2023

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Recommended Citation

D' Bastiani, Camila; Kennedy, David; and Reynolds, Anthony, "CFD Simulation of Anaerobic Granular Sludge Reactors: A Review" (2023). *Articles*. 80.
https://arrow.tudublin.ie/engschmecart/80

Water Research 242 (2023) 120220

Contents lists available at ScienceDirect

Water Research

journal homepage: www.elsevier.com/locate/watres

Review

CFD simulation of anaerobic granular sludge reactors: A review

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ARTICLE INFO

Keywords:
CFD
Anaerobic digestion
Multiphase flow
Granular reactors
Biogas

ABSTRACT

Anaerobic digestion processes can generate renewable energy in the form of biogas while treating organic wastewater. The generation of biogas within anaerobic digestion systems is directly linked to the mixing conditions inside the reactors. In high-rate reactors such as the upflow anaerobic sludge blanket (UASB) reactor, the expanded granular sludge bed (EGSB) reactor and the internal circulation (IC) reactor, the hydrodynamic behaviour will depend on the interactions between the wastewater, the biogas, and the biomass granules. Over the past few years, various researchers have used computational fluid dynamics (CFD) to study the hydrodynamic behaviour in these types of reactors. This review aims to present and critically discuss the state of the art in the use of CFD applied to anaerobic granular sludge reactors (AGSRs). It briefly introduces and discusses the various aspects of modelling. It also reviews the various papers which used CFD to model these reactors and critically analyses the models used for the simulations in terms of general approaches and single-phase vs multiphase studies. The methods used in the validation of the CFD models are also described and discussed. Based on the findings, the challenges and future perspectives for the CFD modelling of AGSRs are discussed and gaps in the knowledge are identified.

1. Introduction

Anaerobic digestion is a natural process of biodegradation of organic matter, which occurs in the absence of oxygen. It has been used for the treatment of human waste since the 1800s. However, with the rise in issues related to energy security, the search for feasible sources of renewable energy has become more crucial. Hence, in recent years the use of anaerobic digestion for waste valorisation has gained increased visibility due to its ability to produce energy from waste in the form of biogas (Kythreotou et al., 2014).

Traditionally, the design process of wastewater treatment plants relies mainly on laboratory-scale testing of the effluent treatability and on empirical relationships to design the reactors to be used. As for the ideal operating conditions and optimisation of the reactors, they are normally adjusted at the pilot-scale or full-scale stages of the project. A problem with this approach is that hydrodynamic conditions such as mixture quality and shear stress change considerably from laboratory scale to industrial scale and have an influence on the treatability of the wastewater as well as on the quality of the treated effluent (Ren et al., 2009). This was demonstrated experimentally by Van Hulle et al. (2014) who studied the influence of mixing on biogas production for various sizes of reactors. They concluded that as the reactors are scaled-up, the mixing conditions play a bigger role in improving biogas production.

In addition, von Sperling (2007) argues that the basis of the biological processes is the effective contact between the microorganisms responsible for the treatment and the organic matter present in the wastewater, which is used as food for the microorganisms. Therefore, the efficiency of the biological unit process depends on the quality of the mixing inside the reactor which is being used. Hence, when dealing with anaerobic digestion processes, an increase in the efficiency of the reactor can often be related to an increase in the generation of biogas (Zhang et al., 2016).

In this context, the use of more advanced techniques for the design and optimisation of wastewater treatment systems such as computational fluid dynamics (CFD) has seen an increase in the last few years as reported by Nopens et al. (2020), Baeten et al. (2019), and Samstag

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List of abbreviations: 2D, Two-dimensional; 3D, Three-dimensional; ADM1, Anaerobic digestion model No.1; AGSR, Anaerobic granular sludge reactor; CFD, Computational fluid dynamics; CSTR, Continuous stirred-tank reactor; EGSB, Expanded granular sludge bed; GPU, Graphics processing unit; HRT, Hydraulic retention time; IC, Internal circulation; ISC, Increasing-size CSTR; MFR, Multiple flow regimes; PIV, Particle image velocimetry; SST, Shear-stress transport; UASB, Upflow anaerobic sludge blanket; VF, Volumetric fraction.

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https://doi.org/10.1016/j.watres.2023.120220
Received 1 February 2023; Received in revised form 6 May 2023; Accepted 11 June 2023

et al. (2016).

CFD modelling involves the use of numerical methods and algorithms to solve the fundamental governing equations of fluid dynamics (i.e. continuity, momentum and energy equations). In traditional CFD software, the solutions to these equations are found by solving a set of partial differential equations called the Navier-Stokes equations. The Navier-Stokes equations describe the motion of a fluid and how pressure, velocity, temperature and density of a moving fluid are related. For a three-dimensional (3D) system, they consist of one continuity equation for the conservation of mass, three equations for the conservation of momentum and one equation for the conservation of energy (Anderson et al., 1995).

The continuity equation is presented in Eq. (1), and it states that the mass in the control volume cannot be created, destroyed or transformed:

$$\frac{D\rho}{Dt} + \rho\nabla\cdot\mathbf{V} = 0 \tag{1}$$

Where ρ is the density, t the time, and $(\nabla\cdot\mathbf{V})$ is the divergence of the velocity vector field.

Traditional CFD packages use finite volume, finite difference or finite element methods to solve the partial differential equations involved in fluid flow. However, the use of advanced methods for the simulation of fluid flows such as the lattice Boltzmann method (Feng and Michaelides, 2004) and the computational fluid dynamics/discrete element method (Norouzi et al., 2017) or meshless methods such as smoothed particle hydrodynamics (Meister and Rauch, 2016) is increasing in the last few years.

The use of CFD to study and optimise slurry anaerobic digesters has already been undertaken by several authors (Dabiri et al., 2021; Wu and Chen, 2008; Wu and Bibeau, 2006). In general, the hydrodynamics of common slurry anaerobic digesters can be simulated adequately by assuming a single-phase (liquid) or two-phase (gas/liquid) flow, as shown in most studies reviewed by Sadino-Riquelme et al. (2018). A common approach to model the rheological behaviour of slurry digesters is to use a non-Newtonian model for the liquid phase. This allows the model to account for the effects of the total solids content in the viscosity of the wastewater without having to include a solid phase in the model, hence reducing the number of phases to be simulated (Wu and Chen, 2008; Shrestha and Lohani, 2022; López-Jiménez et al., 2015). In general, this is a reasonably good assumption as the size of the solids dispersed on the flow is very small compared to the size of the reactors.

However, for high-rate anaerobic granular sludge reactors (AGSRs) such as the upflow anaerobic sludge blanket (UASB) reactor, the expanded granular sludge bed (EGSB) reactor and the internal circulation (IC) reactor, the role of the biogas bubbles in the mixing as well as the effect of the granules should not be underestimated. UASB reactors are considered to be self-mixed by the upflow movement of the biogas bubbles and by the liquid flow through the reactor (Chernicharo, 2007). Moreover, high-rate systems rely on their ability to retain biomass granules (high solids residence time). This is ensured by a combination of reactor design, settling characteristics of the granules, and liquid upflow velocity. An accurate CFD model would include the effects of biogas bubbles on the overall flow characteristics. It would also capture the effects of increased flow rates of wastewater and biogas on the loss of biomass (sludge wash-out). In this context, CFD simulations stand out as a tool capable of aiding in the design and study of AGSRs by allowing for design iterations for optimisations without the need to construct and build reactors.

The use of CFD for the simulation of AGSRs has started in the last two decades, however, multiphase simulations are in general computationally demanding, especially when including a granular (solid) phase. Moreover, a CFD model should only be used to drive real-life design decisions if it has been carefully verified and validated (The American Society of Mechanical Engineers, 2009). Therefore, knowing the state of the art in terms of previous studies and validated models will allow for further research to be developed.

Previously published reviews in the field focused on CFD applied to anaerobic digesters in a more general approach, without focusing on granular reactors (Sadino-Riquelme et al., 2018; Samstag et al., 2016; Batstone et al., 2015; Wu, 2013). Other reviews focused on aspects such as protocols for the simulations and validation of the models (Nopens et al., 2020; Laurent et al., 2014). The use of CFD applied to specific tasks such as modelling of mixing in anaerobic digestion reactors has been the core of some reviews (Li et al., 2022; Leonzio, 2020; Lindmark et al., 2014).

The modelling of anaerobic granular reactors was reviewed by Liotta et al. (2015) and Yang (2020) from a hydrodynamic and general modelling perspective. CFD is mentioned in the reviews as a modelling possibility but the details of the CFD models are not reported. Baeten et al. (2019) reviewed the modelling of granular sludge reactors (aerobic, anaerobic and nitritation-anammox) from a mechanistic modelling perspective (i.e. models that are based on mass balance with transport and reaction terms). The authors report that some papers used CFD to study the transport of liquid, gas and solid phases. While the authors discuss the forces involved in the momentum transfer between the phases no details on the CFD modelling are provided.

