

Technical University of Denmark



## **pH variation and influence in an autotrophic nitrogen removing biofilm system**

An efficient numerical solution strategy

**Vangsgaard, Anna Katrine; Mauricio Iglesias, Miguel; Valverde Pérez, Borja; Gernaey, Krist V.; Sin, Gürkan**

*Publication date:*  
2012

*Document Version*  
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

*Citation (APA):*  
Vangsgaard, A. K., Mauricio Iglesias, M., Valverde Perez, B., Gernaey, K., & Sin, G. (2012). pH variation and influence in an autotrophic nitrogen removing biofilm system: An efficient numerical solution strategy. Poster session presented at IWA Nutrient Removal and Recovery 2012, Harbin, China.

## **DTU Library**

Technical Information Center of Denmark

---

### **General rights**

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

# pH variation and influence in an autotrophic nitrogen removing biofilm system:

## An efficient numerical solution strategy

Anna Katrine Vangsgaard\*, Miguel Mauricio-Iglesias\*, Borja Valverde-Pérez\*, Krist V. Gernaey\*\*, and Gürkan Sin\*

\* Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Lyngby

\*\* Center for Process Engineering and Technology, Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Lyngby

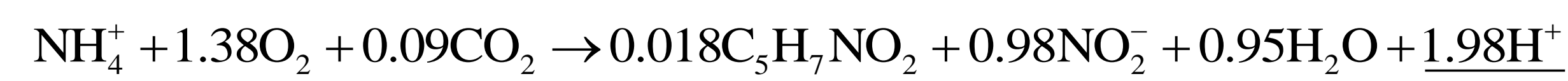
### 1. Introduction

pH impacts the nitrification and anammox processes and vice versa through:

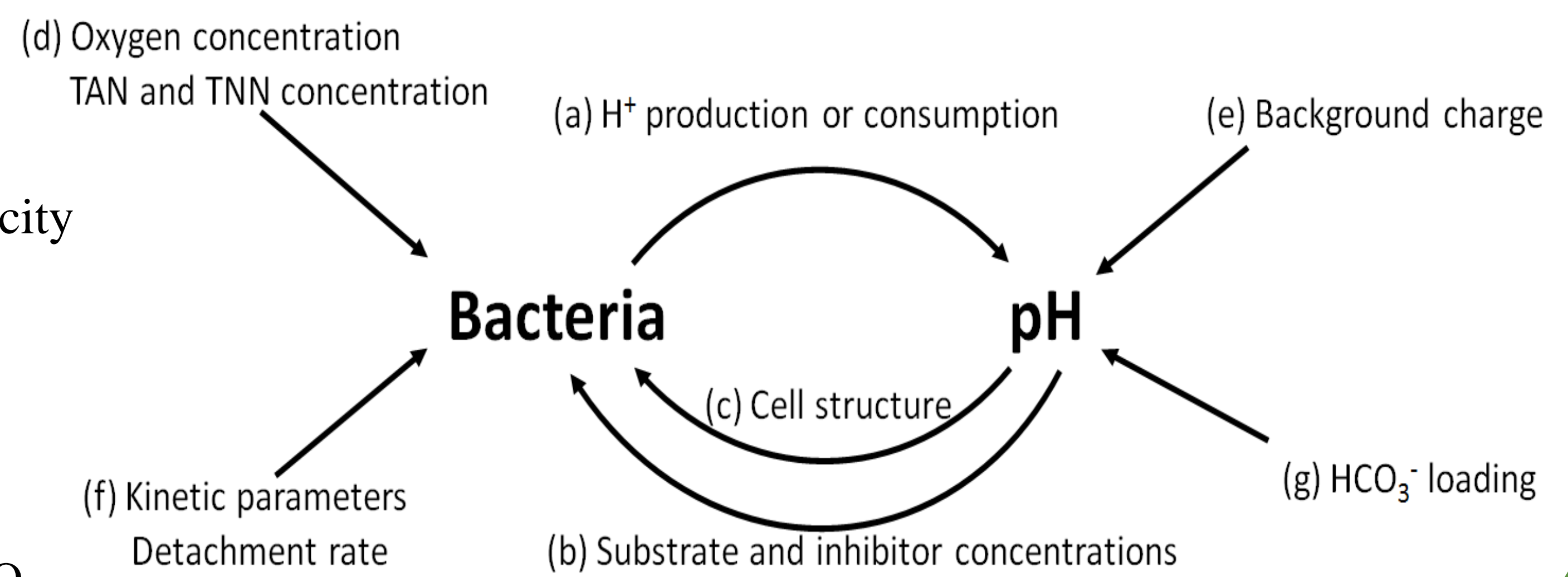
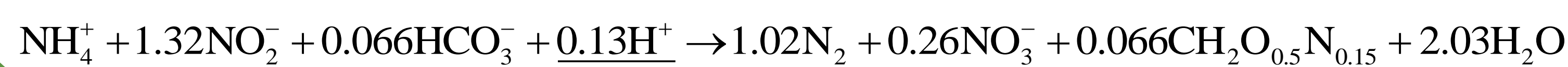
(a) H<sup>+</sup> production/consumption, (b) substrate and inhibitor speciation, (c) cell structure dependency, (d) substrate and inhibitor concentrations, (e) system background charge and distribution, (f) microbial activity, and (g) buffering capacity

