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AUSTRALIA

Modeling N_2O production by ammonia oxidizing bacteria: single pathway or two-pathway models?

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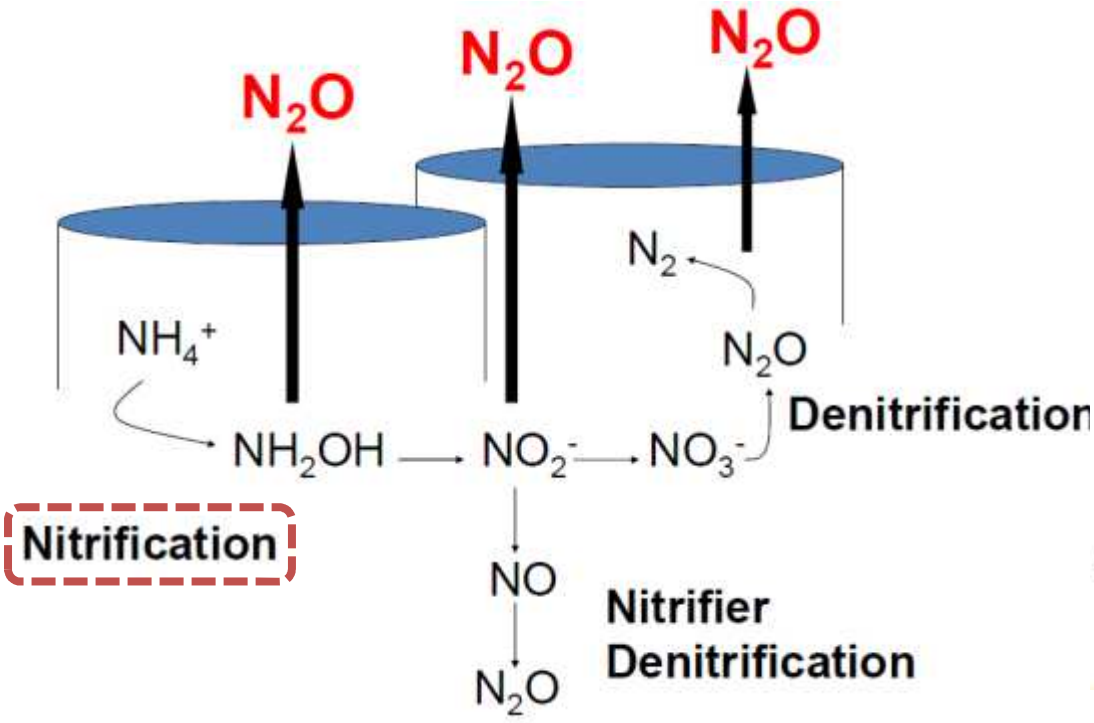
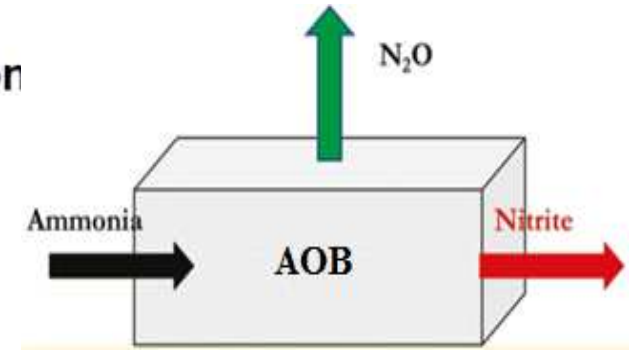
IWA
the international water association