The main motivation to publish this review comes from the need to understand current and future trends, in terms of the multiphase CFD modelling of AGSRs, as well as to elucidate the gaps in knowledge. Moreover, the validation method used for said models is also reviewed, in an attempt to understand how accurate these models are, and hence the possibility of using them in benchmarking studies in the future.

The field of CFD is in constant change and relies on the vast improvements in the technology available, especially in terms ofcomputer hardware. Simulations that were not feasible a few years ago due to high computational costs are becoming more accessible and therefore more complex and detailed models can be simulated in a timely manner with a lower investment in hardware. The increased use of CFD techniques applied to wastewater treatment processes has led to a large increase in papers published in this field in recent years and therefore there is a need for this information to be systematically organised and critically reviewed.

This review aims to present and critically discuss the state of the art in the use of CFD applied to anaerobic granular sludge reactors, with emphasis on UASB, EGSB and IC reactors and their modified versions.

The specific objectives of this paper are:

- To elucidate the gaps in knowledge in the field by analysing the modelling approaches used in various papers.
- To critically review the methods used for the simulation and validation of the CFD models.
- To collect details on the modelling approaches adopted for the multiphase simulation of AGSRs.
- To discuss the challenges and future perspectives in CFD modelling of AGSRs.

2. Scope and introduction to AGSRs

2.1. Scope of the review

This review focuses on the use of CFD models applied to anaerobic granular sludge reactors and it is limited to the application of said models to UASB, EGSB and anaerobic IC reactors and their modified versions. With these selection criteria, this review found 24 papers ranging from 2007 to 2022, which are discussed in detail in Chapter 4.

Around 63% of the papers reviewed focused on simulating UASB reactors and some modified versions of them. UASB reactors were the first generation of granular anaerobic sludge reactors to be developed and are therefore a well-established technology. Anaerobic EGSB reactors are considered an improved version of UASB reactors and papers dealing with CFD modelling of said reactors and their modified versions accounted for around 29% of the works reviewed. Being the latest technology to be developed, anaerobic IC reactors accounted for only around 8% of the papers reviewed (2 papers – including a modified IC reactor).

2.2. *Fluid dynamics of AGSRs*

From a fluid dynamics standpoint, AGSRs consist of complex multiphase flows coupled with bioreactions. The level of complexity of the flow will depend, amongst other factors, on the number of phases involved in the process as well as on the rheology of the influent being treated. The validation of CFD models of multiphase flows can be complex and difficult given that analytical solutions are not available and obtaining high-quality experimental data is not always possible. As mentioned before, this review focuses on three types of anaerobic granular reactors: EGSB, UASB and IC reactors and their modified versions. Each type of reactor has characteristics such as the maximum operating velocities and the expansion of the sludge bed, which are specific to each type of reactor. For instance, UASB reactors have three broad distinguished zones:

- sludge bed zone,
- sludge blanket zone, and
- three-phase separator zone.

The sludge bed zone at the bottom of the UASB reactor is formed by densely packed larger biomass granules, the influent and some biogas, as shown in Fig. 1 (A). Above it, there is the sludge blanket zone, which consists of finely suspended solids in water, and gas. The top zone (the three-phase separator zone) is mainly formed by clear water and gas.

From a modelling standpoint, the three zones are usually described using tank in series derived models (Liotta et al., 2015). Such models might describe the UASB reactor as a combination of only continuous stirred-tank reactors (CSTRs) (Chen et al., 2015) or a combination of CSTRs and other reactors such as the plug flow reactor (Heertjes et al., 1982).

EGSB reactors are regarded as second-generation sludge bed reactors. The main difference from UASB reactors is that the granules are now partially fluidised rather than densely packed as shown in Fig. 1 (B). EGSB reactors are also usually taller than their predecessor. To cause the fluidisation of the sludge bed, higher upflow velocities are needed, hence this reactor operates at higher flow rates. This leads to the washout of finer granules and the retention of larger ones, and better-mixing conditions. These characteristics lead to improved contact between wastewater and granules, hence improving the efficiency of treatment (van Lier et al., 2020).

IC reactors are considered third-generation reactors. They work with an expanded bed at the bottom region, and feature three-phase separators at different heights of the reactor, as shown in Fig. 1 (C). The three-phase separator devices lead the biogas upwards through a pipe (riser) into a degassing tank. The gas/liquid mixture is then separated using a degasifier unit, and the biogas is removed from the system. The liquid/sludge mixture returns to the tank through a pipe (downer) placed inside the reactor, thus generating the internal circulation of wastewater (van Lier et al., 2020).

In EGSB and IC systems the recirculation leads to good mixing conditions within the reactors. For this reason, EGSB reactors are often described using models for completely mixed reactors according to Liotta et al. (2015). A combination of completely mixed regions and plug flow regions was proposed by Zheng et al. (2012) to model an EGSB reactor. IC reactors usually work at high organic loading rates, which also have an impact on their hydrodynamics. Huang et al. (2019) successfully applied an increasing-size CSTR (ISC) model to simulate an IC reactor. Liotta et al. (2015) argue that the exact mixing patterns cannot be generalized for IC and EGSB reactors, and a case-by-case experimental evaluation should be performed.

Although the overall hydrodynamic conditions might not be the same in UASB, EGSB and IC reactors, the three share the multiphase flow aspect. UASB reactors are said to be self-mixed, meaning that the biogas bubbles together with the inlet of the fluid are responsible for the good mixing inside the reactors. Moreover, the solids at the bottom of the reactor create a region of higher resistance for the fluid, similar to what would happen in a packed bed reactor. The mixing in both the IC and the EGSB reactors is also highly impacted by the upward movement of the biogas bubbles within the reactor and the recycling of effluent (either internally or externally).

The biochemical processes in AGSRs are the same as the ones happening in common slurry anaerobic digesters, meaning that the anaerobic digestion model No.1 (ADM1) can also be used in the biokinetic modelling of these reactors (Batstone et al., 2002). However, the hydrodynamic behaviour inside granular reactors is substantially different. That generally translates into the need for more complex models capable of capturing the multiphase dimension in granular reactors.

The relationships between the gas-liquid-solid phases have been previously studied. Zhang et al. (2011) found that the liquid superficial velocity affects the shear rate and the mass transfer, while Wu et al. (2015) showed that the rising biogas bubbles inside a granular anaerobic reactor were responsible for 57% to 97% of the shear rate exerted on the granules. This means that in many cases, the biogas generated within the reactor has a larger potential for causing the breakage of granules than the liquid. From a simulation standpoint, this would also mean that the gas phase should not be neglected when studying the shear rate/shear stress inside a reactor. Zhang et al. (2011) and Wu et al. (2015) observed experimentally that as the rate of biogas production increases, the biogas bubble diameter decreases and concluded that the specific bubble population plays a more important role in the shear rate on granules than the bubble diameter (Wu et al., 2015). Hence, it may be concluded that it is more important to use the correct volumetric gas fraction than to use a bubble-size distribution model in the CFD simulations.

Another challenge when simulating the movement of the granules inside AGSRs is the change in apparent density caused by the bubbles while entrapped/attached to the granule (Zhao et al., 2022). No papers to date were found that reproduced this experimental observation using CFD methods but the adhesion forces between the surface of the granules and the bubbles were studied experimentally by Feng et al. (2020). The results showed a relationship between the velocity of the gas and its Reynolds number with the bubble-attachment on two kinds of anaerobic granular sludge. This type of experimental study could ultimately aid in improving the CFD modelling ofAGSRs by creating the foundations for informed choices of what model simplifications may or may not be assumed when dealing with CFD simulations.

3. Modelling of anaerobic reactors

From a modelling standpoint, a reactor can be divided into:

- biokinetic modelling of the anaerobic digestion processes,
- modelling of the hydrodynamic processes.

The biokinetic modelling of the anaerobic digestion processes focuses on the biochemical and physicochemical reactions happening inside the reactor. It concentrates on understanding and reproducing phenomena such as the degradation of organic matter and the generation of biogas. It also aims to relate those processes to the operating parameters within the reactor, such as pH, temperature, feed concentration, the composition of the biogas, etc. (Batstone et al., 2002).

To date, the most used biokinetic model is the ADM1 developed by Batstone et al. (2002), which can realistically predict the reactor's performance in terms of chemical oxygen demand removal and biogas generation (van Lier et al., 2020).

