CFD Analysis of Turbulence Models to Achieve the Digester Mixing Process

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Abstract

Mixing efficiency defines the features of physicochemical and biological reactions carried out in reactors or digesters. The reason for this influence is because it conditions the heat and mass transfer. That is why the mixing level and intensity become important aspects to study to know the effects they have on the processes. Furthermore, it should be noted that most of the mixing processes are carried out under turbulent conditions. Mixing enhancement evaluation is achieved in two ways, that is, experimentally and performing simulations. Simulations are based on numerical methods approximating solutions to results in line with reality. In this context, turbulence models applied in systems have great influence on the final numerical solution and, therefore, on the interpretation of improved mixing in reactors. It is also necessary to consider the influence of rheology in these simulations, since the working fluid does not always have a linear stress-strain relationship. In this way, an analysis of turbulence models and their applications in mixing characterization and the adequacy of these models to the reactor configuration and operating conditions is carried out. Mention is also made of the experiences around the study of turbulence in mixing tanks.

Keywords: turbulence models, mixing, digester, rheology, dead zones

1. Introduction

The use of biodigesters offers great advantages in energy production. The purpose of anaerobic digestion (AD) is the destruction of volatile solids by microorganisms in the absence of oxygen [1]. The AD is a common process to stabilize and reduce excesses or wastes of a different nature. For example, in a wastewater treatment plant and agricultural holdings, the AD allows a better treatment of animal or vegetable waste, by extracting much of the energy they contain. Besides, the use of biogas to generate electricity gives an additional value to the utilization of bioreactors in agricultural enterprises. The process of anaerobic digestion has several implications, and its effectiveness is based on aspects such as source, pH, temperature, reduction potential, hydraulic retention time (HRT) and mixing characteristics [2].

Mixing is one of the critical activities in the transformation process, a uniform mixture reduces the stratification, allows a better substrate dispersion, and if the mixture is not adequate, the digestion efficiency is reduced [3, 4]. When designing an anaerobic digestion system, the volume to be removed should be considered in relation to pump capacity, hydraulic retention time, sludge inflow rate, velocity gradient which relates the pump power, tank volume and sludge viscosity [1, 5].

Despite the technological advances in organic waste treatment, established mechanisms for design and operation require even more research. The AD is based on a combination of complex processes in which different residues are transformed mainly into a mixture composed of CH_4, CO_2 and H_2, which is called biogas [6].

Hydrodynamic performance of bioreactors is determined by the flow patterns inside. Consequently, biogas production is also conditioned by the reactor design, mainly referred to device dimensions and arrangement inside to favor the fluid movement and thereby generate the desired product [7]. Several models that allow relatively stable operation and provide desirable results have emerged. However, the punctual analysis of fluid movement inside the bioreactor is a complex issue mainly for the fluid characteristics, and of course by the geometry. This problem has been investigated using numerical methods, specifically computational fluid dynamics (CFD).

Digester design process involves several stages. A part is based on the calculation of organic loading rate as a function of temperature and input intensity. However, factors such as sedimentation, biogas, and sludge accumulation can influence on system hydrodynamic behavior and therefore on its removal efficiency. Generally, the predominance of mixed flows inside the reactor and its highly complex description is presumed, reason why a numerical discretization is attempted using CFD.

The evaluation and optimization of designs currently made with CFD allows to reduce the costs of prototype development [8]. Different studies have been conducted on improving hydrodynamic configurations using CFD [9, 10]. The use of CFD has allowed to understand that mixing is one of the most important activities for total solids reduction and biogas production. Despite the low speeds occurring inside a biodigester, it is advisable that the materials be completely mixed, so it is desirable to produce turbulence, which will be a function of rheological characteristics of fluid, flow rate, and dimensions and geometry of bioreactor.

Phenomena involving fluid movement at high velocities or in chaotic patterns can be inferred by turbulence models. Currently, robust turbulence models applicable to most physical processes have been developed. This is shown by the comparison of numerical solutions against experimental results.

With the addition of rheological properties of reaction materials, an appropriate turbulence model application for simulation becomes more complicated, since it is usual to find materials that do not present linear stress-strain behavior when flowing, that is, non-Newtonian fluids [11].

2. Factors affecting mixing

2.1. Geometric characteristics of containers

Flow dynamics of mixing process in anaerobic digesters has been analyzed from different standpoints. In waste degradation for energy generation, there are advances indicating the relevance of mixing process. Although good mixing can favor the material homogenization and exchange process between microorganisms and their environment, excessive mixing may also disrupt biological activities such as trophic processes [12, 13].

