N₂O Mass Transfer Coefficient Calculation from Aeration Field Size and Air Flow

In the aerated reactor the size of the total aeration field (m^2) and the total air flow Q_A (NOTE the unit! m^3s^{-1}) for the aerated reactor is known. The total aeration field (m^2) is measured as the reactor surface where leaving air bubbles are detected visually by on-site inspection.

The superficial gas velocity of the aerated reactor is calculated by dividing the total air flow with the aeration field size:

$$v_{g\ 20°C} \cong \frac{Q_{A\ 20°C}}{Aeration\ field\ size} \quad (1.1)$$

From the superficial gas velocity of the aerated reactor the N₂O mass transfer coefficient k_La_{N2O} can be calculated using the empirical formula 3.2 based on laboratory experiments at 20°C in mixed WWTP liquor[i]:

$$k_L a_{N_2O\ 20°C} = \left\{\frac{D_R}{D_L}\right\}^{-0.49} \times 34500 \times \left(v_{g\ 20°C}\right)^{0.86} \quad (1.2)$$

$$k_L a_{N_2O\ 20°C} = \left\{\frac{D_R}{0.815\ m}\right\}^{-0.49} \times 34500 \times \left(v_{g\ 20°C}\right)^{0.86} \quad (1.3)$$

v_g: Superficial gas velocity of the reactor ($m^3m^{-2}s^{-1}$)   **D_L**: Depth of the laboratory reactor (0.815 m)
D_R: Depth over the diffuser of the reactor (m)   **k_La_{N2O}**: N₂O mass transfer coefficient (d^{-1})

Finally the k_La_{N2O} calculated above is temperature corrected to the process temperature $T_{Process}$:

$$k_L a_{N_2O\ T_{Process}} = k_L a_{N_2O\ 20°C} \times (1.024)^{(T_{Process}-20°C)} \quad (1.4)$$

N₂O Emission Formula

The dissolved N₂O concentration and mixed liquor temperature are measured with the N₂O Wastewater System and values used to calculate the temperature compensated N₂O concentration in the aerated reactor (g-N/m^3). From the input of the air flow Q_A in the aerated reactor the temperature compensated N₂O mass transfer coefficient $k_L a_{N_2O}$ is calculated using equations 1.1- 1.4.

With the values $k_L a_{N_2O}$ and Q_A known the N₂O emission rate per reactor volume can be calculated using the formula below[ii,iii] (NOTE the Q_A unit! m^3d^{-1}):

$$Aerated\ zones:\ r_{N_2O,T_{process}} = H_{N_2O,T_{process}} \times S_{N_2O} \left[1 - e^{-\frac{k_L a_{N_2O}}{H_{N_2O,T_{process}}} \cdot \frac{V_R}{Q_{A,T_{process}}}}\right] \times \frac{Q_{A,T_{process}}}{V_R} \quad (2)$$

$$Non-aerated\ zones:\ r_{N_2O,T_{process}} = k_L a_{N_2O,T_{process}}^{Non-aerated} \times \left[S_{N_2O} - \frac{C_{N_2O,air}}{H_{N_2O,T_{process}}}\right] \quad (3)$$

$r_{N_2O,T_{process}}$: N₂O emission rate (g-N N₂O $m^{-3}d^{-1}$)   **V_R**: Volume of aerated part of reactor (m^3)
$H_{N_2O,T_{process}}$: Henrys constant (dimensionless)   **$k_La_{N_2O}$**: N₂O mass transfer coefficient (d^{-1})
S_{N_2O}: N₂O concentration (g-N N₂O m^{-3})   **$C_{N_2O,air}$** : N₂O concentration in air equilibrium (g-N/m^3)
$Q_{A,T_{process}}$: Total air flow through reactor per day (m^3d^{-1})

The dimensionless Henrys constant $H_{N_2O,T_{process}}$ is like the N₂O Wastewater sensor signal dependent on the process temperature and the temperature correction is calculated using equations 4.1- 4.2.

$$H_{N_2O,T_{process}} = \frac{1}{k_H \cdot R \cdot (T_{process} + 273.15) \cdot 10^3 \frac{L}{m^3}} \, (4.1)$$

$$k_H = k_H{}^\theta \times e^{\left(\frac{-\Delta solnH}{R}\left(\frac{1}{T_{process}+ 273.15} - \frac{1}{T^\theta+273.15}\right)\right)} (4.2)$$

$k_H{}^\theta$: Henrys constant at the std. temp. (mol·L⁻¹·bar⁻¹) $T_{process}$: Mixed liquor temperature (°C)

T^θ: Standard temperature = 25°C   -ΔsolnH/R: The enthalpy of the solution (K)

From literature the N₂O mean values for $k_H{}^\theta$, -ΔsolnH/R and supporting constant numbers are given in the below table:

$k_H{}^\theta$ (mol·L⁻¹·bar⁻¹)	$\frac{-\Delta solnH}{R}$ (K)	$C_{N_2O,air}$ (g-N/m³)	R (m³·bar·mol⁻¹·K⁻¹)	$k_L a_{N_2O\ T_{process}}^{Non-aerated}$ (d^{-1})
0.0247	2675	0.0003	8.314 x 10⁻⁵	2 − 4

[i] Foley, J., de Haas, D., Yuan, Z.,Lant, P. (2010) Nitrous oxide generation in full-scale biological nutrient removal wastewater treatment, plants. Water Res. 44, 831-844.

[ii] Schulthess, R. & Gujer W. (1996) Release of nitrous oxide (N2O) from denitrifying activated sludge: Verification and application of a mathematical model, Water Res. 30, 521-530.

Validation papers:

[iii] Baresel, C., Andersson, S., Yang, J., Andersen, M.H. (2016) Comparison of nitrous oxide (N₂O) emissions calculations at a Swedish wastewater treatment plant based on water concentrations versus off-gas concentrations, Advances in Climate Change Research, 7(3), 185-191.

[iv] Janis E. Baeten, Mark C.M. van Loosdrecht, Eveline I.P. Volcke (2020) When and why do gradients of the gas phase composition and pressure affect liquid-gas transfer? Water Res. 178, 115844

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