ABSTRACT
Models adapt constantly, usually increasing the degree of detail describing physical phenomena. In water resource recovery facilities, models based on mass and/or heat balances have been used to describe and improve operation. While both mass and heat balances have proven their worth individually, the question arises to which extent their coupling, which entails increased model complexity, warrants the supposedly more precise simulation results. In order to answer this question, the need for and effects of coupling mass and heat balances in modelling studies were evaluated in this work for a biological nitrogen removal process treating highly concentrated wastewater. This evaluation consisted on assessing the effect of the coupling of mass and heat balances on the prediction of: (1) nitrogen removal efficiency; (2) temperature; (3) heat recovery. In general, mass balances are sufficient for evaluating nitrogen removal efficiency and effluent nitrogen concentrations. If one desires to evaluate the effect of temperature changes (e.g. daily, weekly, seasonally) on nitrogen removal efficiency, the use of temperature profiles as an input variable to a mass balance-based model is recommended over the coupling of mass and heat balances. In terms of temperature prediction, considering a constant biological heat generation term in the heat balance model provides sufficient information – i.e. without the coupling of mass and heat balances. Also, for evaluating the heat recovery potential of the system, constant biological heat generation values provide valuable information, at least under normal operating conditions, i.e. when the solids retention time is large enough to maintain nitrification.

1. Introduction
Biological processes for nitrogen removal from wastewater have proven effective for minimizing the impact of excess nutrients on our water systems. They are widely applied for the treatment of municipal wastewater as well as specific wastewater streams containing high nitrogen concentrations, e.g. landfill leachate and the thin fraction of manure [1,2]. Models based on mass balances are powerful tools to describe and optimize the operation of these nitrogen removal processes. They are often based on the widely accepted Activated Sludge Models (ASMs) [3] which was developed for municipal wastewater treatment, and have been adapted for specific cases of concentrated wastewater treatment [1,4–7]. Many of the parameters in mass balance models are temperature dependent, e.g. growth rate of microorganisms, so temperature values need to be assumed or provided in some way [8]. Temperature can be considered constant, as a predetermined time profile, or predicted through heat balances. The latter involves coupling mass and heat balances, which implies an increased model complexity. The question arises to which extent this increased complexity is warranted by the expectedly more precise simulation results.

Wastewater treatment plants are nowadays increasingly regarded as resource recovery facilities, an evolution which also requires reconsideration of modelling practices [9]. Heat is one of the most important resources to be recovered [10]. Models based on heat balances calculate the heat fluxes throughout the system, including convection, conduction, and biologically produced heat [11–16]. The biologically produced heat can be considered constant based on an assumed average biological conversion efficiency, or calculated from mass balances which then need to be coupled with the heat balances. Analogous
to the case for mass balance models, but for temperature, the question arises whether or in which cases the increased model complexity caused by coupling mass and heat balances warrants the expected higher precision of the simulation results.

To answer these questions, a pre-denitrification/nitrification system treating wastewater with high ammonium and organic carbon concentrations was described with both mass and heat balances. Wastewater with high ammonium and organic carbon concentrations was taken as an extreme-case scenario, in the sense that a large amount of biological heat is produced, which results in a higher potential need to couple mass and heat balances. In other words, if coupling mass and heat balance models is not required for modelling this type of wastewater treatment, it is also not required for modelling the treatment of less concentrated wastewater. An analysis on three levels was performed to assess which degree of coupling is required depending on the intention of the simulation: (i) Prediction of effluent quality; (ii) Prediction of temperature; (iii) Prediction of heat recovery potential. The overall aim is to select the appropriate model complexity for each of these applications. Indeed, even though computational power nowadays often no longer is the limiting factor, it is important not to make models more complex than needed to meet their objectives, in order to ensure their practical applicability and the straightforward interpretation of simulation results.

