to optimize both the future digester configurations and operating conditions such as mixing, temperature, and hydraulic retention time. The Anaerobic Digestion Model No. 1 (ADM1) for the conversion of biomass into biogas and based on mass transfers was developed by the International Water Association (IWA) task group in 2002 in the aim to harmonize the modeling studies (Batstone et al., 2002). Following this general model, other authors proposed various modified ADM1 (Batstone et al., 2015). Batstone et al. presented a review on the application and future needs concerning the mathematical modeling of AD processes (Batstone et al., 2015). This paper showed an increased demand on mathematical modeling in terms of complexity, and the need to better characterize inputs and their primary conversion processes, as well as supporting models such as the chemistry models. However, an in-depth analysis of the process must be carried out in order to characterize the mixing behavior of anaerobic digesters. The modeling of the mixing behavior is even more important since solid-state digestion is getting importance. Indeed, Zhou and Wen (2019) highlighted that the number of publications with keywords "solid-state AD" has a major increase in interest in this area (Zhou and Wen, 2019). The mixing controls mass and heat transfer through the digester and thus the physicochemical and biological reactions (Lindmark et al., 2014). All these aspects, including the growing need for accurate flow simulations (Van Hulle et al., 2014), justify the development of computational fluid dynamic (CFD) model allowing the study of the fluid flow with greater details and accuracy (Koerich and Rosa, 2016). CFD modeling is based on the fluid mechanics principles. Several transport phenomena, such as multiphase flow, can be analyzed with CFD. Interesting outcomes (dead zone volume, mixing efficiency, effect of solid content, etc.) can be obtained with CFD for AD process, explaining the growing interest for this tool and the recent developments.

The aim of this paper is to provide a comprehensive review on the current advances and future needs of CFD modeling in AD. Indeed, thanks to the advances in numerical calculations, CFD is widely used today on anaerobic digestion applications to optimize and control the process. However, the methods for using CFD as well as the application cases are numerous. In this paper, we present a critical analysis of advances in CFD modeling of anaerobic digesters. The aim of this study is to provide a comprehensive review on the current contributions of CFD in AD modeling; and the lacks and future directions for CFD modeling of AD process.

## 2. Methodology

This review addresses the CFD contributions in AD modeling in order to identify possible developments of these models.

In order to carry out this literature review, we first studied the reviews already published on anaerobic digestion in order to identify the aspects not covered in these works. From these first results, research was carried out on all the parameters related to the development of CFD

models applied to anaerobic digestion. Thus, the first part of our research focused on the contributions of CFD to anaerobic digestion in order to show the contributions of CFD to this field according to the objectives of the studies. The identification of the contributions then allowed us to carry out specific research for each category of contributions in order to clarify the numerical methods implemented, the gaps and the future needs. A detailed analysis is presented on the evaluation of the effects of waste rheology and total content on the flow. Specific studies on biofilm, high anaerobic digesters, multiphase studies, coupling of biochemical and CFD models, turbulence modeling are addressed in this review.

## 3. Contributions of CFD in AD

In this part, we expose the work contributions of CFD modeling studies, carried out from 2005 to 2021. This tool has been widely used for anaerobic digester or stirred tank flow modeling and process optimization. The contributions are manifold. The Fig. 1 shows the proportion and number of works per type of contributions: studies on the effect of rheology and TS content, the turbulent modeling, the bioreactor configuration, the mixing mode and design, the scale-up effect, the settling/suspensions/stratification, the dead zone, the multiphase flow, the coupling of CFD and kinetics models, the high solid digesters, and the biofilm development. Most of the works evaluated the mixing mode or design (75 %), the multiphase study (36 %), and the effect of rheology and total solid (TS) content (27 %), the turbulent modeling (18 %).

The objectives of the CFD simulations are presented in Table 1. The contributions are detailed and analyzed in the following parts.

### 3.1. Technologies of bioreactors, and meshing approaches of mechanical mixing

The mixing mode and design was widely studied, with 64 papers, representing 75 % of the CFD studies (cf. Fig. 1). These investigations are related to the mixing system (mechanical mixing, gas mixing or mechanical pumping) (Wu, 2010c; Dapelo et al., 2015; Meister et al., 2018; Trad et al., 2015; Wu, 2009; Fan et al., 2018), the mixing device (for instance the type of impeller) (Wu, 2011; Wiedemann et al., 2018; Mohammadrezaei et al., 2017; Jahoda et al., 2007; Meister et al., 2018; Zhang et al., 2018; Wu, 2009, 2014; Meroney and Colorado, 2009; Yu et al., 2011; Wu, 2012b; Caillet et al., 2018), the mixing speed in mechanically stirred digesters (Zadghaffari et al., 2009; Cheng et al., 2017; Wu, 2011; Wang et al., 2017; Jian and Zhengming, 2006; Bridgeman, 2012; Wiedemann et al., 2018; Lebranchu et al., 2017; Rasouli et al., 2018; Xie et al., 2019; Trad et al., 2015; Rasool et al., 2017; Xinxin et al., 2018; Zhai et al., 2018; Mishra and Ein-Mozaffari, 2017; Fan et al., 2018; Wu, 2012b; Mohammadrezaei et al., 2018; Wu, 2010d) or liquid/gas velocity inlet of digesters with recirculation mixing (Vesvikar and Al-Dahhan, 2005; Wu, 2010b; Karim et al., 2007; Sajjadi et al., 2016; Leonzio, 2018; Dapelo and Bridgeman, 2018; Wei et al., 2019; Zhang et al., 2018; Fan et al., 2018), and the position of stirring system (Trad et al., 2015; Zhang et al., 2018). The aim of these studies were the optimization of the mixing configuration (dead zone reduction, homogenization, reduction of energy consumption, etc.). In the same context, studies have also been carried out on the bioreactor configurations (Vesvikar and Al-Dahhan, 2005; Karim et al., 2007; Leonzio, 2018; Wu, 2010c; Meister et al., 2018; Rasouli et al., 2018; Meroney and Colorado, 2009; Foukrach et al., 2019; Wu, 2012b, 2010d). The volume of dead zones is a common result obtained from CFD simulations of AD reactors. It characterizes the non-agitated areas within the reactor. Therefore, this parameter allows to compare different mixing strategies and configurations. 10 % of the papers reviewed used the dead volume to analyze the mixing efficiency (cf. Fig. 1).

The Fig. 2 presents the proportion and the numbers of studies for each mixing system between 2005 and 2021. Mechanical mixing was the most commonly studied with 53 papers (62 %). Then, gas mixing and

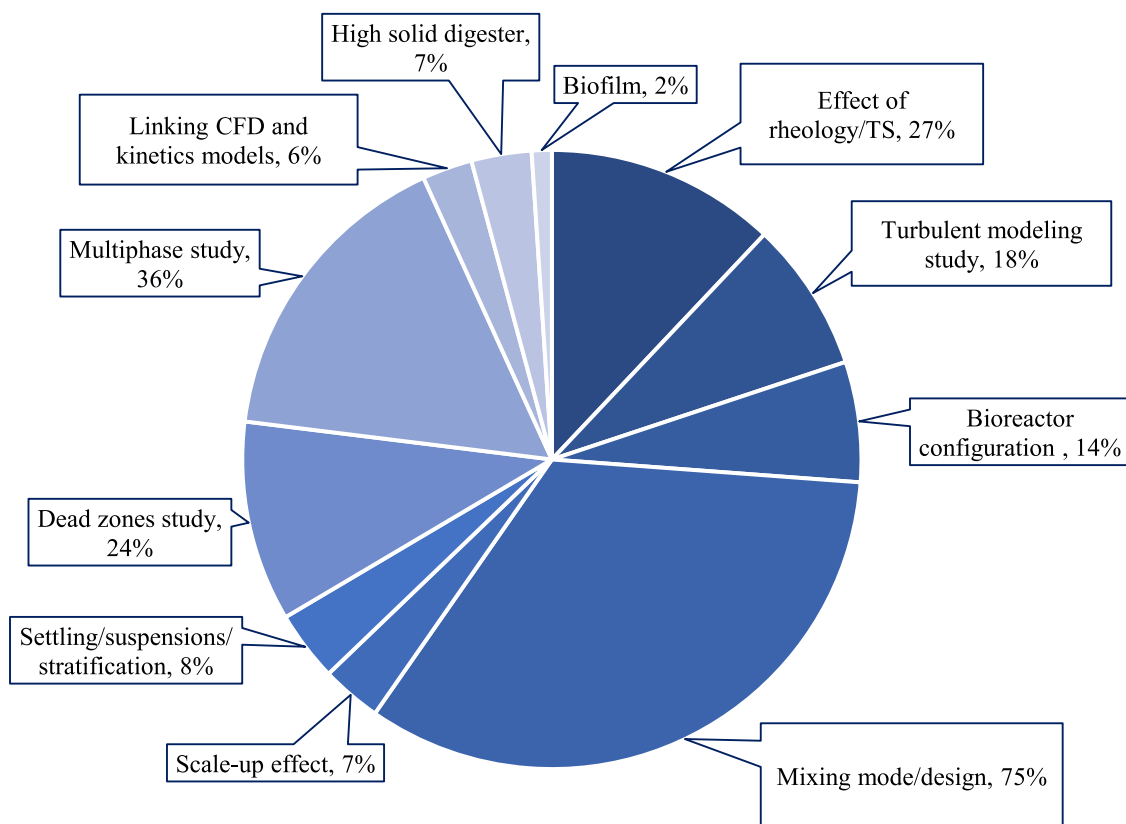


Fig. 1. Contributions of CFD modeling in anaerobic digesters.

mechanical pumping were studied in 16 (19 %) and 16 papers (19 %) respectively.

### 3.1.1. Technologies: geometries and mixing systems

Various digester technologies exist characterized by the mixing mode and the geometry. Technical data concerning mixing mode, reactor type, diameter, mixing speed, flow rate and mixing system are given in Table 2. Caillet et al. detailed a procedure for the analysis of numerical results on the flows of a mechanically stirred reactor (Caillet et al., 2020; Caillet, 2019b). Parameters such as the Reynold number, the mixing energy level, the power consumption, the power and flow numbers, the shear stress, the spatially average characteristic velocity gradient, the circulation time, the dead zone volume, the vorticity, the helicity, the angle between the vorticity vector and the velocity vector, and the Lambda2 field can be evaluated to characterize the flow field and to analysis the turbulence phenomena (Caillet et al., 2020). The uniformity index (UI) allows the prediction of the mixing dynamics (Terashima et al., 2009). The UI is calculated with Eq. 3. The maximum shear stress could be an appropriate parameter in order to determine the appropriate upper agitation of digesters, reducing the loss of productivity (Lebranchu et al., 2017). The shear rate must be evaluated because it impacts the microorganisms involved in the digestion process (Dapelo et al., 2015).

$$V = \sum_{i=1}^m V_i \quad (1)$$

$$C = \frac{\sum_{i=1}^m C_i \cdot V_i}{V} \quad (2)$$

$$UI = \frac{\sum_{i=1}^m \{|C_i - C| \cdot V_i\}}{VC} \quad (3)$$

Where V is the volume of the digester ( $m^3$ ),  $V_i$  is the partial volume for

numerical calculation ( $m^3$ ), C is the average tracer concentration in the digester ( $kg \cdot m^{-3}$ ), and  $C_i$  is the local tracer concentration ( $kg \cdot m^{-3}$ ), UI is the uniformity index.

