Improving the Accuracy of Granular Sludge and Biofilm Reactor Simulations in Aquasim Through Artificial Diffusion

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ABSTRACT: Aquasim is public-domain and user-friendly software that is widely used for biofilm modeling. The program uses built-in process unit blocks, such as biofilm and mixed compartments. In the literature, often several of these compartments are linked with artificial advective flows to represent a single physical well-mixed system, such as a granular sludge reactor. This work shows that caution should be exercised with this popular approach because numerical errors occur when too high artificial advective flows are used. These errors could stay unnoticed if mass-balances of the simulation results are not checked. A solution to this problem is proposed in this work. A new method based on diffusive links between compartments instead of advective links leads to more reliable and faster simulations and is much easier to implement.

KEYWORDS: aerobic granular sludge; anammox; Aquasim; granule size distribution; modeling; numerical error

In the last decade, there has been a strong increase in attention for wastewater treatment processes based on granular sludge because of their compactness and energy efficiency. Anaerobic granulation is already known for a long time, but granulation of aerobic sludge (Prönk et al., 2015), anammox sludge (Lackner et al., 2014), sulfate reducing sludge (Hao et al., 2013), and sulfide oxidizing sludge (Yang et al., 2016) are more recent developments. Models of granular sludge processes are expected to play an important role in the further understanding and optimization of these systems. The goal of this work is to facilitate the development of such models.

AquaSim (Reichert, 1994) is public-domain simulation software widely used for one-dimensional multi-species and multi-substrate biofilm modeling. To represent the physical configuration and transport phenomena in a system, the user can connect biofilm, mixed or other compartments with links that represent either diffusion or advection. Valuable time can be saved with such built-in process unit blocks. For example, the partial differential equations required to calculate the solute and biomass profiles inside the biofilm matrix are automatically solved by the software. However, predefined unit models also imply restrictions. For example, AquaSim does not allow the total volume of a biofilm compartment to change during a simulation. If the biofilm system under study has a fluctuating volume, such as sequencing batch reactors, this cannot be dealt with at first sight. Secondly, a biofilm compartment can only have a biofilm with one, uniform thickness. It therefore seems impossible to consider several biofilm thicknesses or granule sizes within one reactor.

Modelers have found creative ways to overcome the aforementioned limitations of AquaSim by combining different compartments. Beun et al. (2001) was the first to connect the bulk liquid zone of a biofilm compartment to a mixed compartment with advective links to simulate an aerobic granular sludge sequencing batch reactor. Figure 1A shows how this connection can be made. A high advective exchange flow rate is chosen to obtain an equal concentration of all components in both compartments’ bulk liquids, thus adequately mimicking the mixing that occurs in the actual reactor liquid. A similar approach has been used to consider the granule size distribution inside a continuously fed granular sludge partial nitritation-anammox reactor (Volcke et al., 2012). Figure 2A shows how several biofilm compartments with different biofilm thicknesses were linked with each other and with a mixed compartment by large advective exchange flow rates. Many other studies used this approach with artificial flows to model granular sludge and biofilm reactors (Table 1).

Popular the approach with artificial advective exchange flows may be, it can lead to erroneous calculations. Volcke et al. (2012)
noticed that the choice of the advective exchange flow rates, the distribution of the reactor volume between the different compartments, and the configuration of the links is of utmost importance to avoid numerical errors. When no particular attention was paid to these choices, the mass balances were inaccurate, meaning mass is wrongfully created or lost during the simulation. No other publication in Table I mentioned the danger of erroneous calculations. Often they did not specify the advective exchange flow rate, distribution of the reactor volume or the configuration of the links they used, even though these are critical parameters to obtain reliable simulations.

The use of artificial advective links implies a trade-off between mixing and correct mass balances and, therefore, requires a time-consuming manual optimization procedure before reliable simulations can be performed. To illustrate this, the model of Volcke et al. (2012) considering a granule size distribution was used (configuration in Fig. 2A). Figure 3A shows that the inaccuracy in the mass balance (mathematical definition in materials and methods, Equation 2) increases with an increasing advective exchange flow rate. In contrast, the difference between the concentrations in the different compartments (Equation 3) becomes higher at low flow rates. The envisaged perfectly mixed conditions are consequently not realized in this case. Only at around $10,000 \text{ m}^{-2} \cdot \text{d}^{-1}$ there are both acceptable mass balances (1% inaccuracy) and mixing (difference in N$_2$ concentration maximally 0.3%). This flow rate was therefore used in the original publication.

The inaccuracy in the mass balance at artificial high advective flow rates is attributed to numerical errors. These errors are inherent to the data type in which numbers are stored by the software. Real numbers are stored as binary numbers with a fixed amount of significant digits. Because of the finite precision with which numbers are stored, a summation of values with greatly different magnitude leads to errors. In the case of artificial high advective flows, the associated mass transfer rate of a compound

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**Figure 1.** Two possible configurations to model a granular sludge sequencing batch reactor in Aquasim. (A) Traditional approach with advective links to ensure equal concentrations in the bulk liquids (Beun et al., 2001). (B) New approach with diffusive links.