2. Materials and methods

2.1. System under study: biological nitrogen removal from manure

The system under study concerns a biological nitrogen removal process treating the nitrogen-rich thin fraction of pig manure obtained after mechanical separation (centrifugation) – the most applied manure processing technique in Flanders, Belgium (VLM, 2018). The average composition of the thin fraction considered in this study is summarized in Table 1 – determined by averaging the values of five bimonthly samples from a manure treatment plant in Flanders, Belgium – values from May/2014 to January/2015 – and following the fractionation shown in Boursier et al. [17].

Nitrogen removal takes place via nitrification-denitrification over nitrate. During nitrification, ammonium is oxidized over nitrite to nitrate. This process is followed by denitrification i.e. reduction of nitrite and nitrate to nitrogen gas. These processes are established in a pre-denitrification system, consisting of a denitrification reactor followed by a nitrification reactor (Figure 1). This configuration allows to make use of the organic carbon present in the influent for denitrification. A recirculation flow from the nitrification reactor to the denitrification reactor is applied to supply the denitrification process with nitrate produced from nitrification.

The predenitrification system under study is operated as a sequencing batch reactor (SBR) (Figure 1). This SBR operation is characterized by cyclic operation. Each cycle starts with a feeding phase. During this phase, fresh thin manure fraction (Qin,demi; Figure 1) is fed to the denitrification reactor at a fixed flow rate (0.475 m$^3$.min$^{-1}$) for 45.8 min. As both the denitrification and nitrification reactors are interconnected, there is also a flow going to the nitrification reactor (Qout,demi = Qin,nit), which equalized the liquid levels in both reactors. During this feeding phase, the nitrification reactor is aerated continuously. After the feeding phase, the carbon source addition phase takes place (C-source; Figure 1), during which methanol is added to the denitrification reactor (QMeOH), with a typical dose of 3 liter methanol per cubic metre of manure ($\rho_{MeOH} = 792$ kg.m$^{-3}$). Aeration of the nitrification reactor continues during the methanol addition step. After the C-source phase, aeration continues. At the end of the aeration phase, it is checked whether the reactor has reached its maximum capacity (liquid level $H > H_{max}$). In case the maximum capacity of the reactor has not yet been reached, a recirculation step (Qrec = 0.6536 m$^3$.min$^{-1}$) of 153 min is applied and the aforementioned steps (i.e. feeding, C-source, aeration, $H > H_{max}$) are repeated. In case the maximum capacity is reached, the reactor undergoes a settling period (240 min) followed by a draw period (Qout,nit = 0.56 m$^3$.min$^{-1}$) of 350 min. Once

\[
\text{Table 1. Influent characterization.}
\]

<table>
<thead>
<tr>
<th>Influent component (COD fractionation)</th>
<th>COD content (g COD. l$^{-1}$)</th>
<th>Nitrogen content (g N. l$^{-1}$)</th>
<th>Phosphorus content (g P. l$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particulate inerts (29%)</td>
<td>10</td>
<td>0.61</td>
<td>0.067</td>
</tr>
<tr>
<td>Soluble inerts (14%)</td>
<td>5</td>
<td>0.06</td>
<td>–</td>
</tr>
<tr>
<td>Readily biodegradable COD (14%)</td>
<td>5</td>
<td>0.15</td>
<td>–</td>
</tr>
<tr>
<td>Slowly biodegradable COD (43%)</td>
<td>15</td>
<td>0.61</td>
<td>0.085</td>
</tr>
<tr>
<td>Ammonium</td>
<td>–</td>
<td>3.27</td>
<td>–</td>
</tr>
<tr>
<td>Phosphate</td>
<td>–</td>
<td>–</td>
<td>0</td>
</tr>
<tr>
<td>Total</td>
<td>35</td>
<td>4.7</td>
<td>0.152</td>
</tr>
</tbody>
</table>

*Following the fractionation shown in Boursier et al. [17] matching with the values of nitrogen and phosphorus of the wastewater at hand through the nitrogen and phosphorus content of COD (Table S5).
two steps take place (settling and draw), the reactor goes to a recirculation step, and the cycle starts anew.

All of these phases, except the aeration phase, had a fixed duration in the model. The aeration phase was shortened or lengthened to control the average manure influent flow rate ($m^3_{\text{manure.d}^{-1}}$). Shorter aeration phases resulted in shorter cycles and more cycles per day – i.e. a higher amount of manure could be treated.

