Research on Partial Nitrification Based on Mathematical Model

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Abstract: The successful completion of partial nitrification is the basis of good nitrogen removal efficiency in subsequent anammox process. The effects of inorganic carbon, salinity, FA, FNA, DO and other key factors can be predicted and verified through mathematical simulation to determine the most suitable environmental conditions for the partial nitrification.

1. Introduction:
Compared to traditional denitrification process, nitrification-denitrification process, the partial nitrification-anaerobic ammonium oxidation process has the characteristics of saving aeration energy consumption, no additional carbon source, and low surplus sludge production. Based on these characteristics, the partial nitrification-anaerobic ammonium oxidation process has good feasibility on the technical level and the economic level. The smooth progress of partial nitrification (PN) is a prerequisite for the stable nitrogen removal efficiency of anaerobic ammonium oxidation (ANAMMOX). In order to achieve effective partial nitrification, the reactor operating conditions need to be strictly controlled to retain the maximum amount of ammonia-oxidizing bacteria (AOB). \( \text{NH}_4^+ \)-N in wastewater is only oxidized to \( \text{NO}_2^- \)-N, Instead of continuing to oxidize to \( \text{NO}_3^- \)-N, a higher rate of nitrite accumulation (\( \text{NO}_2^-/\text{NO}_x^- \) \( >0.5 \)) is achieved to create a more reasonable substrate environment for the subsequent anaerobic ammonia oxidation process. However, both AOB and NOB are symbiotic, and the growth kinetics of the two bacteria are similar. Their environmental conditions for growth also have many common features. Many studies have shown that in order to maximize the enrichment of AOB, it is necessary to accurately grasp and control the reaction environment such as control of DO, FA, FNA, SRT, PH, temperature, etc. in order to maximize the enrichment of AOB. Mathematical models, laboratory experiments and other scientific researches in the design and operation of the sewage treatment process can effectively predict the test results, have a very rich application value. In summary, the role of the mathematical model of sewage is rough: (1) Design optimization function: In the initial design, different schemes were simulated, and evaluate the advantages and disadvantages of different schemes. (2) Control and optimize the process: It is divided into two categories: static optimization and dynamic optimization. The former refers to designing the experimental conditions ahead of time, and then carrying out the practice in the process, with poor flexibility. Dynamic optimization is more effective. It is based on the dynamic model of online identification and adjusts the static form of the dynamic model, although it will be closer to the actual value, it is more difficult to operate. (3) Benefit optimization: the model is conducive to the operation management of the sewage treatment plant so that the purification effect of the sewage is maintained in an ideal state, and the energy consumption and operation cost of the water plant is reduced. (4) Research Assistance: through the simulation of numerous experiments, the model provides a favorable condition for researchers to study from multiple angles, and provides convenience and help for the
research and development of new domestic sewage treatment process. This article describes the establishment of nitrification models and the experimental results of partial nitrification under different experimental conditions to explore the optimum environment for suitable nitrification processes.

2. The establishment of partial nitrification model

A model was established to investigate the growth and decay rates of different microorganisms during the nitrification process, to a clear understanding and analysis of the partial nitrification process. The nitrification process is divided into two major processes: ammonification and nitrite oxidation. The stoichiometric relationships are shown in the following table, reflecting the proliferation and decay processes of AOB and NOB. $Y_{AOB}$ and $Y_{NOB}$ are the yield coefficients of AOB and NOB. $X_{AOB}$ and $X_{NOB}$ are the concentrations of AOB and NOB respectively. $i_{XB}$ is the content of ammonia nitrogen in microorganisms, $S_{NO2}$, $S_{NO3}$ and $S_{NH4}$ are the concentration of nitrite nitrogen, nitrate nitrogen and ammonia nitrogen, respectively.

| Table 1. Kinetics and chemometric models of two-stage nitrification |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
|                 | $X_I$           | $X_{AOB}$       | $X_{NOB}$       | $S_0$           | $S_{NO2}$       | $S_{NO3}$       | $S_{NH4}$       |
| AOB aerobic     | —               | —               | 1 — $\frac{3.43}{Y_{XAOB}}$ | $\frac{1}{Y_{XAOB}}$ | —               | $\frac{1}{Y_{AOB}}$ — $i_{XB}$ |
| growth          |                 |                 | ($X_{AOB}$)     | ($X_{AOB}$)     |                 | ($X_{AOB}$)     | ($X_{AOB}$)     |
| NOB aerobic     | —               | —               | 1 — $\frac{1.14}{Y_{XNOB}}$ | $\frac{1}{Y_{XNOB}}$ | $\frac{1}{Y_{XNOB}}$ | —               | ($X_{NOB}$)     |
| growth          |                 |                 | ($X_{NOB}$)     | ($X_{NOB}$)     | ($X_{NOB}$)     |                 | ($X_{NOB}$)     |
| AOB attenuation | $f_p$ —1        | —               | $f_p$ —1        | —               | —               | —               | —               |
| NOB attenuation | $f_p$ —1        | —               | $f_p$ —1        | —               | —               | —               | —               |

