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Guideline of Selecting N_2O Models to predict N_2O Production by Ammonia Oxidizing Bacteria

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Summary of key findings

This study tests the predictive ability of two single-pathway models to describe the N_2O data generated by a two-pathway N_2O model and provides theoretical guidance on how to use these models under various conditions. The modeling results suggested that (1) The model based on the AOB denitrification pathway should be used under the conditions with constant dissolved oxygen (DO) concentration and applied either at low DO concentration (< 0.5 mg O_2/L) with any non-inhibitory nitrite (NO_2^-) concentration or at higher DO (≥ 0.5 mg O_2/L) with relatively high NO_2^- but non-inhibitory concentration (≥ 1.0 mg N/L); (2) The model based on the NH2OH oxidation pathway can be applied under the conditions of relatively high DO concentration (≥ 1.5 mg O_2/L) with any non-inhibitory NO_2^- concentration; (3) under other conditions, the two-pathway model should be applied.

Background and relevance

Ammonia oxidizing bacteria (AOB) have been recognized to be the main contributor to N_2O production during wastewater treatment via two main pathways: (i) the reduction of nitrite (NO_2^-) to N_2O via nitric oxide (NO), known as AOB denitrification and (ii) N_2O as a side product during incomplete oxidation of hydroxylamine (NH_2OH) to NO_2^- (Law et al., 2012).

The conceptual structures of three representative N_2O models are presented in Figure 1. The AOB denitrification model (Figure 1A) is based on the AOB denitrification pathway, whilst the NH_2OH oxidation model (Figure 1B) assumes that N_2O production is due to the reduction of NO produced from the oxidation of NH_2OH (Ni et al., 2013a; Ni et al., 2013b). The two-pathway model (Figure 1C) incorporates both the AOB denitrification and NH2OH oxidation pathways (Ni et al., 2014).

The two-pathway model enhanced our ability to predict N_2O production by AOB during wastewater treatment under different conditions, which has been demonstrated to be applicable to various cultures under different DO and NO_2^- conditions (Ni et al., 2014). However, the single-pathway models have simpler structures and fewer parameters, which bring convenience to model calibration, and could be used preferably under certain conditions. However, such conditions have not been established. The aim of this study is to identify under what conditions the AOB denitrification model and the NH2OH oxidation model are able to replace the two-pathway model for practical applications, and under what conditions the two-pathway model has to be applied.

Results and Discussion

The performance of the two single-pathway models for the steady-state simulations was evaluated based on the η_{AOB} variations under various conditions. The estimated values of η_{AOB} for the AOB denitrification model and the NH_2OH oxidation model under different conditions are shown in Figure 2.

With regard to the AOB denitrification model, the following observations are made:

At each NO_2^- level, the value of η_{AOB} in the AOB denitrification model is very sensitive to DO concentration and increases almost linearly as DO increases from 0.05 to 5 mg O_2/L in Figure 2a, suggesting that the AOB denitrification model would only be applicable when DO is constant.

For a constant DO in the range of 0.5 – 5 mg O_2/L, the value of η_{AOB} of the AOB denitrification model drops rapidly as NO_2^- increases from 0.05 to 1.0 mg N/L, indicating that the AOB denitrification

model can not reproduce the two-pathway model outputs with any fixed η_{AOB} values in this region (constant DO in the range 0.5 – 5 mg O_2/L, while nitrite varies in the range 0.05 – 1.0 mg NO_2^--N/L) (Figure 2a). However, η_{AOB} becomes almost independent of nitrite concentration as NO_2^- further increases from 1.0 to 5.0 mg N/L (Figure 2a) and the values of η_{AOB} are within the feasible range (below 1.0). These indicate that the AOB denitrification model is able to reproduce the two-pathway model outputs under these conditions (constant DO in the range of 0.5 – 5 mg O_2/L, while nitrite varies in the range 1.0 – 5.0 mg NO_2^--N/L).

For a constant DO below 0.5 mg O_2/L, η_{AOB} is independent of the NO_2^- concentration and stays in the feasible range (close to 0) (Figure 2a). These mean that the AOB denitrification model can adequately describe N_2O production by AOB in the DO range of 0 – 0.5 mg O_2/L, independent of the nitrite concentration (provided that DO remains constant).

With regard to the NH_2OH oxidation model, the following observation is made:

η_{AOB} of the NH2OH oxidation model remains almost constant when DO is in the range of 1.5 – 5.0 mg O_2/L at all NO_2^- levels (Figure 2b). This means that the NH_2OH oxidation model can be applied at high DO concentrations (> 1.5 mg O_2/L). The η_{AOB} values are in the feasible range (close to 0).

In comparison, in the DO range of 0.05 - 1.5 mg O_2/L, the value of η_{AOB} of the NH_2OH oxidation model varies significantly to substantially with DO (Figure 2b). Further, at each DO level, η_{AOB} also varied with NO_2^- particularly in the range 0.05 to 0.5 mg N/L. This implies that the NH_2OH oxidation model is not a suitable model under low DO conditions (<1.5 mg O_2/L).

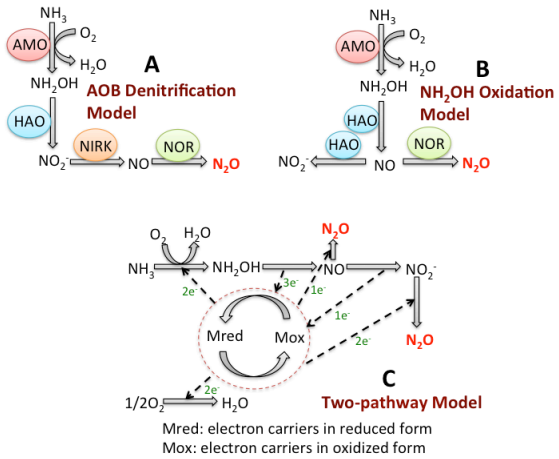

Figure 1. Reaction schemes in the three N2O models evaluated in this study.

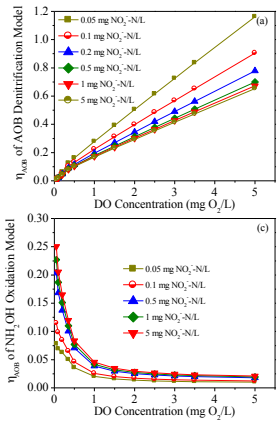

Figure 2. Estimation results of ηAOB of two single-pathway models under various DO and NO2- concentrations.

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