The total volume of the system was $2844 m^3$ (56% nitrification reactor), with a surface area of 547 $m^2$ and a maximum liquid height of $H_{\text{max}} = 5.2 m$. A reference case (RC) was defined, treating an average influent flow rate of $34 m^3.d^{-1}$ is treated (Table S7). The reference operating temperature is 30°C – a common temperature during the summer, as the systems can even require cooling during this period.

2.2. Modelling and simulation set-up

Biological nitrogen removal in the SBR system under study was described through mass balances and heat balances, as detailed in the Supplementary Information S1 and S2, respectively. The denitrification and nitrification reactors were assumed to be ideally mixed at all times, i.e. concentration and temperature gradients within the reactors were neglected. Furthermore, even though time was given in the model for the settling period, no settling was applied – i.e. the solids retention time equaled the hydraulic retention time. The mass and heat balance based models could be linked as shown in (Figure 2).

The mass balance model requires a temperature value in order to evaluate certain parameters (e.g. growth rate). This temperature value was either directly fed into the mass balance model as a constant value, or was predicted by coupling the mass balances with heat balances.

An analogue is also present in the heat balance model. In order to predict the temperature of the system, the heat balance model requires a biological heat value. This biological heat value was either fed directly into the mass balance model as a constant value, or was predicted by coupling the heat balances with mass balances. A summary of the simulations can be found in the Supplementary Information (S3 – Table S7).

All simulations were run to represent a 2 years (730 days) period. Annual averages represent average values from the second year – in order to avoid the effect of initial conditions. Removal efficiency values were calculated with average concentration values in the nitrification reactor during the Draw period (Figure 1).

The mass and heat balance models used in this work were not been validated for the specific system at hand. This was not deemed necessary for the goal of this study, which is to assess the required degree of complexity in terms of (un)coupling mass and heat balance models. Nonetheless, similar models, e.g. Magri and Flotats [5] for the mass balance model and Makinia et al. [14] for the heat balance model, have been successfully used in the past to describe systems for highly concentrated wastewater treatment.

Comparisons are made mainly between the predictions obtained coupling mass and heat balance models (HM; Table S7), and different simulations with uncoupled mass and heat balances, i.e. using constant temperature (CT30, CT20, CT10 in; Table S7), or constant biological
heat generation (CB90 or CB60; Table S7). Coupled mass and heat balance models are expected to give the most precise results, which made this our base for comparison. It was subsequently examined (as detailed below) to which extent uncoupled models could provide the same results regarding three different aspects: effluent quality and temperature, temperature and biologically produced heat, and heat recovery and biologically produced heat.

2.2.1. Effluent quality and temperature

To evaluate the effect of coupling (or not) mass and heat balances on nitrogen removal efficiency prediction, the simulations here were: (i) coupling of mass and heat balance models (HM; Table S7); (ii) [uncoupled] constant temperature (10, 20, 30°C; CT10, CT20, CT30; Table S7). A comparison was made between the nitrogen removal efficiency predicted when considering a constant temperature against the predictions obtained when coupling the mass and heat balance models.

2.2.2. Temperature and biologically produced heat

The reactor temperature predicted by (i) coupling of mass and heat balance models (HM; Table S7) was compared with the one obtained from considering (ii) only heat balances and assuming a constant biological heat production. For (ii), the constant heat production was considered to be either 60 or 90% of the biological heat potential present in the wastewater to be treated (CB60 and CB90, respectively). The chemical heat potential was defined as the heat that would be generated from the oxidation of all biodegradable COD to CO₂ and all ammonium to nitrate, (catabolic reactions only, neglecting biomass production). As for the location of heat production, two scenarios were considered: one with equal volumetric biological heat production distribution, i.e. the same amount of heat per cubic metre of reactor was produced in both the nitrification and denitrification reactors, between the nitrification and denitrification reactors (ii-a). A second simulation (ii-b) was made considering 95% of the heat produced in the nitrification reactor (CB90-95N), i.e. the heat produced per cubic metre in the nitrification reactor was 19 times higher than the one in the denitrification reactor.