Studies on geometry influence in the mixing process include not only the container shape but also the shape of elements to generate movement inside the reactors. Agitation inside the anaerobic digestion containers is carried out mainly in the following three ways: (1) mechanical agitation with impellers, (2) pumped circulation and (3) gas recirculation [4].

The main type of reactor used in anaerobic digestion is the Continuous Stirred Tank Reactor (CSTR), from which various geometry investigations have been carried out, of flat bottom, conical, spherical or even egg-shaped reactors [14, 15]. The scale of the process is also a factor to be considered in the hydrodynamic performance of bioreactors, since there may be differences in performance when moving from a laboratory scale (**Figure 1**) to a full scale.

Large-scale agricultural waste treatment is commonly performed in covered lagoon digesters (**Figure 2**), which are reservoirs with a gas-tight cover mounted for biogas capture [10, 16]. Such reactors are used to exploit the methane production potential of animal waste. In these reactors, methane emission rates may vary depending on the covered lagoon area [17].

2.2. Fluid rheology

Total solids concentration in digestion fluids, besides having effects on degradation rate of organic matter, also has direct effects on rheological properties [14]. The study of fluid rheology entails the adjustment of CFD models to more real conditions [18, 19].

Figure 1. Laboratory-scale anaerobic reactor with pumped circulation.

Figure 2. Covered lagoon digesters for cow manure treatment.

Rheological behavior of fluids can be described by a basic diagram of shear rate against shear stress (**Figure 3**). The time-independent flow behavior is classified as Newtonian and non-Newtonian (shear thinning, shear thickening and yield stress) [11]. The rheological properties of non-Newtonian fluids greatly affect flow patterns, differing from those obtained with Newtonian fluids [19].

The description of nonlinear deformation of non-Newtonian fluids is characterized by generating rheological models, which must match experimental data that help obtain the value of model variables to be used. The rheological model application will depend on behavior and trend of experimental data, as well as the speed ranges achieved by the mixing equipment.

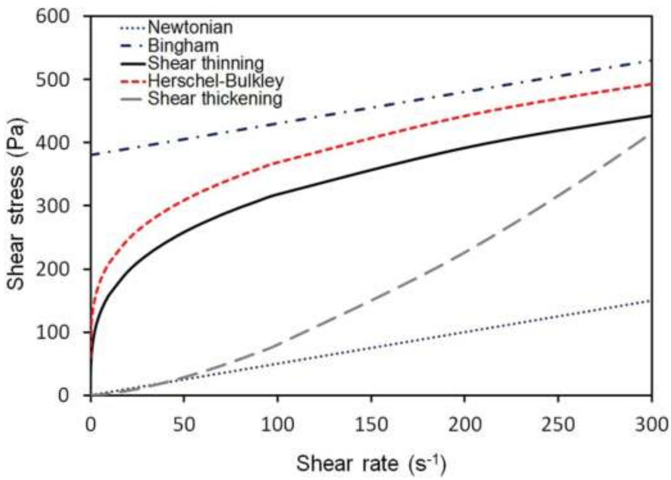

Figure 3. Shear rate versus shear stress for non-Newtonian fluids.

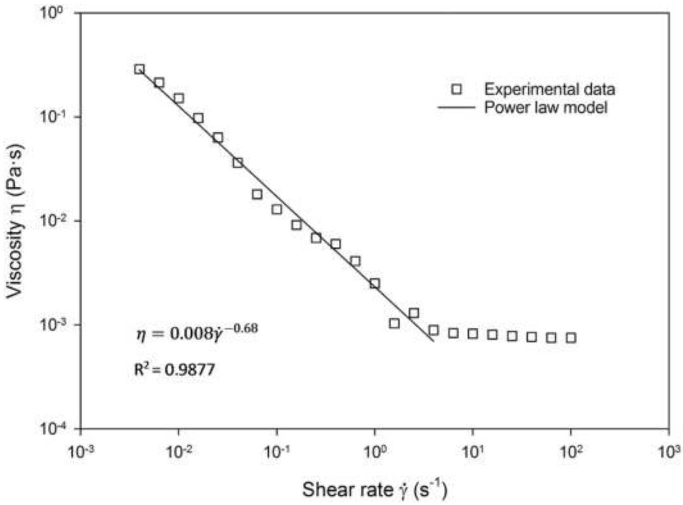

Figure 4. Flow curve of 4% cow manure and power law model fit to experimental data.