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**Figure 2.** Two possible configurations to consider a granule size distribution in Aquasim. (A) Traditional approach with advective links to ensure equal concentrations in the bulk liquids (Volcke et al., 2012). (B) New approach with diffusive links.

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2132 Biotechnology and Bioengineering, Vol. 114, No. 9, September, 2017
transported into a reactor becomes much bigger than the (more realistic) transport and reaction terms. When the software solves the mass balance equations, numbers of greatly different magnitude are therefore added to each other. Consequently, numerical errors occur during this summation. The bigger the artificial flow rate, the bigger the artificial transport terms and so the higher the risk for such errors.

Numerical errors can be avoided by connecting the compartments with diffusive links instead of advective links. The mass transfer rate \( m \) (g·d\(^{-1}\)) of a compound between two diffusively linked compartments is calculated by Aquasm with Equation (1), where \( C_1 \) (g·m\(^{-3}\)) is the concentration in the first compartment, \( C_2 \) (g·m\(^{-3}\)) the concentration in the second one, and \( q_{ex} \) (m\(^3\)·d\(^{-1}\)) a predefined exchange coefficient. This equation follows from Fick’s law of diffusion, assuming a certain distance and area over which diffusion takes place (see Supporting Information for explicit comparison). In Equation (1), the difference in the concentrations \( C_1 \) and \( C_2 \) represents the driving force for mass transfer and \( q_{ex} \) is a scale factor, analogous to the \( k_{a} \) in the well-known gas–liquid transfer model. Diffusive links are interesting because the mass transfer rate \( m \) decreases when the difference in concentrations decreases. When two compartments are linked with a high diffusive exchange coefficient \( q_{ex} \), the concentrations in the compartments quickly grow closer. As such, the driving force and, therefore, also the mass transfer rate decreases. Consequently, the associated transport terms in the mass balances are small and they will not easily lead to significant numerical errors.

\[
m = q_{ex} (C_1 - C_2)
\]

The approach with diffusive links eliminates the trade-off between mixing and correct mass balances. Figure 2B shows this novel method for the case of Volcke et al. (2012), where a granule size distribution is considered. From Figure 3B, it is clear that the nitrogen mass balance fits well (<0.001% inaccuracy), independently of the chosen diffusive exchange coefficient. However, the difference in concentrations between the compartments again becomes high for low values of the exchange coefficient. Altogether, it is now possible to simply use a very high exchange coefficient (e.g., 10,000,000 m\(^3\)·d\(^{-1}\)) to obtain thorough mixing, without significant inaccuracies in the mass balance. Consequently, no tedious trial-and-error optimization procedure to find a suitable flow rate is required here. On top of that the simulations ran 13.7 ± 0.6% \((n = 3)\) faster with diffusive links. Only at extremely high values of the diffusive exchange coefficient, the simulations could not run. In this case, this happened at 10\(^{12}\) m\(^3\)·d\(^{-1}\), which is 10 million times bigger than the minimal required value of 100,000 m\(^3\)·d\(^{-1}\) for sufficient N\(_2\) mixing (Fig. 3B). This means there is a very wide range of applicable diffusive exchange coefficients.

Analogous simulations with a model for an aerobic granular sludge sequencing batch reactor based on advective links (Fig. 1A) showed that the same trade-off between mixing and numerical errors existed (Fig. S1). With this particular model, no suitable exchange flow rate could be found at all, since the mass balance inaccuracy (mathematical definition in Supporting Information, Equation S1) rose far above 1% before an acceptable difference in concentrations (Equation S2) below 1% was reached. The alternative approach with diffusive links (Figure 1B) could again eliminate the problem completely. The simulations ran significantly faster as well (31.7 ± 0.8%, \(n = 3\)). This proves that diffusive links are also better to model the changing reactor volume in sequencing batch reactors with granular sludge compared to the popular approach with advective links. It is therefore strongly recommended to always use this alternative approach when several compartments are used to represent one single physical well-mixed system.