However, the ADM1 model assumes the liquid to be completely

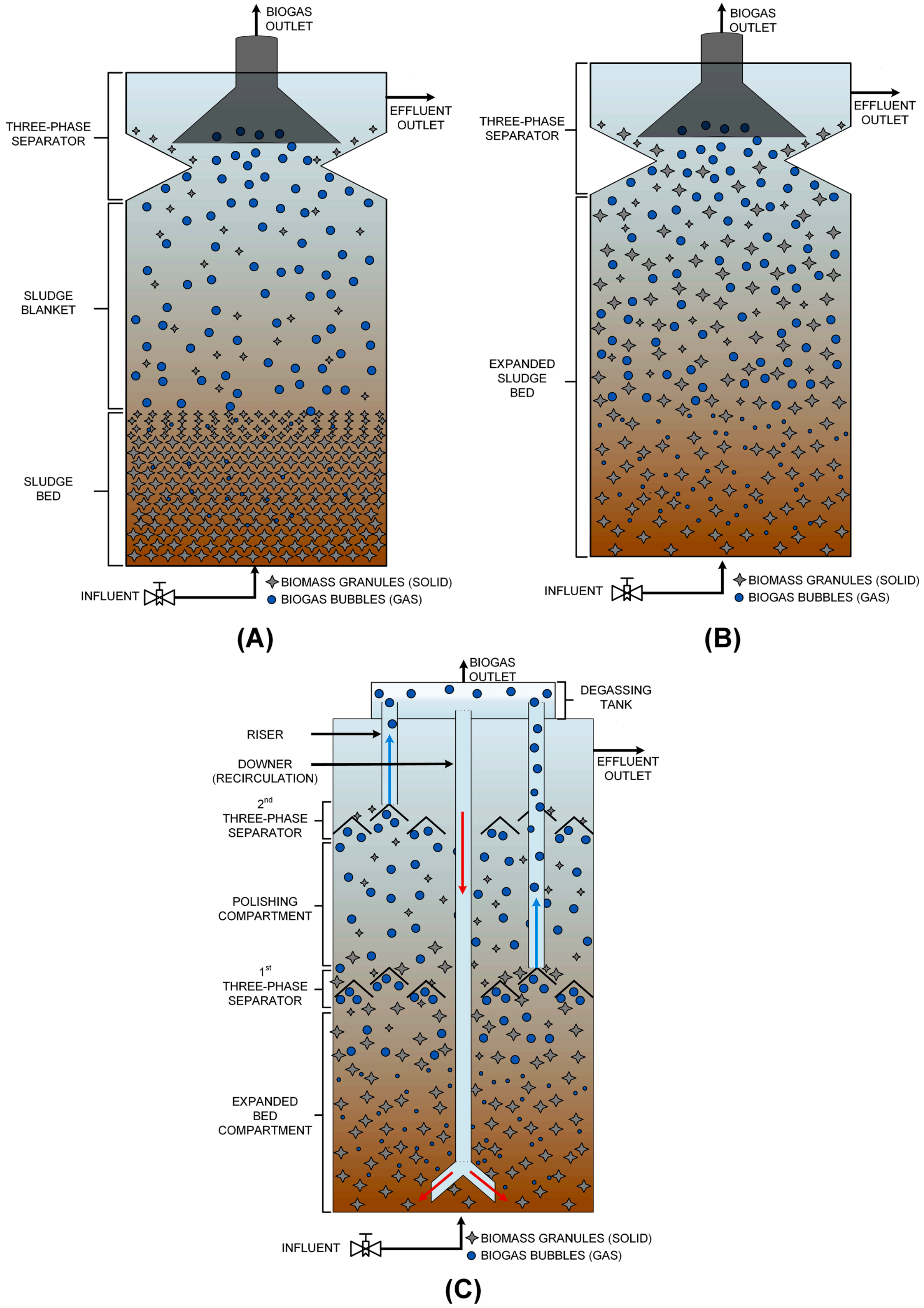

Fig. 1. Schematic representation of (A) UASB reactor (B) EGSB reactor (C) IC reactor.

mixed. Therefore, it does not take into consideration the behaviour of the fluids or poor mixture zones within the reactor. According to van Lier et al. (2020), the system's hydraulics can largely determine the actual kinetics in high-rate anaerobic treatment systems. This is particularly important in granular reactors, where the dynamics inside the reactor are affected by three phases (i.e. solid, liquid and gas).

While the ADM1 model can be solved for different temperatures, it cannot model temperature variations within the reactor. The model assumes the same temperature in all regions of the reactor, which may not be true in large-scale reactors.

Van Lier et al. (2020) argue that while the ADM1 model is useful to predict the performance of reactors, it is not as helpful as a design tool, particularly for full-scale reactors. While the ADM1 model has already been successfully coupled with physicochemical models (Flores-Alsina et al., 2016; Maharaj et al., 2019), the authors mention that the current challenge is to combine the ADM1 model with a fluid dynamics model while also including physicochemical models in an attempt to create a comprehensive design and operation tool to aid the development and application of anaerobic reactors in a dynamic environment.

Some authors have made attempts at combining ADM1 and spatially resolved models, like CFD, using various approaches. For example, Fleming (2002) developed and validated a modelling tool called LagoonSim3D. It was able to dynamically predict the local temperature and biogas production in a covered lagoon digester. The model was developed before the publication of the ADM1 model and therefore used other kinetic models to predict methane production, such as the model developed by Hill (1983). Fleming (2002) mentions that a multiphase approach (gas/liquid or solid/liquid) was not used due to the disparity in time and length scales important to two-phase flows and anaerobic digestion. A biogas bubble diameter is in the order of millimetres while the digester is in the order of tens or hundreds of meters. In the same way, the fluid dynamics involved in multiphase flows such as bubbly flow have time scales in the order of seconds or less, while the biochemistry modelling in digesters changes week-to-week, month--to-month or even seasonally.

Gaden and Bibeau (2011) developed a framework called the coupled reaction-advection flow transient solver for coupling the ADM1 into a spatially resolved model. The framework was verified by the authors but needs to be validated against experimental data. According to Gaden (2013), one of the main challenges when coupling CFD and ADM1 models is the temporal resolution. While the ADM1 biochemistry model requires a time step of hours to days, a flow simulation of the same digester requires a time step on the order of fractions of a second.

Wu et al. (2009) used the CFD software Ansys Fluent to develop a 3D model capable of predicting biogas production in plug-flow anaerobic digesters. The model focused on predicting the temperature and concentration fields in a digester. The authors adopted a steady-state, single-phase approach, neglecting the effects of the biogas rising in the flow field. The model used a first-order kinetic model to predict the biogas generation. The biogas production was modelled using a chemical reaction where glucose was directly converted to methane following the Buswell and Mueller (1952) model. The production of biogas from the model was compared against experimental data from the literature for one measured data point.

A one-way coupling approach was adopted by Tobo et al. (2020a) and Tobo et al. (2020b) when coupling the CFD hydrodynamics and the ADM1 model in such a way as to overcome the time-stepping problem encountered by other authors. A similar approach was adopted by Notari (2022) using the CFD software OpenFOAM to implement the ADM1/CFD model. In this approach, the outputs from the CFD simulations are fed as inputs to the biokinetics models. This allows for a study of how the fluid profiles affect the efficiency of the anaerobic digestion process. However, they do not allow for the study of how those fluctuations (e.g. larger or lower biogas productions) will affect the mixing conditions (and as a consequence the reactor's efficiency). According to Norouzi-Firouz et al. (2022), the one-way approach for coupling hydrodynamic and biokinetic models is suitable when the amount of sludge (and gas in the anaerobic digestion case) and other soluble substrates is so small that it cannot affect the turbulence and momentum equations significantly. In this sense, reactors which rely heavily on self-mixing (i.e. the mixing caused by the biogas production), like the UASB reactor (Chernicharo, 2007) cannot be accurately modelled using a one-way coupling approach. In this case, a two-way approach, which would send the information on the biogas production from the ADM1 model back to the CFD model, would allow for the modelling of how the fluctuations in biogas production affect the mixing in the reactor.

The most common approach used by the authors was a single-phase approach (Fleming, 2002; Wu et al., 2009; Tobo et al., 2020b; Notari, 2022; Tobo et al., 2020a). Some authors chose to use steady-state simulations (Wu et al., 2009; Tobo et al., 2020b) while others made attempts at performing transient simulations, in which case the authors cite time resolution as a big challenge when running time-dependant CFD-ADM1 coupled simulations (Fleming, 2002; Gaden and Bibeau, 2011).

Most of the authors that opted for steady-state and single-phase simulations adopted a one-way coupling by solving the flow fields and then solving the biokinetics model (Wu et al., 2009; Tobo et al., 2020a; Tobo et al., 2020b; Notari, 2022). This meant that the biogas production was estimated as a function of local flow characteristics but the effects of the biogas on the flow were not considered.

To reduce the simulation time and simplify the model, some authors opted for a first-order kinetic model rather than the ADM1 model (Wu et al., 2009; Rezavand et al., 2019) or a partial implementation of the ADM1 model (Tobo et al., 2020b).

For the hydrodynamics simulations, a CSTRbased model was implemented by some authors (Chen et al., 2015; Tobo et al., 2020a).

So far, papers have mainly focused on modelling slurry anaerobic digesters concerning the coupling between CFD and biokinetic models, leaving a clear gap when it comes to the modelling of multiphase granular reactors. In addition, there seems to be a general agreement in the papers reviewed for the need to take into consideration the flow fields and the temperature distribution within the reactor in a way to better predict the biogas output, if the intention is to accurately couple CFD and biokinetics models in the future.