N_2O production processes

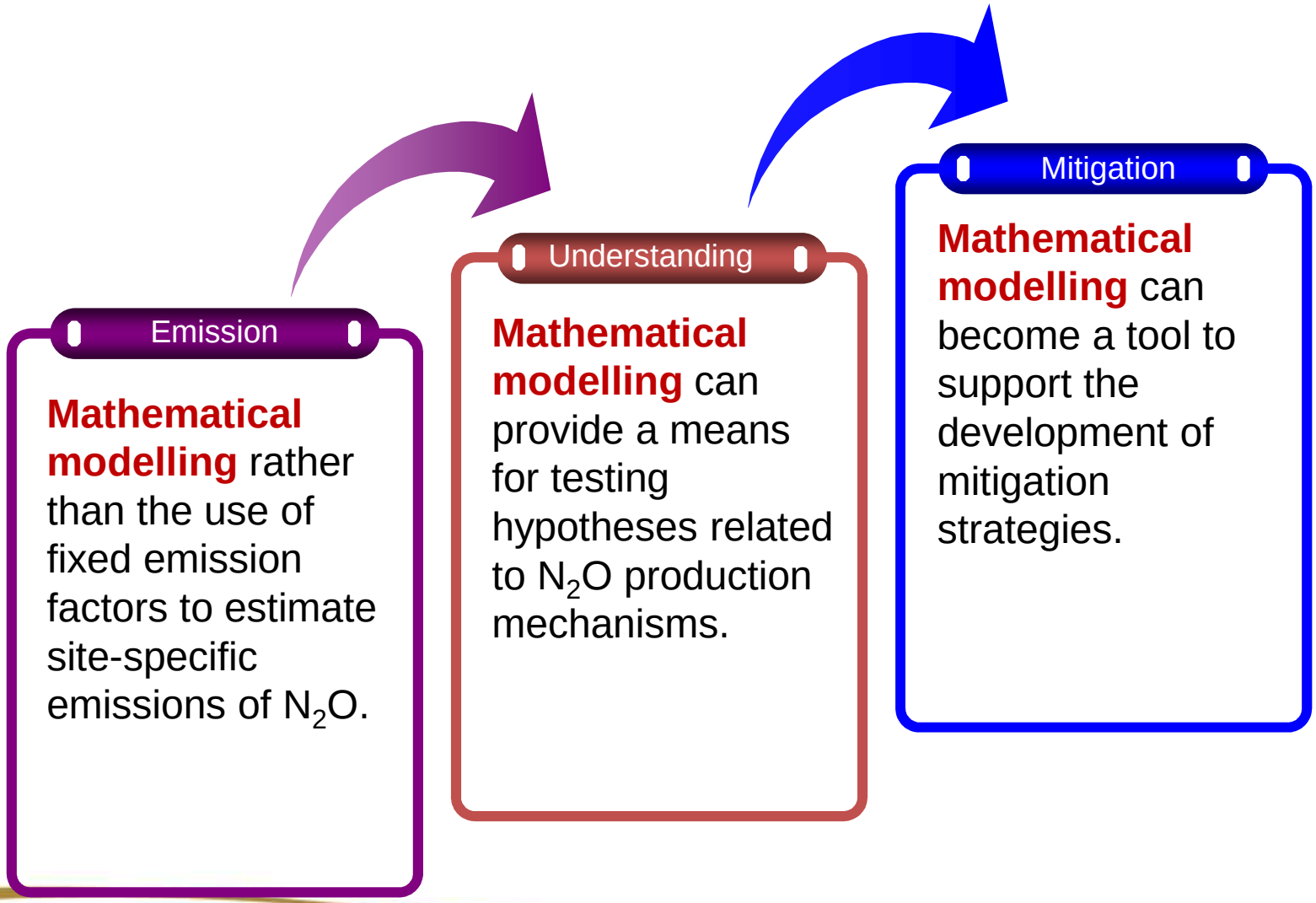


AOB might be the major contributors to N_2O emission

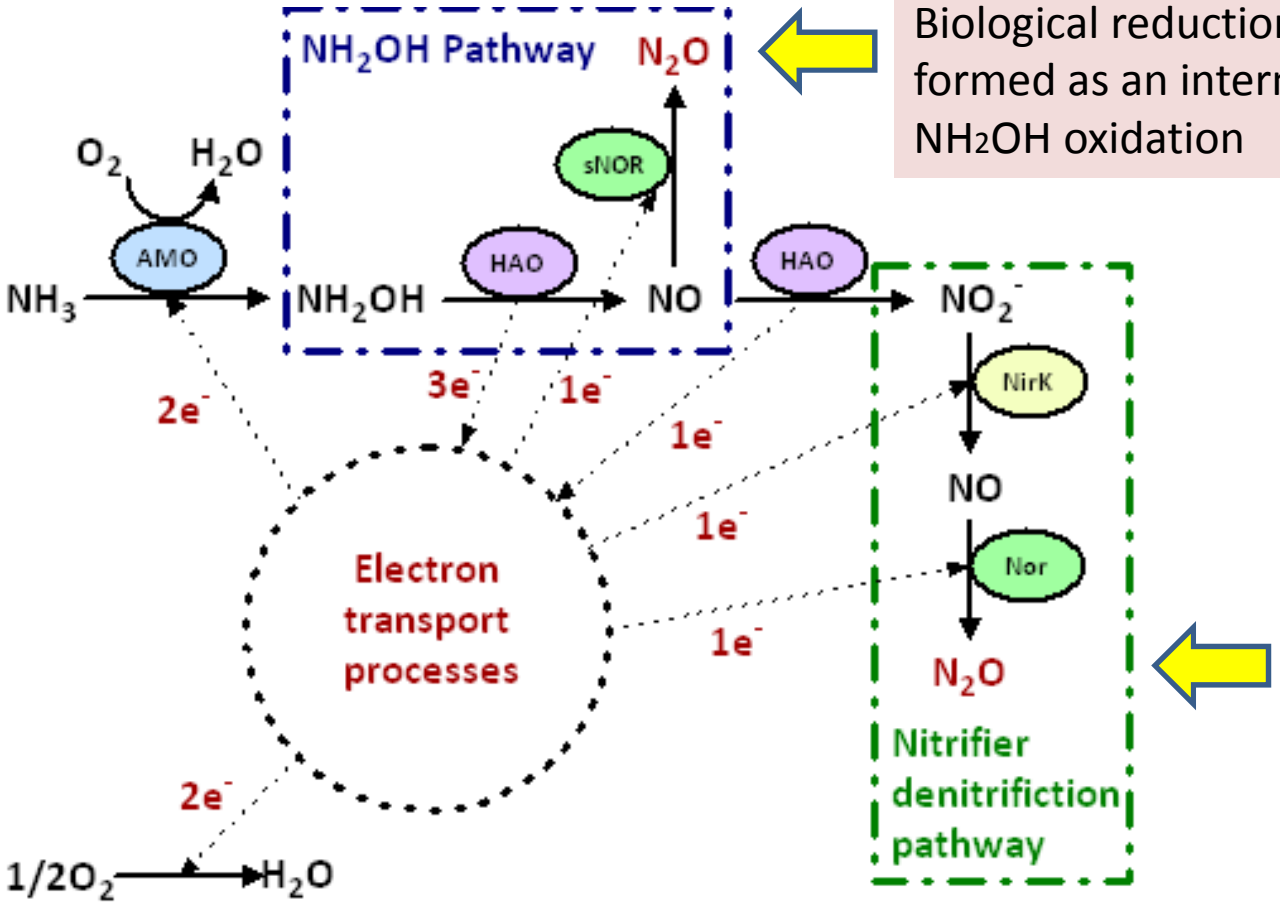


N_2O is produced during biological nitrogen removal typically attributed to autotrophic ammonia-oxidizing bacteria (AOB) and heterotrophic denitrifying organisms.