Various stirring technologies have been tested such as the six-blade Rushton turbine (Zadghaffari et al., 2009, 2010; Jahoda et al., 2007; Ryma et al., 2013; Trad et al., 2015; Foukrach et al., 2019; Alcamo et al., 2005), the Lightnin A310 (Wu, 2012a; Caillet et al., 2020; Yu et al., 2011), and draft tube with different diameters (Wu and Chen, 2007; Vesvikar and Al-Dahhan, 2015; Coughtrie et al., 2013; Terashima et al., 2009). The aim was to determine the most efficient technology, and the appropriate stirring velocity or flow rate to achieve the homogenization of the whole digester. The mixing time in function of the TS content can be evaluated (Terashima et al., 2009). As an example, the study of the mixing speed showed that the increase of the mixing speed improves the solid particles dispersion (Xie et al., 2019). However, high mixing rate can result in a major decrease in methane production (Lebranchu et al., 2017). In addition, CFD simulation allow to propose new shapes of close clearance impellers, based on the analysis of the distribution of flow velocities and the power consumption (Ameur and Kamla, 2021). Other authors studied different types of mixing in order to compare mechanical mixing and gas mixing (Bergamo et al., 2020; Fan et al., 2018).

CFD simulations were carried out for different digesters geometries (cylindrical tanks, egg-shaped digesters, lab-scale digesters, etc.), with diameters varying from 0.10 to 120 m (cf. Table 2). Meroney and Colorado carried CFD simulations on cylindrical anaerobic tanks (diameters of 13.7, 21.3, 30.5 and 33.5 m) in order to evaluate the mixing characteristics (rates of mixing of step, mixture diffusion time, and hydraulic retention time) (Meroney and Colorado, 2009). Washout characteristic was compared in order to numerically identify the presence of partial mixing, dead zone, and short-circuiting or piston flow (Meroney and Colorado, 2009). In a more general way, the adequate mechanical agitation was defined in relation to the homogenization (volume of the dead zone and velocity field) of the digester.

**Table 1**  
Objectives of the CFD simulations.

Sources	Objectives
(Vesvikar and Al-Dahhan, 2005; Zadghaffari et al., 2009; Wu, 2010a; López-Jiménez et al., 2015; Cheng et al., 2017; Conti et al., 2020a; Zarei et al., 2021)	Visualization of flow pattern in anaerobic digestion. Proxy of hydrodynamic parameters, energy efficiency, and study of mixing time.
(Wu, 2010a; Wu and Chen, 2007; Wu, 2011; Vesvikar and Al-Dahhan, 2015; Wang et al., 2017; Yu et al., 2013; Russell et al., 2019)	Study of the scale effect.
(Cheng et al., 2017; Wu and Chen, 2007; Wu, 2011; Vesvikar and Al-Dahhan, 2015; Jian and Zhengming, 2006; Zadghaffari et al., 2010; Bridgeman, 2012; Coughtrie et al., 2013; Madhania et al., 2018; Wiedemann et al., 2018; Wu, 2010b, 2012a; Madhania et al., 2021)	Modeling of the turbulent flow in a stirred tank. Comparison of different turbulent models.
(Zarei et al., 2021; Okiyama et al., 2017; Rezavand et al., 2019; Tobo et al., 2020a, 2020b; Khalil et al., 2021)	Coupling of CFD and kinetics models. Study of the species concentration profiles.
(Wu and Chen, 2007; Karim et al., 2007; Mendoza et al., 2011; Sajjadi et al., 2016; Mohammadrezaei et al., 2017; Lebranchu et al., 2017; Jahoda et al., 2007; Leonzio, 2018; Caillet, 2019a; Bergamo et al., 2020; Caillet et al., 2020; Hu et al., 2021a, 2021b)	Characterization of the mixing, and dead zones and the reduction of the percentage of poorly mixing zone. Study of the liquid homogenization in stirred tank.
(Wu and Chen, 2007; Wang et al., 2017; Bridgeman, 2012; Madhania et al., 2018; Terashima et al., 2009; Wu, 2010c; Craig et al., 2013; Ryma et al., 2013; Dapelo et al., 2015; Meister et al., 2018; Dapelo and Bridgeman, 2018; Rasouli et al., 2018; Xie et al., 2019; Wei et al., 2019; Servati and Hajinezhad, 2020)	Study of the effect of TS content on the rheological properties, the mixing time, the power inputs, the dead zone, and the required impeller torque.
(Wang et al., 2017; Wiedemann et al., 2018; Madhania et al., 2021; Mohammadrezaei et al., 2017, 2017; Lebranchu et al., 2017; Leonzio, 2018; Bergamo et al., 2020; Dapelo et al., 2015; Meister et al., 2018; Dapelo and Bridgeman, 2018; Rasouli et al., 2018; Xie et al., 2019; Zhang et al., 2016a; Dapelo and Bridgeman, 2020; Trad et al., 2015; Rasool et al., 2017; Dabiri and Noorpoor, 2018; Zhang et al., 2018; Xinxin et al., 2018; Zhai et al., 2018; Conti et al., 2019; Ebrahimi et al., 2019; Mao et al., 2019; Zhang et al., 2019; Zhu and Jing, 2019; Foukrach et al., 2020; Aneur and Kamla, 2021; El Ibrahim et al., 2021a; Wu, 2009, 2014; El Ibrahim et al., 2021b)	Study of mixing designs in anaerobic digesters: mode of mixing, type of mixing device, characteristics of mixing (time, period, intensity). Evaluation of the hydrodynamic behavior and performances of the digesters with different mixers. Optimization of the mixing.
(Karim et al., 2007; Leonzio, 2018; Rasouli et al., 2018; Dapelo and Bridgeman, 2020; Meroney and Colorado, 2009; Foukrach et al., 2019; Jegede et al., 2020; Saini et al., 2021; Conti et al., 2020b)	Simulations of different configurations of the bottom of the digester or of the tank. Optimization of the digester geometry.
(Yu et al., 2013; Mendoza et al., 2011; Xie et al., 2019; Zhang et al., 2018, 2017; Brennan, 2001; Mishra and Ein-Mozaffari, 2017; Fan et al., 2018)	Study of the stratification, settling, suspension or granulation in anaerobic digester. Evaluation of the biomass retention physical process.
(Sajjadi et al., 2016; Hu et al., 2021a; Meister et al., 2018; Zhang et al., 2019; Yu et al., 2011; Cui et al., 2021)	CFD study in high solid anaerobic digester.
(Ramírez-Muñoz et al., 2021; Loganath et al., 2020)	Study of the biofilm in anaerobic digesters.

### 3.1.2. Meshing approaches

The modeling of the mechanical mixing by an agitator can be carried out by different methods. In the case of stirred digesters or tanks, two main methods were frequently used: The Moving Reference Frames (MRF) and the Sliding Mesh (SM). In the case of SM, two zones are defined. A mobile zone where the mechanical agitator is located, and a stationary zone. The interface between the zones must be identical for the two regions. Regarding the MRF, we consider a multi-fluid flow, and the rotational velocity is assigned to the moving volume.

Cortada-Garcia et al. did experimental and CFD studies on the power consumption due to mixing of highly viscous shear thinning fluids (Cortada-Garcia et al., 2017). The two main approaches for modeling stirred tanks were the MRF and the SM [178]. The MRF converged fast, but it was only suitable for steady-state flows (Cortada-Garcia et al., 2017). In a stationary frame of reference (stationary relative to the laboratory) the flow in the stirred tank was unsteady. In contrast, SM approach was also suitable for unsteady flows, providing a time dependent solution, but the disadvantages were the significant computational effort and time. In the SM approach, the geometry should have at least two connected non-deforming sections that slide in relation to each other. The SM technique was more accurate, but was much more time consuming than the MRF (Jahoda et al., 2007). Wu also compared the two techniques (Wu, 2010a), the authors preferred the MRF approach in terms of prediction accuracy and computing time.

In conclusion, two meshing approaches exist for the modeling of mixing. Both MRF and SM were used by many authors. The SM approach provided more accurate results but was more time-consuming. Furthermore, the SM approach should be used in case of transient simulations.

The appropriate mesh depends on the requirements of the study, whether extremely precise results or a global description of the flows are required. Studies of different types of mesh have been carried out on mechanical stirred tank: the multiple reference frame, and the sliding mesh. Both the two approaches provide accurate predictions. However, the sliding mesh can be used to model unsteady flows contrary to multiple reference frame, with more accurate results and higher simulation time.

### 3.2. Evaluation of the effects of substrate rheology and TS content

The rheological behavior of the substrate impacts the flows in anaerobic reactors. Rheological models must be implemented in CFD models for each type of waste and the appropriate model depends on the type of waste and the TS content (Caillet and Adelaar, 2023).

