

## Estimation of mass transfer coefficient and emission of N<sub>2</sub>O from surface aerator systems

Like the estimation of the oxygen mass transfer coefficient  $k_L a_{O_2}$ , the nitrous oxide mass transfer coefficient  $k_L a_{N_2O}$  can be estimated. Several different ways are possible to calculate the  $k_L a_{O_2}$  and if measurement methods were available for N<sub>2</sub>O the formulas would be the same as for oxygen in high shear/turbulent systems, like surface aeration and jet aerators. However, N<sub>2</sub>O is very soluble in wastewater, and it is therefore impossible to measure the  $k_L a_{N_2O}$  value directly in full scale wastewater treatment plants.

Oxygen Transfer:

$$OTR = \frac{dC_{O_2}}{dt} = K_L a_{O_2} \times (C_{O_2}^{sat} - C_{O_2}^i)$$

Nitrous Oxide Transfer:

$$NTR = \frac{dC_{N_2O}}{dt} = K_L a_{N_2O} \times (C_{N_2O}^{sat} - C_{N_2O}^i)$$

Above formulas are the volumetric transfer rates (g-N N<sub>2</sub>O m<sup>-3</sup>d<sup>-1</sup>). By multiplying with the tank volume, the total process emission rate is derived.

The only way the mass transfer coefficient for N<sub>2</sub>O ( $k_L a_{N_2O}$ ) can be estimated is from an empirical correlation to the mass transfer coefficient for oxygen ( $k_L a_{O_2}$ ). With  $k_L a_{O_2}$  known for the aerated reactor, the N<sub>2</sub>O mass transfer coefficient  $k_L a_{N_2O}$  at 20°C can be calculated:

$$k_L a_{N_2O\ 20^\circ C} = k_L a_{O_2\ 20^\circ C} \times \sqrt{\frac{D_{N_2O}}{D_{O_2}}} = k_L a_{O_2\ 20^\circ C} \times \sqrt{\frac{1.77 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}}{2.12 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}}} \quad (0.1)$$

$$k_L a_{N_2O\ T_{Process}} = k_L a_{O_2\ T_{Process}} \times \sqrt{\frac{D_{N_2O}}{D_{O_2}}} \quad (0.2)$$

Formula 0.1 above is only valid for high shear systems far away from equilibrium, e.g. bottom aerated tanks are governed by Henrys law type of calculations.

Finally, the  $k_L a_{N_2O\ 20^\circ C}$  calculated above is temperature corrected to the process temperature  $T_{Process}$ :

$$k_L a_{N_2O\ T_{Process}} = k_L a_{N_2O\ 20^\circ C} \times (1.024)^{(T_{Process} - 20^\circ C)} \quad (0.3)$$

With the  $k_L a_{N_2O}$  at the process temperature known, the N<sub>2</sub>O emission rate for the aerated zone(s) can finally be calculated:

$$NTR_{Aerated} \text{ (gN}_{N_2O}\text{/h)} = k_L a_{N_2O\ T_{Process}} \times C_{N_2O}^{process} \times V_{Aerated\ Tank} \quad (0.4)$$

For the non-aerated zones, the N<sub>2</sub>O emission rate is much smaller and can be calculated.

$$NTR_{Non-Aerated} \text{ (gN}_{N_2O}\text{/h)} = k_L a_{N_2O\ T_{Process}}^{Non-aerated} \times C_{N_2O}^{process} \times V_{Non-aerated\ Tank} \quad (0.5)$$

$k_L a_{N_2O\ T_{Process}}^{Non-aerated}$  is usually set fixed to 0.08 – 0.167h<sup>-1</sup> (2 - 4 d<sup>-1</sup>).

## Methods

The determination of  $k_L a_{N_2O}$  constitutes a specific problem in surface aerated treatment systems, as the mass transfer coefficient may be very high locally and can vary with the immersion of the aerators and number of aerators in operation. Below two different ways to extract the overall  $k_L a_{O_2}$  and  $k_L a_{N_2O}$ .

### 1. Calculations based on power consumption

A shortcut to get a fairly precise real-time estimation of the  $k_L a_{O_2}$  is to log the power consumption of the aerators and based on known values for standard aeration efficiency (SAE, kgO<sub>2</sub>/kWh) the  $k_L a_{O_2}$  can be estimated.

