Application of a model-based optimisation methodology for nutrient removing SBRs leads to falsification of the model

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Abstract Recently, a model-based optimisation methodology for SBR operation has been developed and an optimal operation scenario proposed to improve N and P removal in a pilot-scale SBR. In this study, this optimal operation scenario was implemented and evaluated. The results of the implementation showed that the SBR performance was improved by approximately 50 and 40% for total nitrogen and phosphorous removal, respectively, which was better than predicted by the model. However, the long-term SBR performance was found to be unstable, particularly owing to settling problems developed after the implementation. When confronted with reality, the model used for the optimisation of the operation was found to be invalid. The model was unable to predict the nitrite build-up provoked by the optimal operation scenario. These results imply that changing the operation of an SBR system using a model may significantly change the behaviour of the system beyond the (unknown) application domain of the model. This is simply because the mechanistic models currently do not cover all the aspects of activated sludge systems, e.g. settling and adaptation of the microbial community. To further improve model-application practices, expert knowledge (not contained in the models) can be valuable and should be incorporated into model-based process optimisations.
Keywords Modelling; nutrient removal; operation; optimisation; SBR; sensitivity analysis

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Introduction

The early concept of sequencing batch reactor (SBR) technology appeared first during the advent of the activated sludge concept by Arden and Locket (1914) who operated activated sludge in a fill and draw reactor. However, it was only recently (the last two decades) that SBR technology started to receive significant attention as a feasible alternative to the continuously operated activated sludge systems thanks to the pioneering works of Irvine, Wilderer and Goronszy in this field (see Wilderer *et al.*, 2001). SBR technology has been successfully developed and widely used for both nitrogen and phosphorus removal from wastewaters (Manning and Irvine, 1985; Furumai *et al.*, 1999; Demoulin *et al.*, 2001; Keller *et al.*, 2001; Wilderer *et al.*, 2001).

One of the chief advantages of this technology is to offer a high degree of flexibility in operation. This is sometimes considered as a disadvantage because it requires a more complicated operation/control scheme as opposed to simple and robust operation of continuous systems (Wilderer *et al.*, 2001). Nonetheless, this property of SBR technology motivated many researchers to develop optimal operation strategies (Manning and Irvine, 1985; Demuynck *et al.*, 1994; Hvala *et al.*, 2001; Lin and Jing, 2001; Puig *et al.*, 2004), which were mostly tested and evaluated experimentally. For obvious reasons, the number of operational scenarios that can be tested experimentally remained rather limited.

Alternatively, modelling and simulation have also been used to find optimal operation strategies for biological N and P removal in SBRs (Demuynck *et al.*, 1994; Hvala *et al.*, 2001; Artan *et al.*, 2002). Recently, a model-based approach to search systematically for

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an optimal operation of SBRs has been developed and applied to a pilot-scale SBR (Sin *et al.*, 2004). Since the quality of the model to represent the system adequately is central to the above-mentioned approach, a systematic calibration methodology for SBRs was also developed (Insel *et al.*, 2004).

The objective of this study is to evaluate the results from a specific application of a model-optimised SBR operation within the framework of contributing to general experiences and understanding of the usefulness of models for better SBR operation. This contribution is structured as follows: first, the results from the implementation of the optimal operation scenario (see Sin *et al.*, 2004) to the pilot-scale SBR are evaluated in view of the optimisation targets of the previous study. Following that, the model used to find the optimal operation is confronted with the reality observed under this new operation scenario and an improved methodology is proposed.

Materials and methods

The pilot-scale SBR is described in detail elsewhere (Insel *et al.*, 2004). Two operating scenarios, which are shown in Figure 1, were applied to the SBR within this study. In both scenarios, synthetic wastewater was used as influent (Boeije *et al.*, 1998), the volumetric exchange ratio (VER) was fixed at 0.5, the HRT was 12 h, the SRT was 10 days and the total cycle time was fixed at 6 h.