Mathematical Modelling of N_2O Production



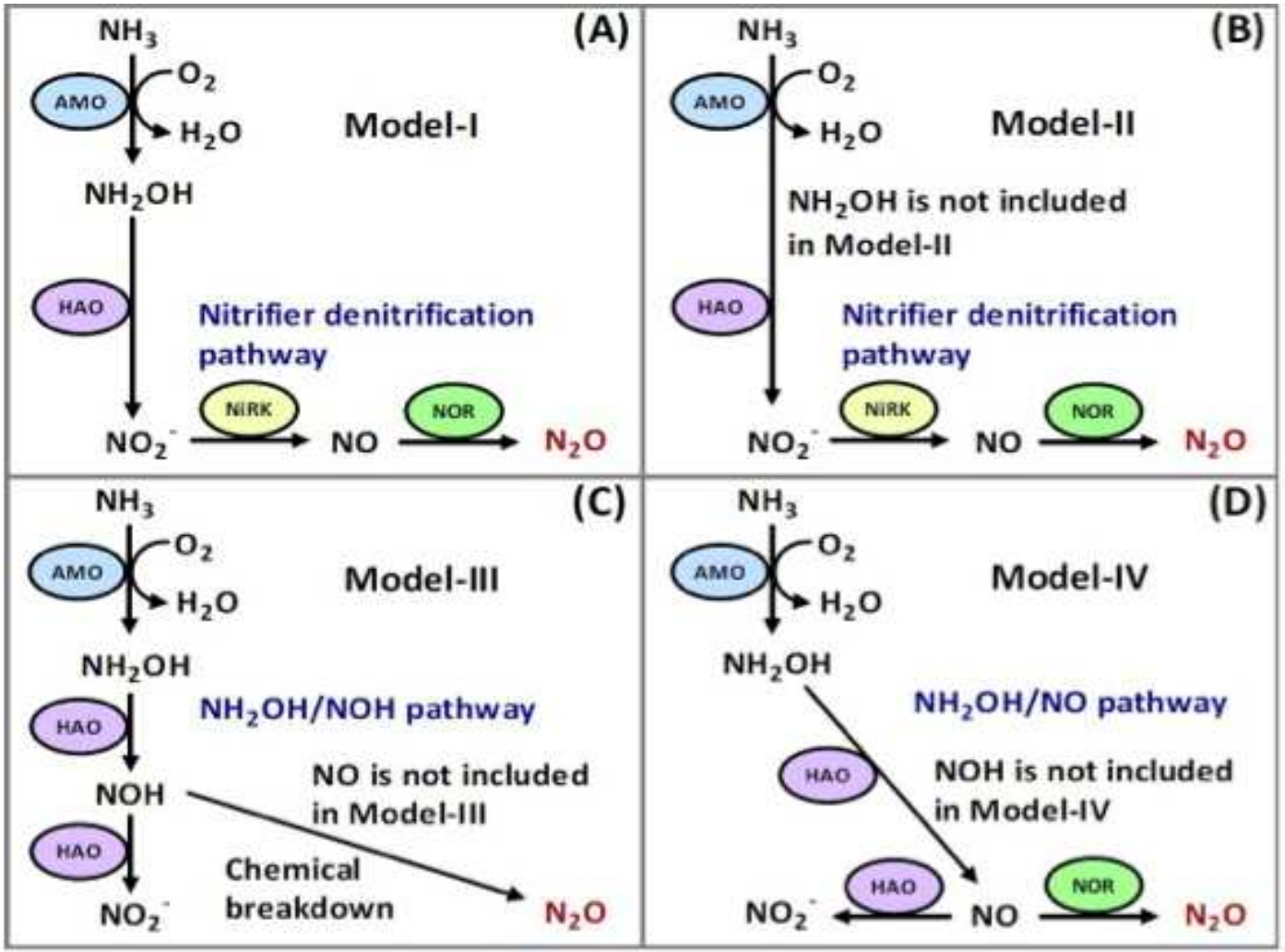
N_2O production pathways by AOB



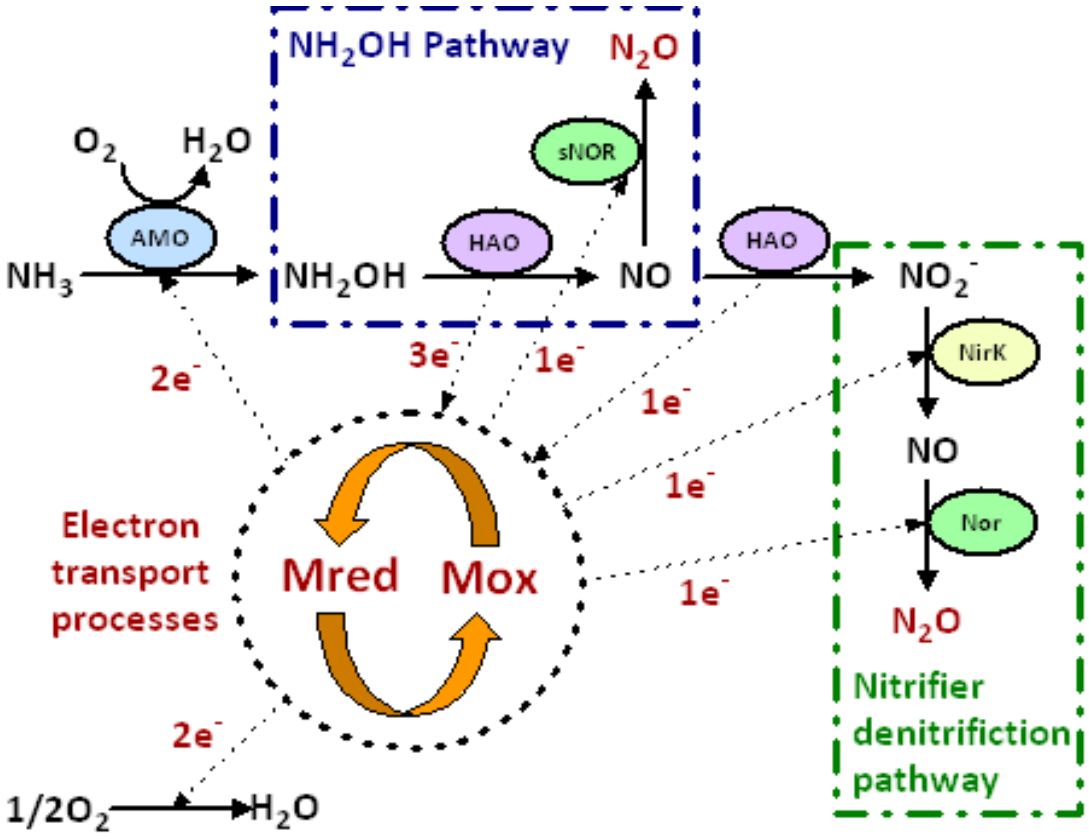
NH_2OH/NO pathway
Biological reduction of NO that is formed as an intermediate of NH_2OH oxidation

Nitrifier denitrification
NO_2^- can be used as terminal electron acceptor instead of O_2 for N_2O production

Single-pathway models for N_2O production by AOB



Two-pathway model for N_2O production by AOB



Mred: electron carriers in reduced form

Mox: electron carriers in oxidised form

- decoupling the oxidation and reduction processes
- electron carriers as new model components
- total level of electron carriers being constant
- electron distribution between O_2, NO_2^- and NO with different kinetics controlling the relative contributions between the two N_2O pathways

Single pathway vs. two-pathway models

Two-pathway model:

- advantages: applicable under varying conditions
- disadvantages: complicated with more parameters

These applicable regions have not been identified!!!

