Validation of computational non-Newtonian fluid model for membrane bioreactor
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ABSTRACT

Membrane bioreactor (MBR) systems are often considered as the wastewater treatment method of the future due to their high effluent quality. One of the main problems with such systems is a relative large energy consumption, compared to conventional activated sludge (CAS) systems, which has led to further research in this specific area. A powerful tool for optimizing MBR-systems is computational fluid dynamics (CFD) modelling, which gives researchers the ability to describe the flow in the systems. A parameter which is often neglected in such models is the non-Newtonian properties of active sludge, which is of great importance for MBR systems since they operate at sludge concentrations up to a factor of 10 compared to CAS systems, resulting in strongly shear thinning liquids. A CFD-model is validated against measurements conducted in a system with rotating cross-flow membranes submerged in non-Newtonian liquids, where tangential velocities are measured with a Laser Doppler Anemometer (LDA). The CFD model is found to be capable of modelling the correct velocities in a range of setups, making CFD models a powerful tool for optimization of MBR systems.

Key words | CFD, MBR, modelling, non-Newtonian, rheology

NOMENCLATURE

\( k \) consistency factor (Pa s\(^3\))
\( n \) power law exponent (-)
PSD particle size distribution (-)
\( r \) radius (m)
\( \text{Re}_{\text{TAN}} \) non-Newtonian radial Reynolds number (-)
\( T_\lambda \) transmittance (-)
TSS total suspended solids (kg m\(^{-3}\))
\( u_f \) friction velocity (m s\(^{-1}\))
\( y^+ \) dimensionless relative distance from wall (-)
\( y \) distance from wall (m)
\( \dot{\gamma} \) shear rate (s\(^{-1}\))
\( \mu \) dynamic viscosity (Pa s)
\( \nu \) kinematic viscosity (m\(^2\) s\(^{-1}\))
\( \omega \) angular velocity (rad s\(^{-1}\))
\( \rho \) density (kg m\(^{-3}\))
\( \tau \) shear stress (Pa)

INTRODUCTION

Membrane bioreactor (MBR) systems as a method for cleaning wastewater have been subject to intensive research in recent years, because of their high quality effluent. MBR systems are a combination of biological processes consuming organic content and nutrients into bigger particles and the filtration performed by the membranes retaining the particles larger than the pore size of the membranes. Fouling of membranes during the filtration, resulting in lower permeate flux through the membranes and thereby lower effectiveness, is one of the major drawbacks for MBR systems. Several principles are used to decrease the fouling of the membranes; one such way to do this is with shear-enhanced systems. The principle is to create a high shear stress at the surface of the membranes, scouring the membranes and thereby minimizing fouling, for example created by rotating cross-flow (RCF) membranes. The increase of the flux through the membranes with higher shear stresses has been proved by experimental setups (Tardieu et al. 1999; Jørgensen et al. 2014). Computational fluid dynamics (CFD) models can be used to determine the shear stresses on the membranes and thereby the antifouling impact. Several sources have described modelling of such systems, e.g. Bentzen et al. (2012) where the model was only validated against measurements of a physical setup with water, and Torras et al. (2006) where the CFD model was
compared with analytical approximations. This implies uncertainties since activated sludge (AS) shows pseudoplastic behaviour, and the shear thinning effect close to the membranes is of great importance where high shear rates are present. For AS the decrease of viscosity by increase of shear rate can be up to a factor of 100 (Rosenberger et al. 2002), hence this clearly affects the hydrodynamics and thereby, e.g. shear stresses. In this work, experiments were carried out with carboxymethyl cellulose (CMC) solutions as a surrogate for AS with shear thinning properties, for validation of the CFD model. The system was modelled with a laminar flow and with use of turbulence models, in order to validate the area of use for the different approaches.

METHODS

For validation of the CFD model, physical experiments were carried out on RCF submerged in CMC-solutions. The choice of non-Newtonian liquid was a high molecular weight CMC solution, since it is a shear thinning liquid like AS, plus the solutions are clear enough for measuring velocities with a Laser Doppler Anemometer (1D Flowlite LDA, Dantec). A shear thinning liquid is characterized by viscosity decreases when higher shear rates are noted; one way to describe such liquids is shown in Equation (2).