The newly proposed approach with artificial diffusion is not only more reliable, but also much easier to implement, which leads to time savings and a lower risk for human mistakes. The implementation is easy because a simple configuration can be used (compare Fig. 2A and B) and because the simulations are
The following steps can be used to implement the new approach:

1. Create a biofilm compartment for every granule size fraction to be considered and create a single mixed compartment.
2. Connect the influent and effluent streams to the mixed compartment and connect every biofilm compartment to the mixed compartment with a diffusive link.
3. Divide the total reactor volume equally among the different compartments. If the reactor liquid volume changes (e.g., sequencing batch reactors), distribute the minimum volume over the compartments and add the maximal additional volume to the mixed compartment, to ensure that the volume of the mixed compartment remains positive during the simulation.
4. Give every soluble and particulate compound the same, low diffusive exchange coefficient for all the diffusive links. \( \frac{1 \text{ m}^3}{\text{C}_1 \text{ d}} \) is a good initial guess.
5. Increase the diffusive exchange coefficient stepwise, each time by a factor 10, until the concentrations of all components in the bulk liquid of the different compartments are nearly identical (in this work, only N\(_2\) concentrations are considered for illustrative purposes). Use a predefined maximal difference (e.g. 1%) or a visual inspection, depending on the required accuracy.
6. To be absolutely sure no numerical errors occur, it is recommended to check the mass balances at steady-state one time before starting the simulations you intend to make. Do this for all quantities that should be conserved, such as nitrogen, COD and phosphorus (in this work, only N is considered for illustrative purposes).

In the light of the new findings, we reconsider the last conclusion of Volcke et al. (2012): “The application of the widespread software package Aquasim for the simulation of one-dimensional biofilm models is limited in terms of taking into account detailed granule size distributions.” The necessary laborious optimization that led to this conclusion is no longer required with the new approach using diffusive links, as...
demonstrated in this work. Aquasim is therefore certainly useful to model size distributions in different types of granular sludge and biofilm reactors. Furthermore, a similar approach with diffusive exchange could be applied in other software platforms like WEST or Biowin to model granule size distributions or granular sludge sequencing batch reactors. Commercial water simulators mostly do not yet offer a granular sludge sequencing batch reactor as built-in process unit block nor the definition of a granule size distribution as a standard option. Since diffusive links are not available as a standard feature in these software platforms, a basic user cannot easily apply the approach described in this work. However, Equation (1) might help software developers to create the source code of these process unit blocks. For simplicity, the diffusive links do not even have to be shown in the user interface.

To conclude, sequencing batch reactors with biofilms and granule size distributions can be modeled with Aquasim by linking different compartments by artificial diffusion processes. This letter showed that advective links have always been used for this purpose up to now, but that erroneous calculations easily occur with this approach. The new method based on diffusive links leads to better fitting mass balances, faster simulations, and is easier to implement. It is therefore recommended to always use the approach described here.

Materials and Methods

The bioconversion model described by Volcke et al. (2010) for a partial nitritation-annamox process was implemented in Aquasim (Reichert, 1994). The granule size distribution was taken into account using the volumetric mean diameters to characterize each size class, as described by Volcke et al. (2012). In a first set of simulations, the configuration presented in Figure 2A was applied, using advective exchange flows and an uneven distribution of the reactor volume among the compartments (Volcke et al., 2012). Advective exchange flow rates between 10 and 500,000 m$^3$·d$^{-1}$ were studied. A constant influent ammonia concentration of 500 g N·m$^{-3}$ was assumed and the simulated time was 20,000 days for all simulations to ensure that a steady state of the process performance and microbial population distribution was reached. In a second set of simulations, the alternative configuration presented in Figure 2B was used, connecting the compartments with diffusive links and with equal compartment volumes. The diffusive exchange coefficient was varied between 10 and 10$^{12}$ m$^3$·d$^{-1}$. The complete implementation in Aquasim for both approaches is described in Supplementary Material.

Two performance indicators were applied to compare the two approaches. The first indicator is the nitrogen concentration in the effluent (g N·m$^{-3}$ ammonium), $C_{in}$ is the total nitrogen concentration in the influent (g N·m$^{-3}$ ammonium), nitrate, nitrite, nitrogen gas, and nitrogen incorporated in all biomass fractions), $Q_{in}$ is the influent flow rate (m$^3$·d$^{-1}$), and $Q_{out}$ is the effluent flow rate (m$^3$·d$^{-1}$), at steady state. This indicator represents the amount of nitrogen that was created or lost during the simulation owing to numerical errors. The second indicator is the maximal difference in the nitrogen gas (N$_2$) concentration between the different compartments’ bulk liquids at steady state (Equation 3). $C_i$ and $C_j$ are the concentrations in two different compartments and $i$ and $j$ go from 1 to 5 to compare the concentrations in all five compartments shown on Figure 2. $N_2$ was selected as indicator component for mixing because it is the main end product of the process.

\[
N \text{ mass balance in accuracy} = \frac{C_{in}Q_{in} - C_{out}Q_{out}}{C_{in}Q_{in}} \\
\text{Difference in N}_2 \text{ concentration} = \frac{\max_{i=1,2,3,4,5} |C_i - C_j|}{\max_{i=1,2,3,4,5} |C_i|} 
\]

An analogous set of calculations was made with a model for an aerobic granular sludge sequencing batch reactor (see Supporting Information for details). The implementation in Aquasim for both approaches can also be found for this model as Supplementary Material.

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References


Supporting Information

Additional supporting information may be found in the online version of this article at the publisher’s web-site.