Full-scale N_2O model calibration using BSM2

N_2O Workshop,
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Content

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1. Problem statement

1.1 Studied model and calibration purposes

- Model building

  ASMN[1]

  AOB denitrification: Mampaey A (Aerobic senario of Mampaey[2])

- Model application

  BSM2: a plant-wide layout, open loop, 609 days influent files

- Model calibration objectives:

  N_2O emission factor: Emitted N_2O-N g / TN-N g load ≈ 0.5%

  Effluent quality (EQI) ≈ value in BSM2[3] (ASM1): 5661

  Operation cost (OCI) ≈ values in BSM2[3] (ASM1): 9208

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1. Hiatt and Grady. Water Environ. Res., 2008, p 2145-2156.
2. Mampaey et al. Nutrient Recovery and Management 2011, p. 997-1009.
3. Nopens et al. Water Sci. Technol., 2010, p 1967-1974.

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1. Problem statement

1.2 Results using parameters suggested in papers

- Default ASMN (using suggested parameter values[1])

  N_2O emission factor: 5.53%

  EQI=7060, OCI=10485

  S_{NO2} concentrations: high potential of N_2O production by AOB

S_{NO2} (gN/m³)	ASU1	ASU2	ASU3	ASU4	ASU5	Effluent
	1.006	0.993	1.016	0.907	0.939	0.976

- Default ASMN[1] + Default Mampaey A[2]

  N_2O emission factor: 16.03%

  EQI=5332, OCI=9719

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2. Model calibrations

2.1 Calibration methods

- In order to reduce N_2O emissions:

1. Reduce N_2O production by ASMN: lower than 0.50%

Because: N_2O_ASMN ≥ 0.5% → full inhibition of AOB denitrification → irrationally large Mampaey A parameters

2. Lower S_{NO2} of ASMN

Because: S_{NO2} is used for AOB denitrification

3. N_2O produced by AOB should be denitrified by heterotrophs

Because: AOB cannot $N_2O \rightarrow N_2$

→ Suggest calibration in 2 steps:

Step1: calibrate ASMN to reduce N_2O emission factor below 0.50% and lower S_{NO2}

Step2: calibrate Mampaey A to meet final N_2O emission requirement

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2. Model calibrations

2.1 Calibration methods

- Calibration target of ASMN

T1. Reduce N_2O emissions from heterotrophic denitrification

→ enhance denitrification (T1.1)

→ increase N_2O denitrification to N_2 (T1.2)

T2. Reduce effluent S_{NH}

→ improve nitrification (T2.1)

→ slow down ammonification rate (T2.2)

T3. limit N_2O production potential of AOB

→ lower S_{NO2} (3.1)

- Calibration target of Mampaey A

T4. Reduce N_2O emissions from AOB denitrification

→ lower AOB denitrification rate (T4.1)

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2. Model calibrations

2.2 Calibration of ASMN (Step 1)

- ASMN[1] vs. ASM1[4]

Different parameter values except: f_P, i_{XB}, i_{XP}, K_S, η_h

- Parameter adjustment

T1.1: increase K_{OH} (ASM1); increase η_g (ASM1>ASMN)
T1.2: decrease K_{N2O}, K_{I5NO}, K_{S5}
T2.1: decrease K_{FNA}
T2.2: decrease k_a (ASM1), K_X (ASM1<ASMN);
increase k_h, η_h (ASM1>ASMN)
T3.1: decrease K_{FNA}, K_{I9FA}, K_{I9FNA}

- Results of calibration (ASMN calibration)

N_2O emission factor: 0.35% ☺ EQI=5690, OCI=9852 ☺

S_{NO2} (gN/m^3)	ASU1	ASU2	ASU3	ASU4	ASU5	Effluent
	0.208	0.128	0.096	0.069	0.083	0.092

☺

1. Hiatt and Grady. Water Environ. Res., 2008, p 2145-2156.
4. Jeppsson. A General Description of the IAWQ AS Model No. 1.

2. Model calibrations

2.3 Calibration of ASMN + Mampaey A (Step 2)

- Results of ASMN_calibration + default Mampaey A[2]

N_2O emission factor: 0.62% ☹

→ Decrease AOB denitrification (T4.1): Mampaey A_calibration

Increase $K_{NH\_AOBdenitr}$ (1→2 mgN/L), $K_{OH\_AOBdenitr}$ (0.5→1 mgO_2/L)

- Results of ASMN_calibration + Mampaey A_calibration

N_2O emission factor: 0.50% ☺
EQI=5575, OCI=9852 ☺

2. Mampaey et al. Nutrient Recovery and Management 2011, p. 997-1009.

2. Modeling and control of GHG emissions

2.3 Calibration of ASMN + Mampaey A (Step 2)

- Potential problems

  Further decreasing N_2O emissions may require even higher K values which is no longer rational

- Solutions

  S1. Growth inhibition factor η_{AOB} for AOB denitrification

  S2. Competitive inhibition term of DO

  Research showed that N_2O production by AOB denitrification happened only under low DO

  → Competition between N_2O and NO_3^- : at higher DO, more NO_2^- is oxidized to NO_3^-, less for N_2O production

  or

  → High DO has an inhibition effect → Competitive kinetic term

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2. Modeling and control of GHG emissions

2.3 Calibration of ASMN + Mampaey A (Step 2)

- AOB denitrification rate by Mampaey A[2]

$$r_{\mathrm{AOBden}} = \mu_{\mathrm{AOB}} \cdot \frac{S_O}{S_O + K_{O\_AOB}} \cdot \mathrm{A}$$

A: a multiplication term of X_{AOB} and inhibition terms of NO_2^- (NO) and NH_4^+