2.2.1. Power law model in rheology

The power law model (Eq. (1)) has been employed to adjust experimental data and to describe the rheological behavior of anaerobic digestion fluids [19].

$$\eta = k\dot{\gamma}^{n-1} \tag{1}$$

where η is viscosity, k is consistency coefficient, $\dot{\gamma}$ is shear rate and n is power law index.

Commercial CFD programs incorporate the power law model function for viscosity of non-Newtonian fluids. This model only fits to shear thinning region (**Figure 4**).

2.2.2. Herschel-Bulkley model

The capacities of the Herschel-Bulkley model (Eq. (2)) to show the sludge behavior before the flow occurs (very low shear stress) and when it begins to flow (shear stresses that exceed yield) make these yield stress models preferable in anaerobic digestion applications [20].

$$\tau = \tau_y + k\dot{\gamma}^{n} \tag{2}$$

where τ is shear stress, τ_y is yield stress, $\dot{\gamma}$ is shear rate, k and n are model factors.

2.2.3. Cross and Carreau viscosity models

The Cross (Eq. (3)) and Carreau (Eq. (4)) models are suitable to describe the shear dependence of aqueous dispersions [11].

$$\eta = \eta_\infty + \frac{\eta_0 - \eta_\infty}{1 + (K\dot{\gamma})^n} \quad (3)$$

$$\eta = \eta_\infty + \frac{\eta_0 - \eta_\infty}{[1 + (\lambda\dot{\gamma})^2]^N} \quad (4)$$

where η is non-Newtonian viscosity, η_∞ is viscosity in the lower Newtonian region, η_0 is viscosity in the upper Newtonian region, K and λ are time constants related to the relaxation times and n and N are dimensionless exponents.

These models have been employed to describe the flow curve of anaerobic sludge and model fluids with similar characteristics [21]. Although some commercial CFD packages have included rheological model functions, some authors have preferred to use user-defined functions (UDF) to incorporate them.

2.2.4. Use of model fluids

Fluid dynamics validations in anaerobic reactors usually use model fluids, which have rheological characteristics like digestion fluids, with the advantage of being translucent to allow the application of optical techniques for fluid movement visualization.

Xanthan gum solutions are non-Newtonian fluids that exhibit similar properties to various media used in anaerobic digestion [22]. The use of rheometers for determination of flow curves (**Figure 5**) is essential when determining the upper and lower Newtonian plateaus.

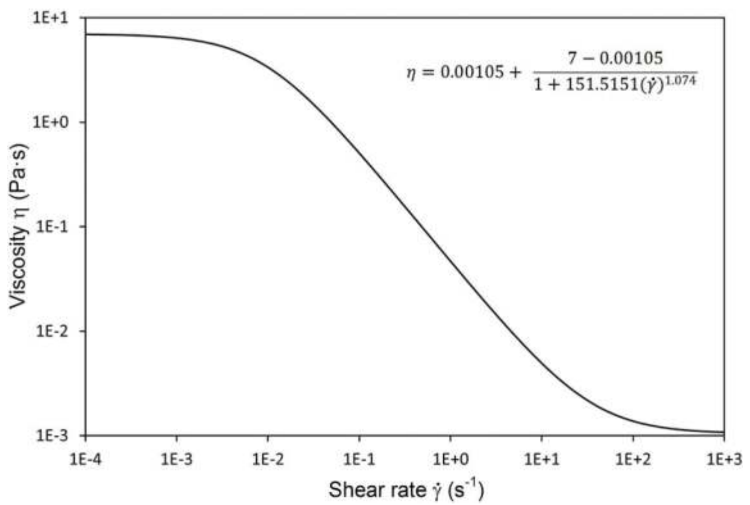

Figure 5. Flow curve of 0.05% xanthan gum solution and Cross viscosity model equation.

3. Turbulence models applied in characterization of mixing in bioreactors

Flow velocity, characteristic length and fluid properties are, among others, factors that define the flow type. Differences between the dynamic and kinematic viscosities can cause a turbulent flow, which in turn leads to the appearance of eddies whose description allows to infer mixing processes; however, due to the wide range of length and time scales that interact with each other, dynamic analysis is complex [23].