Even though xanthan gum (XG) has been described as a better surrogate to describe the rheology of AS than CMC (Buetehorn et al. 2010), it could not be used in this experiment due to the low clarity level of the liquid. The transmittance of the liquids at a given wavelength is given from the relation between incoming intensity of radiation $I_0$ and the intensity $I$ coming out of the sample, described by Equation (1).

$$ T_{\lambda} = \frac{I}{I_0} $$  

The transmittance was determined for solutions with both CMC and XG for light with a wavelength of 633 nm (the wavelength of LDA) and the results are illustrated in Figure 1. Due to the low transmittance of the XG solutions they could not be used for the measurements with the LDA.

Experimental setup

The setup for the experiments consisted of a box with two ceramic membranes, mounted on a shaft, connected to a frequency-regulated motor facilitating the rotation of the membranes with an angular velocity of 120 rpm. Three different setups were used for validation of the model, including two different geometric setups and three different concentrations of CMC. The first setup was with a concentric location of the membranes and a solution of CMC with a concentration of 2.0 g/l. To make sure the model was valid in a wide range of setups, the physical model was also made with an eccentric location of the membranes, illustrated in Figure 2(c) with CMC solutions of 1.5 g/l and 3.0 g/l.

The LDA measures the velocity at a given point (with a diameter of approximately 1 mm) in a given direction by the reflection from the particles in the fluid passing this point. The velocity profiles are determined along a line with the same distance to both membranes with different radial positions, and as a profile from membrane to membrane in a radius of 178 mm.

It was not possible to mount the membranes perfectly on the shaft. This resulted in small oscillations, which induced an uncertainty when determining the location of the measurement points for the velocity profile in radius of 178 mm in the size of ± 1 mm. The velocity normal to the membranes’ surface from the oscillations was, however, much smaller than the tangential velocity and was therefore not included in the CFD model.

The measurements were carried out at a room temperature of 20 °C.

The velocity profiles from the different setups were compared with the modelled velocities for the corresponding lines in the CFD model.
Rheology of surrogate

It is generally agreed that AS shows non-Newtonian behaviour and has shear thinning properties, but a consensus of how to describe the rheology has not yet been reached (Ratkovich et al. 2013). The most important parameters for the rheology of active sludge are the concentration of total suspended solids (TSS) and the particle size distribution (PSD), where the PSD will change over time due to flocculation/deflocculation in the AS (Naessens et al. 2012). Nevertheless, the rheology of AS is often described as a time independent liquid by the power law where the viscosity ($\mu$) is determined from the shear rate ($\dot{\gamma}$), the consistency factor ($k$) and the power law exponent ($n$).

$$\mu = k \cdot \dot{\gamma}^{n-1}$$ (2)

The wall shear stress ($\tau$) is described as:

$$\tau = k \cdot \dot{\gamma}^n$$ (3)

This expression is, for example, used in Rosenberger et al. (2002) where $k$ and $n$ are assumed to depend only on the TSS concentration, where the constants are described as:

$$k = 0.001 \cdot \exp (2 \cdot \text{TSS}^{0.41})$$ (4)

$$n = 1 - 0.23 \cdot \text{TSS}^{0.37}$$ (5)

The model surrogates for AS used for the experiments were CMC solutions with the concentrations 1.5, 2.0 and 3.0 g/l, which can also be described with the power law. The rheology of the solutions was measured with a rotating cylindrical rheometer, with a gap size of 2.05 mm. A further description of the rheometer can be found in Sørensen et al. (2015).

The measurements were carried out at room temperature, approximately 20 °C, which was also the temperature for the physical setup with the membranes. The measurements were conducted with shear rates starting at about 20 s$^{-1}$ and then after a two-minute measurement the shear rate was increased,
with maximum shear rates at 2000 s\(^{-1}\). Furthermore an analysis of the rheological time dependency of CMC solutions was made by measuring the viscosity as described above, after which the shear rate was incrementally decreased, and the viscosity was measured at each increment again.

**Modelling of the system**

The CFD model for the system was made with STAR CCM + v9.06.009.