As an example, the widely used oxidation ditch systems fitted with surface aeration rotors can be used:

$$SAE = \frac{SOTR}{P} \quad (1.1)$$

$$OTR = k_L a_{O_2} \times (C_{O_2}^{Sat} - C_{O_2}^{Process}) \times V_R \quad (1.2)$$

$$OTR = \alpha \times \beta \times SOTR \quad (1.3)$$

Where:

SAE	= Standard Aeration Efficiency (kgO <sub>2</sub> /kWh)
SOTR	= Standard Oxygen Transfer Rate (kgO <sub>2</sub> /h)
P	= Power Consumption (kWh)
$C_{O_2}^{Sat}$	= Oxygen Saturation Concentration (kgO <sub>2</sub> /m <sup>3</sup> )

$$C_{O_2}^{Sat} = \frac{1 \text{ kg}}{1000 \text{ g}} \times (14.65 - 0.41 * T_{Process} + 0.0049 * T_{Process}^2 + 0.0000778 * T_{Process}^3)$$

$C_{O_2}^{Process}$	= Oxygen Process Concentration (kgO <sub>2</sub> /m <sup>3</sup> )
$k_L a_{O_2}$	= Mass Transfer Coefficient (h <sup>-1</sup> ).
$\alpha$	= Correction from clean water to process conditions (-).
$\beta$	= Change in saturation concentration from clean water to process conditions (-)
$V_R$	= Volume of process tank (m <sup>3</sup> )
F	= Fouling factor, usually 1 for surface aerator rotors (-).

Actual  $k_L a_{O_2 T_{Process}}$  values under process conditions can be determined from combining the above equations:

$$SOTR = SAE \times P \quad (1.4)$$

$$OTR = \alpha \times F \times SOTR \times \frac{(\beta \times C_{O_2}^{Sat T_{Process}} - C_{O_2}^{Process})}{C_{O_2}^{Sat 20^\circ C}} \times 1.024^{(T_{Process} - 20^\circ C)} \quad (1.5)$$

$$k_L a_{O_2 T_{Process}} = \frac{AOTR}{(C_{O_2}^{Sat} - C_{O_2}^{Process}) \times V_R} \quad (1.6)$$

Once the  $k_L a_{O_2 T_{Process}}$  is known the  $k_L a_{N_2O T_{Process}}$  can be calculated using formula 0.2. Finally, the  $N_2O$  emission rate using (0.4). Note that formula (1.5) and (1.6) results in a process temperature corrected  $k_L a_{O_2}$  and  $k_L a_{N_2O}$  can be derived directly using formula (0.2).

As an example:

SAE = 1.8 kgO<sub>2</sub>/kWh and Power = 66 kWh.

$\alpha = 0.9$  - generally accepted value for surface aeration rotors.

$\beta = 0.95$  and  $F = 1.0$

$C_{O_2}^{Sat T_{Process}}$  at 20°C = 0.00903 kg/m<sup>3</sup>

$C_{O_2}^{Sat T_{Process}}$  at e.g. 22°C = 0.00883 kg/m<sup>3</sup>

$C_{O_2}^{Process} = 0$  mg/L

$C_{N_2O}^{process} = 0.1$  mgN/L

$V_R = 4000$  m<sup>3</sup>

$$SOTR = 118.8 \text{ kgO}_2/\text{h} \quad (\text{Formula 1.4})$$

$$OTR = 104.12 \text{ kgO}_2/\text{h} \quad (\text{Formula 1.5})$$

$$k_L a_{O_2 T_{Process}} = 2.9479 \text{ h}^{-1} \text{ or } 70.75 \text{ d}^{-1} \quad (\text{Formula 1.6})$$

$$k_L a_{N_2O T_{Process}} = 2.6938 \text{ h}^{-1} \text{ or } 64.65 \text{ d}^{-1} \quad (\text{Formula 0.2})$$

$$NTR = 1077.5 \text{ gN}_{N_2O}/\text{h} \text{ or } 25.86 \text{ kgN}_{N_2O}/\text{d} \quad (\text{Formula 0.4})$$

The SAE can be estimated from re-aeration tests combined with power measurements. As example, the reaeration test made at the Silkeborg Utility, Denmark. In the below plot (Figure 1), the oxygen transfer and power usage has been measured as a function of the rotor immersion.