Turbulent flows are numerically simulated using methods such as Reynolds Average Navier-Stokes (RANS), Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES). Although the most accurate method is DNS, it has the disadvantage of being computationally more expensive. The RANS simulation method is the most used in turbulent flow simulations in bioreactors; however, another method that could be appropriate to model the turbulent mixing in bioreactors is the embedded LES [4].

In CFD applications, the effectiveness of several turbulence models has been evaluated to mixing characterization of non-Newtonian fluids in anaerobic digesters, such as the standard k-ε model, RNG k-ε model, realizable k-ε model, standard k-ω model, SST k-ω model and the Reynolds Stress Model [8, 24].

3.1. k-ε turbulence models

The k-ε turbulence model is widely used in commercial CFD programs. This model has been tested under different flow conditions and is numerically robust and computationally less expensive [25]. Applications include studies on mixing performance improvement in CSTR used in anaerobic digestion [26, 27]. The transport equations of the model are shown as follows [28]:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\varepsilon \tag{5}$$

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_i}(\rho\epsilon u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + C_{1\varepsilon}\frac{\varepsilon}{k}\left(G_k + C_{3\varepsilon}G_b\right) - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} \tag{6}$$

where ρ is liquid density, t is time, u is velocity, μ is viscosity, μ_t is turbulent viscosity, k and ε are turbulent kinetic energy and specific dissipation rate respectively, σ_k and σ_ε are turbulent Prandtl numbers, G_k represent the turbulent kinetic energy generation due to mean velocity gradients, G_b is turbulent kinetic energy generation due to buoyancy, $C_{1\varepsilon}$, $C_{2\varepsilon}$ and $C_{3\varepsilon}$ are constants.

3.2. k-ω turbulence models

The k-ω model has been applied to predict flow characteristics during the mixing of anaerobic sludge [8, 24]. This model is recommended when modeling the flow of non-Newtonian fluids to low Reynolds numbers [29]. The governing equations for turbulent kinetic energy and the specific rate of dissipation are as follows [30]:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}\left(\rho u_j k\right) = \rho \tau_{ij} \frac{\partial u_i}{\partial x_j} - \beta^* \rho k \omega + \frac{\partial}{\partial x_j}\left[\left(\mu + \sigma^* \frac{\rho k}{\omega}\right) \frac{\partial k}{\partial x_j}\right] \quad (7)$$

$$\frac{\partial}{\partial t}(\rho \omega) + \frac{\partial}{\partial x_j}\left(\rho u_j \omega\right) = \alpha \frac{\omega}{k} \rho \tau_{ij} \frac{\partial u_i}{\partial x_j} - \beta \rho \omega^2 + \sigma_d \frac{\rho}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} + \frac{\partial}{\partial x_j}\left[\left(\mu + \sigma \frac{\rho k}{\omega}\right) \frac{\partial \omega}{\partial x_j}\right] \quad (8)$$

where p is static pressure, τ_{ij} is the Reynolds stress tensor, β and σ are body forces and k and ω are turbulent kinetic energy and specific dissipation rate, respectively.

4. Phenomenology of the CFD process applied in mixing of bioreactors

Mixing consists of making a uniform combination of two or more components, so it is present in many processes [31]. When analyzing air change rates of natural ventilation in buildings designated for agricultural or livestock production, the mixing is present.

In industrial processes where chemical reactions are carried out, mixing promotes contact between the reactants improving process efficiency. Particularly in bioreaction processes, mixing influences substrate and product transport toward and from the location of conversion by microorganisms [32].

The effect of different modes of mixing on biogas production has been studied [3]. The main modes of mixing in biodigesters are as follows: biogas recirculation, impeller mixing and pumped circulation [33]. The mixing methods have greater impact when dealing with higher solids content materials. Often, the increase in the concentration of total solids in digestate generates important rheological changes.

4.1. Temperature and density gradients in fluid modeling

Fluid motion can occur on a temperature gradient and, consequently, mass transport phenomena by convection. Two models are basic for the analysis of this phenomenon: flotation model for natural convection, which considers the variation of density as a function of temperature and the Boussinesq model (Eq. (9)) that has given adequate results [34].

$$\rho = \rho_i\left[1 - \beta(T - T_i)\right] \quad (9)$$

where ρ is density, β is the thermal expansion coefficient and T is temperature.