3. Impact of environmental factors on Partial Nitrification

3.1 Inorganic carbon

The effect of inorganic carbon on AOB obeys the Monod equation but has little effect on the activity of NOB. Therefore, the difference in the activity of inorganic carbon can be utilized to provide sufficient inorganic carbon to promote the activity of AOB and formed a competitive advantage over NOB to achieve partial nitrification. Li Dong et al. restored SNAD reactors that collapse due to excessive accumulation of nitrate, he found that only with the increase of inorganic carbon concentration, the temperature and apparent gas velocity remained stable during the experiment, indicating that sufficient inorganic carbon has a significant effect on the inhibition of NOB in the SNAD process. Before and after the addition of inorganic carbon, the aerobic ammonia oxidation activity (AOR) and anaerobic ammonia oxidation activity (ANR) increased from 0.0614 and 0.0406 g/(g·d) to 0.0811 and 0.0659 g/(g·d), respectively, it shows that inorganic carbon can effectively promote the activity of AOB and ANAMMOX. Liao Dexiang found that when the concentration of inorganic carbon is low (1.0g/L), the activity of ANAMMOX bacteria is inhibited, and when the concentration of inorganic carbon is increased to 1.5g/L, the removal rates of ammonia nitrogen and nitrous acid nitrogen rapidly increase from 41.6%, 46.2% to 83.6% and 100%, further indicating the inhibitory effect of inorganic carbon on NOB.
3.2 Salinity
Li Lingling[3] et al. found that the inhibition rate of salinity began to be 10~15gNaCl/L and 50~70gNaCl/L, and nitrification was completely inhibited. The acclimated activated sludge still has good nitrification efficiency in a high salt environment of 35g NaCl/L. Salts are severely inhibited by non-acclimated nitration systems. Even domesticated systems cannot withstand the effects of excessively high salt concentrations and are not suitable for salted wastewater with concentrations >5%. After the experimental analysis, Liu[4] suggested that NOB is more easily inhibited by salt. When the concentration is >20gNaCl/L and the survival rate of NOB is <1%, the survival rate of AOB is reduced by 50%. Different levels of inhibition of AOB and NOB by high salinity will lead to the accumulation of nitrite and change to the type of partial nitrification and denitrification.

Xu Hanli[5] et al. have reached some conclusions about the effect of salt concentration on the nitrification efficiency. Some of them are even contrary, and the main reasons are: (1) Differences in reaction systems and experimental conditions (temperature, pH-inhibiting compounds); (2) The way of adding salt is different, and the gradual increase is conducive to the adaptability of microorganisms to high salinity; (3) Inoculation of sludge source, microbial species, domestication; (4) Inoculation of sludge source, microbial species, domestication; different reactor operating modes, such as continuous flow or SBR, PF or CSTR, affect the retention of biomass, the uniformity of the matrix and oxygen, and so on.

3.3 FA
FA has different inhibitory concentrations for AOB and NOB. The former can be more than tens of times larger than the latter, so that the FA concentration can be adjusted to a reasonable value. When the NOB is almost completely suppressed, only a small amount of AOB is affected. Ji Min[6] analyzed the removal of NH₄⁺-N and the production of NO₃⁻-N. The NOB (FA inhibitory concentration of 6.6 mg/L) was more sensitive to FA than AOB (FA inhibitory concentration of 9.3 mg/L) and was more susceptible to inhibition. Before the inhibition, as the concentration of FA increased, the activity of both increased, indicating that FA also has a certain role in promoting. Vadivelu[7] et al. determined the oxygen uptake rate (OUR) of two microorganisms when Nitrosomonas and Nitrobacter were used under different concentrations of FA and FNA and when the aeration contained CO₂. In addition, when the inorganic carbon source (CO₂) is sufficient, the microorganism is simultaneously anabolic and catabolic, but when the inorganic carbon source is lacking, bacteria only undergo catabolism without anabolic. With this feature, the synthesis and catabolic activity of AOB and NOB at different FA concentrations were evaluated to further discuss the effect of FA on two different bacteria. It was found that for Nitrosomonas, the oxygen uptake rate increased with FA concentration when FA concentration was lower than 4 mg NH₃/L. When the concentration exceeds 4 mg NH₃/L, no increase in the oxygen uptake rate was observed even if the FA concentration increased (up to 16 mg NH₃/L). This means that even if FA reaches 16 mg NH₃/L, Nitrosomonas will not be inhibited. Hawkins[8] stabilized the pH at 8.0 and adjusted the FA concentration from 0.2 to 181 mg/L. It was found that the NOB inhibition rate only increased by 4%, while maintaining the FA at 2.2 mg/L, increasing the pH from 7.1 to 8.0, and the NOB inhibition rate consisted of 0.18 rose to 0.60.