The effects of substrate rheology and TS content on the flow pattern were evaluated in 27 % of the papers reviewed (cf. Fig. 1). These works examined the impact of TS and the rheology of the substrate on the hydrodynamics of anaerobic digester, and so on the power input (cf. Table 1). The stagnant zone below the six-blades Rushton turbine as well as the shear rate increased with the viscosity (Ryma et al., 2013). Four viscosity were tested: 1.002, 16, 22 and 3 CPS ( $10^{-3}$  Pa.s). As expected, the mixing is more efficient for lower viscosity because the frictional forces and resistance forces are smaller. Dead zone is observed below the mixing device, and this zone is larger with higher viscosity. It is therefore mandatory to characterize the fluid viscosity in order to design the mixing system. Wu and Chen (2007) investigated the flow field in function of the TS concentration of the liquid manure (2.5 %, 5.4 %, 7.5 %, 9.1 % and 12.1 %), in order to determine the optimal power inputs (0.5–2.0 HP) as well as to reduce the dead and low velocity zones (Wu and Chen, 2007). The liquid manure is a Non-Newtonian fluid and the viscosity range from 0.006 Pa.s (TS=2.5 %) to 0.25 Pa.s (TS=12.1 %). In this paper, the authors classified four velocity zones:

- dead zone: < 0.001 m/s
- low velocity zone: 0.001–0.01 m/s,
- medium velocity zone: 0.01–1 m/s,

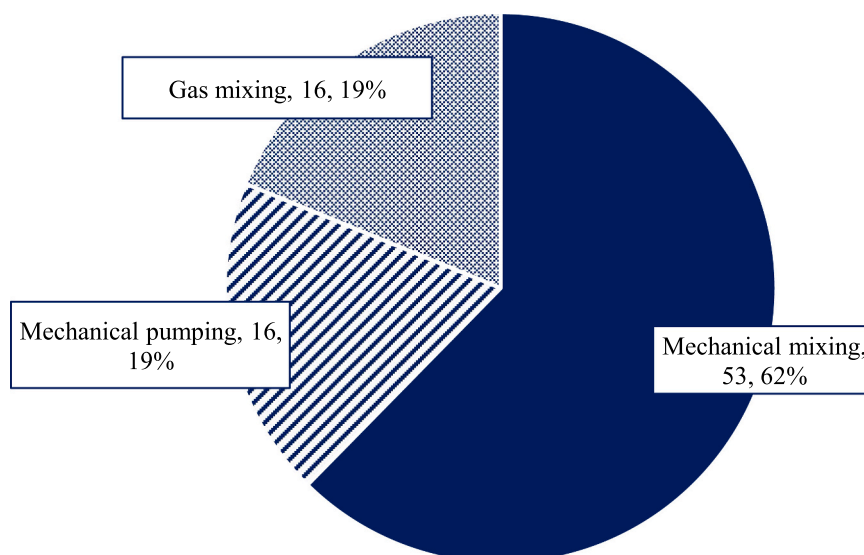


Fig. 2. Proportion and number of studies for each mixing systems Gas mixing, Mechanical pumping, and Mechanical mixing.

- high velocity zone: > 1 m/s.

The low velocity zone did not change in function of TS and the power input. The impact of TS on medium velocity zone was small. The greatest impact is observed for the high velocity zone with a decrease of this volume from 17.0 % (TS=0) to 8.8 % (TS=12.1 %) with a power input of 2 HP and from 28.8 % (TS=0) to 17.7 % (TS=12.1 %) with a power input of 3 HP. These results show this importance of characterize different velocity zones in order to analyze the results. The study of the dead zone is not sufficient to characterize the effect of TS on the flows.

The mixing time increased non-linearly with the TS content increase (Wu, 2010a). However, the dead zone volume cannot be avoided by the increase of the power input (Dapelo et al., 2015). A relation between the sludge concentration (X), the ratio of the homogenization time ( $T_H$ ), and the internal recirculation time ( $T_R$ ) was proposed (Terashima et al., 2009):

$$\frac{T_H}{T_R} = 0.0132X + 0.840 \quad (4)$$

High shear rates, involving significant viscous torque, were observed at the impeller level (Craig et al., 2013). A strategy was proposed in order to improve mixing for different sludge rheology (Dapelo and Bridgeman, 2018). As a result, the shear rate increase leads to the decrease of the viscosity. The flow should be enhanced in the low-viscosity zones and reduced in high-velocity area, leading to inhomogeneous medium. Homogenization in anaerobic process is sought in order to foster the contact between the organic matters and microorganisms (Caillet et al., 2021). It appears that it is preferable to homogenize the viscosity of the medium. CFD is an appropriate tool to provide a local description of the viscosity within anaerobic digesters. In addition, the radial component velocity is more impacted by the viscosity changes than the axial component of velocity (Ryma et al., 2013). The dissolution rate of the solid particles was reduced with the increase of the viscosity (Xie et al., 2019). Madhania et al. carried out CFD simulations of the mixing of miscible liquid (water-molasses) with important viscosity difference in a stirred tank equipped with a side-entry Marine propeller (Madhania et al., 2018). The density variations, the power number and the flow direction were impacted by the numerical approaches (turbulence modeling and meshing approach). LES and RANS approaches were evaluated. RANS approach is based on ensemble averaged governing equations, hence, cannot predict the local unsteadiness in the flow. LES approach which is based on spatially filtered governing equations can capture the large-scale flow structures based on

the filter size. The standard k-epsilon and the realizable k-epsilon turbulent model were studied. Concerning the velocity flow pattern, the direction of the flow was different the simulation with LES with the SM. In addition, the density contour was similar for RANS simulations with standard k-epsilon and realizable k-epsilon turbulence model. However, the density contour was lower with LES (MRF and SM). The density of the mixture was predicted in function of the time (1.5–181.5). The mixture density barely decreased in function of time with RANS approach. However, the mixture density decreased from 1280 to 1270  $\text{kg}\cdot\text{m}^{-3}$  with LES-MRF approach, and from 1280 to 1240  $\text{kg}\cdot\text{m}^{-3}$  with LES-SM approach. These results highlight the importance of the numerical solution as well as the confrontation of simulations and experimental measurements in order to choose the adequate numerical approach.

### 3.3. High solid anaerobic digester study

High solid anaerobic digesters were poorly studied. Only 7 % of the studies identified addressed this topic. As a matter of fact, few rheological data on solid waste (TS greater than 10 %) were published (Caillet and Adelard, 2023). The particularity of solid waste is its non-Newtonian behavior as well as its lower water content (Baroutian et al., 2017; Bhattacharya and Rastogi, 1998; Zhang et al., 2016b). However, the description of mixing conditions in anaerobic digesters dedicated to solid waste treatment is worthy of interest due to the energy costs of the stirring system. Furthermore, the viscosity of the medium is greater, thus the presence of dead zones is more frequent. In dead zones, substrate digestion can be incomplete, reducing the biogas production (Caillet et al., 2020). Yu et al. carried out CFD simulations on high solid anaerobic digester mechanically mixed with the impeller A-310 and the helical ribbon (Yu et al., 2011). Simulations were carried out with the impeller A-310 for 5 % and 10 % of TS. Qualitatively, the digester with 5 % TS was well agitated, and the digester with 10 % was agitated only at the impeller level. The helical ribbon was more appropriate to mix this solid substrate (sludge with TS of 10 % and 20 %). A slight reduction of the velocity intensity was observed with 10 % TS in comparison with 20 % TS. The mixing speed should not be too high (Re greater than 100) because it would induce high shear rate, affecting the bio-structure growth. Impeller A-310 induces low wall shear stress but a large shear rate. Contrariwise, helical ribbon results in large wall shear stress and small shear rate. Therefore, the impeller A-310 is adapted to low viscosity and turbulent flow and the helical ribbon to higher viscosities and laminar flow. Comparing two mixing systems (double-bladed and

**Table 2**  
Mixing system, meshing approach, reactor type, diameter, agitation speeds or flow rate, and mixing technologies.

Sources	Mixing system	Meshing approach	Reactor	Feedstock or fluid	Reactor diameter	Intensity / Inlet velocity / flow rate	Stirring technology
(Vesvikar and Al-Dahhan, 2005)	Gas mixing	-	Mimic anaerobic digester	Dilute slurry (physical properties of water); air	0.2032 m	0.027, 0.048, 0.072 cm/s	Draft tube
(Zadghaffari et al., 2009)	Mechanical mixing	MRF and SM	Fully baffled stirred vessel	Water	0.30 m	225, 300, 400 rpm	Two six-blade Rushton turbines
(Wu, 2010a)	Mechanical mixing	MRF and SM	Full-scale anaerobic digester	Liquid manure	0.147 m	600 rpm	Rushton turbine
(López-Jiménez et al., 2015)	Mechanical pumping	-	Ontinyent Wastewater Treatment Plant anaerobic digester	Sludge	15 m		"HEATMIX": 2 tubes (31 mm internal diameter)
(Cheng et al., 2017)	Mechanical mixing	MRF	Stirred tank	Water, immiscible kerosene oil & air	0.24 m	170, 220, 300, 400, 425, 440, 500, 540 rpm	Rushton turbine (0.08 m diameter)
(Wu and Chen, 2007)	Gas mixing	-	Stirred anaerobic digester	Water & slurry	0.12, 1, 1.26, 1.44, 1.6, 1.72 m	2, 5 m/s	Draft tube
(Wu, 2011)	Mechanical mixing	MRF	Lab-scale and full-scale (model application) anaerobic digester	Liquid manure	0.9 m and 12 m	60, 150, 250, 350, 800 rpm	Pitched blade turbine (Lightnin A310 and PMSL 3LS39)
(Vesvikar and Al-Dahhan, 2015)	Gas mixing	-	Gas-lift loop anaerobic digester (lab-scale & pilot-scale)	Slurry (water density)	6 & 18 in.	2.74 & 4.5 mm/s respectively	Draft tube
(Wang et al., 2017)	Mechanical mixing	MRF	Continuously stirred tank reactor (CSTR)	Mixture of food waste and activated sludge	0.25 m	20, 60, 100, 140 rpm	Six-blade radial Rushton turbines
(Yu et al., 2013)	Gas mixing	-	Lab-scale and pilot-scale anaerobic digester with conical bottom	Wastewater	0.0762 m and 0.117 m	1.24 m/s	Jet agitation
(Jian and Zhengming, 2006)	Mechanical mixing	SM	Stirred tank	Water	0.476 m	150, 180, 260, 300 rpm	3-narrow blade hydrofoil CBY impeller
(Zadghaffari et al., 2010)	Mechanical mixing	MRF and SM	Baffled tank	Water	0.30 m	250 rpm	Six-blade Rushton turbine
(Bridgeman, 2012)	Mechanical mixing	-	Lab-scale cylindrical vessel	Sewage sludge	0.160 m	30, 50, 100, 200 rpm	2 six-blades paddles
(Coughtrie et al., 2013)	Gas mixing	-	Bench-scale anaerobic gas-lift digester	Slurry	0.2032 m		Central draft-tube
(Madhania et al., 2018)	Mechanical mixing	MRF and SM	Stirred tank with conical bottom	Water, molasses (miscible liquids with high viscosity difference)	0.28 m	1000 rpm	Side-entry Marine propeller (0.036 m diameter)
(Wiedemann et al., 2018)	Mechanical mixing	MRF	Cylindrical anaerobic digester	Non-Newtonian fluid	18 m (CFD), 1.5 (experiments)	60, 80 rpm	3 types of mechanical mixers (propeller and paddle)
(Wu, 2010b)	Mechanical pumping	-	Full-scale anaerobic digester	Liquid manure	12, 13.74, 15.12, 16.29, 17.31 m	0.138–0.209 m/s	Pumped circulation
(Wu, 2012a)	Mechanical mixing	MRF and SM	Cylindrical anaerobic digester with conical bottom	Liquid manure	0.152 m	500 rpm (model validation)	Lightnin A310
(Okiyama et al., 2017)	Mechanical pumping	-	Lab-scale up-flow anaerobic packed bed reactor (APBR)	Sugarcane vinasse	0.08 m	4.6 l/day	Pumped circulation
(Karim et al., 2007)	Gas mixing	-	Gas-lift digester	Sewage sludge	0.2032 m	28.32, 56.64, 84.96 l/h (superficial gas velocities: 0.02, 0.05, 0.07 cm/s)	Draft tube (4.4 cm internal diameter)
(Mendoza et al., 2011)	Mechanical pumping	-	Full-scale anaerobic digester	Sewage sludge	30.5 m	-	2 nozzles DINOMIX system (jet)