#### Stoichiometry of microbial processes

Nitrification:

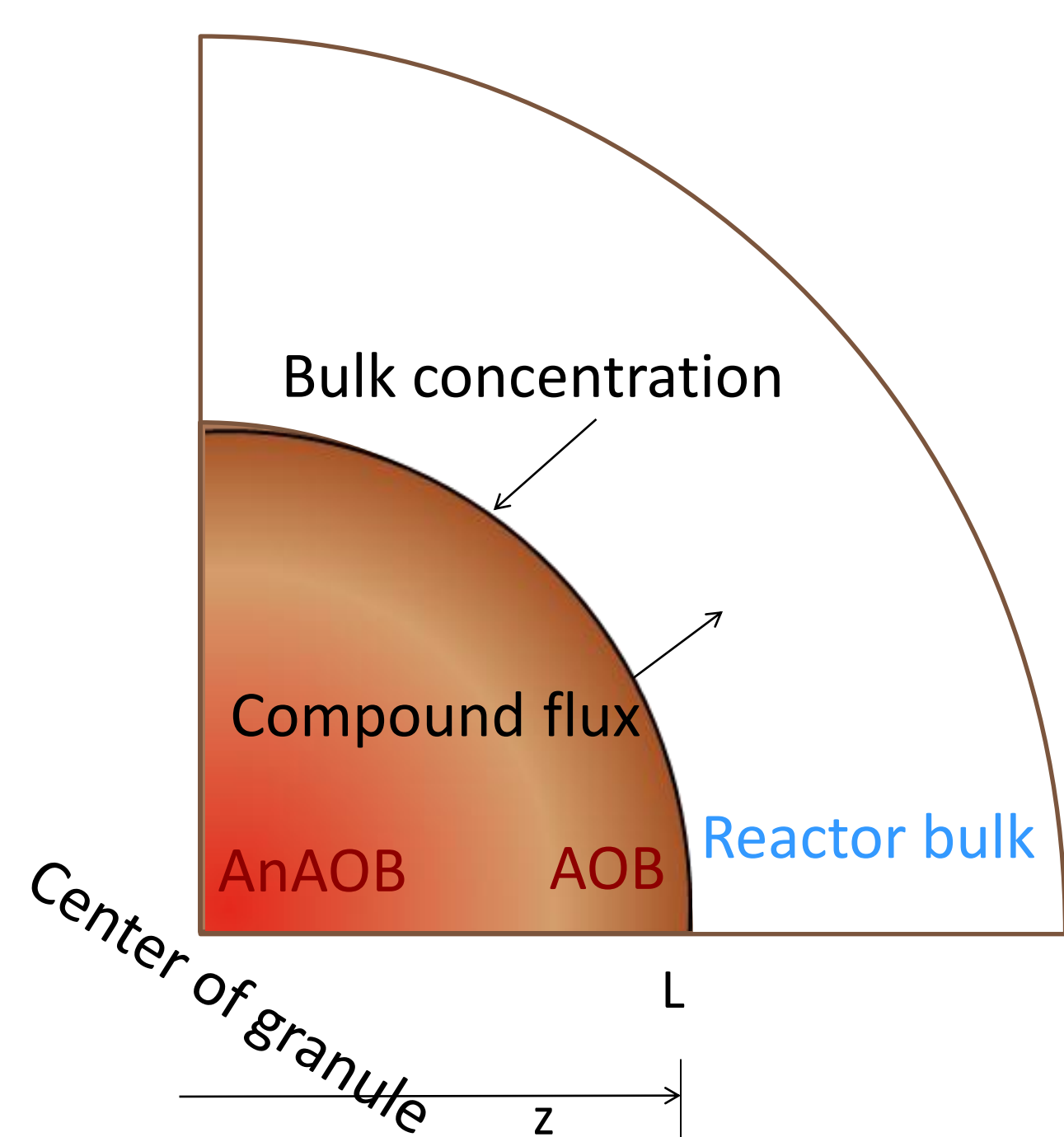


Anammox:



### 2. Methods and solution strategy

#### Model description



#### Biofilm mass balance

$$\frac{\partial(C_i V)}{\partial t} = \frac{\partial(j_i A)}{\partial z} dz + r_i dV$$

#### Reactor mass balance

$$\frac{dC_{i,bulk}}{dt} = \frac{Q_{in} C_{i,in} - Q_{out} C_{i,bulk}}{V_{react}} - j_{Ci} \frac{A}{V_{react}} + r_{i,bulk}$$

i = soluble or particulate compound

j = substrate flux

z = radial distance from the center of the granule

r<sub>i</sub> = microbial growth and conversion

Q = flow

V<sub>react</sub> = reactor volume

A = biofilm surface area

#### New and fast numerical solution for pH calculation

A system of nine nonlinear equations was solved by a multi-dimensional Newton-Raphson method adapted from Luff et al. (2001) coupled with the granular biofilm model (left).

$$0 = \text{TAN} - (\text{NH}_4^+ + \text{NH}_3)$$

$$0 = \text{TNN} - (\text{HNO}_2 + \text{NO}_2^-)$$

$$0 = \text{TIC} - (\text{CO}_2 + \text{HCO}_3^- + \text{CO}_3^{2-})$$

