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ESTIMATION OF THE SPATIAL DISTRIBUTION OF SUBSTANCES IN ANAEROBIC DIGESTION TANKS WITH CFD

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Abstract

Anaerobic digestion (AD) is used in wastewater treatment plants (WWTPs) to decompose organic matter. Highly efficient AD tanks are able to mix biochemical substances within the tank, and – in order to assess such spatial distribution of substances - a proper modelling method is necessary. Computational fluid dynamics (CFD) is a simulation tool for modelling fluid flows in WWTPs, but there is a lack of studies on CFD modelling of hydrodynamics together with an integrated modelling of bio-kinetics due to the complexity of biochemical reactions in AD processes. The current study aims at estimating the distribution of biochemical components within an AD tank. For doing this, an integrated modelling of hydrodynamics and bio-kinetics is conducted, in order to assess mixing quality. The novelty of the work is the derivation of a new AD-related solver in an open source CFD platform.

As the first step, the hydrodynamics of the fluid flow in our WWTP are estimated through iterative solution of fluid flow equations, and subsequently, by fixing the obtained velocity vector field, bio-kinetic equations are applied to the flow field. The bio-kinetics in our solver are based on ADM1, the state of the art transient model for AD process. The validation of our developed solver is done by comparing the results to a fully-mixed digester in an experimental setup. Then, the results of our hydrodynamic modelling are shown as the velocity profile and streamlines. Subsequently, regarding bio-kinetics, the concentrations of substances are estimated and plotted during the simulation time. In order to evaluate the distribution of the organic material within the tank, the uniformity index for the substances is analysed.

Keywords
wastewater treatment plant modelling, computational fluid dynamics, anaerobic digestion modelling, ADM1 modelling.

1 INTRODUCTION

Anaerobic digestion (AD) is often used in wastewater treatment plants (WWTPs) to decompose organic matter. Based on organic loading rate, mixing and the geometry of digesters, the distribution of biochemical components can vary. Mixing in anaerobic digestion (AD) tanks is of importance, to assure proper stabilizing organic wastes and efficient biogas production [1]. Computational fluid dynamics (CFD) are a valuable tool for investigating the flow field within digesters [2]. However, how to set proper initial and boundary conditions has always been an important question. e.g., the inlet configuration is an important issue in case of sludge recirculation [3]. Although many CFD investigations have been done to model the behaviour of mixers and gas injection in bioreactors, fluid recirculation specifications need to be investigated as well [4]. Additionally, mixing time should be analysed to give insight about the effect of the inlet configuration. Thus, we need to model a transient setup in real-scale to investigate sludge recirculation. In order to assure a homogeneous distribution of substrates, a proper modelling method is necessary.

Computational fluid dynamics (CFD) is a simulation tool for modelling fluid flows in AD tanks [5, 6]. CFD modelling of hydrodynamics together with an integrated modelling of bio-kinetics makes a recipe for a comprehensive modelling method in AD tanks. However, due to complexity of biochemical reactions in AD process, current CFD modelling studies usually focus mainly on the fluid flow within the digester, rather than the bio-kinetics [7, 8]. Thus, this study aims at estimating the distribution of biochemical components within an AD tank, which employs a sludge recirculation system, through an integrated modelling of hydrodynamics and bio-kinetics.

In the following, investigate the behaviour of the real world AIZ wastewater treatment plant in Tyrol, Austria represented by means of a full-scale model. The sludge is recirculated within the AD tank and through our two-step method the distribution of the biochemical material is estimated in 100 days, by using the CFD tool, OpenFOAM. The non-Newtonian characteristics of the sludge and proper turbulent enclosure are taken into account. The novelty of our project is applying ADM1 bio-kinetics to an open source CFD solver, which promotes the potential use of ADM1 in CFD platforms, in order to assess mixing quality in WWTPs.

2 METHOD

2.1 Procedure

In this study, initially, the hydrodynamics of the sludge recirculation is evaluated through an iterative solution of fluid flow equations (the geometry, meshing procedure, and the mixing simulation are also published in [9]), and subsequently, by fixing the obtained velocity field, bio-kinetic equations are applied to the velocity field. This is because there is a huge difference between of the required simulation time steps for fluid flows and in biochemical reactions.

2.2 Hydrodynamics modelling

Our case study is an egg-shaped AD tank, whose diameter reaches up to 15.4 m at the middle. The height of the sludge level is about 22.9 m. The outlet tube is 0.2 m in diameter, located at the bottom of the digester and extended from inside to the outside of the tank. According to [9], the splashing inlet configuration is investigated as emulating the sludge recirculation within the tank.