(continued on next page)

Table 2 (continued)

Sources	Mixing system	Meshing approach	Reactor	Feedstock or fluid	Reactor diameter	Intensity / Inlet velocity / flow rate	Stirring technology
(Sajjadi et al., 2016)	Mechanical pumping	-	Cylindrical tank	Highly viscous xanthan gum solution for simulating municipal wastewater	0.19 m	0.6, 1.3, 2.6 l/min	Jet agitation
(Mohammadrezaei et al., 2017)	Mechanical mixing	MRF	Full-scale anaerobic digester (1200 l)	Cow manure	-	30 rpm	Six-blade turbine, four-blade turbine, six-flat-blade disc turbine
(Lebranchu et al., 2017)	Mechanical mixing	SM	Stirred tank	Cow manure digestate	0.136 m	10, 50, 90 rpm & 22, 66, 110 rpm	Double helical ribbon & six-blade Rushton turbine
(Jahoda et al., 2007)	Mechanical mixing	MRF and SM	Stirred tank	Water	0.29 m	300 rpm	Six-blade 45° pitched blade turbine, standard Rushton turbine
(Leonzio, 2018)	Mechanical pumping	-	Anaerobic continuously stirred digester	Liquid manure	8 m	Inlet velocity: 0.5–1 m/s	External pumps
(Caillet et al., 2020)	Mechanical mixing	MRF	Cylindrical tank with conical bottom	Vinasse	0.152 m	500 rpm (model validation)	Lightnin A310
(Terashima et al., 2009)	Mechanical pumping	-	Egg-shaped anaerobic digester	Sludge	11 m	0.2 m <sup>3</sup> /min	Draft tube mechanical mixer
(Wu, 2010c)	Gas mixing & Mechanical pumping & Mechanical mixing	-	Cylindrical tank with conical bottom	Liquid manure	12 m	7.6 m/s	Draft tube (0.66 m diameter)
(Craig et al., 2013)	Mechanical mixing	MRF	Full-scale anaerobic digester	Sewage sludge	13.5 m	500 rpm	Impeller situated in a centrally-located draft tube (0.61 m diameter)
(Ryma et al., 2013)	Mechanical mixing	MRF	Stirred tank	Addition of variable quantity of CMC (carboxymethylcellulose) in water	0.36 m	250 rpm	six-blade Rushton turbine (0.1243 m diameter)
(Dapelo et al., 2015)	Gas mixing	-	Lab-scale digester	Addition of variable quantity of CMC in water	0.20 m	2.05, 5.30, 8.63 ml/s	-
(Meister et al., 2018)	Mechanical mixing & Mechanical pumping	MRF	Cylindrical & egg-shaped digesters	Slurry	20.10 m	840 rpm	Impeller (helical & 4PBT 45) rotating within a mechanical draft tube.
(Dapelo and Bridgeman, 2018)	Gas mixing	-	Full-scale unconfined anaerobic digester	Sewage sludge	14.63 m	4.717.10 <sup>-3</sup> m <sup>3</sup> /s per nozzle	12 nozzles
(Rasouli et al., 2018)	Mechanical mixing	MRF	Novel prototype radial mixed semi-continuous plug-flow reactor (PFR)	Cow dung	0.73 m	20, 50, 100 rpm	32 blades impeller
(Xie et al., 2019)	Mechanical mixing	-	Stirred tank	PPD (p-phenylenediamine) solution, solid PMDA (pyromellitic dianhydride anhydride)	0.146 m	100, 200, 250, 300 rpm	Stirring paddle
(Wei et al., 2019)	Gas mixing	-	Gas-lift anaerobic digester (7.2 l)	Water and sludge	0.2032 m	28.32, 56.64, 84.96 l/h (superficial gas velocities: 0.02, 0.05, 0.07 cm/s)	Gas injection pipe (0.5 cm diameter) & draft tube (4.4 cm diameter)
(Zhang et al., 2016a)	Mechanical mixing	-	Stirred tank reactor (STR)	Cattle manure & corn stover	0.20 m	80 rpm	Three-layered 45° pitched blade (0.17 m diameter)
(Trad et al., 2015)	Mechanical mixing & Mechanical pumping	MRF	Anaerobic submerged membrane bioreactor	Lignocellulosic waste	0.170 m	100, 150, 200, 400 rpm	Four-blade disk Rushton turbine (56 mm) & three-blade, 45° pitched blade turbine (82 mm)
(Rasool et al., 2017)	Mechanical mixing	MRF	Fully baffled stirred tank	Water	0.30 m	60–135 rpm (step 15 rpm)	three-blade impeller
(Zhang et al., 2018)	Mechanical mixing	-	Spiral symmetry stream anaerobic bioreactor (SSSABR)	Wastewater and sludge granules	0.08 m	Inlet velocity: 2.0 * 10 <sup>-3</sup> m/min	cutting angle set to 30°, 45°, 60°
(Xinxin et al., 2018)	Mechanical mixing	MRF	Full-scale anaerobic digester	10 % TS fluid	16 m	200, 250, 300, 400, 450 500 rpm	Side-entering agitator

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Table 2 (continued)

Sources	Mixing system	Meshing approach	Reactor	Feedstock or fluid	Reactor diameter	Intensity / Inlet velocity / flow rate	Stirring technology
(Zhai et al., 2018)	Mechanical mixing	-	Cylindrical pilot-scale anaerobic digester (1m3)	Dairy manure (14 % TS)	1.2 m	50, 100, 150 rpm	Double disc 45° six pitched-blade turbine impeller (6PBT-45)
(Wu, 2009)	Mechanical mixing & Mechanical pumping	MRF	Full-scale anaerobic digester	Liquid manure	12 m		(1) Mechanical pumping by two propellers in two external draft tubes, (2) mechanical stirring by two side-entry propellers, (3) mechanical pumping by one propeller in an internal draft tube, and (4) mechanical stirring by one top-entry propeller.
(Wu, 2014)	Gas mixing	-	Cylindrical tank	Power-law fluid	10 m	7.6 and 8.0 m/S	Unconfined mixing by 2 bottom diffusers, confined mixing by one draft tube, unconfined mixing by 2 cover mounted lances, confined mixing by 2 bubble guns
(Meroney and Colorado, 2009)	Mechanical pumping	-	Full-scale circular anaerobic digester tank	Water	13.7, 21.3, 30.5, 33.5 m	395 l/min	Single and multiple draft impeller tube mixers (jet mixing)
(Foukrach et al., 2019)	Mechanical mixing	MRF	Cylindrical, polygon (without/with baffles), circular tanks	Water	0.6 m	-	Six-blade Rushton turbine
(Zhang et al., 2017)	Mechanical mixing	MRF	Stirred tank	Distilled water, floating particles and sinking particles	0.20 m	80 rpm	4 two-blade impellers
(Mishra and Ein-Mozaffari, 2017)	Mechanical mixing	SM	Stirred tank (experiment: cylindrical vessel)	Slurry	0.40 m	180–600 rpm	Maxblend impeller (250 mm diame+A42: I42ter)
(Fan et al., 2018)	Mechanical mixing & Gas mixing	SM	Aerobic stirred tank	Water	0.165 m	100, 250, 300 rpm & 450, 925 L/h	Plastic cuboid baffle agitator & diffuser (3 cm diameter)
(Yu et al., 2011)	Mechanical mixing	MRF	Cylindrical anaerobic digester with conical bottom	Liquid manure and waste slurries	0.152 m	500 rpm	A-310 impeller (62 mm diameter) and helical ribbon (120 mm diameter)
(Wu, 2012b)	Mechanical mixing	-	Cylindrical tank and rectangular lagoon	Crude oil and wastewater	40.844, 64.618, 71.932, 86.564, 65, 120 m	400, 416, 425, 420, 440 rpm	6 impellers (3 blades)
(Mohammadrezaei et al., 2018)	Mechanical mixing	MRF	Full-scale anaerobic digester (1200 l)	Cow manure	1 m	0, 40, 80, 120 rpm	45° six-blade turbine (0.3 m diameter)
(Wu, 2010d)	Mechanical pumping	MRF	Egg-shaped and cylindrical shape anaerobic digester	Liquid manure	20.1 m	400, 450, 500, 550, 600, 650, 700, 750 rpm	Draft tube (pumped recirculation)
(Wu, 2012c)	Mechanical pumping	-	Egg-shaped plug-flow anaerobic digester	Cow manure	-	-	-

ribbon impellers) in high-solid anaerobic digester, Cui et al. also concluded that the ribbon impeller was more relevant for high-solid digestion (Cui et al., 2021). Sajjadi et al. (2016) developed a model of the high solid anaerobic digester with jet mixing, experimentally validated, in order to study the cavern structure and the cavern size (Sajjadi et al., 2016). A cavern is a well-mixed zone surrounded and enclosed by a dead zone. The effect of rheological properties was also investigated. The bilaterally symmetrical structure of the cavern depended on rheological properties and the position of the outlet, and showed an effect on the volume fraction of active/inactive zones. Bridgeman carried out CFD modeling of mechanically mixed sewage sludge anaerobic digester, and showed that the increase of the solid content of sewage sludge impact significantly the velocity magnitude and the volume of stagnant zone

(Bridgeman, 2012). The effects of mixing in high solid anaerobic digester (14.3 % solid content) on the dead zone reduction were also evaluated by Hu et al. (Hu et al., 2021a). The radial mixing was impacted by the impeller diameter, the axial mixing by the distance between the impellers, and the rotating speed had a slight effect on the mixing range. The relationship between solids content and the volume of dead zones can be described by a second order polynomial function (Bridgeman, 2012):

$$y = 0.3053x^2 + 0.2469x \quad (5)$$

Meister et al. (2018) modeled a real-life high solids anaerobic digester (2.5 m<sup>3</sup>) mixed by pumped recirculation and helical impeller within a draft tube; with Newtonian and non-Newtonian fluids (Meister

et al., 2018). This study showed that the pumped recirculation did not expand the mixing, but interrupted the symmetry properties of the flow pattern. It was suggested to increase the impeller agitation speed of 1000 rpm for a TS content of 12.1 %. However, such mixing speed leads to high shear rate, and it is not recommended for anaerobic digestion process (Yu et al., 2011). Therefore, it is crucial to carried out experimentations on the anaerobic digestion process in order to confront the mixing performances obtained with CFD simulations and the biogas production reached during experimentations. Zhang et al. (2019) studied different mixing strategies based on CFD simulations and experiments (Zhang et al., 2019). Intermittent mixing of 2 mins/hour was the optimal mixing allowing the homogenization of the reaction mixture. Intermittent mixing is a promising mode of mixing allowing to reduce energy costs and suitable for anaerobic digesters showing good

performances (biogas production) (Zhai et al., 2018; Caillet et al., 2021; Caillet and Adelaar, 2020). CFD is a useful tool for choosing the most suitable agitation system in the case of high solid anaerobic digesters, in order to provide a detailed analysis of the optimum position and type of agitation system. The helical ribbon impeller appears as a good solution for mixing in high solid anaerobic digesters. However, additional works and comparison with experimental studies on the process should be carried out in order to deeply analyze the CFD results and to optimize the biogas production through proper selection and sizing of the agitation system (position, dimension, mixing speed and duration, number, etc.).