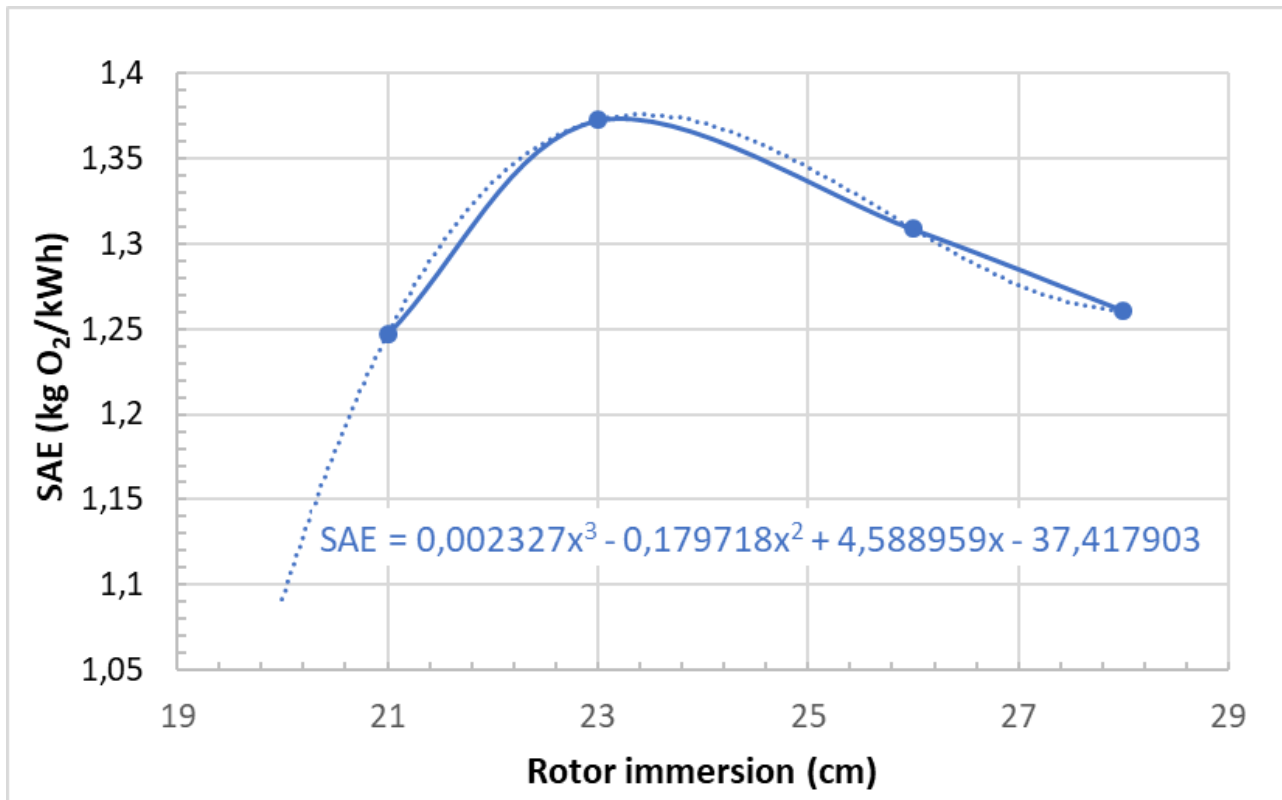


Figure 1. The SAE measured as a function of the rotor immersion depth at a standard surface aerated wastewater plant. Raw data from a DHI report from 2013.

In the second plot (Figure 2), the oxygen transfer and power usage has been measured as a function of rotor immersion. The SAE measured as a function of the frequency setpoint for variable frequency drive (VFD) for the rotor.

Hz	SAE kg O <sub>2</sub> /kWh
40	1,295
45	1,291
48	1,202
50	1,31
53	1,158
55	1,115
60	1,023

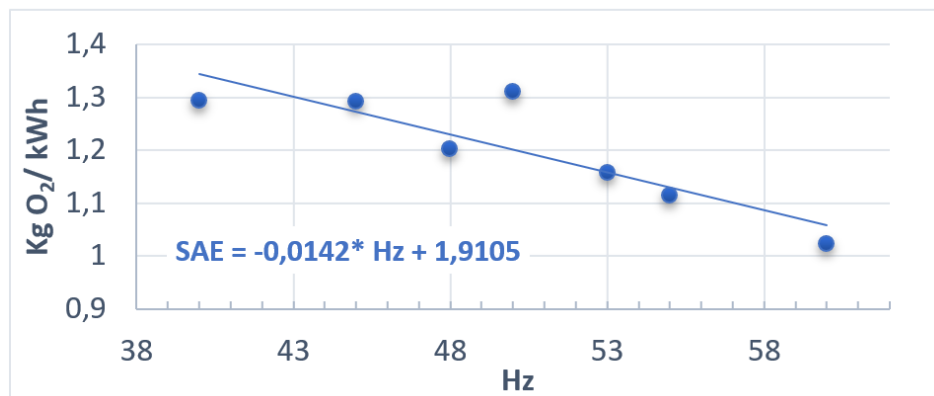


Figure 2 The SAE measured as a function of the frequency setpoint for variable frequency drive (VFD) for the rotor at a standard surface aerated wastewater plant, data redrawn from a DHI report 2013.