Reference operation scenario

In this operation, each SBR cycle consisted of 60 min fill/anaerobic, 150 min aerobic, 60 min anoxic, 30 min aerobic and 60 settling/draw phases (see Figure 1 top). The total volume of the SBR was 80 L and the 40 L of influent was supplied to the reactor during the fill/anaerobic phase. The DO set-point was 2 mgO_2/L. It is important to note that step-feed of the influent was not applied in this operation.

Optimal operation scenario

The optimal operation scenario, shown in the lower part of Figure 1, was found by a large number of model simulations in Sin *et al.* (2004). To improve the P-removal capacity of the system, it mainly aimed at reducing effluent nitrate at the end of the cycle. Since part of the effluent nitrate (depending on the volumetric exchange ratio of the SBR) is recycled back to the initial anaerobic phase of the cycle, it competes via denitrification with the phosphorus-accumulating organisms (PAO) for fresh readily biodegradable substrate in the influent. As a result, the optimal operation was found to impose (1) four intermittent aeration frequencies (IAF4), i.e. four alternating aerobic and anoxic conditions during the react

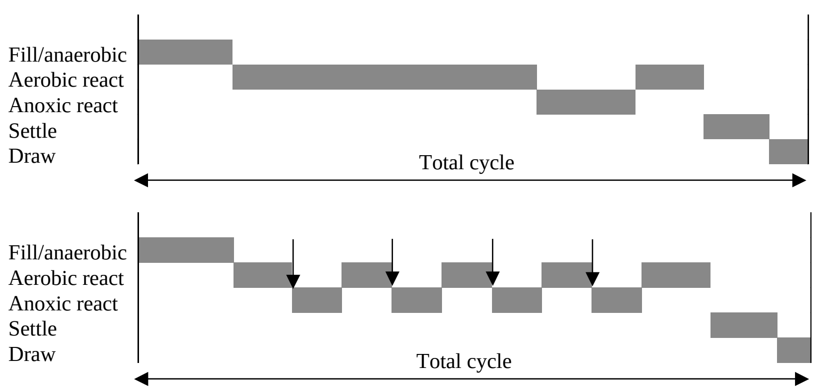

Figure 1 Operation of the SBR reactor: The reference operation configuration (top), the optimal operation scenario with IAF4 configuration. The arrow indicates the instant of step-feed (Sin *et al.*, 2004) (bottom)

phase; (2) low oxygen concentrations during the alternating aerobic sub-phases to stimulate simultaneous nitrification and denitrification; and (3) step-feed of the influent to the anoxic sub-phases to increase the rate of denitrification.

The optimised operation of one SBR cycle therefore consisted of a 60 min fill/anaerobic phase, four alternating 32.5 min aerobic and 20 min anoxic sub-phases, respectively, a 30 min final aerobic sub-phase and a 60 min settling/draw phase. The optimal DO set-point was 0.5 mg/L. The total volume of the SBR was 68 L (volumetric exchange ratio remained fixed at 0.5 as mentioned above). In total, 34 L of the SBR influent was fed into each cycle. Twenty-four litres of the influent was supplied during the fill/anaerobic phase of the cycle and the remaining 10 L was equally step-fed to the anoxic phases, i.e. 2.5 L per each anoxic phase (see Figure 1).

Simulations were performed using WEST® (Hemmis NV, Kortrijk, Belgium) dedicated software for the modelling of wastewater treatment plants (WWTP) that contains a scenario analysis module.

Results and discussion

Evaluation of the implementation of the optimal operation scenario

The optimal operation scenario was implemented on 17 December 2003 and the SBR system behaviour for the subsequent 2.5 months (until 2 March 2004) is reported here. Nitrogen (total and nitrate), phosphorus, MLSS and SVI were measured daily during the monitoring period while ammonium nitrogen was only measured twice a week since complete nitrification was consistently achieved over a long-term period in the SBR. The results are shown in Figure 2.