**Table 3**  
Multiphase CFD studies.

Sources	Phases	Fluids	Multiphase approach	CFD Software
(Vesvikar and Al-Dahhan, 2005)	Liquid-Gas	Dilute slurry (physical properties of water); air	Eulerian approach for each phase	CFX 5.5
(Cheng et al., 2017)	Liquid-Liquid-Gas	Water, immiscible kerosene oil & air	Eulerian approach for each phase	open source CFD platform OpenFOAM
(Vesvikar and Al-Dahhan, 2015)	Liquid-Gas	Slurry (water density), biogas	Eulerian approach for each phase	CFX 5.7
(Wang et al., 2017)	Liquid-Gas	Mixture of food waste and activated sludge (homogeneous & incompressible, continuous phase), biogas (dispersed phase)	Eulerian approach for each phase	CFX 10.0
(Yu et al., 2013)	Liquid-Gas-Solid	Wastewater, biogas, and solids (dairy manure fiber and biomass particles)	Eulerian approach for each phase	Fluent 6.3.26
(Coughtrie et al., 2013)	Liquid-Gas	Slurry, biogas	Euler-Lagrange	Fluent 13.0sp2 OpenFOAM
(Madhania et al., 2018)	Liquid-Liquid	Water, molasses (miscible liquids with high viscosity difference)	Lagrangian approach (Mixture model multiphase flow)	Fluent 17.1
(Sajjadi et al., 2016)	Liquid-Liquid	Highly viscous xanthan gum solution for simulating municipal wastewater (power-law model, continuous phase), and liquid injected (similar rheological properties of the first phase)	-	Fluent v.13.5
(Hu et al., 2021b)	Gas-Liquid & Gas-Liquid-Solid	Two-phase flow: air and water Three-phase flow: air, water, and polymethyl methacrylate (PMMA) particles	Eulerian approach for each phase	OpenFOAM
(Wu, 2010c)	Liquid-Gas	Liquid manure, biogas	Eulerian approach for each phase	Fluent 12.0
(Ryma et al., 2013)	Liquid-Gas	Addition of variable quantity of CMC (carboxymethylcellulose) in water, biogas	Eulerian approach for each phase	Fluent
(Dapelo et al., 2015)	Liquid-Gas	Addition of variable quantity of CMC in water, biogas	Euler-Lagrange	-
(Dapelo and Bridgeman, 2018)	Liquid-Gas	Wastewater sludge, biogas	Euler-Lagrange	-
(Rasouli et al., 2018)	Liquid-Gas	Cow dung, biogas	Eulerian approach for each phase	Fluent 6.3
(Xie et al., 2019)	Liquid-Solid	PPD solution (liquid phase), solid PMDA (solid phase)	Eulerian approach for each phase	Fluent 15.0
(Wei et al., 2019)	Liquid-Gas	Liquid phase (water, sludge1, sludge2), Gas phase (air)	Euler-Lagrange	Fluent 16.2
(Zhang et al., 2016a)	Liquid-Liquid	Cattle manure & corn stover (incompressible, pseudo-plastic)	-	Fluent 14.0
(Dapelo and Bridgeman, 2020)	Liquid-Gas	Non-Newtonian sludge (Lagrangian continuous phase), biogas (Eulerian dispersed phase)	Euler-Lagrange	-
(Trad et al., 2015)	Liquid-Gas	-	Eulerian approach for each phase	RTD Phoenics (SHAM Ltd.)
(Zhang et al., 2018)	Liquid-Gas-Solid	Wastewater (primary phase), gas and sludge granules (second phase)	Eulerian approach for each phase	Fluent 6.3.26
(Wu, 2014)	Liquid-Gas	Power-law fluid, biogas	Eulerian approach for each phase	Fluent 14.5
(Jegade et al., 2020)	Liquid-Liquid-Gas	Manure 12 % TS, manure 15 % TS, biogas	Eulerian approach for each phase	COMSOL Multiphysics code
(Zhang et al., 2017)	Liquid-Solid-Solid	Distilled water, floating particles & sinking particles	Eulerian approach for each phase	Fluent 14.0
(Mishra and Ein-Mozaffari, 2017)	Liquid-Solid	Slurry (water is used in experiment)	Eulerian approach for each phase	Fluent 15.4
(Fan et al., 2018)	Liquid-Gas	Water, air bubbles	Eulerian approach for each phase	Fluent 15.4
(Chen et al., 2019)	Liquid-Gas	Non-Newtonian fluid (TS > 5 %), biogas	-	Fluent 16.0
(Sarkar et al., 2016)	Liquid-gas	Newtonian fluid, biogas	Eulerian approach for each phase	Fluent 14
(Amirafzabi et al., 2021)	Gas-Liquid	NaCMC (rheological characteristics of digested sludge), and bubble gas	Eulerian approach for each phase	Fluent 19.1

#### 4. Multiphase models

36 % of the CFD studies considered multiphase modeling (cf. Fig. 1), such as for gas mixing digesters (Dapelo et al., 2015; Wu, 2014), or mechanical pumping digesters (Zhang et al., 2016a; Trad et al., 2015). In addition, it was used to model the settling phenomena's (Yu et al., 2013).

Different ways exist in order to model the digestion medium. First, we can consider one liquid phase, regrouping both liquid part and particles, neglecting the biogas. This assumption was largely chosen for the study of mechanical mixing. Second, liquid-solid two-phase flow (Zhang et al., 2017; Mishra and Ein-Mozaffari, 2017) or liquid-gas-solid three-phase flow (Yu et al., 2013) were used to study the settling and suspensions phenomena. Third, two-phase flow can be considered: liquid-liquid or liquid-gas. These approaches were used for the study of mechanical pumping and gas mixing, respectively.

##### 4.1. Numerical approaches

We summarize in Table 3 the multiphase studies with the considered phases, the mixing system, the mathematical model the turbulent model, the fluids, and the multiphase approach. Three multiphase approaches to describe the fluid motion have been used: the Euler-Euler approach (Vesvikar and Al-Dahhan, 2015; Wang et al., 2017; Yu et al., 2013; Wu, 2010c; Rasouli et al., 2018; Xie et al., 2019; Zhang et al., 2018; Wu, 2014; Zhang et al., 2017; Mishra and Ein-Mozaffari, 2017; Fan et al., 2018), the Lagrange-Lagrange approach (Madhania et al., 2018) and the Euler-Lagrange approach (Coughtrie et al., 2013; Dapelo et al., 2015; Dapelo and Bridgeman, 2018; Wei et al., 2019). In an Eulerian approach, each phase is mathematically considered as interpenetrating continua. Each phase volume is defined. The sum of all volume fractions is equal to one. The fluid properties are written in function of space and time. In the Lagrangian approach, the fluid flow is modeled by following the motion and the properties of the individual particles. No study has focused on the comparison between the Eulerian and Lagrangian approaches. The Eulerian approach is computationally less expensive than the Lagrangian method (Vesvikar and Al-Dahhan, 2015). In the case of the Lagrangian approach, calculation times depend on the number of particles considered (Dapelo et al., 2015). Thus, if the number of particles is relatively small, computation times remain reasonable, with a gain in accuracy for the results. The three methods provided accurate results. The Euler-Euler approach was largely used for the multiphase modeling of anaerobic digesters in particular because the calculation times are shorter. Indeed, CFD simulations based on an Eulerian approach provide a global vision of the flows within a reactor and are sufficient for the design of the stirring system. More detailed modeling will only be necessary if we are interested in more precise elements such as the degradation reactions of the material and the movements of the populations of microorganisms within the reactor. The studies carried out are detailed in the Sections 4.2, 4.3 and 4.4, where we detail the approaches as well as the results obtained.

##### 4.2. Two-phase flow in anaerobic digestion CFD modeling

Most multiphase anaerobic digestion models were two-phase flow, involving the fluid flow of a mixture of two distinct phases. Two-phase flow were liquid-gas (Vesvikar and Al-Dahhan, 2005, 2005; Wu, 2010c; Ryma et al., 2013; Dapelo et al., 2015; Wei et al., 2019; Dapelo and Bridgeman, 2020; Fan et al., 2018; Chen et al., 2019), liquid-liquid (Madhania et al., 2018; Sajjadi et al., 2016; Zhang et al., 2016a), or liquid-solid (Xie et al., 2019; Mishra and Ein-Mozaffari, 2017) (cf. Table 3).