Single-pathway

- ✓ advantages: sir d fewer parameters
- ✓ disadvantages: ertain conditions

Methodology – model evaluations

Two-pathway model generate simulation data for calibration of single-pathway models

- **Steady-state calibration:**

1) calibrated η_{AOB} is constant, independent of the DO and nitrite levels;

2) η_{AOB} is in a feasible range (0 – 1.0) under any conditions.

- **Dynamic verification:**

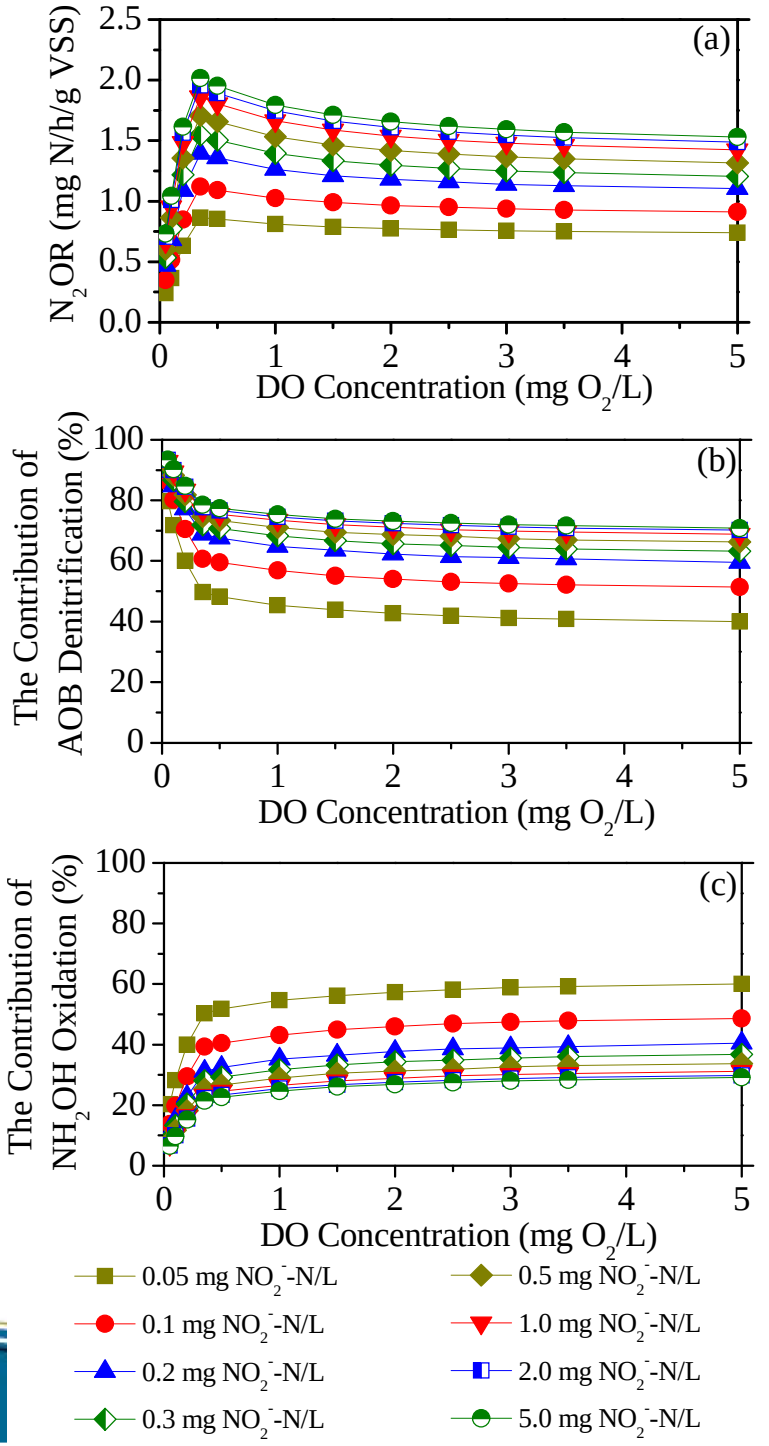
1) $$F(p) = \left(\sum_{i=1}^{n}\left(y_{TM,i} - y(\eta_{AOB})_i\right)^2\right)^{\frac{1}{2}}$$