2.2.3. Heat recovery and biologically produced heat

The effect on heat recovery prediction was assessed for the same scenarios, adding heat recovery, i.e. coupling mass and heat balance models (HM-HR) compared with heat balances and assuming constant biological heat production (CB90-HR and CB60-HR; Table S7). The year average heat recovery potential was used for the comparison. For the heat recovery potential, a critical temperature (T_{crit} = 20°C) was defined, above which heat was recovered from the reactors.

3. Results and discussion

3.1. Reference case – SBR cycle overview

The dynamic response of the SBR to the constant influent composition of the reference case is displayed in Figure 3. In this figure, the last repetition of the SBR cycle is shown, i.e. H is greater than H_{max} and the cycle goes to the settling, draw and recirculation steps (Figure 1). This is the reason why the ‘initial’ and ‘final’ concentrations shown in the graph do not match (it takes nine feeding steps to reach H_{max}). During the feeding phase, the ammonium concentration increases in both the nitrification and denitrification reactor. The ammonium concentration increases in both the nitrification and denitrification reactor. The increase in the denitrification reactor (approx. 50 g N.m⁻³) is larger than in the nitrification reactor (<5 g N.m⁻³), where ammonium is oxidized at the same time. During this period, oxygen concentrations in the nitrification reactor remain low (<0.1 g O.m⁻³), as oxygen is being used for ammonium oxidation.

Aeration in the nitrification reactor remains on once the feeding is stopped, both during and after C-source addition in the denitrification reactor. The ammonium concentration in the nitrification reactor decreases and the oxygen concentration increases. The first small
increase in the oxygen concentration corresponds with organic carbon (COD) depletion (results not shown) – ammonium is incorporated into the biomass, and simultaneous nitrification and denitrification occur. This is followed by a continuous increase in the oxygen concentration along with the consumption of ammonium, during which also nitrite accumulation is observed, followed by nitrate formation. While nitrate accumulates during the whole aeration phase, nitrite reaches a maximum value and decreases by the end of the aeration phase. In the denitrification reactor, nitrite and nitrate concentrations remain close to zero at all times, indicating a good denitrification performance. The total nitrogen removal efficiency amounted to 83%.

During the settling phase, aeration is turned off and some denitrification is observed in the nitrification reactor: the nitrate concentration decreases, resulting in some nitrite accumulation which eventually is converted as well. During the draw period, the ammonium concentration in the nitrification reactor steeply increases – since effluent is withdrawn from the nitrification reactor, water flows from the denitrification reactor to the nitrification reactor.

The effluent values for nitrogen removal efficiency were calculated as the average value of the concentrations in the nitrification reactor during the draw phase. For the reference case, the effluent ammonium concentration during the draw phase increased from 5.6 to 39.8 g N m⁻³, with an average of 22.7 g N m⁻³. The effluent nitrite concentration was 0.1 g N m⁻³; nitrate was virtually not present in the effluent.

3.2. Effect of temperature on nitrogen removal efficiency

A mass balance-based model is set up to describe the nitrogen removal efficiency, as typically done. The effect of temperature on nitrogen removal is discussed first. The added value of considering heat balances simultaneously for this purpose will be discussed next.

3.2.1. Constant temperature

When the temperature decreases, the ammonium concentration in the effluent increases and the total nitrogen removal efficiency decreases. For an average influent flow rate of 34 m³ manure d⁻¹, the average ammonium concentrations in the effluent were 22.7, 240, and 1080 g N m⁻³ at 30, 20, and 10°C, respectively (Figure 4(A)). The corresponding SBR concentration profiles in the nitrification reactor are given in Supplementary Information (Figure S1). At 10°C and 30°C, some nitrite accumulation was observed during the cycle (Figure S1). However, the accumulated nitrite is denitrified during the settling phase, which is why nitrite is virtually not present in the effluent (draw phase). The corresponding nitrogen removal efficiency amounted to 83, 77 and 62%, for 30, 20 and 10°C, respectively (Figure 5(C)).