After designing the geometry a mesh analysis study is a necessity, in order to implement a proper mesh, which is explained in [9]. The final mesh network consists of 404878 elements.

For obtaining the hydrodynamics, a steady-state solver, simpleFoam, for incompressible flow is employed in OpenFOAM, which is an open source CFD software, based on finite volume method. This solver utilises the equations of conservation for mass (continuity) and momentum (Navier-Stokes).

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{V}) = 0 \tag{1}$$

$$\frac{\partial (\rho \vec{V})}{\partial t} + \vec{\nabla}(\rho \vec{V} \vec{V}) = -\vec{\nabla} \mathrm{p} + \vec{\nabla} \cdot (\bar{\bar{\tau}}) \tag{2}$$

where t is the time (for transient simulation), ρ is the density of the fluid and $\vec{V}$ is the fluid velocity, p represents the static pressure and $\bar{\bar{\tau}}$ is the stress tensor

In addition, since we have a high Reynolds number, we need to use a turbulent enclosure sub-model, which in this case we choose as k-ε model due to its robustness. Additionally, for modelling the non-Newtonian behaviour of the sludge, the power law equation is used, taking into account the total solids (TS) concentration of 5% (see [9]).

2.3 Bio-kinetics modelling

The bio-kinetics within an AD tank are based on ADM1, a comprehensive dynamic model for AD processes [10]. The concentration of ADM1 components are estimated through scalar transport equations [11]. ADM1 equations are classified in the following. With the start of the digestion process, the biomass (X_c) is disintegrated:

$$\frac{dX_i}{dt} = k_{dis}X_c \tag{3}$$

where X_i is the either carbohydrates, proteins or lipids, and k_{dis} is disintegration rate. Then, the first step in AD is the hydrolysis of the material, which is calculated as follows:

$$\frac{dS_{sub}}{dt} = k_{hyd,i}X_i \tag{4}$$

where S_{sub} is the concentration of produced substrate and $k_{hyd,i}$ is the hydrolysis rate. Afterwards, the uptake rate of each soluble substrate depends on its own concentration:

$$\frac{dS_{sub}}{dt} = k_{m,i}\frac{S_{sub}}{K_{S,i} + S_{sub}}X_{bac}I \tag{5}$$

where $k_{m,i}$ and $K_{S,i}$ are the Monod maximum rate of uptake and half saturation value for the process i. X_{bac} is the bacteria and I represent the inhibitions, which are classified as pH, nitrogen, ammonia and hydrogen inhibitions. The decay rate of bacteria should be considered as follows:

$$\frac{dX_i}{dt} = k_{dec,i}X_i \tag{6}$$

where $k_{dec,i}$ is the decay rate for each degrader bacteria.

The hydrodynamic equations are solved through an OpenFOAM solver, simpleFoam in steady-state, and the bio-kinetic equations are solved via a developed solver that we denote as passivScalarADMFoam.

3 VALIDATION

3.1 Hydrodynamics validation

As we have conducted our model in 2D, a two-step simulation set should be conducted for comparing the 2D and the 3D results, which has been done and explained in [9].

Moreover, regarding validation of hydrodynamics, the velocity profile at the centre of the AD tank as computed by OpenFOAM is compared to a previously validated ANSYS Fluent simulation results – see [9]. Both OpenFOAM and ANSYS results depict a good match, with differences less than 1%.

3.2 Bio-kinetics validation

With regard to modelling the bio-kinetics within the AD tank, the model is validated by a previous experimental set in a fully-mixed lab-scale digester [12] as suggested by Wu [13]. They conducted a set of experiments at mesophilic temperature in a 25-day period. The digester had 0.06 m3 volume and was fed daily with 0.63 kg COD/m^3 of biomass.

As the model is fully-mixed - for validation purposes - we can remove the spatial variation in our calculation domain and reduce the mesh network to a single cell with an inlet and an outlet. A single vector represents the velocity field within the cell, the amount of which corresponds to the 25-day HRT in the tank. *Figure 1* shows the results of our passiveScalarADMFoam solver, compared to Fatolahi experiments [12], where only 9% of difference is observed between the biogas yield in our solver and Fatolahi experiments, which validates the efficiency of our developed solver.