Vesvikar and Al-Dahhan performed CFD simulations in order to visualize the flow pattern in a mimic anaerobic digester mixed by gas recirculation (Vesvikar and Al-Dahhan, 2005). The simulations were in good agreement with experimental data (flow pattern, dead zones

location, and velocity profiles trends), but the model should be improved in order to predict the velocity data accurately. Concerning the aspects related to the modeling of the flows of fluids with high viscosity, the Eulerian-Eulerian approach was not adequate due to the presence of a highly concentrated and unrealistic gas phase distribution (Wei et al., 2019). Other work focused on models based on an Euler-Lagrange approach. Coughtrie et al. proposed a multiphase model based on the Euler-Lagrange approach, and compared the simulations results obtained with multiphase and single phase models (Coughtrie et al., 2013). The main differences provided by these two solutions were the inlet velocity profile and the outlet velocity profile with an average velocity at the draft tube outlet for the single-phase model more than twice that of the multiphase model. The multiphase model provided more accurate results. Sarkar et al. successfully predicted the size distribution of bubbles, which impacts mixing and liquid-gas transfer, as a function of process parameters such as the volumetric flow rate (Sarkar et al., 2016). In fact, the interfacial surface area is related to the bubble size. The Multiple Size Group (MUSIG) was used by Fan et al. in order to determine the bubble size distribution, as well as to simulate the bubble coalescence and breakup phenomena in stirred and aerated bioreactors (Fan et al., 2018). Thanks to this model, it was possible to consider the diameters of 18 bubble groups from 0.3096 to 19.200 mm. The flow pattern of the reactor, equipped with a plastic cuboid baffle agitator, was evaluated for different rotational velocities and superficial gas velocities. The increase of the rotational speed had a more significant impact to gas holdup, liquid velocity, shear rate, bubble size distribution than the increase of superficial gas velocity. Wei et al. (2019) proposed a two-phase flow model (liquid and gas) using an Euler-Lagrange approach and underlined that the bubble size, the interactions forces, and the liquid rheology strongly impact the digester hydrodynamics (Wei et al., 2019). The flow pattern was impacted by the bubble size, and therefore experimental measurements of the bubble size were needed in order to improve CFD simulations, and to validate the numerical outcomes (Dapelo and Bridgeman, 2018; Wei et al., 2019). The bubble size increased with the apparent viscosity of the fluid. In addition, the phase interaction forces is an important parameter to be determined because it strongly impacts the distribution of the gas phase, and the liquid flow. Three dimensional CFD simulations of the mixing in mechanically stirred tank of two miscible liquids with different viscosities were performed (Madhania et al., 2018). For this purpose, a liquid-liquid multiphase model was developed. The main results were the density contours in function of the mixing time for different solution strategies (turbulence model and meshing approach). Sajjadi et al. also considered the liquid-liquid two-phase flow in order to study the mixing performance of an anaerobic digester mixed with recirculating jets (Sajjadi et al., 2016). The first phase was municipal wastewater and the second phase was the liquid injected with similar rheological properties as the first phase. These simulations allowed to analyze the caverns (formation, growth, structure, and volume) the influence of the fluid rheology and the specific power input. The outcomes were in good agreements with experimental data, expected at the flow regimes transition points. The liquid-solid two-phase flow CFD model developed by Mishra and Ein-Mozaffari (2017) provided an accurate description of the particle distribution (concentration profiles) in the stirred tank equipped with the Maxblend impeller (Mishra and Ein-Mozaffari, 2017). The applications of this model are manifold, such as the study of the impact of mixing speed and the particle characteristics (concentration, diameter, specific gravity) on the mixing performances. In this work, the solid particles were uniformly suspended at the impeller speed of 360 rpm, while at lower speeds, the particles accumulated in the lower phase.

A number of studies have been carried out on two-phase reactor modeling, in order to better understand and describe flows. The results obtained are more accurate than those obtained by modeling flows as a single phase. The choice of two phases is multiple. We can consider two liquid phases if the two liquids are immiscible, which are then considered as two distinct phases. The two phases can be liquid and gaseous.

This strategy enables the study of reactors stirred by gas recirculation and, in particular, the optimization of this stirring mode. It also allows the biogas produced to be taken into account and integrated into the model. The latter may have an impact on flows. At a later stage, in the case of coupling a CFD model with a material degradation model, we could integrate the biogas produced into the CFD modeling. Finally, the two phases can be liquid and solid. This configuration offers the possibility of considering solid particles within the reactor. Indeed, one of the challenges is to re-suspend solid particles in order to promote contact between micro-organisms and biodegradable materials. In addition, the concentration of solid particles in one part of the digester favors the creation of dead zones, which we aim to avoid in these processes. In the future, liquid-solid modeling could also be used to study the development of biofilms on solid particles and their movement within the reactor.

#### 4.3. Three-phase flow in anaerobic digestion CFD modeling

Three-phase flow are liquid-gas-solid (Yu et al., 2013; Hu et al., 2021b; Zhang et al., 2018), liquid-liquid-solid (Zhang et al., 2017), and liquid-liquid-gas (Cheng et al., 2017; Jegede et al., 2020). Three-phase flow was poorly used for anaerobic digester modeling.

Yu et al. (2013) (Yu et al., 2013) and Zhang et al. (2017) (Zhang et al., 2017) studied the settling and suspensions phenomena, which are detailed in the next section. Two and three-phase CFD simulations of slurry polymerization and fuel production were carried out (Hu et al., 2021b). The simulation outcomes were validated with experimental data in literature (Hu et al., 2021b; Ford et al., 2008; Shewale and Pandit, 2006). However, the Hu et al. underlined that no experimental data were available in literature on the gas-liquid-solid system despite its interest (Hu et al., 2021b). Concerning the bubble gas diameter, the simulations (at 700 rpm) were in good agreements with experiments for 0.5 mm bubble diameter at the impeller region, and 1.5 and 2.5 mm outside of this region. These observations signified that the bubble size distribution was non uniform within the reactor, due to the bubbles break-up at the impeller region. The impact of the addition of the solid phase was analyzed. The addition of solid particles strongly modified the water flow pattern, in particular the disappearance of the radial-pumping flow pattern replaced by an upward circulation at the impeller level. Chen et al. studied the mixing throughout a flat-bottomed stirred tank equipped with the Rushton turbine using an Eulerian approach (Cheng et al., 2017). A liquid-liquid-gas three-phase flow was considered, with water, immiscible kerosene oil and air. The simulations were validated with experimental data. As this study only focused on flow analysis, the numerical approach is transposable to an anaerobic digestion case.

Liquid-liquid-gas Chinese dome digester was modeled using three-phase CFD (Jegede et al., 2020). The considered phases were two liquid phases (manure at 12 % TS and manure at 15 % TS), and the biogas. The traditional Chinese dome digester is mixed by the feeding and the flow back of the slurry into the reactor when the biogas stored in the headspace is used. The aim was the optimization of mixing of a modified Chinese dome digester including two baffles at the top and bottom. The velocity field and the recirculation rate were compared for the two configurations. The hydraulic characteristics were improved in the second configuration.

Few numerical studies have considered three phases, whereas in the case of anaerobic reactors, we often find three or more phases:

- In the case of a liquid (TS < 10 %) or solid (TS > 10 %) reactor, there are liquid phase, solid particles and biogas. The solid and liquid fractions will differ according to the TS.
- In the case of co-digestion reactors (liquid or solid), each substrate could constitute a phase, plus biogas. CFD can be used to analyze the homogeneity of the reaction medium. Studies in the literature have focused on reactors with two substrates with different TS. Nowadays,

the rise of co-digestion which improves biogas yields (e.g. food waste and garden waste) (Lebon et al., 2019; Adeldard et al., 2015), makes it necessary to model several phases in order to describe flows accurately.

- Stratification of the digestion medium is also common, especially in poorly stirred reactors (Caillet et al., 2021). In this case, several phases will also have to be considered in order to accurately model the process.

However, to reduce calculation time, it's worth simplifying the model, and therefore the number of phases considered. There must therefore be an interest in modeling three phases. Considering three phases enables to achieve more accurate results and to better describe and understand reactor flows.

#### 4.4. Study of the settling, the suspensions, and the stratification phenomena in bioreactors

One of the interests of multiphase models is the study of the settling, the suspensions, and the stratification phenomena within stirred tanks. Yu et al. developed a multiphase (liquid gas and solid) three-dimensional CFD for describing the settling and suspension in anaerobic digester and evaluating the biomass retention physical process (Yu et al., 2013). The multi-fluid model developed use Kinetic Theory of Granular Flow (KTGF), which is a recognized approach for studying particle flow. The laminar flow was used for the settling process modeling while the turbulent was used for the suspension process modeling. The mechanism of a high rate digester was described by separating the solid retention time (SRT) from HRT to retain more microorganisms in the anaerobic digester. The determination of the optimum SRT was allowed thanks to biomass retention evaluation. Ramin et al. (2014) developed a settling velocity model to describe secondary sedimentation (Ramin et al., 2014). Mendoza et al. carried out a CFD study on the flow inside a digester in order to study the dead zones, and the stratifications in the digester (Mendoza et al., 2011). As an assumption, the particles with a velocity lower than  $0.001 \text{ m.s}^{-1}$  will sediment. Zhang et al. evaluated the effect of the diameter and width of the impeller on sinking and suspensions, using CFD and a Eulerian-Eulerian multiphase model, in order to optimize the impeller geometry (Zhang et al., 2017). This study provided a description of the solid distribution and the axial velocity vector, however the effect of these two parameters on the AD process was not investigated. A similar work on an anaerobic digester equipped with the Maxblend impeller was done, and the optimal mixing speed in relation with the operating conditions (homogeneity and mixing index) was determined (Mishra and Ein-Mozaffari, 2017). The influence of the specific gravity and the size of solid particles on the slurry reactor homogeneity was highlighted. CFD simulations have also been carried out on a stirred aerobic digestion in order to model the aerobic sludge granulation in function of rotation speeds and superficial gas velocities (Fan et al., 2018). The flow pattern with the vortices formation, the liquid velocity, the bubble size distribution, and the shear rate were investigated. Although this study was conducted on an aerobic digester, it presents an interesting approach for the modeling of granulation. Moving away from studies conducted strictly for application to anaerobic digestion, Xie et al. focused on the development of a CFD model in order to simulate the distribution of the solid particles considering the polymerization reaction and interface mass transfer in polymerization-stirred tank reactor with high viscosity (Xie et al., 2019). Major results were that the mass transfer flux was inversely proportionality to the particle size square, and the increase of the dissolution rate of the solid particles with the decrease in particle size. It would be interesting to conduct similar work on anaerobic digesters to evaluate the relationship between hydrodynamics and biochemical reactions.

## 5. Turbulence modeling

The turbulent modeling study is worth of interest. In fact, turbulent flow generally appears with stirring. Hence, 18 % of CFD studies for anaerobic digester modeling focused on the turbulent model evaluation.

Turbulence can be modeled by three different methods:

- Direct Numerical Simulation (DNS): this method is the most expensive in terms of calculations. Indeed, all scales of turbulence are calculated. The results are thus extremely precise and the mesh must be very fine;
- Large Eddy Simulation (LES): this method remains expensive in calculation time even if a part of the turbulence scales is not calculated (turbulence scales smaller than the smallest mesh size of the mesh). Uncalculated scales are modeled. The results obtained are precise but the necessary mesh size remains large;
- Reynolds Averaged Navier-Stokes (RANS): it is the least expensive method in calculation and allows the use of a less fine mesh. Indeed, the turbulence is mathematically modeled. In this case, we are interested in average quantities. For this purpose, the ensemble-average operator is applied to the instantaneous equations by carrying out the Reynolds decomposition on the unknowns of the problem. RANS methods are less precise than DNS and LES methods. However, these methods have the advantage of computing complex configurations with large Reynolds numbers (Coughtrie et al., 2013).

The turbulence model studied in the literature, and the respective sources are presented in the Table 4. In general, the main RANS and LES turbulence models studied in the literature were:

- RANS models: Standard k-epsilon, Realizable k-epsilon, Re-Normalization-Group (RNG) k-epsilon, Reynolds Stress Model (RSM), Standard k-omega, SST k-omega;
- LES models: Smagorinsky-Lilly, Smagorinsky-Van Driest, Wall-Adapting Local Eddy-Viscosity (WALE), Kinetic Energy Transport (KET).