It can be seen that the change of the SBR operation resulted in an immediate effect on the SBR performance (see Figure 2 top and-middle). This immediate effect was positive both for effluent total nitrogen, nitrate and also for phosphorus (see Figure 2 top and middle). The average effluent concentrations of the total nitrogen and the nitrate nitrogen were 8.6 mgN/L and 3.1 mgN/L respectively (see Table 1). This means that the optimal operation resulted in ca 50% improvement in the total nitrogen and 76% improvement in the nitrate nitrogen removal compared with the reference operation state of the SBR (see Table 1). As for the P-removal, the optimal operation was able to improve the previous SBR performance by 43%. However, the effluent concentration was still around 3.8 mgP/L, which is higher than the legal treatment targets (e.g. EC Directives, 91/271/EEC).

On the other hand, the ammonia concentration in the effluent was observed to increase from 0.1 to 1.1 mgNH4-N/L during the optimal operation period, indicating that the nitrification process could no longer be completely achieved (see Table 1 and Figure 2 top). It is important to note that the high NH_4-N concentrations appearing in the effluent around 1 February were due to a technical problem with the SBR operation, which caused the loss of some biomass from the system. The nitrification activity was affected most by this incident (see Figure 2 top).

The SBR performance was observed to be fluctuating both for nitrogen and phosphorus removal. A certain trend can be observed between the effluent nitrate nitrogen and phosphorous profiles (see Figure 2 middle): the effluent phosphorus concentrations decrease following a decrease in the effluent nitrate nitrogen. This indicates the well-known competition between the PAOs and denitrifying heterotrophs for readily biodegradable substrate.

As expected, an immediate effect in the trends of the MLSS and SVI was not observed (see Figure 2 bottom). The MLSS and the sludge volume index (SVI) were also following a dynamic pattern within the observation period (see Figure 2 bottom). After switching the operation, a gradual increase in the SVI profile was observed in the first two weeks. In the