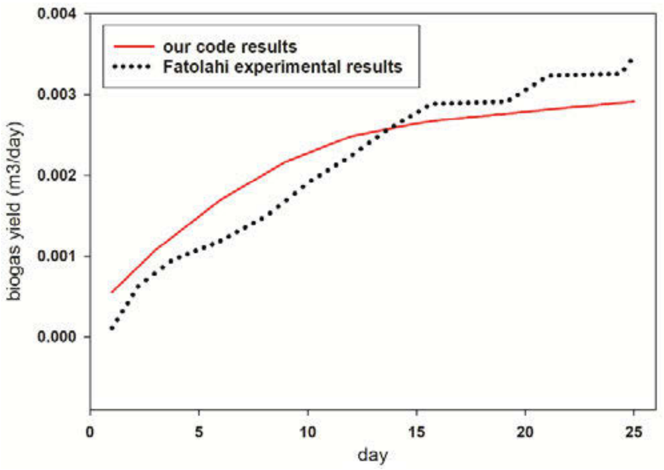
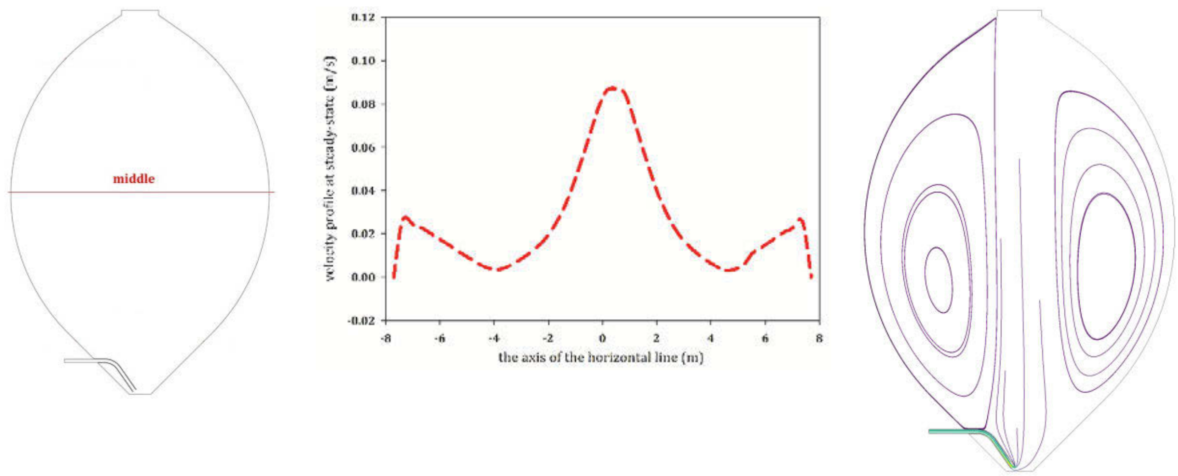


Figure 1 comparing the results of our passiveScalarADMFoam solver to Fatolahi experiments

4 RESULTS AND DISCUSSION

4.1 Hydrodynamics results

Regarding the hydrodynamics of the model, the results of the steady-state simulation are depicted as velocity profiles at the central line at the middle of the digester, 11 m from the bottom. Moreover, the streamlines of the fluid flow are displayed, in order to give an insight on the behaviour of the fluid flow within the tank. *Figure 2*(a) shows the velocity profiles at the central horizontal line and the streamlines.