2) ANOVA to evaluate the fit

N_2O production by AOB

two pathway model

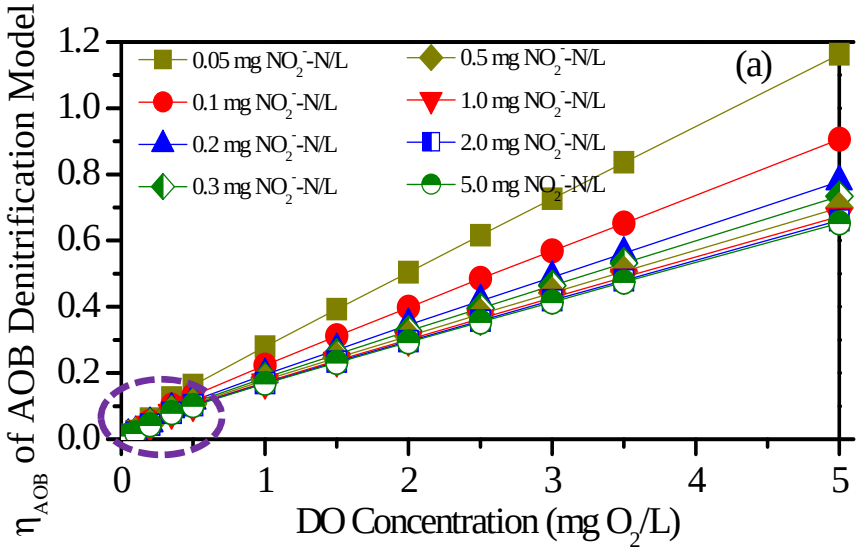
- ✓ Biomass specific N_2OR increases rapidly as DO increases from 0.05 to 0.35 mg O_2/L, and then decreases as DO further increases to 5.0 mg O_2/L.
- ✓ At each DO concentration, the simulated biomass specific N_2OR increases as NO_2^- increases.
- ✓ **The contribution of AOB denitrification pathway decreases with the increase of DO, but increases with the increase of NO_2^-, accompanied by opposite changes in the contribution of NH_2OH oxidation pathway.**

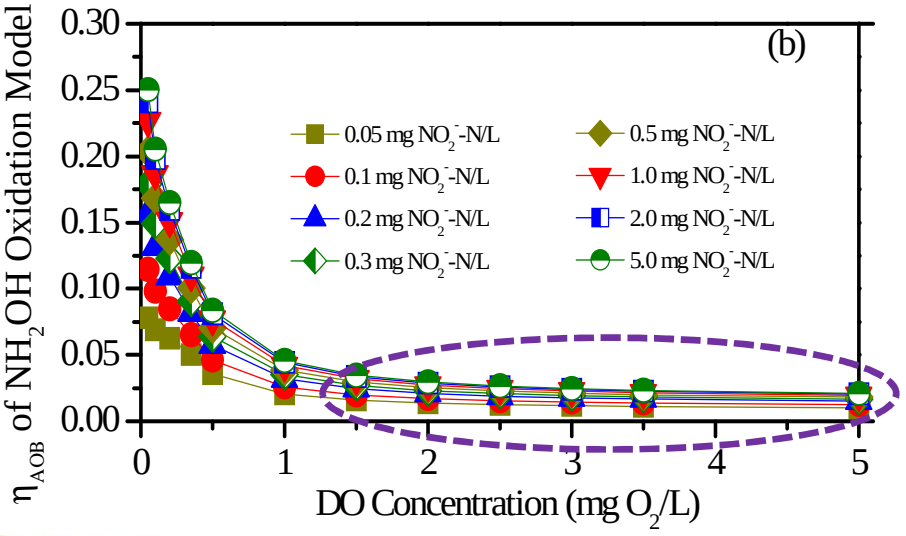


Steady-state calibration of single-pathway model

- ✓ The AOB denitrification model would only be applicable when DO is constant: 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; in the DO range of 0 – 0.5 mg O_2/L, independent of the nitrite concentration

- ✓ NH_2OH oxidation model can be applied at high DO concentrations (> 1.5 mg O_2/L), which is not a suitable model under low DO conditions (<1.5 mg O_2/L).