The fluid movement assumes a mixture of liquid, vapor and nonconsumable gases. The standard equation governing the mixing model and the mixing turbulence model describing the flow of the mass vapor fraction (f) can be written as follows [35]:

$$\frac{\partial}{\partial \varepsilon}(\rho f) + \nabla\left(\rho \vec{v}_V f\right) = \nabla(\gamma \nabla f) + R_e - R_c \quad (10)$$

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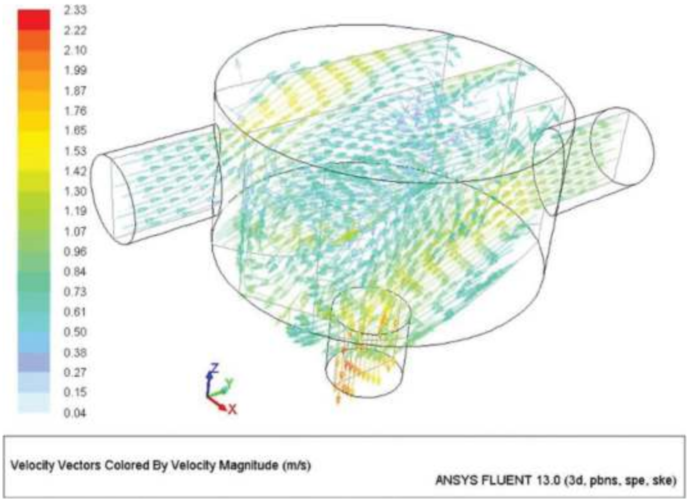

Figure 6. Detail of the velocity vectors in the container (m s^{-1}).

where v is velocity vector, γ is the effective exchange coefficient and R_e and R_c are terms included in the steam generation and condensation rate (rate of phase change).

Figure 6 shows the spatial distribution of velocity vectors, which leads to the entry of two solutions, under different fluid characteristics. According to the hypotheses presented, it is a turbulent flow whose centrifugal forces favor the separation of emulsions. Velocity increase at the exit of digester causes a change in mixture viscosity and consequently its ability to flow.

Because of the boundary conditions and flow characteristics, temperature distribution and corresponding density are shown in **Figures 7** and **8**, respectively. A parameter to qualify the process is the uniformity in the mixing, which in turn will be in function of the content of the solutions.

4.2. Flow patterns in single-phase models

To evaluate hydrodynamic performance of anaerobic reactors, single-phase CFD models have been used [14, 19]. In these models, it is assumed that multiphase effects such as sedimentation of solids, bubble formation and biogas flow in the aqueous phase are negligible.

4.2.1. Covered lagoon digester

The treatment of large-scale organic wastes is carried out in covered lagoon reactors (**Figure 9**). In these reactors, it is usual to find stagnant zones, where the flow velocity is very low and affects the anaerobic digestion process efficiency. Reduction of stagnant areas in covered lagoon reactors is a challenge that has been addressed through the CFD model generation.

The flow model consists of continuity (Eq. (11)) and Navier-Stokes equations for linear motion conservation (Eq. (12)) in its vector form at steady state, incompressible and isothermal flow [36].

$$\nabla \cdot \vec{v} = 0 \tag{11}$$

$$\rho[\nabla \cdot (\vec{v}\vec{v})] = -\nabla \cdot P + \nabla \cdot (\overline{\overline{\tau}}) + \overline{\overline{F}} \tag{12}$$

where $\overline{\overline{\tau}}$ is defined by Eq. (13).

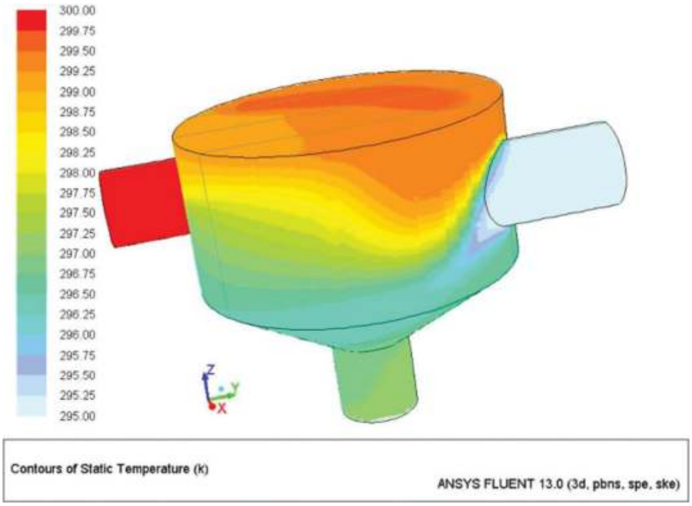

Figure 7. Temperature contours (*K*) in mixing reactor.