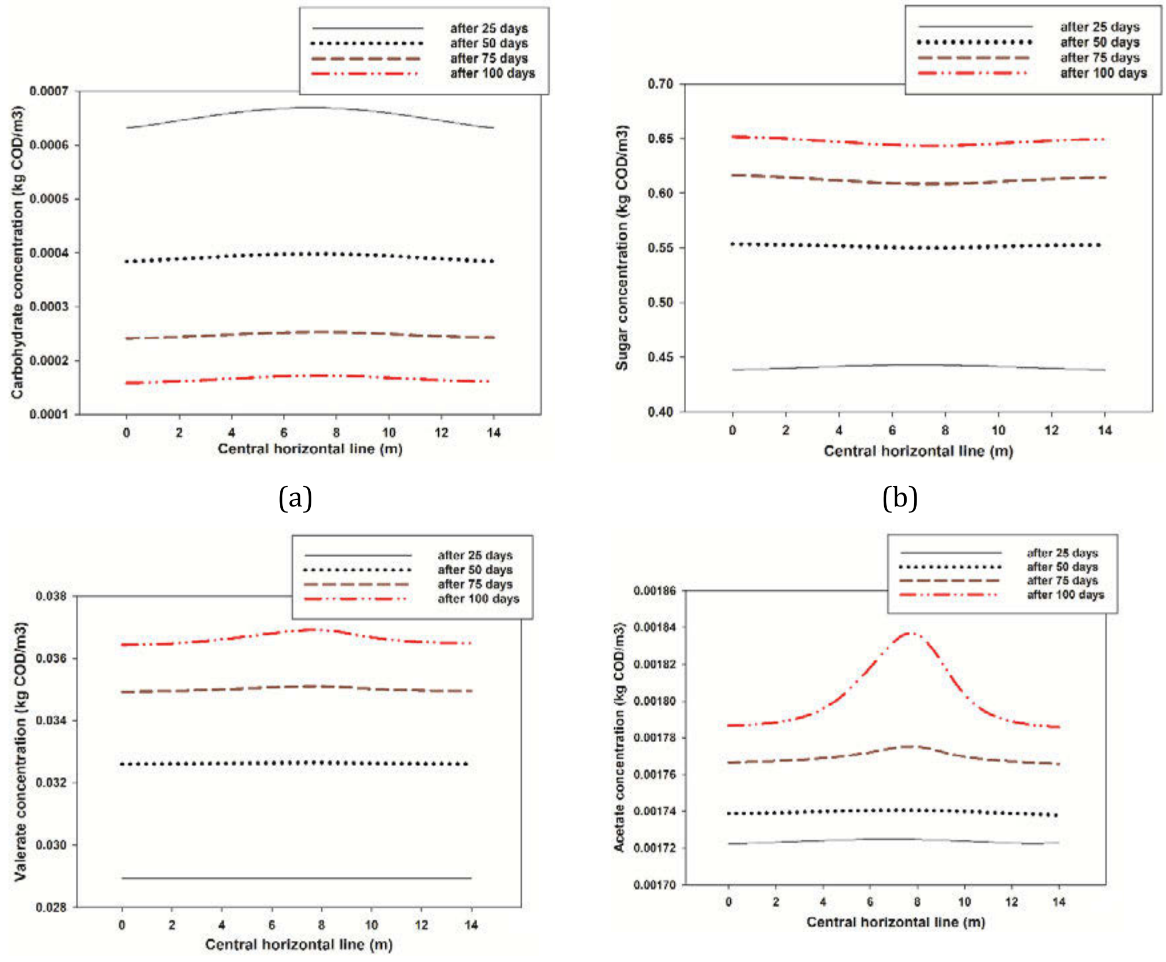
(a) (b) (c)

Figure 2 the central horizontal line (a), the velocity profile at the central horizontal line (b), the streamlines within the tank (c)

Figure 2(a) shows the location of the central line, which later is used for showing the concentration of bio-kinetic substances. The velocity profile along the central line in *Figure 2*(b) depicts that the maximum velocity at the centre is about 0.085 m/s. The plot also shows that a higher velocity range is formed at the center of the tank, while a smaller increase in at the regions close to the wall represent the upward flow regime at the two lateral sides. This is better shown in *Figure 2*(c), where the streamlines illustrate the creation of two circular flow regime within the tank. Still, the downward flow in the tank is more dominant than the upward flow near the walls.

4.2 Bio-kinetic results

The concentration of the substances is plotted for each component along the central line of the digester (located 11 m from the bottom). Here, we display only the concentration of the substances that are representative of the various steps of the AD process. The first step is the disintegration of the biomass, from which hydrocarbons are produced. Thus, *Figure 3*(a) shows the amount of hydrocarbons concentration along with the central line during a constant distributed times within 100 days of ADM1 simulation, that is, after 25, 50, 75 and 100 days. The next step is hydrolysis, and one of its products is sugar. Hence, sugar is also plotted in *Figure 3*(b). Similarly, the concentrations of valerate, as the product of acidogenesis, and the concentration of acetate, as the product of acetogenesis is plotted within the mentioned times, and shown in *Figure 3*(c) and *Figure 3*(d), respectively.



(a) (b) (c) (d)

Figure 3 the substrates concentration along with the central horizontal line in the tank

From the four substance concentration profiles at the horizontal line located at the centre of the tank it is clear that there is little variation along the central line, that is, the distribution of the materials are almost evenly within the tank. However, after 100 days the distribution of the acetate is less homogenous as compared to other plotted substances. *Figure 3*(a) shows that the concentration of carbohydrates decreases during the simulation time. After 25 days, it is more than $6*10^{-4}$ kg COD/m^3, while it decreases to less than $6*10^{-4}$ kg COD/m^3 after 100 days. Carbohydrate, as the product of disintegration, is the only substance which decreases along the time. Sugar (from 0.44 to 0.65 kg COD/m^3), Valerate (from less than $2.9*10^{-2}$ to more than $3.6*10^{-}$

2 kg COD/m3) and Acetate (from 1.72*10-3 to more than 1.78*10-3 kg COD/m3) increase during the time.