4. CFD modelling of anaerobic granular sludge reactors

Classical approaches to the hydrodynamic modelling of AGSRs, such as the serial tanks model and the ISC model, can be effective tools when studying aspects such as hydraulic retention time (HRT), residence time distribution and dead zones inside UASB and EGSB reactors (Ren et al., 2009; Abyaneh et al., 2022). However, these models are not capable of showing the local characteristics of the flow. CFD can be used to analyse local velocities, pressure, and shear stresses that can aid in the design and operation of reactors.

CFD has already been recognized as an emerging tool for the modelling of wastewater treatment processes (Batstone et al., 2015; Samstag et al., 2016). Samstag et al. (2016) highlight CFD as a tool that can aid in the upscale of wastewater treatment processes. However, its application to granular reactors still poses a considerable number of challenges, such as the accurate modelling of the interfacial momentum transfer between the phases and the validation of the CFD models.

This chapter summarises and critically analyses the papers found, giving an insight into the various aspects of the CFD modelling applied to AGSRs and the approaches adopted in the papers reviewed.

4.1. General CFD modelling approaches

The papers reviewed in the present work are summarised in Tables 1 and 2. For the CFD simulations, all the authors that mentioned the software they used adopted commercial software packages, rather than in-house developed codes. Various releases of the Ansys Fluent software

Table 1
Summary of the papers reviewed.

Reactor	Phases	Results validated?	Software	Multiphase approach	Steady /Transient	Time Simulated	2D/ 3D	Turbulence modelling	Reactor size	Mesh size (cells)	Author
UASB	L	Yes	Ansys Fluent	NA	NM	NM	3D	NM	V. = 30 L H. = 1.10 m D. = 0.20 m	NM	Wongnoi et al. (2007)
EGSB	S/L/G	Yes	Ansys Fluent	E-E	Steady	NA	2D	Turbulent (k-ε model)	V. = 3.35 L H. = 1.20 m D. = 0.06 m	5,540	Wang et al. (2009)
UASB	S/L/G	Yes	Ansys Fluent	E-E	Transient	22 s	3D	Turbulent (k-ε model)	V. = 7.50 L H. = 0.88 m D. = 0.10 m	NM	Ren et al. (2009)
EGSB	S/L/G	Yes	Ansys Fluent	E-E	Transient (time step = 0.001 s)	3 s	2D	Turbulent (k-ε model)	V. = 3.35 L H. = 1.20 m D. = 0.06 m	14,440	Wang et al. (2010)
UASB	S/L/G	Yes	Ansys CFX	E-E	Steady	NA	2D	Turbulent (k-ε model)	V. = 3,000 L H. = 4.5 m D. = 1 m	41,344	Lima et al. (2011)
UASB	S/L/G	No	Ansys Fluent	E-E	Transient	32.7 s	2D	Turbulent (k-ε model)	NM	120,000	Kundu and Mishra (2013)
UASB	S/L/G	Yes	Ansys CFX	E-E	NM	NM	3D	Turbulent (k-ε model)	V. = 6,000 m^3	2,265,975	Ruttithiwapanich et al. (2013)
IC	S/L	No	NM	E-E	Steady	NA	2D	Turbulent (model not specified)	V. = 20 L H. = 2.5 m D. = 0.15 m	4,460,636	Wang et al. (2014b)
EGSB	S/L	Yes	Ansys Fluent	E-E	Transient	NM	3D	Turbulent (k-ε model)	H. = 0.8 m D. = 0.1 m	NM	Wang et al. (2014a)
UASB	L	No	COMSOL	NA	NM	NM	3D	Turbulent (k-ε model)	NM	80,347	Pereira et al. (2015)
EGSB	L*1	Yes	COMSOL	NA	Steady	NA	3D	NM	NM	NM	Yang et al. (2015)
UASB	S/L	No	COMSOL	E-E	Transient	600 s	2D and 3D	NM	V. = 160 L H. = 1.7 m D. = 0.28 m	2D - 4,400 3D-70,000	Cruz et al. (2016)
EGSB	S/L/G	Yes	NM	E-E	Transient (time step = 0.02 s)	50 s	2D	Turbulent (k-ε model)	H. = 1 m D. = 0.09 m	41,536	Pan et al. (2017)
UASB	G/L	No	COMSOL	NM	Transient	3,600 s	2D	Laminar	H. = 1.35 m D. = 0.1065 m	60,272	Paiva et al. (2017)
UASB	L	Yes	Ansys Fluent	NA	Steady	NA	3D	NM	NM	NM	Márquez-Baños et al. (2018)
UASB	S/L/G	No	Ansys Fluent	Mixture model	Steady	NA	2D	Turbulent (k-ε model)	H. = 0.7 m Square base = 0.07 m side	49,100	Das et al. (2018)
IC	G/L	Yes	STAR-CCM+	MFR model	Transient	22 s	3D	NM	D. = 1.75 m	NM	Wang et al. (2019)
UASB	S/L/G	No	Ansys CFX	E-E	NM	NM	3D	Turbulent (k-ω SST model)	H. = 5 m Rectangular base = 1.2 × 1 m	NM	Hao and Shen (2019)
UASB	G/L	Yes	Ansys Fluent	E-E	Transient	235 s	3D	Laminar	H. = 1.75 m D. = 0.3 m	528,000	D' Bastiani et al. (2020)
UASB	S/L/G	Yes	Ansys Fluent	E-E	Transient	268 s	3D	Laminar	H. = 1.75 m D. = 0.3 m	528,000	D' Bastiani et al. (2021)
UASB	L	Yes	Ansys Fluent	NA	Transient	120 s	3D	Turbulent (k-ε and k-ω SST model)	V. = 41 m^3 H. = 8.1 m D. = 2.5 m	2,796,190	Cisneros et al. (2021)
EGSB/ UASB	S/L/G	NM	Ansys CFX	E-E	Steady	NA	3D	Turbulent (k-ω SST model)	NM	NM	Hao and Shen (2021)
EGSB	L*2	NM	Ansys Fluent	NA	Transient	6,000 s and 1,500 s	3D	Turbulent (k-ε model)	V. = 2,100 m^3 H. = 30 m	1,929,204	Abyaneh et al. (2022)
UASB	L/G*1	NM	Flow 3D® version 11.1.1	NM	NM	NM	3D	NM	*V* = 2 L	204,768	Hernández-Rodríguez et al. (2022)

S = Solid; *G* =Gas; *L* = Liquid.
NA = Not Applicable.
NM = Not Clear or Not Mentioned.
V. = Volume; H. = Height; D. = Diameter.
E-E = Eulerian-Eulerian.
MFR = Multiple Flow Regimes.
SST = Shear-Stress Transport.
*1 The papers treated the sludge bed as a porous media.
*2 The papers simulated the liquid as Newtonian and Non-Newtonian.

Table 2
Summary of the main goals of the studies reviewed in the present work.

Reactor	Author	Main goal/application of the model in the studies
UASB	Wongnoi et al. (2007)	Investigate the influence of a new three-phase separator configuration on the performance of a modified UASB.
EGSB	Wang et al. (2009)	Analyse hydrodynamics information in an EGSB reactor.
UASB	Ren et al. (2009)	Visualise the phase holdup, explore the flow patterns in UASB reactors, and compare it with an ISC model.
EGSB	Wang et al. (2010)	Visualise and analyse flow patterns in an EGSB reactor, by incorporating a reaction kinetics model (production of hydrogen) into a CFD model.
UASB	Lima et al. (2011)	Study the fluid dynamic behaviour of a UASB reactor theoretically and experimentally.
UASB	Kundu and Mishra (2013)	Analyse hydrodynamics information in a UASB reactor.
UASB	Ruttithiwapanich et al. (2013)	Identify the cause of granular sludge washout inside an industrial-scale UASB reactor using CFD.
IC	Wang et al. (2014b)	Study the flow characteristics in a modified internal circulation reactor under different flow rates of external circulation.
EGSB	Wang et al. (2014a)	Investigate the impact of the water distribution system on the internal flow field in an EGSB reactor.
UASB	Pereira et al. (2015)	Analyse hydrodynamics information in a UASB reactor.
EGSB	Yang et al. (2015)	Analyse the effect of influent distribution in the reactor hydrodynamics and integrate CFD and biokinetics models in an EGSB reactor.
UASB	Cruz et al. (2016)	Investigate the impact of water distribution configurations on the internal flow field in a UASB reactor.
EGSB	Pan et al. (2017)	Investigate the impact of baffle angle on the separation efficiency and the hydraulic characteristics in a three-phase separation zone in an EGSB reactor.
UASB	Paiva et al. (2017)	Analyse hydrodynamics information in a UASB reactor.
UASB	Márquez-Baños et al. (2018)	Analyse hydrodynamics information in a UASB reactor.
UASB	Das et al. (2018)	Compare the flow patterns and mixing of a modified UASB reactor against a conventional UASB reactor.
IC	Wang et al. (2019)	Investigate the flow patterns, internal circulation flow rate, gas holdup, and frictional pressure drop of the vertical riser in an IC reactor.
UASB	Hao and Shen (2019)	Evaluate the effects of the overlapping rate of baffle plates on the separation of the three phases in a UASB reactor.
UASB	D' Bastiani et al. (2020)	Study the fluid dynamic behaviour of a UASB reactor theoretically and experimentally using gas/liquid simulations.
UASB	D' Bastiani et al. (2021)	Study the fluid dynamic behaviour of a UASB reactor theoretically and experimentally in solid/gas/liquid simulations.
UASB	Cisneros et al. (2021)	Investigate the impact of water distribution configurations on the internal flow field in a UASB reactor.
EGSB/ UASB	Hao and Shen (2021)	Study the performance of a novel gas-liquid-solid separator for UASB and EGSB rectors.
EGSB	Abyaneh et al. (2022)	Evaluate the mixing of a special EGSB reactor with internal circulation
UASB	Hernández-Rodríguez et al. (2022)	Analyse hydrodynamics information in a UASB reactor and the influence of the gas bubbles on the flow at two different temperatures.