The works using RANS approaches, and LES approaches are presented in the following parts.

### 5.1. RANS approach

RANS approach was widely used by many authors for turbulent flow modeling. In fact, this approach requires less fine meshes, and is therefore less time-consuming. In the case of the settling and suspension model, the standard k-epsilon turbulence model was used for modeling the suspension process (Yu et al., 2013). Just as the previous model, the CFD models (López-Jiménez et al., 2015; Wu and Chen, 2007) employed the standard k-epsilon turbulence model. Indeed, this turbulence model has been successfully used by many researches for similar problems as we can see in Table 4 (López-Jiménez et al., 2015). The k-epsilon model was also used for the liquid phase modeling of the mimic anaerobic digester (Vesvikar and Al-Dahhan, 2005). The realizable k-epsilon model was used for mixing simulations in anaerobic digesters realized by Wu, Wu and Zhai et al. (Zhai et al., 2018; Wu, 2009, 2010d). The model developed by Yu et al., which concerned the high solid anaerobic digesters, considered laminar flow, assuming that the turbulent flow was suppressed by high viscosity (Yu et al., 2011). The standard k-epsilon model was used when the Reynolds number was upper to 1000, the low-Re-k-epsilon model was used when the Reynolds number was comprised between 10 and 1000, and the laminar model was used when the Reynolds number was inferior to 10. The RNG k-epsilon turbulence model was used in many studies as specified in Table 4. It was appropriate for studying the sinking and floating behavior of suspending particles (Zhang et al., 2017). To achieve this objective, this model includes the effect of swirl on turbulence (Mao et al., 2019). Wu conducted a study on turbulence models. The studied turbulent models were the standard k-epsilon model, the RNG k-epsilon model, the realizable

k-epsilon model, the standard k-omega model, the SST k-omega model and the RSM. It was found that the realizable k-epsilon model and the standard k-omega model were the most appropriate models through comparing power and flow numbers (Wu, 2011). Craig et al. used the SST k-omega turbulence model for the turbulent closure (Craig et al., 2013), supported by previous authors experiences and recommendations (Wu, 2010b; Craig et al., 2013; Bakker et al., 2009). The results from the RSM and SST k-omega turbulence model were compared (Craig et al., 2013). In conclusion, the outcomes were adequately closed to justify the use of the cheaper SST k-omega turbulence model. In addition, the turbulent flow of the CFD model developed by Wu (Wu, 2014) was also modeled by the SST k-omega model, as proposed in a previous work (Wu, 2010c).

Coughtrie et al. (2013) tested four RANS turbulence models (RNG k-epsilon, k-omega SST, Linear RSM, and SST Transition) for a gas-lift loop reactor modeling (Coughtrie et al., 2013). They concluded that the turbulence model had an impact on the flow predictions. Moreover, the SST transition turbulence model provided the most accurate predictions for velocity, separation and reattachment, and overall flow-field, whereas the k-omega SST and RSM provided the most accurate results with inaccuracies with velocity and separation and reattachment predictions. A study was carried out by Koerich and Rosa (2016) to compare different models of turbulence (Spalart-Allmaras, transition SST k-omega, k-epsilon, realizable k-epsilon, and RSM) for low Reynolds flow (Koerich and Rosa, 2016). The isotropic models could underestimate the turbulence phenomenon, and the RSM model provided the most accurate predictions. In their review, Karpinska and Bridgeman presented a comparison between the standard k-epsilon model, the RNG, the realizable k-epsilon model, the standard k-omega model, the SST k-omega model and the RSM (Karpinska and Bridgeman, 2016). The standard k-epsilon model was more stable than RNG model. The different turbulence models were adapted to different case studies. For instance, the realizable k-epsilon model was suitable for planar and rounded jet. Moreover, the SST k-omega model was less efficient for free shear flows. The RSM provided accurate results but was computationally expensive. They concluded that RANS/URANS closed by the standard k-epsilon model was the most computationally efficient scenario for the modeling of activated sludge tanks.

### 5.2. LES approach

Different authors explored the LES approach to compare the two approaches, and to improve the accuracy of the simulations. Works have been carried out to compare LES and RANS approaches in different case studies. The recommended turbulent model in literature are presented in the Table 4.

Hartmann et al. carried out LES and RANS simulations on the flow in a baffled mixed reactor (Hartmann et al., 2004). Smagorinsky and Voke (modified Smagorinsky) sub grid-scale (SGS) models in LES simulations, and numerical Lattice-Boltzmann scheme for Navier-Stokes equation discretization were used. Both models provided an accurate representation of the flow field compared to experimental data. It was concluded from the comparison of simulations and experiments that LES provided better results than RANS in terms of the structure and levels of the turbulent kinetic energy in the impeller discharge flow. The upward directed radial impeller outflow was properly described by the LES model but not found with the RANS model. Thereby, LES provided more accurate results than RANS simulations. Jian and Zhengming performed LES simulations with Smagorinsky-Lilly SGS model of mixing process in a stirred tank (Jian and Zhengming, 2006). Better results were obtained (power demand and mixing time) with this approach than with RANS approach (with the standard k-epsilon model) compared with experimental predictions. Moreover LES was a good tool to investigate the unsteady and quasi-periodic behavior of the turbulent flow in stirred tanks. Jahoda et al. compared RANS with standard k-epsilon model (with MRF and SM techniques), and LES with Smagorinsky-Lilly (SL)

**Table 4**  
Turbulence modeling approaches of 3D CFD models.

Sources	Mathematical model	Turbulence model	Recommended turbulent model
(Vesvikar and Al-Dahhan, 2005; López-Jiménez et al., 2015; Wu and Chen, 2007; Wang et al., 2017; Mendoza et al., 2011; Sajjadi et al., 2016; Mohammadrezaei et al., 2017; Leonzio, 2018; Caillet et al., 2020; Ryma et al., 2013; Xie et al., 2019; Zhang et al., 2016a; Meroney and Colorado, 2009; Foukrach et al., 2019; Mishra and Ein-Mozaffari, 2017; Fan et al., 2018; Mohammadrezaei et al., 2018; Zhang et al., 2016a; Sajjadi et al., 2016; Wang et al., 2017; Mohammadrezaei et al., 2017)	RANS	Standard k-epsilon	-
(Vesvikar and Al-Dahhan, 2005, 2015)	RANS	Zero-equation model (gas phase)	-
(Zadghaffari et al., 2009, 2010)	LES	Smagorinsky-Lilly	-
(Wu, 2010a)	RANS	Standard k-epsilon RNG k-epsilon Realizable k-epsilon RSM	Realizable k-epsilon
(Cheng et al., 2017)	RANS	Standard k-epsilon model RSM	RSM
(Jian and Zhengming, 2006)	RANS & LES	Standard k-epsilon Smagorinsky-Lilly	LES Smagorinsky-Lilly
(Wu, 2011)	RANS	Standard k-epsilon RNG k-epsilon Realizable k-epsilon Standard k-omega SST k-omega RSM	Realizable k-epsilon and Standard k-omega
(Bridgeman, 2012)	RANS	Standard k-epsilon Realizable k-epsilon RNG k-epsilon Standard k-omega RSM	RSM (MRF)
(Coughtrie et al., 2013)	RANS	SST k-omega RNG k-epsilon Linear RSM Transition-SST	Transition-SST
(Vesvikar and Al-Dahhan, 2015; Wiedemann et al., 2018)	RANS	Standard k-epsilon Standard k-omega	-
(Madhania et al., 2018)	RANS & LES	Standard k-epsilon Realizable k-epsilon Smagorinsky-Lilly	LES Smagorinsky-Lilly
(Wu, 2010b, 2010c)	RANS	Three high-Reynolds-number k-epsilon Six low-Reynolds-number k-epsilon Two k-omega RSM	Chang-Hsieh-Chen low-Reynolds-number k-epsilon and standard k-omega (Wu, 2010b) 3 low-Reynolds-number k-epsilon (Abid, Abekondoh-Nagano, Chang-Hsieh-Chen) for TS = 2.5 % (Wu, 2010c) Chang-Hsieh-Chen for TS = 5.4 % (Wu, 2010c)
(Wu, 2012a)	LES & RANS	Smagorinsky-Lilly Wall-Adapting Local Eddy-Viscosity (WALE) Kinetic Energy Transport (KET) 6 RANS turbulence models	LES KET
(Yu et al., 2013; Lebranchu et al., 2017; Terashima et al., 2009)	Laminar flow model	Laminar	-
(Jahoda et al., 2007)	RANS & LES	Standard k-epsilon Smagorinsky-Lilly	LES Smagorinsky-Lilly
(Craig et al., 2013; Wu, 2014)	RANS	SST k-omega	-
(Dapelo et al., 2015)	RANS	Reynolds stress model (RSM)	-
(Meister et al., 2018)	RANS	Realizable k-epsilon Standard k-omega	Realizable k-epsilon
(Rasouli et al., 2018; Wei et al., 2019; Rasool et al., 2017; Zhang et al., 2018; Xinxin et al., 2018; Zhang et al., 2017)	RANS	RNG k-epsilon	-
(Trad et al., 2015)	RANS	Standard k-epsilon RNG k-epsilon Chen-Kim k-epsilon	Chen-Kim k-epsilon
(Zhai et al., 2018; Wu, 2009, 2012b, 2010d)	RANS	Realizable k-epsilon	-
(Yu et al., 2011)	RANS	Standard k-epsilon (Re>1000) Low-Reynolds-k-epsilon (10 <Re<1000) Laminar (Re<10)	-
(Alcamo et al., 2005)	LES	Smagorinsky-Van Driest	-

SGS model (with SM technique) approaches (Jahoda et al., 2007). LES was the most time-consuming method but the results on flow patterns and liquid homogenization were closer to reality. By comparing results from LES and RANS simulations and experimentations, the predictions can be substantially improved with LES (Zadghaffari et al., 2010). Three turbulent models were compared in CFD simulations: Standard k-epsilon, Realizable k-epsilon and Smagorinsky-Lilly (Madhania et al., 2018). The simulation results were compared with experimental data from a previous study conducted by Wu and Patterson (Wu and Patterson, 1989). The experimental data allowed to compare the mixing time in function of the impeller revolution, the radial profile of turbulent kinetic energy dissipation rate at impeller center line, the power number, and the velocity in impeller stream of Rushton turbine. The LES approach with the Smagorinsky-Lilly SGS model was recommended. In other study, the free SGS models investigated were SL model, WALE model and KET model (Wu, 2012a). The three models gave very similar results for flow fields. The comparison between simulated and measured axial velocities showed that the LES shapes were in general agreement with the experimental data but they differed clearly in velocity magnitudes. Concerning the impeller power and flow numbers, the SGS models and the KET model provided the accurate results. The author also compared the results with six RANS turbulence models (realizable k-epsilon model with SM, standard k-omega model with SM, Reynolds stress model with SM, realizable k-epsilon model with MRF, standard k-omega model with MRF, Reynolds stress model with MRF).