One of the most critical parameters in reactor design for nitrogen removal is the solids retention time required to maintain nitrification. In the system under study, the solids retention time (SRT) equals the hydraulic retention time (HRT), which is inversely proportional to the influent flow rate. The effect of the influent flow rate on the yearly average effluent concentrations of ammonium, nitrite, and nitrate of the system is summarized in Figure 4, for different temperatures (10, 20, and 30°C – corresponding to simulations CT10, CT20 and CT30 in Table S7). At low influent flow rates (high SRT), the influent ammonium concentration was relatively constant. As the influent increases (SRT decreases), a minimum ammonium concentration was reached, followed by a rapid increase of ammonium concentration at higher influent values as nitrification diminishes.

While a similar ammonium effluent concentration profiles in terms of the influent flow rate was observed at all temperatures, the influent flow rate beyond which the effluent ammonium concentration increased, was lower for lower temperatures. This reflects the increasing minimum solids retention time required for nitrification with decreasing temperature. In order to avoid nitrification failure, the reactor should be sized...
for the lowest temperature expected to be encountered.

A nitrite peak was observed at increasing influent flow rates, just below the critical influent flow rate for nitrification (Figure 4(B)). This nitrite peak indicates that nitrification becomes critical and nitrite oxidizing bacteria (NOB) are washed out before ammonium oxidizing bacteria (AOB). It was observed that the higher the temperature, the broader the nitrite peak (in terms of average influent, $m^3_{\text{manure.d}^{-1}}$). This could be explained by the fact that the maximum growth rate of AOB increases more with increasing temperature than the one of NOB [18]. The nitrate concentration profile complemented the one for nitrite, reaching a peak value at low influent values, which was higher at lower temperatures (Figure 4(C)).

The total nitrogen (TN) removal efficiency predicted as a function of the average influent flow rate displayed a similar behaviour at all three constant temperatures (10, 20, and 30°C; Figure 4(D)). The influent flow rate at which the maximum nitrogen removal efficiency was achieved increased with increasing temperature, following the increased minimum influent flow rate required for nitrification: at 10°C, the maximum TN removal efficiency was 79% at $31 m^3_{\text{manure.d}^{-1}}$ (SRT = 91.7 d); at 30°C, the maximum removal efficiency was 83% at $34 m^3_{\text{manure.d}^{-1}}$ (SRT = 83.6 d). This is the point where the reactor behaves at its full denitrifying potential. At lower influent loads, less simultaneous nitrification/denitrification occurs in the nitrification reactor. This can also be seen on the heat production distribution (Figure 5).

The solids retention time (SRT) at which nitrification starts diminishing at each temperature may seem rather high. At 30, 20, and 10°C, nitrification starts markedly diminishing at around 37, 34, and $33 m^3_{\text{manure.d}^{-1}}$, which corresponds with an SRT of about 76, 84 and 87 d, respectively – the reactor volume being 2844 m$^3$.

If the ammonium oxidizers would grow at their maximum growth rate (1.4, 0.6, 0.2 d, respectively;
Table S3), which is temperature dependent, the minimum SRT required for nitrification would be 1.5, 3.7, and 9.6 d, at 30, 20, and 10°C, respectively. However, one needs to account for the effect of ammonium and oxygen limitation, ammonium and nitrite inhibition, and pH on the growth rate of AOB (as expressed in Table S2). For example, considering the prevailing oxygen concentration of 0.15 g.m⁻³, already brings the minimum SRT’s up to 7.7, 18.5, and 47.4 d – at 30, 20, and 10°C, respectively. This is five times more than the minimum SRT calculated accounting only for the temperature in the reactor. Therefore, for reactor volume requirement calculations, it is recommended to use the minimum expected temperature and a mass balance model to evaluate the point at which nitrification diminishes.

3.2.2. Coupling mass and heat balances

The yearly average TN removal efficiency with the model coupling mass and heat balances (HM; black line in Figure 4(D)) has a similar behaviour as the results obtained at constant temperatures (CT10, CT20 and CT30; Figure 4(D)). The removal (yearly average) predicted with the coupled model was close to the one predicted at 20°C, which matches with the yearly average temperature predicted with the couple model (approx. 18°C).