**3D geometry and model**

The geometry of the system was designed in Rhino 3.0 CAD software. The 3D model was meshed using Star CCM + CFD software yielding a grid of 1.2 million polyhedral cells, with the elements size ranging from 3 to 8 mm. For precise description of the flow in the viscous sublayer in the near wall region, the mesh was refined at the boundaries through generation of the prism layer, so that the distance of the first mesh cell from the wall satisfies the condition of \(y^+ < 1\). The \(y^+\) is defined as:

\[
y^+ = \frac{y \cdot u_t}{v}
\]

where \(y\) is the distance from the wall, \(u_t\) is the friction velocity and \(v\) is the kinematic viscosity. All the boundaries are set as smooth walls with no-slip condition.

The grid was made by dividing the mesh into two volumes, illustrated in Figure 3(b). One volume was outside the membranes, where the cell size was kept at 8 mm. The volume between the membranes, and close to the membranes, was tested with cell sizes at 2, 3, 4, and 5 mm, from which it was found that the velocity profile between the membranes was independent from 2 to 3 mm and a mesh size of 3 mm was chosen.

**Numerical setup**

The velocity fields were determined by solving the steady and unsteady Reynolds-averaged Navier-Stokes (RANS and URANS) equations in 3D for a homogeneous single-phase liquid. The modelling of the non-Newtonian properties was incorporated in the solution of the velocity fields with the power law model, where the apparent viscosity is given as:

\[
\mu_{\text{app}} = \begin{cases} \mu_{\text{min}} & \text{if } k \cdot \dot{\gamma}^n < \mu_{\text{max}} \leq \mu_{\text{min}} \\ \mu_{\text{min}} & \text{if } \mu_{\text{min}} < k \cdot \dot{\gamma}^n < \mu_{\text{max}} \leq \mu_{\text{max}} \\ \mu_{\text{min}} & \text{if } \mu_{\text{min}} = \mu_{\text{max}} \end{cases}
\]

where the \(k\) and \(n\) values are the ones given in Table 1, and minimum viscosity \(\mu_{\text{min}}\) was not set while the maximum viscosity \(\mu_{\text{max}}\) was set to 3 Pa s to avoid instability. The highest modelled viscosities were around 0.4 Pa s.

The motion induced by the rotating membranes was modelled both as a steady solution with moving reference frame and an unsteady approach with a moving mesh. For both methods the volume was divided into two regions with an interface in radius of 190 mm.

The stationary solution was chosen since it required less computational power.

The rotation speed of the membranes was set to 120 rpm in the CFD model as well as in the experiments. For the transient solution the time step was set to 0.00138 s.
corresponding to 1 degree per time step with 10 inner iterations per time step.

For determining whether the flow is turbulent or laminar the radial non-Newtonian Reynolds (Re_{rNN}) number can be used. For non-Newtonian liquids with the density (\rho) with a single submerged infinite disc rotating with angular velocity (\omega) in a given radius (r), the non-Newtonian radial Reynolds number can be described as (Andersen et al. 2001):

$$\text{Re}_{rNN} = \frac{\rho (\omega r)^2 - n}{k}$$  (8)

where the flow is laminar if Re_{rNN} < 1 \cdot 10^5 (Torras et al. 2009). This is the case for all the experimental setups, where the highest radial Reynolds number is Re_{rNN} = 2 \cdot 10^4. However this is not conclusive evidence that the flow is laminar, since the described Re number is determined from a single plate under given assumptions, which will not be completely correct for the given setup, as well as the fact that the two membranes increase the pumping effect and thereby change the velocity field. Due to this, the system is modelled both as a laminar flow and by use of turbulent approaches. The turbulence models used are the Realizable (Two-Layer All-\gamma^+ Wall Treatment) k-\varepsilon model, and the SST (Menter) k-\omega also with Two-Layer All-\gamma^+ Wall Treatment. The SST k-\omega is a hybrid using k-\varepsilon in the far field and k-\omega near the wall and should therefore be better for describing the transition zone.

RESULTS

Rheology of surrogate

Figure 4 illustrates the results of the measurements and the fitted curves from the power law where the CMC solutions are very well described by the power law with the lowest R^2 being 0.98.

The k and n values for the CMC solutions are found from the fit in Figure 4 and are listed in Table 1.

The determined k and n values did not exactly correspond to AS, which tended to have more shear thinning properties, which was clear from the comparison with Rosenberger et al. (2002) in Figure 4(a). From the measurements illustrated in Figure 4(b), the solutions were assumed to be time independent, also differing from AS, which often is time dependent (Ratkovich et al. 2015). Despite the less shear thinning properties when compared to AS, it will increase the validity of the model even when compared to only conducting the experiments with Newtonian liquids, and will justify the use of the model with other shear thinning fluids like AS with associated k and n values.