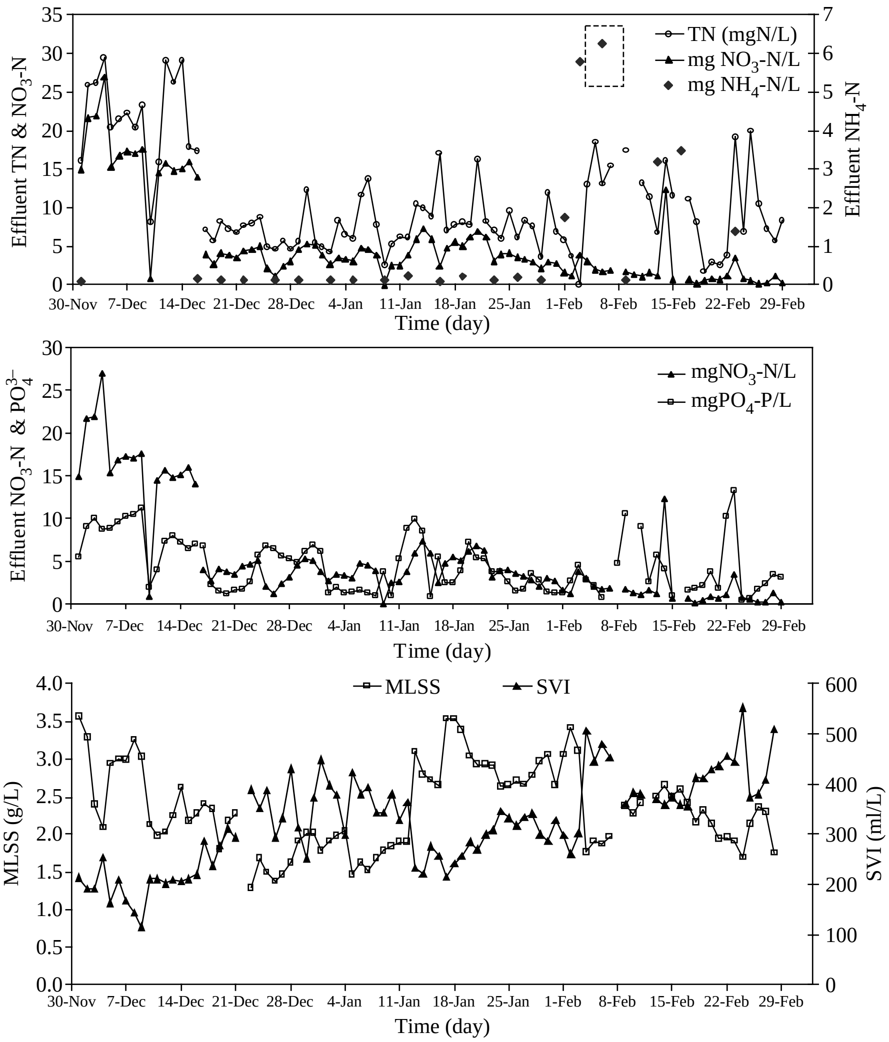

Figure 2 Results of the optimal SBR operation (the arrow indicates the time of implementation): effluent nitrogen species (top); effluent nitrate versus phosphorus (middle); MLSS in the reactor and SVI (bottom). The dashed box (top) indicates the days where the SBR operation was interrupted due to a technical problem

next two weeks the SVI recovered but then the SVI resumed an increasing trend towards full bulking (see Figure 2 bottom). The MLSS was found to be inversely correlated to the trend observed in the SVI due to washout of biomass (see Figure 2 bottom). In short, a long-term steady state could not be achieved in the SBR system.

Confrontation of the model with reality: model validation

The model used in the previous study to find the optimal operation was compared with the new data to check the validity of the model. The so-called ASM2dN model was developed in the previous study by modifying the ASM2d of Henze *et al.* (2000) with the hydrolysis of organic nitrogen processes of ASM1 of Henze *et al.* (2000) (see Insel *et al.*, 2004).

Considering the long-term SBR performance data considered above, the model prediction of the total effluent nitrogen appears to be correct whereas there is approximately 100% deviation between the modelled and measured nitrate nitrogen. In a positive sense,

Table 1 The SBR performance before and after the optimal operation versus the model prediction

	Total Nitrogen mgN/L	NH_4-N mgN/L	NO_3-N mgN/L	PO_4-P mgP/L
Influent	60	5	0	11
Effluent concentrations				
Model prediction	8.4	1.7	6.7	1.5
Reference operation	18.1	0.1	12.5	6.6
Optimal operation	8.6	1.1	3.1	3.8
Removal efficiency				
Reference operation	70%	–	–	48%
Optimal operation	86%	–	–	65%
Improvement	+53%	–	+76%	+43%

in real-life the optimal operation provided an even better effluent nitrate concentration than that which the model had predicted (see Table 1). With respect to the phosphorus removal, however, the model failed to predict reality since the effluent phosphorous concentration was approximately 100% higher than the model had predicted (see Table 1).

To understand better the underlying reason for these discrepancies between the model and reality, a new measurement campaign was performed to monitor the dynamics within one cycle of SBR operation (on 29 January 2004). This measurement campaign was set up to validate and eventually recalibrate the model as proposed in the systematic protocol of Sin *et al.* (2004). The results are shown in comparison with the dynamic model predictions in Figure 3.

It becomes clear from Figure 3 that the model is unable to explain or reasonably predict the dynamics of ammonia and nitrate during the various phases of the cycle. For example, the measured ammonia nitrogen at the end of the anaerobic phase is around 19 mgNH_4-N/L, which is twice as high as the model prediction (see Figure 3 left). These results indicate that the hydrolysis process of organic nitrogen into ammonium nitrogen is no longer a limiting step in the system, whereas it was clearly limiting during the reference operation.

Under limited aeration conditions (the DO set-point was 0.5 mg/L) the nitrification process was observed to occur with nitrite build-up, indicating that the activity of the nitrite oxidisers was slower than that of the ammonia oxidisers. In hindsight, this result was not surprising since the oxygen affinity constant of the nitrite oxidisers is known to be higher than the oxygen affinity constant of the ammonia oxidisers (Hao *et al.*, 2002). It is also important to note that the nitrification (both the first and the second step) is actually just completed at the end of the last aerobic phase (see Figure 3). This indicates that the system was running close to its limits in terms of nitrification capacity, which may explain the significant fluctuations observed in Figure 2.

