9th IWA Symposium on Systems Analysis and Integrated Assessment
14-17 June 2015, Gold Coast, Australia

Modeling of N_2O Production by Ammonia Oxidizing Bacteria: Integration of Catabolism and Anabolism

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Keywords: N_2O model; inorganic carbon; ATP/ADP

Summary of key findings

In the developed N_2O model of this work, inorganic carbon (IC) effect on both ammonia oxidation and N_2O production is explicitly considered, energy transportation is coupled to electron transfer and the catabolism and anabolism of ammonia oxidizing bacteria (AOB) are linked through ATP/ADP pool. The calibration and validation of the model are conducted using experimental data from a nitrification system. The model satisfactorily describes the N_2O data under varying IC conditions. In addition, the model also predicts the impact of IC on N_2O production via the AOB denitrification pathway and the hydroxylamine (NH_2OH) oxidation pathway.

Background and relevance

Ammonia oxidizing bacteria (AOB) have been recognized as the main contributor to nitrous oxide (N_2O) production from wastewater treatment plant. The N_2O production by AOB is attributed to two different pathways: (i) the reduction of nitrite (NO_2^-) to N2O via nitric oxide (NO), known as nitrifier or AOB denitrification and (ii) N_2O as a side product during incomplete oxidation of hydroxylamine (NH_2OH) to NO_2^- (Law et al., 2012).

So far, the proposed N_2O models based on either of the two known pathways managed to predict N_2O emission from wastewater treatment plants (WWTPs) under certain dissolved oxygen (DO) and NO_2^- conditions (Ni et al., 2013a). However, as N_2O production by AOB linearly depends on inorganic carbon (IC) concentration (Peng et al., 2015), the previously proposed N_2O models (Ni et al. 2013b) may not be able to estimate N_2O emissions caused by the IC variations in one WWTP or among different type of WWTPs.

Most studies on the biochemistry of AOB have dealt with the ammonia oxidation and N_2O pathways, but little attention has been paid to the coupling of electron transfer, energy generation and carbon assimilation of AOB. The impact of IC availability (substrate for cell synthesis of AOB) on NH_3 oxidation activity, N_2O production and its production pathways has not yet been fully described. Therefore, we aim to develop a new mathematical model incorporating both anabolism and catabolism in AOB metabolism by lumping them into oxidation and reduction reactions through electron carriers and ATP/ADP pools. The model is tested by comparing simulation results with measured data from two different nitrifying cultures and under different IC conditions.

Results and Discussion

We develop a new mathematical model that synthesizes all relevant reactions involved in the consumption and production of NH_3, NH_2OH, NOH, NO_2^-, NO, N_2O, O_2, and CO_2 by AOB (Figure 1). The coupling between catabolism and anabolism is elucidated via the reactions involving electron carriers and energy-rich intermediates. Particularly, Mred (reduced mediator) and Mox (oxidized mediator), defined as the reduced and oxidized forms of electron carriers, respectively, are introduced in the model to link the electron transfer from oxidation to reduction (Figure 1). ATP and ADP are involved in this model to link the energy transfer (Figure 1).

The calibration of the N_2O model involved optimizing key parameter values for the ammonia oxidation and N_2O production via the two pathways by fitting simulation results to batch test data. The model predictions and the experimental results in all batch tests are summarized in Figures 2. The evaluation results show that the model can well describe the linear relationship between N_2OR and IC, which supports the validity of the developed N_2O model. The model also innovatively reveals that IC plays an important role in regulating the shift of the two known N_2O pathways in the nitrifying system. With the increase of IC, the N_2O production from AOB denitrification pathway increased with a decreasing rate, while N_2O production from NH_2OH oxidation pathway (NOH) increased almost linearly. The AOB denitrification pathway was the dominant pathway at tested IC concentration range of 0.5 - 9.5 mmol C/L, whilst the NH_2OH oxidation pathway became main pathway after IC further increased from 9.5 to 11.6 mmol C/L.

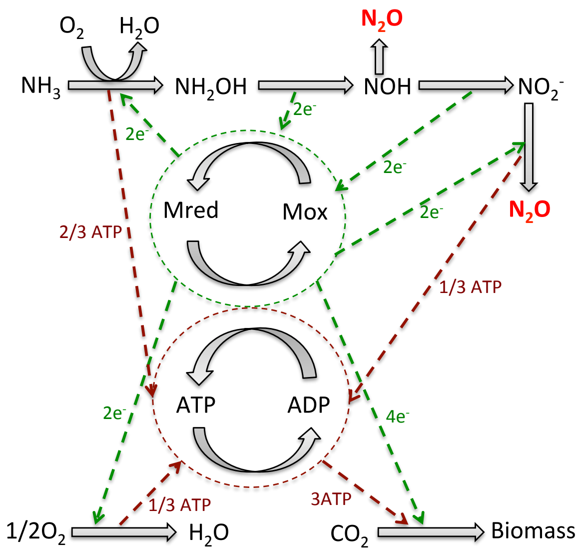

Figure 1. Simplified representation of the biochemical reactions associated with N_2O production by AOB, coupled with electron and energy transportation.

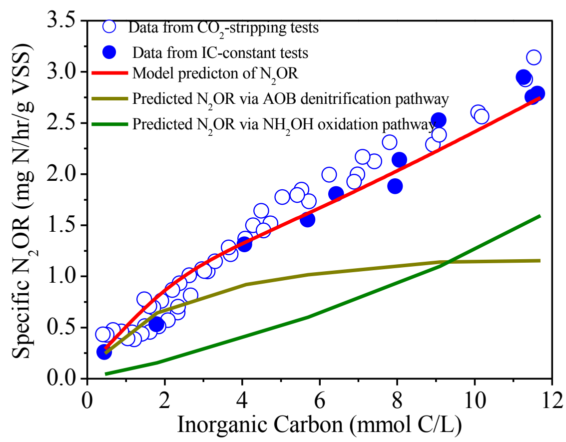

Figure 2. Model evaluation results using experimental data from the nitrifying culture.

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