Tangential velocity profiles

Due to the transiency of the system the results varied over time, not only for the transient solution but also for the steady solution where non-periodic vortices occurred.

Table 1 | Determined k and n values for different concentrations of CMC

<table>
<thead>
<tr>
<th>Concentration [gCMC/l]</th>
<th>k [Pa s^n]</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5</td>
<td>0.0323</td>
<td>0.847</td>
</tr>
<tr>
<td>2.0</td>
<td>0.0551</td>
<td>0.800</td>
</tr>
<tr>
<td>3.0</td>
<td>0.1454</td>
<td>0.725</td>
</tr>
</tbody>
</table>

Figure 4 | (a) Measured viscosities of different CMC solutions and fitted viscosities described by the power law and viscosity of sludge (Rosenberger et al. 2002). (b) Measured viscosities by first increasing the shear rate and then decreasing it.
Since the measured velocities were mean velocities over a longer time period (minutes), a mean was also used for the modelled results.

For the steady solution, it was not possible to find a solution corresponding to the measured velocities, since the position of the membranes was fixed. For taking into account the changes caused by vortices a mean of 1,000 iterations after the model has converged was used.

For the transient solution the values were a mean, where a period of 1 s equalling two rotations was used. Figure 5 illustrates the results of the two methods where it also becomes clear that the steady solution has a problem describing the flow close to the middle due to the different positions of the nave.

From the modelling by the different methods for the movement it became clear that the steady solution was inducing errors in the area just outside the membranes where the interface is located (see Figure 5). The figure also shows large errors close to the middle which is due to fixed position of the nave with this method. The largest maximum error for the steady state was 22%, compared to 13% for the transient solution with moving mesh. Based on this, a transient solution should be used when modelling such
systems, which will also be the case for the rest of the results. Furthermore the study showed large errors when using Newtonian liquid with a viscosity of 0.020 Pa s.

In Figure 6, the results of both the laminar and turbulent models were compared with the measured velocities. The laminar model has shown a great ability of modelling the mean velocities between the membranes, where the flow was confined by the membranes, with a 17.8 mm gap between them. Close to the edge and outside the area confined by the membranes, the precision of the model was lower. This might be due to more turbulence presented in these areas. However, the turbulent models did not seem to provide a significantly better result than the laminar, and the difference between the results of the laminar and the turbulent models was, in most cases, small. The SST $k$-$\omega$ model was chosen due to its capability in the transition zone, though this model seemed to provide the worst result exemplified in Figure 6(a) where the flow diverged from the measurements. From Figures 6(b) and 6(c) it is clear that the modelled velocity was too high close to the edge of the membrane for all the different models. This is the area where the interface for the moving mesh is located, which might also be the reason for the inaccurate results. The error was in general around 20% outside the area of the membranes with a maximum error of 36% for the SST $k$-$\omega$ model. Despite this, the shape of the velocity profile between the membranes in this area as illustrated in Figure 6(d) were well described.

**CONCLUSION**

The experiments have shown that CMC solutions is a suitable surrogate for shear thinning liquids for validation of CFD models which due to the clarity allows velocity measurements with a LDA to be made.

It was possible to include the non-Newtonian parameters for the liquids in the CFD model and thereby model the flows of the system with a moving mesh, while the moving reference frame gave inaccurate results near the interface.

In the areas with the lowest turbulence the flows were well described while the areas with more turbulence were poorly described, also with turbulence models. The CFD model was made with both SST (Menter) $k$-$\omega$ and $k$-$\varepsilon$ turbulence models to validate whether either of these was capable of modelling the correct flow. The $k$-$\varepsilon$ model was used because of its better performance in the transition zone but was found to perform poorly, especially in the concentric setup. This could mean that the turbulence models used were not capable of describing the turbulence in such systems, thus further studies should be made in this area. Furthermore, the simulations made it clear that the non-Newtonian properties were of great importance for modelling the correct velocities in the system. This has clarified the importance of validating non-Newtonian systems with non-Newtonian liquids since the flow clearly differs from the flow of a Newtonian liquid.

**REFERENCES**