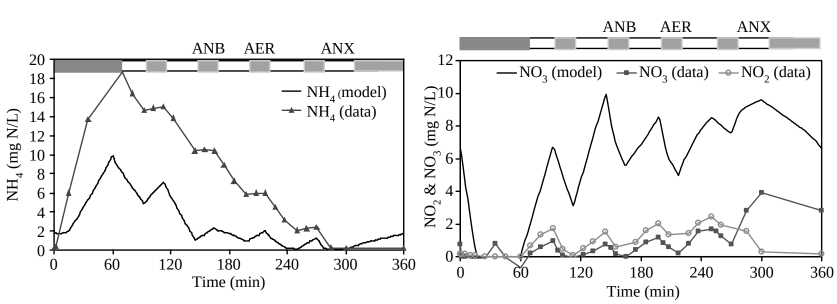

Figure 3 Comparison of the model simulations (ASM2dN) with the results obtained after the optimal operation scenario: in-cycle NH_4-N dynamics (left) NO_3-N and NO_2-N dynamics (right).

The system was observed to denitrify using not only NO_3-N but also the NO_2-N as electron acceptor under anoxic conditions (see Figure 3 right). Moreover, performing a nitrogen mass balance during the aerobic sub-phases, it was found that around 30–40% of the NH_4-N nitrified was not recovered as NO_2-N and NO_3-N. This indicates that the difference was lost as N_2 gas as a result of the simultaneous nitrification and denitrification (SND) process. However, this was expected to prevail under the limited (0.5 mgO_2/L) aeration conditions (Sin *et al.*, 2004). The combined effect of SND and the nitrite route (nitrification to nitrite and direct denitrification to N_2 gas) considerably increased the N-removal capacity of the system. This explains why the optimal operation resulted in a better nitrate removal than that which the model had predicted (see above).

With respect to bio-P performance, the measured maximum P-release concentration at the end of the anaerobic phase is considerably lower (around 10 mgP/L difference) than the model had estimated (see Figure 4). This indicates that the model had overestimated the PAO activity, which again falsifies the prediction. In short, the model is clearly unable to explain the changed behaviour of the SBR system.

From the evaluation of the implementation results, it becomes clear that the optimal operation has considerably shifted the SBR system to a point where the model used to represent the system is no longer valid. This shifting of the SBR behaviour is probably caused by a selection of an activated sludge community with different kinetics/stoichiometric properties than the reference system. The molecular monitoring of the SBR microbial community by DGGE confirmed the gradual shift in the population dynamics during the optimal operation (Sin *et al.,* 2005). Consequently, the model, which was developed based on the properties of the activated sludge community of the reference SBR system, becomes naturally irrelevant to the new SBR system. Indeed, the resulting mechanistic model lacked the description of the adaptation phenomena and the observed change in the community structure. This outcome was in fact foreseen in the previous study (Sin *et al.*, 2004). To overcome this seemingly probable consequence of model-based process optimisation, it was proposed in that earlier contribution to iterate the methodology until the system's performance converged to the targets specified in the optimisation study.

Understanding the filamentous bulking provoked by the optimal operation

The change in activated sludge community also led to the settling problems characterised by excessive filamentous bulking (see Figure 2 bottom). Although several theories have been proposed, there is no unified theory to explain the filamentous bulking in activated

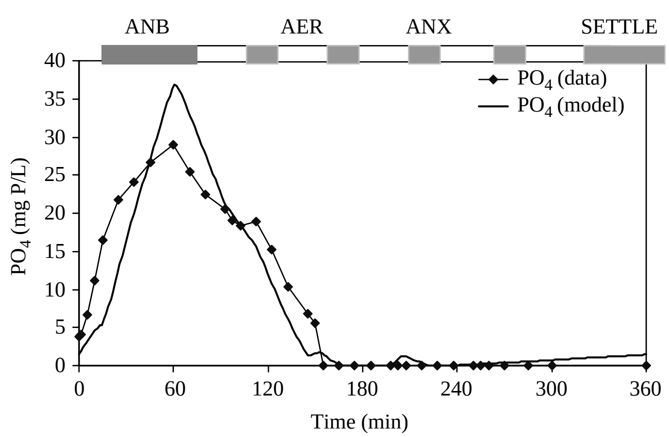

Figure 4 Comparison of the model simulations (ASM2dN) with the results obtained after the optimal operation scenario: in-cycle phosphorus dynamics

sludge systems (Martins *et al.*, 2004). Some of the theories relevant to the studied SBR are discussed below.