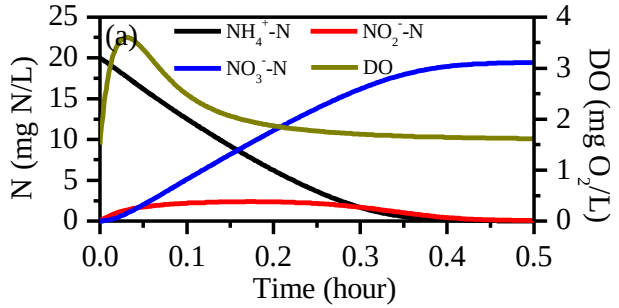


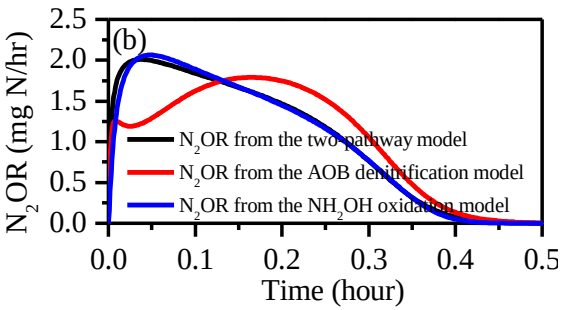


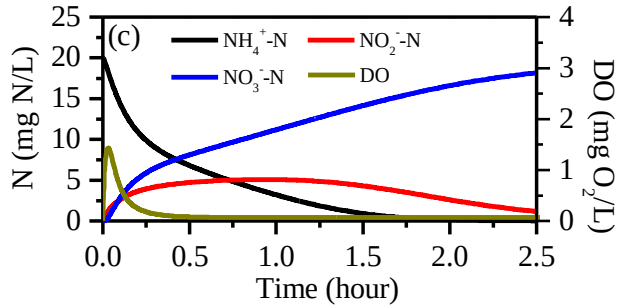
Dynamic verification of the steady-state results

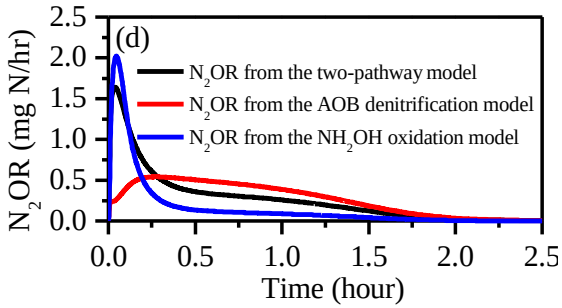
- DO varies between 1.5 – 3.5 mg O_2/L and NO_2^- accumulates to around 2.5 mg N/L.
- DO varies between 0 – 1.5 mg O_2/L and NO_2^- accumulates to approximately 5 mg N/L.

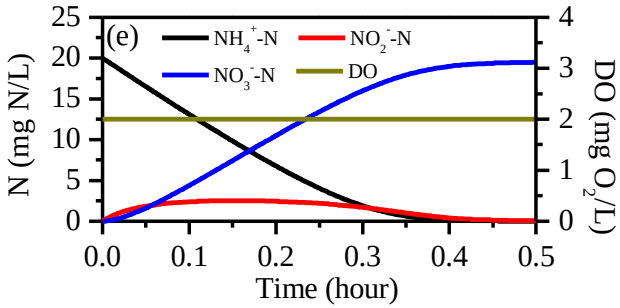
- Constant DO of 2.0 mg O_2/L and nitrite accumulation of 2.5 mg N/L
- Constant DO (0.2 mg O_2/L) and without nitrite accumulation (below 0.5 mg N/L)