Regarding the homogeneity of the substances in the tank, the uniformity index is suggested in [14], which is calculated as follows:

$$\gamma = \left(1 - \frac{\sum_{i=1}^{n}(|\varphi_i - \bar{\varphi}|A_i)}{2\bar{\varphi}\sum_{i=1}^{n}(A_i)}\right) * 100 \qquad (7)$$

where A_i and φ_i are the area of the ith cell and its corresponding scalar variable, respectively, and $\bar{\varphi}$ is the mean value for each variable on the surface.

In order to have a good mixing quality, the uniformity index of all the substances should be high enough. This is true for most of the components. *Figure 4* shows the uniformity index of the analysed material during the 100 days of the simulation time. Since it is assumed that the materials initially are distributed equally at the beginning of the simulation, the uniformity index is 100% at the first day. Among the plotted substances, the uniformity index of sugar and Valerate stays above 95%, however the uniformity index of carbohydrates reaches only above 80%. The uniformity index for acetate does not goes below 70%. These values prove that the recirculation system of the AD tank accounts for an almost even distribution of the material i.e., for a proper mixing of tank.

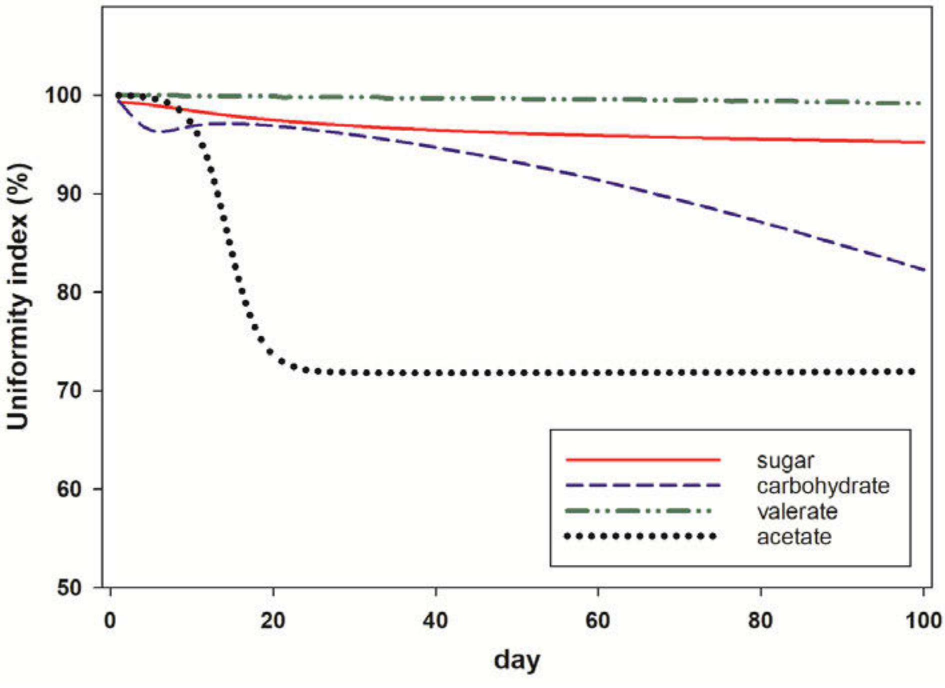


Figure 4 the uniformity index of the analyzed substances during the 100-day period

5 CONCLUSIONS

This paper promotes the potential use of ADM1 in CFD platforms, by applying ADM1 to an open source CFD platform (OpenFOAM). The developed solver is called passiveScalarADMFoam and is employed exemplarily for assessing the mixing quality of sludge recirculation system in the real world case study AIZ WWTP, located in Austria. After calculating the hydrodynamics of mixing and the validation of the solver via experimental case-studies, the following points are concluded:

- The velocity at the centre of the investigated tank does not exceed 0.085 m/s, and it is higher at the center than the regions near the walls.
- Two circular flow regimes are formed within the tank, due to the sludge recirculation (see *Figure 2*(c)).
- The results of passiveScalarADMFoam solver are compared to Fatolahi experiments. Due to low difference in the resulting biogas yield, we conclude the efficiency of our developed solver.
- Carbohydrate, as the product of disintegration, decreases along the time, but other investigated substances, i.e. sugar, valerate and acetate increase.
- The uniformity index of the substances within the tank is not lower than 70%, which proves the efficiency of the recirculation mixing strategy in our studies WWTP.

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