$$0 = K_w - \text{OH}^- \cdot \text{H}^+$$

$$0 = K_{e,NH4} \cdot \text{NH}_4^+ - \text{NH}_3 \cdot \text{H}^+$$

$$0 = K_{e,HNO2} \cdot \text{HNO}_2 - \text{NO}_2^- \cdot \text{H}^+$$

$$0 = K_{e,CO2} \cdot \text{CO}_2 - \text{HCO}_3^- \cdot \text{H}^+$$

$$0 = K_{e,HCO3} \cdot \text{HCO}_3^- - \text{CO}_3^{2-} \cdot \text{H}^+$$

$$0 = Z^+ - \text{NO}_3^- - \text{HCO}_3^- - 2 \cdot \text{CO}_3^{2-} - \text{NO}_2^- - \text{OH}^- + \text{NH}_4^+ + \text{H}^+$$

Because the above system was computationally heavy to solve and prone to errors, the pH was determined offline for the complete expected range of TAN, TNN, TIC and NO<sub>3</sub><sup>-</sup>, prior to simulation. A lookup table was therefore constructed using multi-dimensional interpolation tools in the Matlab software.

Four scenarios representing different operating points were defined and simulated:

(1) Default (2) High oxygen loading (3) Smaller granules (4) High strength wastewater → N and oxygen loadings

### Findings

• pH solver was successfully constructed and implemented in the MATLAB software.