If the goal is to assess the yearly average TN removal efficiency of a system, the use of constant temperature values is sufficient. One should try to use a temperature close to the expected temperature average of the system, as this would provide better results. In our case, the average temperature encountered when mass and heat balances were coupled (HM) was approximately 18°C; Figure 4(C) shows that if a constant temperature of 20°C is used, average TN removal efficiency values are very similar. This would require some previous knowledge of the system to be evaluated, but an idea of the maximum and minimum temperatures in similar systems should be enough to obtain an average constant temperature value. Furthermore, a more important temperature to evaluate could be the lowest expected temperature, as this remains the most important one in relationship to choosing the volume required for the system [19].

Another goal, besides reactor design, can be to evaluate the performance of the system throughout a certain period of time, considering variations in temperature, such as diurnal or seasonal variations. For this, the use of influent characteristics files, such as the one presented by Garnaey et al. [20], is recommended. If these were not to be available, informing with similar installations about maximum and minimum values can provide sufficient information to create influent characteristic files.

3.3. Effect of biologically produced heat on reactor temperature

In this section, the temperature predicted by a heat balance model when coupled with a mass balance model (HM; predicted – dynamic biological heat production; Figure 2) is compared to the temperature predicted when a constant biological heat production is used. In the case of constant biological heat production, two cases are analyzed, that with equal volumetric biological heat production (90 and 60% of the biological heat potential; CB90 and CB60; Table S7) and one where 95% of the heat is generated in the nitrification reactor (90% of the biological heat potential) – as it is here where most of the heat is expected to be generated (CB90-95N).

3.3.1. Dynamic biological heat production

Dynamic biological heat prediction is the coupling point from the mass to the heat balances (HM), i.e. the microbial activity predicted in the mass balance model is multiplied by the corresponding heat of reaction to obtain the dynamic biological heat prediction (input for the heat balance model; Figure 2). Therefore, the coupling can predict how much heat is generated and where (Figure 5). At low influent rates (higher SRT), a higher percentage of the potential heat content in the manure is generated (Figure 5). The values obtained at regular operation, i.e. with a good TN removal efficiency, where 80-85% of the potential heat being generated. This value decreases at higher influent values (lower SRT), as nitrification diminishes.

Biological heat generation occurs in both the nitrification and denitrification reactors. At all flows, most of the heat is generated in the nitrification reactor (Figure 5), as oxidation reactions generate more heat. At low influent flows (26–31 m³.d⁻¹), some heat is generated in the denitrification reactor. The heat generated in this region in the denitrification reactor was 26–6% of the total energy production (74–94% of energy generated in the nitrification reactor; Figure 5).

At high average influent flows (>32 m³/manure.d⁻¹), virtually all heat is generated in the nitrification reactor. At first, due to simultaneous nitrification/denitrification in the nitrification reactor and then due to loss of nitrification, i.e. only COD oxidation generates biological heat. This spatial differentiation of where biological heat is generated translates in temperature differences between both reactors, the nitrification reactor is warmer than the denitrification reactor (Figure S2).
3.3.2. Temperature prediction – constant biological heat production vs. dynamic biological heat production prediction

In this section, we consider the temperature predicted with mass and heat balances coupled (HM; Table S7) as the best temperature prediction. Therefore, the comparison of the temperature predicted when using constant biological heat production is directly compared to the one predicted with dynamic biological heat production prediction. For this, an average temperature difference (ΔT$_{year\;average}$) was defined as the year average of (T$_{dynamic\;heat}$-T$_{constant\;heat}$), i.e. the average of the values in Figure S3. Therefore, a positive value means that a higher temperature was predicted by the coupled model, and values as close to zero as possible are desired.