package were used in most of the papers. The Ansys CFX and COMSOL Multiphysics software packages were used in several papers. The software package STAR-CCM+ was adopted by Wang et al. (2019) and the software package Flow 3D® version 11.1.1 was adopted by Hernández-Rodríguez et al. (2022). Open-source software, such as OpenFOAM, was not used in any of the papers reviewed. The ease of use of commercial software packages due to their available graphical user interface, combined with the documentation available (i.e. manuals, tutorials, video guides) and the fact that the codes are previously verified by a development team, hence removing the need for code verification, makes them a common choice for the application of CFD to wastewater treatment problems. On the other hand, the user is limited to the models available within the software, which might make it challenging to include specific models, such as biokinetics models. The main disadvantages of commercial software packages are:

- the cost,
- the limitations of the academic version, and
- the software's code is usually not provided.

When dealing with multiphase simulations, the Eulerian-Eulerian approach was the most commonly used as shown in Table 1. In this approach the phases are treated as interpenetrating continua, i.e. they share a volume, with a volume fraction of each phase present in said volume. Das et al. (2018) used the mixture model available in Ansys Fluent, which is a simplified version of the full Eulerian-Eulerian model. A MFR model was developed by Wang et al. (2019) combining the advantages of Eulerian-Eulerian and volume of fluid models using STAR-CCM+. The Eulerian-Lagrangian approach (e.g. the Lagrangian discrete phase model) was not used in any of the papers reviewed. In this approach, the dispersed phase should occupy a low volume fraction, and particle-particle interactions would be neglected, given the distance between them. Considering the high concentration of solids inside the reactor and in the sludge bed, such an approach would probably lead to unfeasible computational times if used to model the granular phase. On the other hand, the application of a Lagrangian approach to simulate the gas phase might prove to be feasible as investigated by Dapelo et al. (2015).

The simulations of common slurry anaerobic digesters, in general, require a non-Newtonian modelling approach for the liquid phase to model the effect of the total concentration of solids in the mixture. In granular reactors, most of the papers adopted a Newtonian approach for the modelling of the liquid phase, as the solids (granules) are considered to be a separate phase altogether instead of part of a mixture (Cisneros et al., 2021; D' Bastiani et al., 2021; Wang et al., 2014a). Abyaneh et al. (2022) described the simulation of the liquid phase as a non-Newtonian fluid when modelling the flow using a single-phase model. None of the papers reviewed mentioned an experimental characterisation of the wastewater in terms of its rheology.

The effects of temperature on anaerobic processes and the generation of biogas are broadly known (Enitan et al., 2015). For example, the operation of reactors at mesophilic (25 – 40 °C) or thermophilic (50 – 65 °C) conditions may lead to higher or lower biogas production (Moset et al., 2015; Schultz et al., 2015). Climate conditions may affect the temperature distribution inside the reactor, leading to poor temperature distribution within the vessel. Moreover, maintaining a constant temperature may require energy input and good insulation in cold climate regions, which impacts the design and operational costs of a wastewater treatment plant. In the papers reviewed, the energy conservation equation was neglected, hence the temperature fields inside the reactors and the heat losses to the surroundings were not calculated in the simulations. Therefore, the processes were considered to be isothermal (Hao and Shen, 2021; Ren et al., 2009) and adiabatic. Considering that the biokinetics modelling is intrinsically linked to the temperature inside the reactor, any future inclusion of these models would be positively impacted by solving the energy conservation equation for the system.

Given the low upflow velocities of the liquid in the designed reactor, D' Bastiani et al. (2021), D' Bastiani et al. (2020), and Paiva et al. (2017) assumed the flow to be laminar to simplify the model. However, they did not consider the increment in velocities caused by the biogas phase when calculating the Reynolds number of the reactors. The preferred turbulent model choice in most papers reviewed was the realizable k-ε model for the continuous phase (liquid). Cisneros et al. (2021) compared the results for the realizable k-ε model against the k-ω SST model applied to single-phase flow in a UASB reactor. The results from both these turbulent models were compared against experimental tracer experiments, and it was concluded that for the single-phase flow, the realizable k-ε model showed a better fit. The k-ω SST model has been used in some papers to predict the flow in multiphase (gas/solid/liquid) flows (Hao and Shen, 2019; Hao and Shen, 2021). Further research on the most suitable model for the multiphase flow simulation followed by the validation of the model would allow for more accurate results.

Transient simulations with a simulated time between 3 s and 100 min were reported in most of the papers reviewed. The choice between steady and transient simulations depends on the objectives of the study and the limitations of the modelling strategy or the validation method chosen. A time-step independence test, to verify the largest time step that could be used without impacting the results was performed by Pan et al. (2017). This allowed for better use of the available resources without compromising the results.

While full-scale and pilot-scale reactors were simulated in some papers (Abyaneh et al., 2022; Cisneros et al., 2021; Hao and Shen, 2019; Ruttithiwapanich et al., 2013; Lima et al., 2011) others simulated bench or laboratory scale reactors (Wang et al., 2009; Wang et al., 2010; Das et al., 2018). The liquid upflow velocity is one of the most important design parameters in AGSRs, given that it dictates the expansion of the bed. Therefore, when simulating these reactors, if the intention is to keep this velocity constant as well as the diameters of the granules and bubbles, the size of the reactor to be simulated is directly related to the mesh size. This means that keeping the mesh density constant is important. The impact of the size of the reactor and if the geometry was 2D or 3D on the mesh size can be seen in the papers which performed a mesh convergence test (Abyaneh et al., 2022; Cisneros et al., 2021; D' Bastiani et al., 2021, 2020; Pan et al., 2017; Lima et al., 2011; Wang et al., 2009). Performing a mesh convergence test allows for the use of adequate mesh density in the simulations, hence reducing errors due to the coarseness of the mesh and reducing computational effort due to an over-refined mesh. The grid convergence index method was the preferred method in the most recent papers (Abyaneh et al., 2022; Cisneros et al., 2021; D' Bastiani et al., 2020, 2021).

A biokinetics model was excluded in the majority of the papers reviewed. Papers that did include some level of biokinetics modelling did not use the ADM1 model, but other simplified models. Yang et al. (2015) included the models for butyrate, propionate and acetate degradation. Hydrogen production from ethanol-type fermentation was modelled by Wang et al. (2010).

When dealing with CFD modelling, it is common to assume simplifications in the geometry and/or in the model to reduce computational time. The most common assumptions in the simulation of AGSRs were symmetries at the centre of the reactor or 2D axisymmetric models (D' Bastiani et al., 2020, 2021; Paiva et al., 2017; Lima et al., 2011; Wang et al., 2010). Simulating specific regions of the reactor, such as the reaction zone or the three-phase separator zone, was a common strategy and allowed for the study of specific regions or components of the reactor while reducing the computational effort required (Abyaneh et al., 2022; Hao and Shen, 2021; Pan et al., 2017; Cruz et al., 2016; Wang et al., 2009). Lima et al. (2011) simplified the two-dimensional (2D) three-phase CFD model by simulating only the region above the sludge bed, where the concentration of solids is very low. This allowed for faster simulation of the multiphase model.