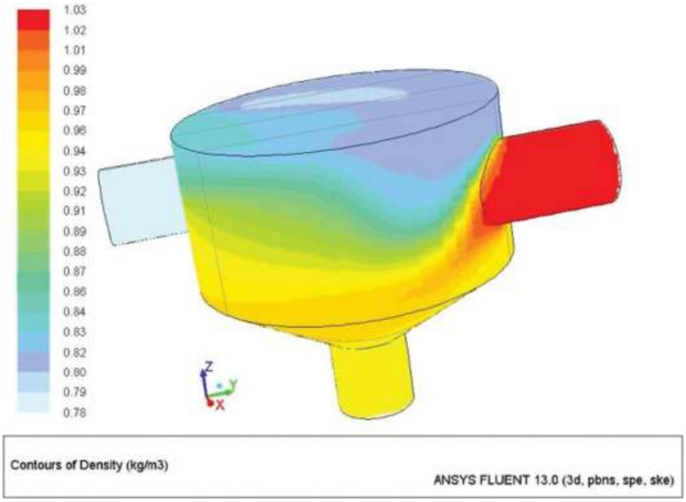

Figure 8. Density contours (kg m^{-3}) in mixing digester.

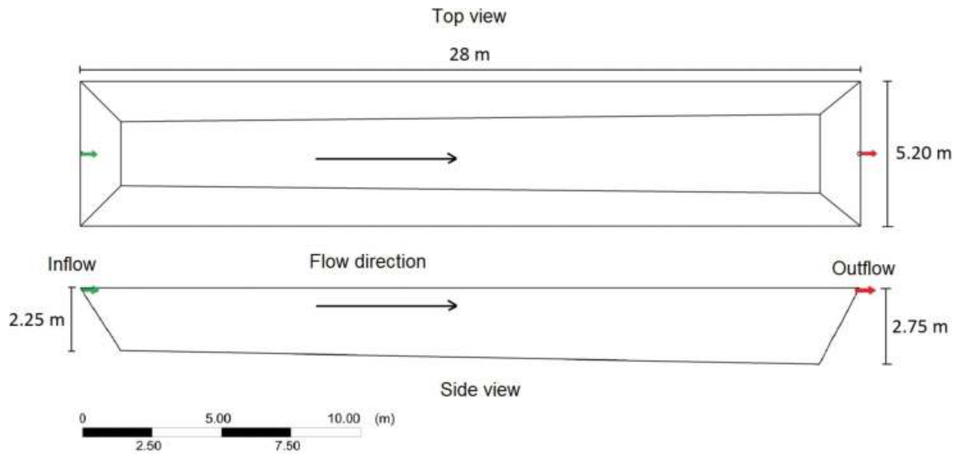

Figure 9. Covered lagoon digester model.

$$\overline{\overline{\tau}} = \mu \left[(\nabla \cdot \vec{v} + \nabla \cdot \vec{v}^{T}) - \frac{2}{3} \nabla \cdot \vec{v} I \right] \tag{13}$$

For the local turbulence calculations, transport equations for turbulent kinetic energy (k) and specific dissipation rate (ω) must be solved (Eqs. (7) and (8)). The incorporation of the Cross viscosity model to define the fluid rheology is done by programming and importing a user-defined function (UDF).

The hydrodynamic performance enhancement is achieved by recirculation incorporation in strategic sites. Streamlines (**Figure 10**) in the original configuration have two large swirls at the inflow; however, in most of the reactor, very low speeds are encountered. Vectors (**Figure 11**) show a velocity increase at the top and middle of the reactor when a recirculation is employed, which improves mixing and sludge digestion.

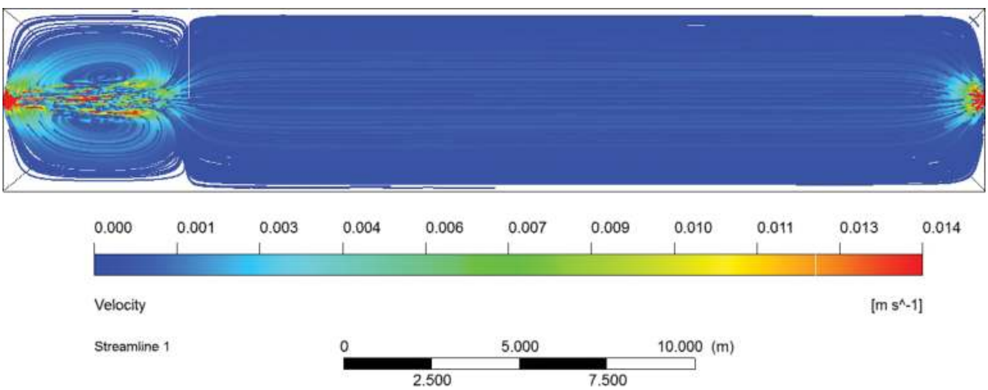

Figure 10. Streamlines in a top view of covered lagoon reactor.