The turbulence modeling is a key parameter in CFD modeling. It has been shown that LES models provide the more accurate outcomes with higher computation time than RANS models. The literature review showed that more studies have been carried out with RANS approaches than with LES approaches. This is explained by the fact that the computational time are faster with CFD simulations using RANS models than LES models. Nevertheless, LES models provide more accurate outcomes. In conclusion, the choice of the approach must be done according to the expected accuracy of the results and the computation time. Various RANS turbulence models have been studied. The standard k-epsilon model and the realizable k-epsilon model are used by many authors, both the models provide accurate results. Moreover, the SST k-omega model is also recommended by other authors. The RSM provides the more accurate results but with the more computation-time. Therefore, the choice of the turbulence model must be done according to the aim of the study, the expected accuracy of the results, and the computation-time.

## 6. Modeling of heat transfer

AD proceeds at a precise optimal temperature, therefore some models were developed in the aim of providing the temperature profiles in digesters. These models allowed several thermal optimization such as the configuration, the energy performance (El Ibrahim et al., 2021a, 2021b), and the process optimization (Kegl and Kovač Kralj, 2020).

Different models were useful in cold climates where the temperature difference between the internal and external environment is significant. Indeed, it is in this context that the losses can be important and need to be reduced. The mathematical model developed by Gebremedhin et al. (2004) described the heat exchange between the anaerobic digester and the environment during the year [250]. Perrigault et al. aimed to optimize tubular digester in cold climates with the development of a one-dimensional and time-dependent heat transfer model (Perrigault et al., 2012). In this model, Radiative, convective, and conductive heat transfer phenomena were considered. The model was validated with experimental data, with a standard error of 2 %. Merlin et al. developed a steady-state heat transfer model in order to predict the biogas production taking into account the ambient air and the temperatures variations of the content in a continental climate context (Merlin et al., 2012). The uncertainty of the model predictions compared to experimental measurements was about 10 %. The heat transfer should be

considered at the conception phase, especially in the case of unheated digesters, which are more sensitive to external temperature conditions. Terradas-III et al. developed a thermal one-dimensional model adapted to unheated, buried and fixed-dome digester in order to predict the biogas production considering the impact the heat transfer (Terradas-III et al., 2014). This model could be used for assessing the methane production and for improving the digesters during cold period. Hreiz et al. developed a zero-dimensional transient thermal model is proposed for predicting temperature variations in semi-buried anaerobic digesters as a function of climatic conditions (ambient temperature, rain level, and solar irradiation) (Hreiz et al., 2017). This model provided the identification of phenomena leading to major energy losses from the reactor, and thus proposed technical solutions in order to reduce these heat losses. This model can therefore be used as a decision-making tool during the design phase (choice of materials, dimensions, etc.). Furthermore, it may be coupled with the ADM1 for predicting biogas production as a function of environmental conditions. The outcomes revealed that the required heat to warm the inputs and radiations to the cover constitute the major heat losses, each one accounting for about 30 % of the total thermal energy lost by the digestate. Besides, heat transfer to the ground and to the biogas constitute each one for about 15 % of the heat lost by the digestate.

Other works aimed to model the heat transfers within the reactor in order to predict the exact temperature of the digestion process, since this parameter has a considerable impact on the digestion kinetics. Gomez et al. developed a two-phase (liquid-gas) mathematical model of auto-thermal thermophilic aerobic digesters (Gomez et al., 2007). Wu carried out numerical simulations of heat transfer and biochemical reaction kinetics within anaerobic stirred tank (Wu, 2012c). The main hurdle for coupling these phenomena is to solve the physical-biological interactions concurrently using the small-time interval required for the mixing and heat transfer. The approach consisted in the development of a two-stage simulation strategy that predicts the temporal biological process using a large time step based on steady fluid flow and heat transfer, where a computational cell was physically treated as an individual bioreactor with its own residence time and temperature. In conclusion, the temperature was the most important physical condition for bacterial growth, residence time determined the duration of digestion by anaerobes, and pH regulated the microbiological process.

Thermal models have been developed essentially in the case of cold climates. Indeed, as the temperature affects the digestion process, variations of process temperature are avoided. The simulations have shown that the environmental conditions affect the process temperature, especially during winter period. The authors agree on the hypothesis that thermal transfers due to chemical reactions are negligible. Moreover, some thermal models are coupled with biochemical models or CFD models. Thermal models can be used to optimize digesters.

## 7. Integration of biological reactions in CFD models and biofilm studies

### 7.1. Biofilm studies

Recent studies have been carried out on biofilms. Ramírez-Muñoz et al. focused on the development of the biofilm in an anaerobic inverse fluidized bed reactor (Ramírez-Muñoz et al., 2021). The numerical results were compared with experimental data in order to validate the 2D and 3D simulation outcomes. CFD allowed to evaluate the final porosity of the bed in relation to the bed expansion in function of the inlet liquid velocities and initial bed heights. The bed porosity is an important factor because it is linked to the organic matter residence time, and thus to the pumping cost (Diez Blanco et al., 1995). The results and experimental data were closed for lower velocities but showed discrepancies for higher velocities. With low inlet velocities, the excessive biofilm growth could affect the operation and the control of the digester. The hydrodynamic parameters (flow patterns, solid bed profiles, shear stress,

effect of biofilm growth on the porosity of the bed, and bed porosity) were evaluated. It was shown that the solid particles are uniformly distributed in the bed, and recirculation zones were observed this position, implying high shear stress. The consequence could be the detachment of the biofilm from the support. Another study dealt with the biofilm selection for a Hybrid Up-Flow Anaerobic Sludge Blanket (HUASB) digester (Loganath et al., 2020). The aim of this paper was to bring solution to clogging in the biofilm using CFD. Experimentations were carried out at laboratory scale with a working volume of 4.2 L. The hydrodynamic movement of the fluid before and after feeding was shown. CFD simulations could allow to choose or design biofilms for anaerobic digesters.

## 7.2. Integration of biological reactions in CFD models

CFD models describing the flows in a stirred reactor are nowadays well mastered. Indeed, various numerical variants have been studied: mathematical models, turbulence models, meshes, dimensions, types of fluids, multiphase models, etc. However, the integration of kinetic models is still very much under study. The advancement of knowledge but also the technological advances in particular in numerical computation allow the development of increasingly complex models and requiring more and more important computing capacities. In this context, models coupling CFD and biophysical-chemical reactions are gradually being developed. The objective is to study the impact of flows on chemical reactions and thus the degradation of organic matter and the production of biogas. Wu et al. developed a three-dimensional model for the prediction of the biogas production of liquid manure (Wu et al., 2006). The authors neglected the momentum and turbulence, considering very low flow rate. The model was based on the mass conservation equation, the energy equation, the species transport equations, and the chemical reaction equations. The simulations results were validated with experimental data. Tobo et al. aimed to understand the impact of advection-diffusion transport on the homogenization (Tobo et al., 2020a), and proposed an approach to link the part of ADM1 (hydrolysis of carbohydrate, protein, and lipids to soluble sugar, amino acids, and long chain-fatty acid, and growth of biomass) and CFD using a compartmental model (Tobo et al., 2020a, 2020b). The integration of kinetic model improved the description of the digester hydrodynamics (analysis of the homogeneity) with the concentration profiles (Tobo et al., 2020a). The compartmental approach is based on the division of the reactor volume into sub-volume based on the velocity distribution obtained by CFD simulations, species concentration, turbulence, or temperature (Jourdan et al., 2019). Tobo et al. divided the reactor in function of the velocity distribution, using a compartmental approach allowing to reduce the computational resources (Tobo et al., 2020b). This technique allowed to characterize the local special variations of substrate, biogas production, pH biochemical processes. The model implemented the ADM1 model in each compartment in order to evaluate the effect of non-uniformity on the performances of the reactor. The coupling of these two categories of models allows to bring accuracy for the characterization of the reactors, the understanding of the phenomena, and the optimization of the process. In addition, it was demonstrated that the performances of the reactor were significantly different for the two approaches (compartmental model considering non-uniformity and continuously stirred tank reactor). This study demonstrates the benefits of coupling CFD and ADM1 models to provide a better understanding of the impact of flows on substrate degradation kinetics. Moreover, as reactions are impacted by shear stress, it would be interesting to integrate this parameter into the ADM1 model in order to consider shear stress as a process inhibitor. In addition, as these parameters are local, it would be interesting to integrate them during the coupling of a CFD and ADM1 model, following the compartmental approach which considerably reduces calculation duration.

Many authors recommended to consider biochemical phenomena in numerical simulations of flows. Few works focused on the coupling of

CFD models and biochemical models. Given the scientific and technical advances in numerical modeling, the next step in the development of models of anaerobic digestion will be the full integration of biochemical processes within the CFD models. This approach will allow to provide a fine description and a local understanding of the digester environment in order to adapt the operating parameters to optimize the biodegradation of the organic waste and to limit the energy consumption. Moreover, this type of model also allow to know the distribution of microorganism's populations within the reactor, and to study the impact of the flows on their development, their death, the local degradation kinetics, as well as on the formation of biofilms.

## 8. Conclusions and future research directions

In conclusion, the objectives and benefits of CFD modeling are numerous. Indeed, this category of models provides a local description of the process and constitutes a promising tool to design AD units. A detailed review on the CFD model developments were described and analyzed in this paper. CFD modeling allowed to study the numerical strategies (turbulence models, meshing approach, multiphase approach, etc.), the bioreactor configuration (dimensions, shape, etc.), the mixing devices (type of devices, dimensions, etc.), the effect of the rheology properties of the substrate, the effect of TS content (liquid and solid waste), the settling and suspension phenomena, the biofilm, the multiphase flows (two-phases and three-phases flow), the high solid digester, the scale-up effect, and the thermal phenomena.

Nevertheless, few studies concerned the coupling of biochemical and CFD models, allowing to consider both the bio-physicochemical aspects and the flows. This strategy is promising because it will provide local insights into the degradation process and the effects of hydrodynamics during anaerobic digestion of waste. Future research should focus on microbiological aspects as well as the full integration of biochemical reactions in CFD models. In addition, future models will have to perform shorter simulations in order to be able to take into account a larger number of parameters in a single simulation. It is important to be able to study the phenomena in the same simulation and not in different simulations in order to study the simultaneous impact of different phenomena/parameters on the process. The main difficulty will concern the validation of such model given the difficulty of producing local experimental data.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Data Availability

No data was used for the research described in the article.

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