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Review

Recent advances in mathematical modeling of nitrous oxides emissions from wastewater treatment processes

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ABSTRACT

Nitrous oxide (N_2O) can be emitted from wastewater treatment contributing to its greenhouse gas footprint significantly. Mathematical modeling of N_2O emissions is of great importance toward the understanding and reduction of the environmental impact of wastewater treatment systems. This article reviews the current status of the modeling of N_2O emissions from wastewater treatment. The existing mathematical models describing all the known microbial pathways for N_2O production are reviewed and discussed. These included N_2O production by ammonia-oxidizing bacteria (AOB) through the hydroxylamine oxidation pathway and the AOB denitrification pathway, N_2O production by heterotrophic denitrifiers through the denitrification pathway, and the integration of these pathways in single N_2O models. The calibration and validation of these models using lab-scale and full-scale experimental data is also reviewed. We conclude that the mathematical modeling of N_2O production, while is still being enhanced supported by new knowledge development, has reached a maturity that facilitates the estimation of site-specific N_2O emissions and the development of mitigation strategies for a wastewater treatment plant taking into the specific design and operational conditions of the plant.

Contents

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1. Introduction

Nitrous oxide (N_2O) not only is a significant greenhouse gas, with an approximately 300-fold stronger warming effect than carbon dioxide (IPCC, 2007), but also reacts with ozone in the stratosphere leading to ozone layer depletion (Portmann et al., 2012). It can be produced and directly emitted from wastewater treatment systems (Foley et al., 2010; Ahn et al., 2010a, 2010b; Ye et al., 2014). Although N_2O emission factors reported for full-scale systems are relatively low, from 0.01% to 1.8% of influent total nitrogen (TN) (Ahn et al., 2010a), N_2O emissions can contribute substantially to the carbon footprint of wastewater treatment plants (WWTP). It should be noted that an emission factor of 1.0% would already increase the carbon footprint of a WWTP by approximately 30% (de Haas and Hartley, 2004; Law et al., 2012). Therefore, the development of reliable predictive tools for quantifying and mitigating N_2O emission is important for achieving greenhouse gas neutral wastewater treatment (Ni et al., 2013a, 2013b).

The N_2O emission data collected from wastewater treatment plants (WWTPs) to date show a huge variation in the N_2O emission factor (the fraction of influent nitrogen load emitted as N_2O), ranging between 0.01% and 1.8%, and in some cases even higher than 10% (Kampschreur et al., 2009; Ahn et al., 2010a, 2010b; Foley et al., 2010; Wang et al., 2011). A high degree of temporal variability in N_2O emission has also been observed within the same WWTP (Ahn et al., 2010a; Ye et al., 2014). The observed variability is in clear contrast with the fixed emission factors currently applied to estimating N_2O emissions from wastewater treatment as recommended by the United Nation's Intergovernmental Panel on Climate Change (IPCC) and various governments (IPCC, 2007; EPA, 2012). A major problem with the use of fixed emission factors is that the link between emissions and process configurations and operating characteristics is not considered. As such, the estimates do not account for the variable process conditions in different plants and do not encourage mitigation efforts (Ni et al., 2013a).

Mathematical models have been widely applied to the prediction of nitrogen removal in wastewater treatment, and are gaining more attention for the prediction of N_2O accumulation and emission during nitrification and denitrification processes (CH2MHill, 2008; Ni et al., 2011; Corominas et al., 2012; Pocquet et al., 2013; Guo and Vanrolleghem, 2014; Harper et al., 2015). The ability to predict N_2O production by modeling provides an opportunity to include N_2O production as an important consideration in the design, operation and optimization of biological nitrogen removal processes (Ni et al., 2011, 2013a). Furthermore, mathematical modelling should be a more appropriate method for estimating site-specific emissions of N_2O than the over-simplified model with fixed N_2O emission factors (Corominas et al., 2012; Ni et al., 2011, 2013a; Mampaey et al., 2013; Pocquet et al., 2013; Guo and Vanrolleghem, 2014). In addition, mathematical modeling provides a method for verifying hypotheses related to the mechanisms for N_2O production, and thus serves as a tool to support the development of mitigation strategies (Ni et al., 2013b).

N_2O modelling has evolved rapidly in the past few years, with models based on various production pathways proposed. These models have been calibrated with data obtained from laboratory reactors and full-scale wastewater treatment plants operated under various conditions. Each of these models has its underlying assumptions and has been calibrated/validated to various degrees based on the understanding of the processes of the distinct model creators, which displayed various predictive abilities (usually good fit with own data but fail with foreign data). Despite the obvious importance of N_2O modeling, and the increasing number of publications, there has never been any attempt to summarize all the modeling information in a comprehensive review. Therefore, this review aims to clarify, to compare, and to provide guide for the use of these models. The existing mathematical models describing all the known microbial pathways for N_2O production as well as their underlying assumptions are reviewed, discussed and compared, including the single-pathway and two-pathway models of AOB, the N_2O models of heterotrophic denitrifiers, and the integrated N_2O models by both AOB and heterotrophic denitrifiers. An overview of the model evaluations using lab-scale and full-scale experimental data is also presented to provide insights into the applicability of these N_2O models under various conditions.

2. N_2O production pathways in wastewater treatment

N_2O is produced during biological nitrogen removal in wastewater treatment, typically attributed to autotrophic AOB (Tallec et al., 2006; Kampschreur et al., 2009; Chandran et al., 2011) and heterotrophic denitrifiers (Kampschreur et al., 2009; Lu and Chandran, 2010; Pan et al., 2012). Although N_2O might be potentially produced through chemical pathway (Schreiber et al., 2009; Harper et al., 2015), there are three main microbial pathways involved in N_2O formation (Fig. 1), namely the NH_2OH oxidation, nitrifier (AOB) denitrification, and heterotrophic denitrification pathways (Wunderlin et al., 2012, 2013).

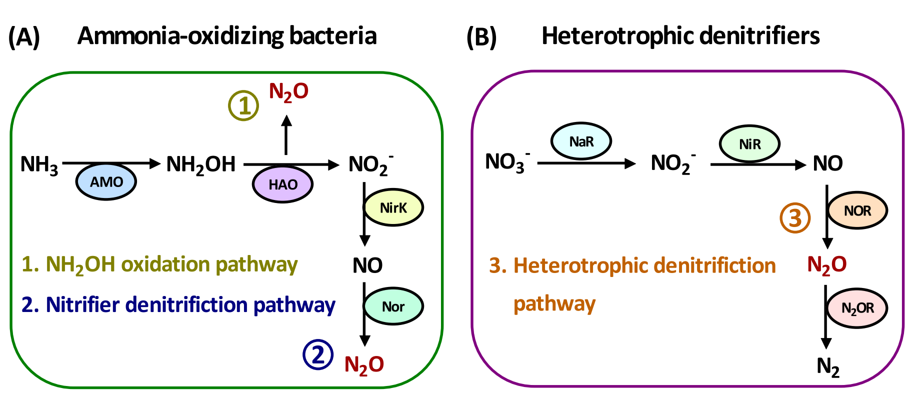

Fig. 1. Simplified representation of the three N_2O production pathways by ammonia oxidizing bacteria (A) and heterotrophic denitrifiers (B): nitrifier denitrification, NH_2OH oxidation and heterotrophic denitrification pathways.