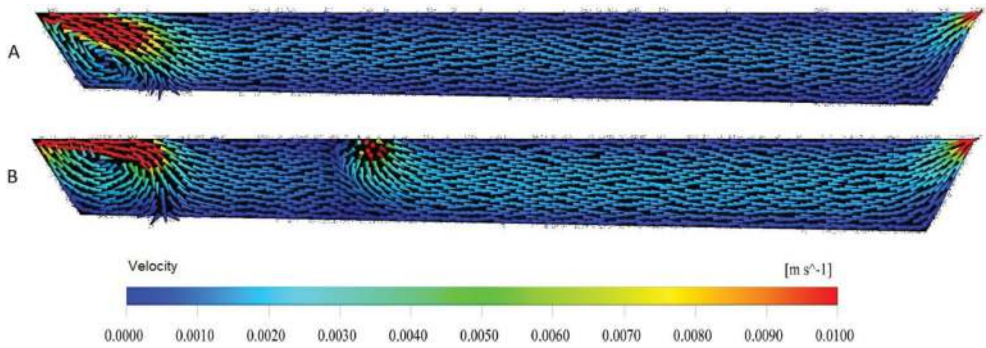

Figure 11. Velocity vectors in configuration A (without recirculation) and B (with recirculation).

4.2.2. Anaerobic reactor with recirculating jets

Currently, the mixing by recirculating jets (**Figure 12a**) is used in industrial digesters to treat organic wastes. Usually these are containers provided with submerged jets pointing downward and have the function of recirculating the digestion fluid by the action of a pump [15]. For single-phase CFD model development, the geometry is simplified by delimiting the part corresponding to the liquid (**Figure 12b** and **c**).

The inflow pipe length influences the velocity distribution within the container. **Figure 13** shows that higher velocity is at reactor bottom, whereby a better homogenization is achieved because the bottom sediments are entrained by the generated stream and are dispersed throughout the reactor.

4.3. Multiphase flow

Although mixing modeling has been approached considering that flow in reactor is a single phase, cases in which the multiphase effect is considerable have also been considered [37].

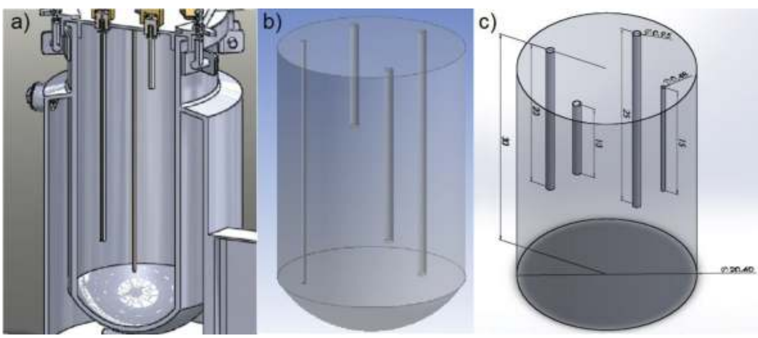

Figure 12. (a) The inside of a reactor with recirculating jets, (b) configuration of the jets in the liquid phase and (c) different jet configuration.