The coupling between multiphase CFD models and biokinetic models capable of predicting the amount of biogas generated inside the reactor has not been successfully achieved so far. Therefore, to model the biogas phase inside the reactor in CFD simulations it is necessary to use techniques to artificially add the biogas phase into the reactor in the CFD simulations, emulating the biogas being generated in an operational reactor. In the studies reviewed, various approaches have been adopted to model the biogas generated inside the reactor. When dealing with transient Eulerian-Eulerian simulations, some papers have assumed an initial volume fraction of biogas (around 3% to 6%) to be trapped inside the sludge bed at the initial simulation time (i.e. at $t = 0$ s); this gas phase was then released from the sludge bed during the simulation and moved upwards (Pan et al., 2017; Wang et al., 2009). The simulated results were validated against experimental results for the axial velocity. However, this approach does not assume a constant volume flow rate of biogas being generated within the reactor. This means that in a transient simulation, the biogas distribution inside the reactor is not constant, limiting the application of this approach. This also affects the expansion of the bed and the mixing inside the reactor. Another common approach was the injection of gas from the bottom of the reactor (either using the same inlet as the liquid or a separate virtual surface) or from a surface at the reaction zone. The biogas flow rate in those cases was based on calculated or measured biogas flow rate results (D' Bastiani et al., 2020, 2021; Hao and Shen, 2019; Hao and Shen, 2021; Wang et al., 2019; Das et al., 2018; Ren et al., 2009). Hernández-Rodríguez et al. (2022) injected a certain number of bubbles per second into the reactor, based on experimental results. While the authors do not mention if a Lagrangian framework was adopted, or how the injection point was set, this was the only approach where the individual biogas bubbles could be visualised.

As shown in Table 2, the aim of most of the studies was to understand the hydrodynamics in the AGSRs and validate said models. Moreover, many approaches adopted in the papers reviewed so far served the purpose of aiding in the design and development of new technologies such as modified versions of UASB, EGSB and IC reactors and new designs for the inlet of fluid into the rectors. However, no single model has been used as a standalone tool for the design of said reactors, especially given the lack of coupling between CFD and biokinetics models.

4.2. *Single-phase vs multiphase approaches*

As mentioned before, the flow inside UASB, EGSB and IC reactors are all characterised by the presence of three distinct phases:

- gas (biogas),
- solid (granular sludge), and
- liquid (wastewater).

As three-phase simulations using CFD tools can be computationally expensive (as they need to account for the interphase interactions), a simpler single-phase (only liquid) approach was adopted in some papers. The use of single-phase modelling was adopted most commonly when using CFD as a support tool to compare the flow profile in modified designs of granular reactors, by analysing overall flow characteristics (Cisneros et al., 2021; Wongnoi et al., 2007). A single-phase model was used by Abyaneh et al. (2022) to study the mixing conditions in an industrial EGSB reactor and to compare Newtonian vs non-Newtonian modelling approaches for the liquid phase, together with simpler hydraulic models such as equally sized CSTRs, ISCs, and a compartment model, against residence time distribution experiments. Single-phase CFD simulations were also used in some papers as a general tool to study the flow profile in reactors or to compare against experimental residence time distribution curves (Pereira et al., 2015; Márquez-Baños et al., 2018).

A simplified biokinetic model, predicting the degradation of butyrate, propionate and acetate was coupled with a CFD single-phase model by Yang et al. (2015) and three influent distribution systems at the bottom of the reactor were studied. To account for the effects of the expanded bed, they adopted a simplified approach by defining the region as a porous media, with a specified porosity and permeability. This approach does not allow for the prediction of sludge washout, or for future coupling with biokinetic models capable of predicting the generation and destruction of biomass, but it does allow to predict the effects of sludge bed in the overall flow profiles.

In all the cases mentioned previously, the main objective was not the most accurate CFD modelling of the reactor, but rather the use of CFD as a support tool for various purposes, such as the assessment of modifications in the design of the reactors. In addition, all the papers that included validation of the model used tracer experiments, mostly to generate residence time distribution curves, which were compared against the CFD simulations (Cisneros et al., 2021; Márquez-Baños et al., 2018; Yang et al., 2015; Wongnoi et al., 2007). The accuracy of the models used (e.g. the turbulence model) was not assessed. On the other hand, the use of simpler single-phase approaches allowed for t3D simulations, and in some cases for full-scale reactors to be simulated (Abyaneh et al., 2022; Cisneros et al., 2021). This might not be computationally viable when dealing with complex multiphase simulations.

Some papers adopted a two-phase flow approach considering either a gas/liquid flow (D’ Bastiani et al., 2020; Wang et al., 2019; Paiva et al., 2017) or a solid/liquid flow (Cruz et al., 2016; Wang et al., 2014a, 2014b). The two-phase flow approach was applied to various configurations of reactors. The solid/liquid approach was used to study various inlet configurations and recirculation flow rates. According to Cruz et al. (2016), the two-phase (solid/liquid) approach allows for the study of preferential paths within the sludge bed, which can have an impact on the HRT. The presence of preferential paths can lead to lower HRT, which means a reduced contact time between wastewater and biomass and therefore lower efficiency of treatment and biogas production. A gas/liquid approach was adopted in preliminary studies of UASB reactors (D’ Bastiani et al., 2020; Paiva et al., 2017) as well as in the study of the gas holdup and superficial liquid velocity in the riser of an IC reactor (Wang et al., 2019). As the complexity of the models increased to deal with multiphase problems, 2D simulations were adopted (Paiva et al., 2017; Wang et al., 2014b) or simplifications of the geometry such as symmetry boundary conditions or simulations of only certain zones of the reactor (D’ Bastiani et al., 2020; Cruz et al., 2016) to reduce the computational effort. When adopting single- or two-phase simplifications, the rationale behind the choice of how many and which phases were modelled was not always clear. Wang et al. (2014b) mention that a three-phase system would be too complex to model.

A three-phase approach was adopted in most papers modelling the gas, liquid and solid phases. A 2D geometry was used in more than half of the papers reviewed (Das et al., 2018; Kundu and Mishra, 2013; Lima et al., 2011; Wang et al., 2010, 2009; Pan et al., 2017), while simplifications of the geometries were adopted in the majority of papers using 3D simulations (Hao and Shen, 2021; D’ Bastiani et al., 2021). The use of 2D models or simplified boundary conditions (such as symmetry conditions applied at the centre of the reactor) while not realistic, considering the 3D, asymmetric nature of multiphase flows (D’ Bastiani et al., 2021), and the irregular generation of gas within the reactor, have been deemed acceptable so far, given the computational effort needed to perform three-phase, 3D simulations using commercial software running on state-of-the-art computers.

To reduce computational time, the use of Graphics Processing Units (GPUs) to run the models in parallel would be an alternative, but no papers discussing the speed-up of the simulations using such technology were found to date. Furthermore, no evidence of the use of advanced CFD methods such as the lattice Boltzmann method and the computational fluid dynamics/discrete element method or meshless methods such as the smoothed particle hydrodynamics in the modelling of AGSRs was found. No papers using machine learning methods or neural networks on the simulation of AGSRs as a tool to speed up the simulations were found.

When dealing with multiphase flow simulation, an important step is to define the characteristics of the phases involved. For the simulation of multiphase flows in AGSRs, in general, the liquid phase was considered to be pure water at a specified temperature. Wang et al. (2010) adopted a different approach. The liquid phase was considered to be a mixture of pure water and glucose to account for the degradation of glucose into hydrogen when including the biokinetics model.

Table 3 summarises the characteristics used for the gas and solid phases. In general, in the papers reviewed, the gas and solid phases were modelled as spheres with a constant diameter. No papers using distribution models, such as the population balance model, were found in this literature review. No papers mention that the bubble coalescence effect was considered. The growth and/or breakage of granules was not simulated in any of the papers studied. Only two papers mentioned the approach to granular modelling; both Wang et al. (2010) and D’ Bastiani et al. (2021) used the kinetic theory of granular flow to model the solids. This theory predicts the collisions of the particles and the resultant energy dissipation caused by these collisions. It also shows how transport properties, such as the particulate viscosity, can be obtained from measurements of random particle oscillation velocities (Gidaspow et al., 2004). It is an extension of the classical kinetic theory of gases but applied to granular flows. In this approach, the thermal temperature is replaced by a concept called the granular flow temperature, which measures the random oscillations of particles (Gidaspow et al., 2004; Ding and Gidaspow, 1990). Both, the viscosity and stress of the solids are a function of the granular temperature (Ding and Gidaspow, 1990). This model has been extensively applied to fluidisation problems (Gidaspow et al., 2004), and therefore it is understood to be suitable to model the expansion and fluidisation of the sludge bed in AGSRs.

From Table 3 it can be seen that there is a general agreement that the acceptable diameter of the granules is between 1 and 3 mm, which is in line with published experimental data (e.g. D’ Bastiani et al., 2021; Liu et al., 2007; Trego et al., 2020; Wu et al., 2015). An experimental density of 1,050 kg/m^3 for the granules was reported in two different papers (D’ Bastiani et al., 2021; Pan et al., 2017).

For the biogas, it was observed that most papers use data from the literature for the simulations. No evidence of experimental data on the bubble diameter for UASB, EGSB or IC reactors producing biogas was found in the reviewed papers. Some papers defined the viscosity and density of the biogas by calculating the properties of a gaseous mixture of methane (CH_4) and carbon dioxide (CO_2). Many of the papers reviewed either do not mention the values used or the sources (experimental or from literature) for the properties of the phases chosen for the simulation. Therefore, it is possible to conclude that more experimental data is needed from granular reactors concerning the characteristics of the three phases involved in the flow to be used in more accurate CFD simulations.