First, the optimal operation imposed low oxygen concentrations (0.5 mgO_2/L). This is commonly listed as one of the conditions giving rise to the proliferation of filamentous organisms. It can be explained by the substrate diffusion and also by the kinetic selection theories (Martins *et al.*, 2004). Accordingly, under low nutrient (oxygen) concentrations microgradients occur inside the flocs due to substrate diffusion. This favours growth of the filaments (K-strategist) since they have easier access to the oxygen outside the flocs owing to their outward growth.

Second, the optimal operation employed intermittent aeration, i.e. fast alternating aerobic and anoxic conditions in the SBR system. According to the hypothesis of Casey *et al.* (1992), the requirement of switching between aerobic and anoxic metabolism provides competitive advantages to filamentous organisms. The presence of nitric oxide (NO), a denitrification intermediate during denitrification of nitrite, causes an inhibitory effect on floc-formers in the subsequent aerobic conditions (Casey *et al.*, 1992). Since most filaments denitrify nitrate only to nitrite, they do not suffer from NO-toxicity and proliferate in a system operated with intermittent aeration and under incomplete denitrification similar to the optimal operation presented here.

As a third factor, the feeding pattern of the influent was also demonstrated to influence the settling properties of activated sludge in SBRs (Manning and Irvine, 1985). The feeding pattern determines the extent of the substrate gradient inside the flocs: slow feeding causes low substrate concentrations (substrate microgradient), whereas instantaneous feeding establishes high concentrations (substrate macrogradient) in the medium. Referring to the above-mentioned theories, the filaments will be favoured with a slow feeding pattern. Since the optimal operation scenario employed a high fill-time ratio (slow feeding), it is probable that the combined effect of the low oxygen, the alternating aerobic and anoxic conditions and the feeding pattern caused the settling problems in the SBR.

Incorporation of expert knowledge to the model-based optimisation methodology of Sin *et al.*

This study revealed that an ASM-type mechanistic model was unable to take into account all aspects of the SBR system under study, particularly regarding the settling properties as well as the change in the microbial community structure. The model-based optimisation therefore led to conditions for which the model no longer held. To circumvent this problem, it is suggested that expert knowledge about activated sludge settling (particularly filamentous bulking) be incorporated into the decision-making step of the optimisation methodology of Sin *et al.* (2004). For instance, no scenarios would be allowed with too low DO, nitrite presence at the end of an anoxic phase (and prior to aerobic conditions) would be checked, and fill-time ratio would be made small enough. In this way, it is expected indirectly to make up for possible inadequacies associated with the model predictions of future states of a system. Ultimately, it is desired to support and improve the choice of a best scenario among a multitude of scenarios to optimise the operation of the SBR systems.

Conclusions

The optimal operation found using a model-based approach in a previous study (Sin *et al.*, 2004) was implemented to the pilot-scale SBR and evaluated. The experimental results showed a remarkable (better than expected) improvement in the total nitrogen (53%), nitrate nitrogen (76%), and phosphorus (43%) removals from the system. However, long-term stable performance could not be achieved due to a severe filamentous bulking problem induced by the optimal operation conditions.

The comparison of the model with reality falsified the model. Particularly, the model was unable to predict the nitrite build-up caused by the low oxygen concentration (0.5 mgO_2/L) and fast alternation of the aeration conditions in the system. To appropriately describe this new behaviour of the system, the model structure has to be extended to include two-step nitrification and two-step denitrification processes as described in Sin and Vanrolleghem (2005).

Overall this study showed that currently mechanistic modelling does not describe all aspects of SBR systems, including the settling and adaptation of the underlying microbial community to new operational conditions. Taking into account these limitations properly is important to ensure a good model-application practice.

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