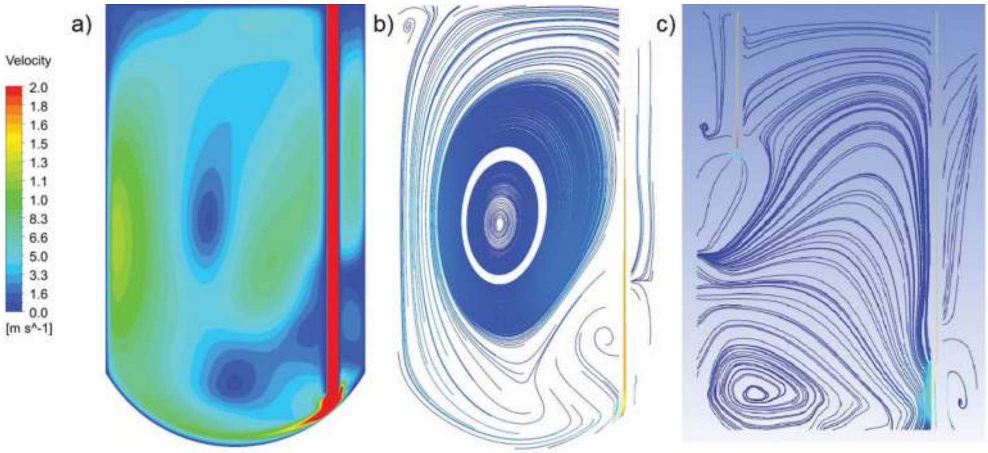

Figure 13. (a) Reactor velocity contours with recirculating jets, (b) streamlines generated by spherical bottom and (c) streamlines on changing reactor bottom and jets length.

Mixing modeling in anaerobic digestion processes should be approached considering the multiple phases involved in the process. The approaches used for multiphase flow description can be grouped into two types: the Eulerian approach and the Lagrangian approach [33].

4.4. Dead space in mixing vessels

Mixing dead zones detection is performed to improve mixing in digesters. Recirculation incorporation causes disturbances and material movement inside the digester and reduces dead spaces, increasing biogas production due to a better microorganism distribution in material.

To define a dead space (**Figure 14**), the concept of hydraulic retention time (HRT) has been used, that is, the time it takes the material to perform the path from inflow to outflow of digester [38]; mathematically, it is defined as follows:

$$HRT = \frac{V}{Q} \tag{14}$$

where V is total volume of digester and Q is volumetric flow at the digester inlet.

Volumetric flow (Q) causes the material to have a certain mean velocity within the digester, whose magnitude is a result of the velocity vector ($\vec{v}$), which has components in x, y, z (u, v, w). Therefore, to calculate the limit velocity to define a dead space, the following mathematical relationship is used.

$$v_{dead\ zone} \leq \frac{reactor\ lenght}{\sqrt{3}\ (HRT)} \tag{15}$$

Those regions where the velocity is less than or equal to the limit velocity ($\vec{v} \leq v_{dead\ zone}$) are considered as dead space.

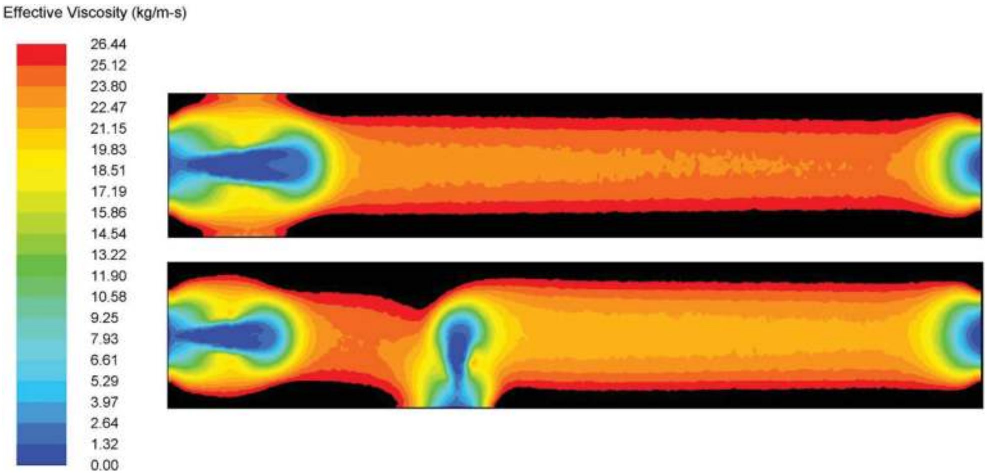

Figure 14. Dead space (black area) in different inflow configurations.

5. Conclusions

The mixing processes in anaerobic reactors are influenced not only by the inlet and outlet flows but also by the rheological properties of the fluid and the geometric characteristics of the reactor. There is an optimum mixing intensity that can maximize energy production with the lowest energy input possible for mixing. Beyond a point, there are no returns in terms of methane generation with increasing energy input. The variability of anaerobic digestion involves the application of different turbulence models of turbulence, which must be analyzed to determine the adjustment of results obtained with reality.

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