- Modified AOB denitrification kinetic equations

Modification1 (S1)

$$r_{\mathrm{AOBden}} = \mu_{\mathrm{AOB}} \cdot \boxed{\eta_{\mathrm{AOB}}} \cdot \frac{S_O}{S_O + K_{O\_AOB}} \cdot \mathrm{A}$$

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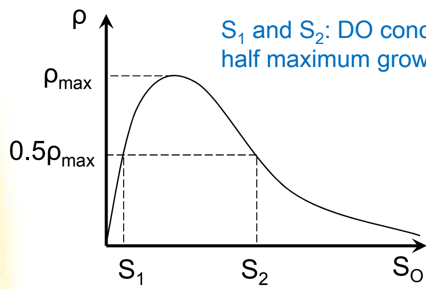
2. Modeling and control of GHG emissions

2.3 Calibration of ASMN + Mampaey A (Step 2)

- Modified AOB denitrification kinetic equations
  Modification2 (S1+S2)

$$r_{AOBden} = \mu_{AOB} \cdot \boxed{\eta_{AOB}} \cdot \boxed{\frac{K_{comp} \cdot S_O}{K_{so\_AOB} + S_O + S_O{}^2 / K_{IO\_AOB}}} \cdot A$$



S_1 and S_2: DO concentrations for half maximum growth rate

$$K_{comp} = \frac{1}{1 - 2 \cdot \sqrt{K_{SO\_AOB}/K_{IO\_AOB}}},$$

$$K_{SO\_AOB} = \frac{S_1 \cdot S_2}{K_{IO\_AOB}},$$

$$K_{IO\_AOB} = \frac{\left(\sqrt{S_1} - \sqrt{S_2}\right)^2}{K_{comp}}.$$

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2. Modeling and control of GHG emissions

2.3 Calibration of ASMN + Mampaey A (Step 2)

- Results of ASMN_calibration + Mampaey A_modification1

  η_{AOB}=0.6, other Mampaey A parameters kept to the defaults
  N_2O emission factor: 0.49%

- Results of ASMN_calibration + Mampaey A_modification2

  η_{AOB}=0.8, S_1=0.5 g / m^3, S_2=1 g/m^3,
  other Mampaey A parameter keep defaults
  N_2O emission factor: 0.50%

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2. Modeling and control of GHG emissions

2.3 Calibration of ASMN + Mampaey A (Step 2)

	BSM2	ASMN_cal + Mam. A_cal	ASMN_cal + Mam. A_mod1	ASMN_cal + Mam. A_mod2
N_2O emission factor	NULL	0.50%	0.49%	0.50%
EQI (poll/day)	5661	5575	5577	5599
S_{NO3} (gN/m^3)	7.47	7.37	7.37	7.45
S_{NH} (gN/m^3)	1.65	1.79	1.79	1.80
TN (gN/m^3)	11.20	11.18	11.18	11.27
TSS (gCOD/m^3)	15.90	14.50	14.50	14.50
COD (gCOD/m^3)	50.06	48.28	48.28	48.28
BOD5 (gBOD/m^3)	2.77	2.34	2.34	2.34
OCI (poll/day)	9208	9852	9852	9852

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3. Discussion

3.1 Comparison on N_2O production and stripping rate

Averaged kinetic rate (g N/d)	ASMN_cal + Mam. A_cal	ASMN_cal + Mam. A_mod1	ASMN_cal + Mam. A_mod2
Net N_2O produced	5848	5717	5790
by heterotrophs	-9109	-8848	-5611
by autotrophs	14957	14565	11400
N_2O stripping	-5757	-5624	-5703

- All have similar total net N_2O production and stripping rates
  → similar emission factor
- The 1st and 2nd have similar heterotrophic and autotrophic N_2O net production rates, but are different from 3rd.

! Impossible to measure N_2O production by a specified organism group
BUT: production rate in each tank can be measured

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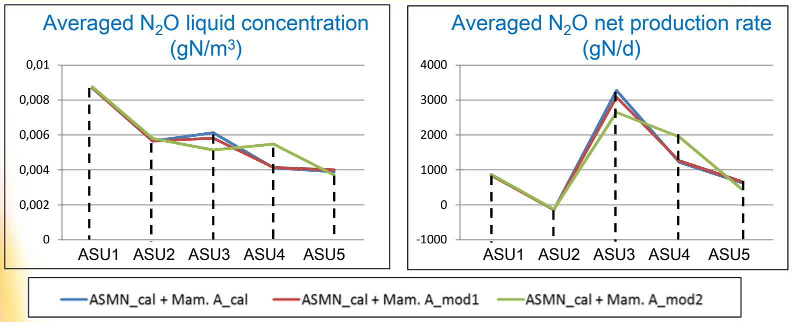
3. Discussion

3.2 Comparison of distributions in tanks



- The 1st and 2nd have similar trends, but are different from 3rd.

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4. Conclusions and perspectives

4.1 Conclusions

- The default parameter values suggested in the reference papers should be calibrated
- Calibration method:
  - a. reduce N_2O emitted by ASMN
    → increase the heterotrophs' ability to denitrify N_2O to N_2
  - b. reduce N_2O sourced from AOB denitrification
→ reduce S_{NO2}
→ lower AOB denitrification rate
- Three calibrated models:
  - Meet requirement on: N_2O emissions, effluent quality, OCI
  - Different profiles of: spatial distributions of N_2O liquid concentration and production rate.

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4. Conclusions and perspectives

4.2 Perspectives

Further calibration requires:

- More measurements on:
  - N_2O liquid concentration and production rate
  - Different zones (spatial distribution)
- Parameter sensitivity analysis

Thanks and questions?

Canada Research Chair in Water Quality Modelling

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