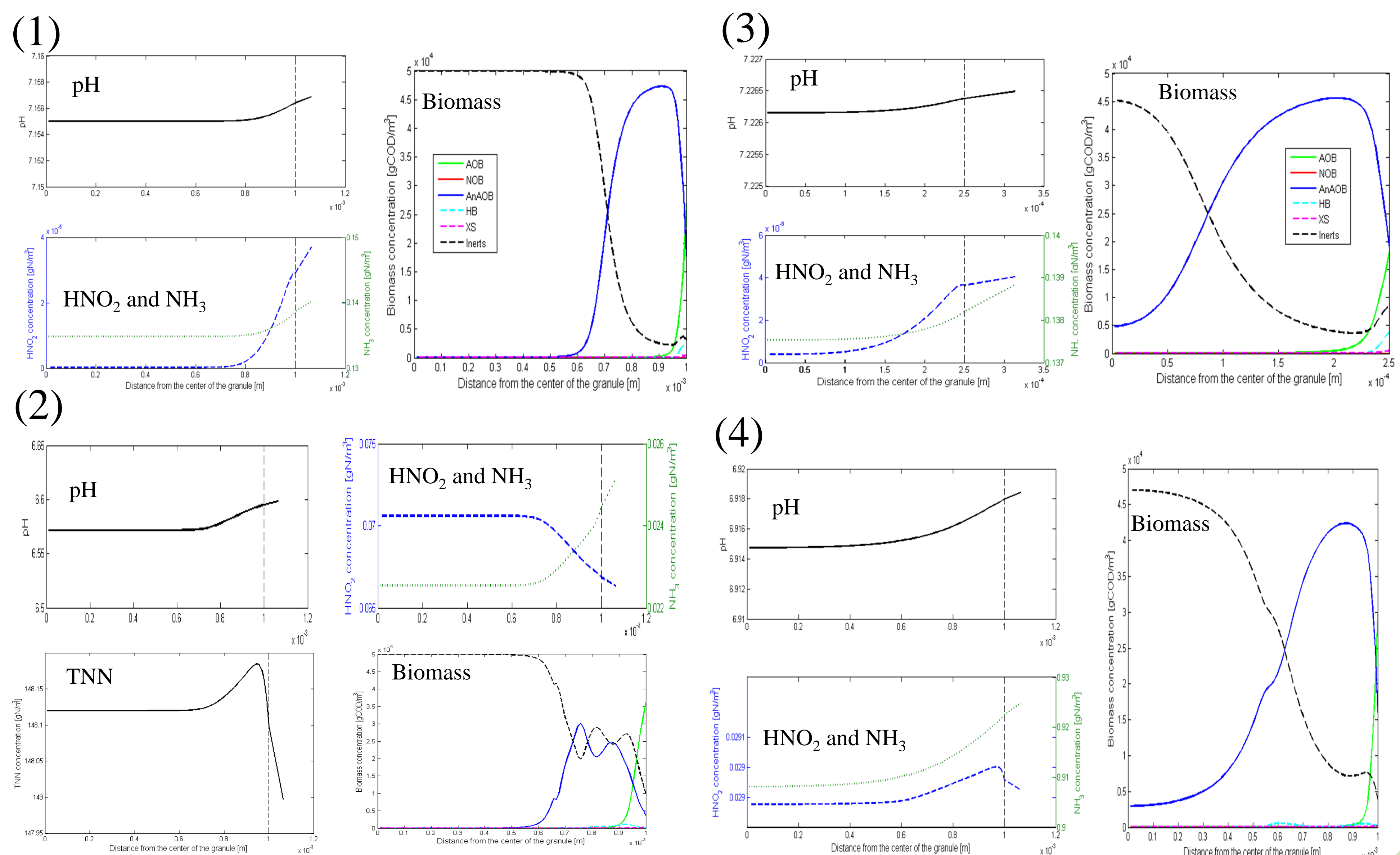
• Approximations of cell structure dependency on pH and the value of the background charge were needed to solve the model.

• The predicted pH profile showed decreasing pH with increasing depth into the biofilm in all scenarios, due to AOB presence in the outer layers.

• The background charge was found to have a great impact on the value and shape of the pH profile.

• More info on background charge effect and cell structure dependency, supported by experiments, is needed to make further progress.

### 3. Results and discussion



#### References:

1. R. Luff et al. Comput. Geosci. 27(2), 157-169 (2001).

Contact: Anna Katrine Vangsgaard (akv@kt.dtu.dk)

#### Acknowledgements:

DSF for funding through the Research Centre for Design of Microbial Communities in Membrane Bioreactors (EcoDesign MBR)