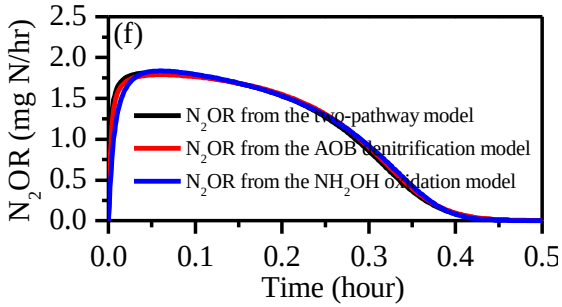


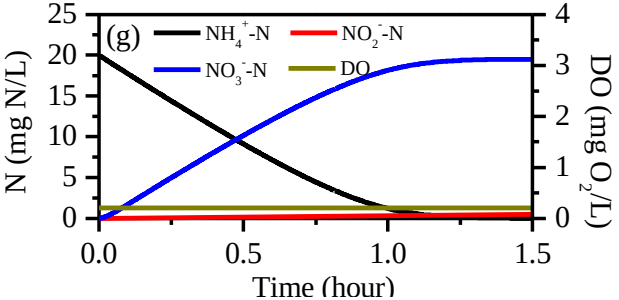


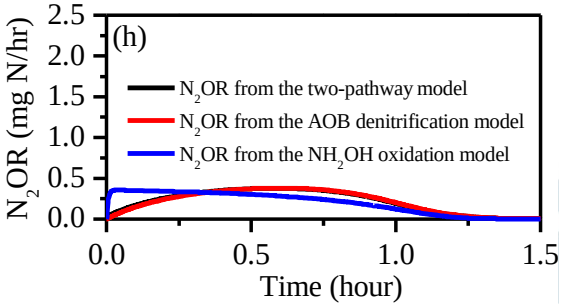






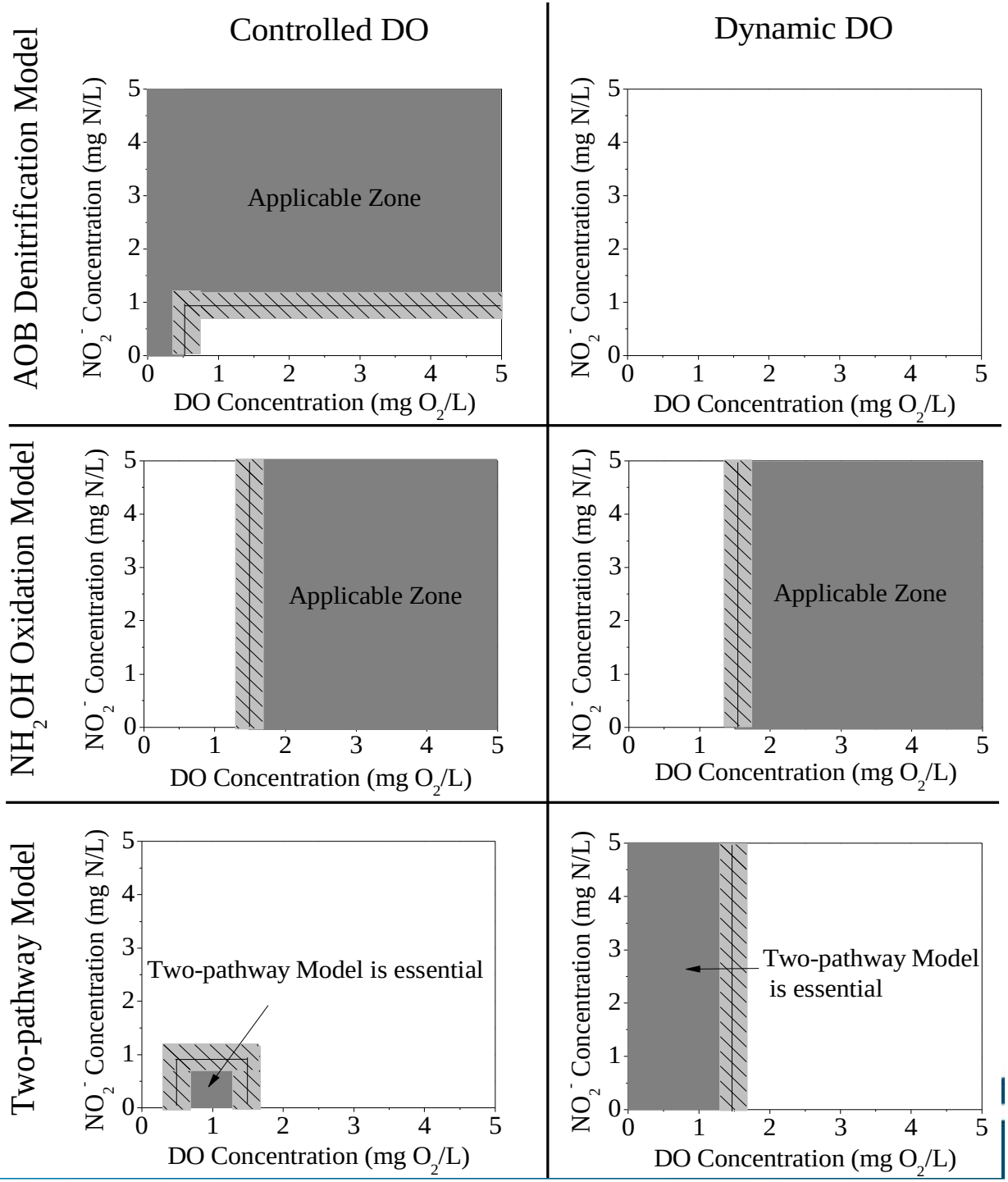






Effect of model parameter of two pathway model?

The applicable regions were generally insensitive (below ±10%) to the variations of key parameter values by ±50% of the two-pathway model



Key messages of this work

- AOB denitrification model: DO is well controlled at a constant level, either at low DO concentration (<0.5 mg O_2/L) with any investigated NO_2^- concentration (0 – 5 mg N/L) or at high DO (≥ 0.5 mg O_2/L) with significant NO_2^- accumulation (≥ 1.0 mg N/L).

- NH_2OH oxidation model can be applied under high DO conditions (≥ 1.5 mg O_2/L), controlled or varying, with any NO_2^- concentration investigated (0 – 5.0 mg N/L).

- Under other conditions, the two-pathway model should be applied.

Thank you!