4.3. Validation of the models

A critical issue when using CFD to model AGSRs is the validation of the models. According to The American Society of Mechanical Engineers (2009), “There can be no validation without experimental data with which to compare the result of the simulation”. Table 4 summarises the methods used in the papers that performed some form of validation of their results.

The American Society of Mechanical Engineers (2009) provides guidelines for verification and validation in CFD and heat transfer. The Verification and Validation Standard suggests approaches to the validation of CFD simulations, and for the analysis of errors and uncertainties, and gives useful examples. The section on “Code Verification and Solution Verification” deals mainly with the uncertainty caused by numerical errors. This section also suggests the use of the grid convergence index method for the mesh independence study. Methods and examples for the analysis of the uncertainty of experimental results, the effect of input parameters on the simulation and the validation

Table 3
Properties of the solid and liquid phases used in the papers reviewed.

Reactor	Granules (Solid)			Bubbles (Gas)			Volumetric fraction (VF) of solids and gas	Source of the data for the phases	Author
	Diameter (mm)	Viscosity (Pa s)	Density (kg/m3)	Diameter (mm)	Viscosity (Pa s)	Density (kg/m3)			
EGSB	1	*1	1,460	0.1 *2	*1	1.225	Solids: VF of 0.55.*3 Gas: accumulated into the sludge blanket. *4	*1	Wang et al. (2009)
UASB	2	0.005	1,070	0.1	1.9×10^{-5}	1.139	Solids: VF of 0.5.*3 Gas: based on the biogas volume flow rate.	Literature (Yu and Mu, 2006) *2	Ren et al. (2009)
EGSB	1	*1	1,460	0.1 *2	*1	1.225	Solids: VF of 0.5.*3 Gas: based on the hydrogen volume flow rate.	*1	Wang et al. (2010)
UASB	3	0.0001295	1,020	3	1.114×10^{-5}	0.72	In the upper region, the concentration was: 3% solids, 6% gas, and 91% liquid. *5	Bubble diameter: from literature (Narnoli and Mehrotra, 1997) Granules diameter: from literature (Hulshoff Pol et al., 2004)	Lima et al. (2011)
UASB	2	0.005	1,070	0.1	1.9×10^{-5}	1.139	Solids: VF of 0.6.*3 Gas: based on the biogas volume flow rate.	Literature: (Ren et al., 2009)	Kundu and Mishra (2013)
UASB	2	0.18	1,042	1	1.83×10^{-5}	1.185	Solids: VF of 0.18.*3	Literature: solids density and viscosity were based on literature data (Panneerselvam et al., 2009) and (Welty et al., 2008)	Ruttithiwapanich et al. (2013)
IC	*1	0.00001794	1,050	*6	*6	*6	Solids: VF of 0.6.*3	*1	Wang et al. (2014b)
EGSB	2	*1	1,250	*6	*6	*6	Solids: VF of 0.6.*3 The sludge bed's original height was 0.2 m out of the 0.8 m total height.	*1	Wang et al. (2014a)
UASB	1	*1	1,460	*6	*6	*6	Solids: VF of 0.35×^{3} up to the height of 0.7 m.	Literature. *1	Cruz et al. (2016)
EGSB	1	*1	1,050	0.1	*1	*1	Solids: VF of 0.55.*3 Gas: accumulated into the sludge blanket. *4	Granules density measuring method from literature (Schuler and Jang, 2007) Biogas diameter from literature (Wang et al., 2010) The biogas was regarded as a mixture of CH_4 and CO_2.	Pan et al. (2017)
UASB	1	0.005	1,250	0.1	1.087×10^{-5}	0.6679	Solids: VF of 0.3.*3	The biogas was assumed as pure CH_4.*1	Das et al. (2018)
UASB	2	*1	1,050	2	1.984×10^{-5}	0.8578	Solids: VF of 0.60×^{3} Gas: based on the biogas volume flow rate.	Granules density and diameter: experimental data. Bubble diameter: from literature (Narnoli and Mehrotra, 1997). *6	D' Bastiani et al. (2021)
UASB	*6	*6	*6	2	1.984×10^{-5}	0.8578	Gas: based on the biogas volume flow rate.	Bubble diameter: from literature (Narnoli and Mehrotra, 1997). *7	D' Bastiani et al. (2020)
UASB	*6	*6	*6	*1	*1	*1	30 and 45 bubbles per second	Number of bubbles per second obtained experimentally by the authors	Hernández-Rodríguez et al. (2022)

*1 Information not available or not clear.
*2 Characteristics of the gas refer to hydrogen-producing anaerobic reactors.
*3 Volume Fraction of solids is given at the sludge bed, at the start of the simulation.
*4 The initial gas phase was assumed to be accumulated into the sludge blanket. It was assumed that the gas would be released when the force balance between the gas and solid phases broke up.
*5 The sludge bed region was neglected. Gas density and viscosity were calculated for a mixture of 70% methane and 30% carbon dioxide.
*6 Not available, as the model was only gas/liquid or solid/liquid.
*7 The gas density and viscosity were calculated for a mixture of 65% methane and 35% carbon dioxide.

uncertainty are also covered in the standard.

Tracer experiments have been used in many studies as a simpler way to achieve a level of validation of the CFD models (Cisneros et al., 2021; Márquez-Baños et al., 2018; Yang et al., 2015; Ren et al., 2009; Wongnoi et al., 2007). While capable of yielding general data about the hydrodynamics in the reactor, tracer experiments are limited, as they are not capable of measuring local data, such as local velocities.

The pressure at various points inside the reactor has also been used as a validation strategy (Lima et al., 2011). The results showed good agreement between CFD and experimental results. However, the simulated region did not include the sludge bed (the biogas accounted for 6% and the solids for 3% of the volume fraction of the region simulated),

Table 4
Summary of the validation methods used in the papers reviewed.

Reactor	Phases	Method used for validation	Tracer	Measured/compared variables	Reactor feed	Comments	Author
UASB	L	Tracer experiments.	Colourful dye.	The dye flow pattern was observed to confirm that a spiral pattern was formed within the reactor.	Wastewater from a fruit-canning factory.	Biogas-producing reactor. It is mentioned in the paper that the CFD results showed good agreement with experimental data. In both cases, spiral flows were observed in the new three-phases separator.	Wongnoi et al. (2007)
EGSB	S/L/G	PIV.	Glass microspheres.	Dimensionless water velocity vs dimensionless lateral distance.	Wastewater from a local pharmaceutical factory	Hydrogen-producing reactor. Water velocity in the reaction zone was measured at four different HRTs.	Wang et al. (2009)
UASB	S/L/G	Tracer experiments.	Solution containing 594 mg/L Li_2SO_4 (Tracer Li^+).	Dimensionless tracer concentration vs time at the outlet and three different heights.	Synthetic sucrose-rich wastewater with a chemical oxygen demand of 9,900 mg/L.	Hydrogen-producing reactor. The paper did not validate the CFD model, but the hydraulic ISC model. The ISC model was then compared against the CFD simulations.	Ren et al. (2009)
EGSB	S/L/G	PIV.	Glass microspheres.	Dimensionless water velocity vs dimensionless axial distance.	NM	Hydrogen-producing reactor. Water velocity in the reaction zone was measured at various HRTs.	Wang et al. (2010)
UASB	S/L/G	Manometers located inside the reactor were monitored weekly.	NA	Pressure at five points inside the reactor at various heights (CFD vs experimental)	Domestic wastewater.	Biogas-producing reactor.	Lima et al. (2011)
UASB	S/L/G	Particle tracking experiment.	Plastic beads.	Solid distribution frequency was analysed statistically.	Liquid-solid flow experiment using plastic beads and tap water.	Not an operational reactor. The chi-square method was used to compare experimental and simulated solid distribution frequency.	Ruttithiwapanich et al. (2013)
EGSB	S/L	Expansion of the sludge bed.	NA	Expanded height of the sludge bed for three water inlet conditions.	NM	The effects of the gas phase were not considered.	Wang et al. (2014a)
EGSB	L*[1]	Tracer experiments.	A solution containing $CaCl_2$ (Tracer Ca_2^+).	Tracer concentration vs time at the outlet.	Clearwater.	Not an operational reactor. Tracer experiments were performed while there was no sludge present in the reactor (single-phase).	Yang et al. (2015)
EGSB	S/L/G	PIV	Glass microspheres.	Water velocity vs axial relative position.	NM	Not clear what phases were present in the reactor used in the validation.	Pan et al. (2017)
UASB	L	Tracer experiments.	NM	Dimensionless tracer concentration vs dimensionless time	NM	The experimental procedure used is not very clear.	Márquez-Baños et al. (2018)
IC	G/L	Analytical validation.	NA	Calculated gas holdup as a function of the Martinelli parameter (CFD vs analytical solution).	NA	No experimental validation, only analytical validation was performed.	Wang et al. (2019)
UASB	G/L	PIV and shadowgraphy	Fluorescent 20–50 µm tracer particles.	Upflow axial liquid velocity at various heights. Liquid velocity contours at the centre. Gas velocity.	Liquid/gas flow experiment using water and air.	Not an operational reactor. The mean bubble size was also measured.	D' Bastiani et al. (2020)
UASB	S/L/G	PIV	Fluorescent 20–50 µm tracer particles.	Average liquid velocity. Liquid velocity contours at the centre. Average gas velocity.	Solid/liquid/gas flow experiment using water, air, and plastic beads.	Not an operational reactor. The mean bubble size was also measured.	D' Bastiani et al. (2021)
UASB	L	Tracer experiments.	A solution containing 1,500 mg/L of NaCl.	Resident time distribution curve (dimensionless tracer concentration vs dimensionless time).	Water	Four tracer tests were conducted.	Cisneros et al. (2021)