3.4 FNA
The control effect of FNA on partial nitrification is similar to that of FA. Li Huijuan[9] et al. used control DO and FA respectively (ammonia nitrogen loading 1kg/m³·d, PH=8, DO=0.5~1mg/L, FA concentration far exceeds NOB threshold 40mg/L) and DO, FNA(Ammonia nitrogen loading 1kg/m³·d, PH=7, DO=0.5~1mg/L, the corresponding FNA concentration reached 0.14 mg/L, far exceeding the NOB inhibition threshold of 0.023 mg/L) two suppression strategies, this two strategies can eliminate NOB and enriched AOB. After comparison, DO and FNA inhibited the enrichment time, the AOB activity was high, and the system stability was strong. NOB has the adaptability to the inhibitory effect of FNA, in order to ensure the stable accumulation of NO₂⁻-N, DO needs to be
reduced. Although AOB has a greater affinity for DO, the NH₄⁺-N oxidation rate is also limited at low DO, as a result, the NH₄⁺-N concentration increases and the pH increases. In order to prevent the increase of pH induced FA inhibition of AOB, the proportion of influent NH₄⁺ and HCO₃⁻ can be changed to maintain the system pH at around 7.0.

3.5 DO
Bao Peng[10] et al. thought that for the nitrification sludge containing AOB and NOB, the high dissolved oxygen conditions favor the growth of Nitrospira belonging to the genus Nitrospirae and Nitrosomonas belonging to the genus Proteobacteria, and low dissolved oxygen conditions will lead to increased microbial diversity in the sludge flora. Liu Hong[11] et al used intermittent aeration mode (single-cycle alternating aerobic: hypoxia = 30min: 30min), separately control aeration volume 120, 100, 80, 60L/h, partial nitrification sludge that has been on hold for two months for recovery, recovery cycles are less than 45 cycles. When the aeration rate was 120L/h, NOB activity in the first 12 cycles gradually increased, and the increase was significantly higher than that in AOB. Afterwards, it gradually decreased. After the 25th cycle, the activity was lower than AOB. When the aeration volume was 80 and 60L/h, the NOB activity recovery was lower than that of AOB, and basically showed a gradually decreasing trend after 5 cycles.

Vincent[12] et al. used 1.5L air-lift granular sludge reactors, observed that changes in residual ammonia concentration could quickly cause changes in nitrate concentration within hours. If the residual ammonia concentration is increased, the rate of ammonia oxidation will increase even if the DO content is properly reduced. Oxygen penetration depth will decrease with increasing ammonia nitrogen concentration, so even when the ammonia concentration is high, there will be a stable partial nitrification process even if the DO fraction increases. When the system DO/ NH₄⁺-N concentration ratio is less than one, the NOB inhibition is more effective.

AOB and NOB have large differences in dissolved oxygen affinity. It is generally believed that the oxygen saturation coefficient of AOB is greater than the oxygen saturation coefficient of NOB, when maintaining a low dissolved oxygen concentration level, the activity of NOB can be largely inhibited with a little inhibition of AOB activity, preventing the nitrite from being continuously oxidized by NOB, thereby obtaining an ideal nitrite accumulation process. Xu Ting[13] et al used mathematical models to simulate the variation of NH₄⁺-N and NO₂⁻-N with time under different DO concentrations and found that the DO concentration was reduced to 0.8 mg/L when compared with DO=4 mg/L, the degradation rate of NH₄⁺-N in the system decreased significantly, by measuring the half rate constant of dissolved oxygen, it was found that Kₒ,AOB were higher than Kₒ,NOB.

4. Conclusion
Using mathematical simulations, you can predict the results of biological experiments that take months to complete in a short period, which can save a lot of time, it is also more economical. It is not difficult to see that the adjustment of factors such as inorganic carbon, salt, FA, FNA, and DO largely determines the operating effect of the partial nitrification system. For FA and FNA inhibitory concentrations, the conclusions drawn by different researchers are quite different and still need to be gradually refined. At the same time, the reasons for the accumulation of nitrate in the low DO concentration need further studies.

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