In general, the temperature predicted in the denitrification reactor with the coupled model (HM) was lower than the one predicted with constant biological heat production (Figure 6; CB90 and CB60). The opposite was true for the nitrification reactor, as higher temperatures were predicted with the coupled model in comparison to the constant biological heat cases (in general). The ΔT$_{year\;average}$ range with 60% constant biological heat productions was within −1.5 to 0.2°C/1.9 to 2.8°C for the denitrification/nitrification reactor; with 90% it was −3.3 to −1.2°C/−0.1 to 1.1°C.

As mentioned above, most of the heat is generated in the nitrification reactor (coupled model; Figure 5). When this spatial differentiation of heat generation is considered (CB90-95N; Table S7), i.e. considering most heat being generated in the nitrification reactor (90% of the generated heat), the temperature predicted approaches more that of the dynamic biological heat model (Figure 6 and S5.3). The ΔT$_{year\;average}$ in this case ranged from −1.0 to 0.8°C/−0.4 to −1.6°C for the denitrification/nitrification reactor.

Using constant biological heat production values to calculate the temperature of the reactor provided results with an average yearly temperature difference of maximum 3.3°C – year average. Considering the results in the previous section (Figure 4), this can provide enough information to evaluate the process, e.g. nitrogen removal efficiency and seasonal dynamics. In order to select which percentage of the potential heat to be used in the simulations, it is recommended to either test the biodegradability of the wastewater at hand, or search for it in literature. If the simulations show that a loss of nitrification is possible at the retention times applied, one should also lower the biological heat generation value used – as mentioned in the previous section, this is a characteristic of the wastewater [19].

If one is studying spatially separated reactors, and using constant biological heat generation values, temperature prediction can be improved by taking into consideration where heat is most likely to be generated (Figures 5 and 6, and Figure S3). In our case, for example, we can make a distinction between aerobic and anoxic reactions. Heat generation should then be considered to be mainly taking place in the aerobic reactor.

3.4. Effect of biologically produced heat on heat recovery potential

3.4.1. Constant biological heat production

When heat generation value corresponding to 90% of the potential (chemical) heat was used (CB90-HR; Table S7), the heat recovery potential could be overestimated by more than 50% in comparison to the coupled model with dynamic biological heat prediction (Figure 7). This overestimation, occurs mainly at the point where nitrification diminishes – i.e. at larger average influent values, lower SRT. In contrast, using a heat generation value corresponding 60% of the potential heat (CB60-HR), results in an underestimation of less than 35% of the heat recovery potential.

The highest errors encountered took place at high flow rates, as nitrification diminishes. Nonetheless, operation under these conditions should be avoided in a water resource recovery system – from design to operation. Therefore, if the modeller has an idea of the biodegradability of the wastewater at hand, and as a result its potential heat generation, constant biological heat
generation values can provide valuable information in this regard. Especially in general assessments of the heat recovery potential of a system.

4. Conclusions

The relevance of coupling mass and heat balance based models for nutrient removal and temperature predictions in biological nitrogen removal systems was assessed. The system under study concerned a predenitrification system treating wastewater with high N concentrations. The following conclusions were drawn regarding the predictions obtained with the models:

- Constant temperature values provide good insights on expected average total nitrogen removal efficiency.
- Temperature can be predicted well without coupling mass and heat balances – i.e. from heat balances, using constant biological heat generation values.
- The biodegradability of the wastewater (biodegradable COD and N content) should be tested to have good constant biological heat generation values.
- With spatially separated reactors, it is important to take into account where heat is most likely to be generated. In this study, significantly more heat was generated in the aerobic reactor than in the anoxic one.
- The heat recovery potential of a system can be assessed with constant biological heat generation values under normal operation conditions – i.e. when nitrogen removal is maintained.

Acknowledgements

Luis Corbala-Robles’ work was supported by the Ghent University Special Research Fund through a Doctoral Scholarship (BOF14/DOC/046).

Disclosure statement

No potential conflict of interest was reported by the author(s).

Funding

This work was supported by Ghent University [grant number BOF14/DOC/046].

ORCID

L. Corbala-Robles http://orcid.org/0000-0002-1981-0287

E.I.P. Volcke http://orcid.org/0000-0002-7664-7033

References