S = Solid; *G* =Ggas; *L* = Liquid.
NA = Not Applicable.
NM = Not Clear or Not Mentioned.
*[1] The paper treated the sludge bed as a porous media.

hence they had little impact on the pressure (Lima et al., 2011). Although pressure can be considered an important parameter in the validation of CFD models, it might be better to use it in conjunction with other methods for validating a complex multiphase model, considering the low velocities inside UASB reactors, and the limited information generated by this method (changes in local velocity profiles cannot be captured when using the pressure method for the validation).

Particle image velocimetry (PIV) is a non-intrusive optical measurement technique, capable of yielding quantitative as well as qualitative data about the flow field (Raffel et al., 2018). The use of high-quality experimental data found in the literature to validate CFD test case models is a common practice, as many researchers do not have access to adequate facilities to perform their experiments. Wang et al. (2009), (2010), and Pan et al. (2017) mention the use of PIV techniques applied to a reactor to obtain water velocity data. However, no details are given on the PIV experimental setup, the operating parameters or the collection, and processing of the data. Moreover, simulated vs experimental results are compared in terms of the dimensionless velocity, but the non-dimensional equations used are not provided. It is also not clear for what height of the reactor the results were collected. Therefore, the lack of details would make it challenging for other authors to use these experimental results for the validation of future CFD models.

Ren et al. (2009) used experiments to validate a hydraulic ISC model. A CFD model was used to study the flow patterns inside the reactors and to prove the discontinuity in the mixing behaviour within the reactor (decrease in dispersion along the axis). Therefore, the CFD model itself was not the object of study and validation, but rather a tool to aid the study of the ISC model.

The American Society of Mechanical Engineers (2009) mentions that validation would ideally cover a range of conditions within a domain of interest. In this context, some papers focused on validating the interphase momentum transfer between the phases by using solid, liquid and gas phases with similar properties to the ones of an operational reactor (D' Bastiani et al., 2020, 2021; Ruttithiwapanich et al., 2013). This allowed for the study of the phases using imaging methods such as PIV, shadowgraphy and particle tracking thanks to the transparent fluid used. One of the biggest challenges in this approach is how to inject the gas in a way that will mimic the biogas being generated inside the reactor and thus expand the bed (D' Bastiani et al., 2021).

Simplified two-phase models were used in some papers to study different design approaches (Wang et al., 2014a). Experimental limitations in the laboratory led some papers to perform single-phase validations (Yang et al., 2015).

As observed in Tables 1,2,3 and 4 there is very little agreement amongst the various papers on the best approach to simulate UASB, EGSB and IC reactors. Although one of the papers dates from 2007, most of the papers were published post-2013. The lack of high-quality, replicable data that can be used for the validation of CFD models is still a challenge in the development of validated AGSRs CFD models. While in some cases single-phase flows may be verified using analytical equations, three-phase flows cannot be verified analytically due to the complexity of the governing equations involved. Therefore, creating guidelines for the modelling and validation of UASB, EGSB and IC reactors would help advance the state of the art, allowing more focus to be put on the application of such models rather than on the development of said models. The creation of a database with validated test cases, and experimental data would also be of benefit. This challenge has also been highlighted by Nopens et al. (2020). They suggest the creation of a database containing successful cases of CFD validation, together with all the data, metadata as well as settings used in the CFD model. Moreover, they argue that the level and type of validation required should be linked to the modelling objective.

Looking ahead, it is worth thinking about what technologies are available for the validation of such models that have not been explored so far. While PIV experiments can yield valuable results, their applicability to opaque liquids is limited, which makes the collection of local velocities in operational AGSRs a challenge. One option would be the use of the ultrasonic velocity profiler technique, which can be applied to opaque fluids (Sardeshpande et al., 2011). The temperature at the outlet of the reactor has also been used as a support tool for the validation of CFD models when dealing with opaque flows (López-Jiménez et al., 2015) this method can be used as a support tool combined with other experimental data or when including heat transfer effects into the simulation.

To summarise, not all papers validate the CFD models used, and amongst the ones that do present some kind of validation, little to no reproducible/usable experimental data on operational reactors was provided. A bigger effort in providing enough details on papers to allow for the reproducibility and benchmarking of simulations is desirable for furthering the research and having more realistic CFD models of anaerobic granular sludge reactors.

5. Challenges and future perspectives in modelling AGSRs

The use of validated CFD models to predict the multiphase flow, accounting for the interfacial momentum transfer between the three phases present in anaerobic granular sludge reactors is still a challenge. It is generally accepted that the ultimate goal of having validated multiphase CFD models is the coupling with biokinetics models for accurate modelling of the biogas generation within the reactors, once hydrodynamics and biochemical effects are interdependent in this type of reactor. A functional coupled CFD-biokinetics model would allow for the scale-up of processes while correctly predicting the generation of biogas, and also taking into consideration realistic mixing conditions within the reactor. Some of the main challenges and hence opportunities for future work towards this end goal are listed hereafter.

The first and more complex challenge is the inclusion of the ADM1 model to predict biomass degradation as well as biogas generation. For that to be possible, a three-phase model must be used to account for the biomass as well the biogas inside the reactor.

The granules' apparent density is not fixed, as it is linked to the biogas generated. Including the effects of the granular apparent density changes due to bubble entrapment/attachment would lead to a better prediction of the movement of the granules in the sludge bed as well as the effects of granular wash-out. Thus, leading to a more accurate prediction of loss of biomass.

The inclusion of granule growth and breakage modelling would allow for the dynamics of the sludge bed to be studied in more detail.

The complexity of the multiphase models, in particular the modelling of the granular phase, leads to large computational times. More effort should be put into developing strategies to reduce the computational time required, in a way that their use in the daily activities of design and analysis of reactors would be feasible. These possibilities could include the application of advanced and novel methods which have not been explored yet in the simulation of AGSRs such as:

- the lattice Boltzmann method,
- meshless methods such as smoothed particle hydrodynamics,
- machine learning methods applied to CFD,
- parallelisation of codes using GPUs.

Most papers reviewed applied the Eulerian-Eulerian approach to the multiphase simulations. However, considering the low volumetric fraction of the gas phase, creating gas injection sites within the sludge bed by adopting a Lagrangian approach for the modelling of the gas phase could allow for a more realistic approach to the generation of biogas within the sludge bed than the approaches adopted so far. The feasibility of using this approach still needs to be researched further.

Including the effects of the heat transfer in the modelling would allow for the study of heat losses and the temperature distribution within the reactor in regions of cold weather.

Research on the most suitable models for the multiphase flow simulation would benefit the entire community, as not much research has been done on what approaches better describe the interaction between the phases in terms of:

- interfacial momentum transfer modelling,
- turbulence models, and
- time discretisation.

Furthermore, the application of techniques already used for other types of bioreactors, such as dynamic compartment models (Nadal-Rey et al., 2021), to couple CFD and biokinetics models can be investigated in future research. In addition, the scaling of the processes aided by CFD and experimental data can also be an alternative to reducing the simulation and modelling time when studying large reactors, as proposed by Haringa et al. (2017).

However, the biggest gap in knowledge remains the validation of the models using good-quality experimental data. No papers so far have reported the validation of a three-phase model against an operational biogas-generating reactor by showing a clear comparison between experimental and CFD results for each of the phases. The collection and dissemination of such experimental data would allow for the furthering of the state of the art in modelling AGSRs by enabling the validation of CFD models. Only by having high-quality experimental data to compare against, an in-depth study on possible model simplifications (e.g. geometry, 2D vs 3D, transient vs steady-state simulations) aiming to increase simulation speeds without losing accuracy will be possible. This will make it possible to quantify the loss in accuracy created by the simplifications. A question that remains is "What benefits the added layers of modelling will bring to the results?". It is important to highlight that the level of accuracy desired is directly linked to the objective of the simulation, and one should carefully analyse in what ways it will impact the final decisions supported by the results of the CFD simulations.

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.

Acknowledgements

The authors would like to acknowledge the Fiosraigh Scholarship Programme, Technological University Dublin and the Environmental Sustainability and Health Institute (ESHI) for facilitating the completion of this work.

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