The fitted functions can be used in the SCADA system to yield the SAE value at any given depth or frequency.

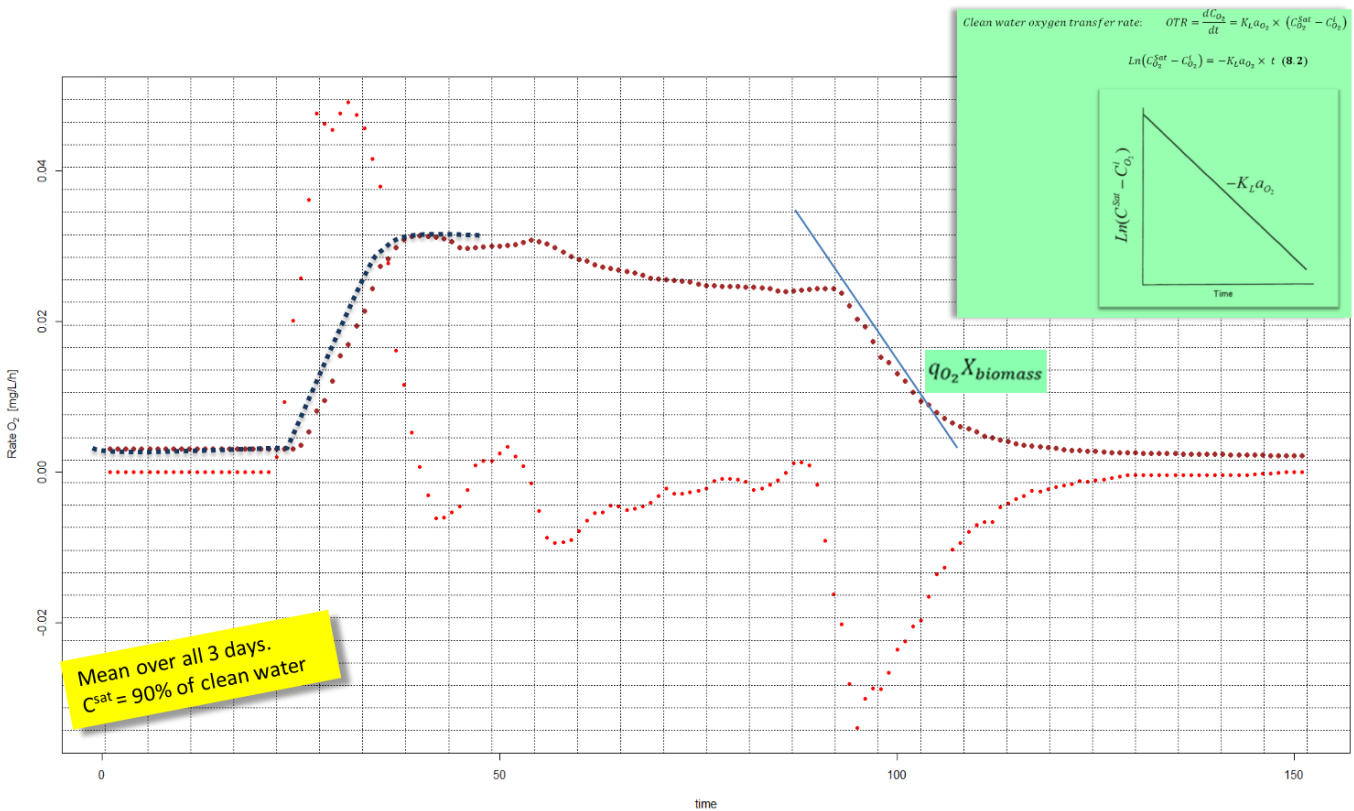
## 2. Calculations based on online $k_L a_{O_2}$ estimation

In-process calculations are possible using several methodologies depending on the trends and quality of the oxygen data measured and logged in the SCADA systems on the wastewater treatment plant.

In a first case the  $k_L a_{O_2}$  can be estimated for the whole aerated tank by calculating the oxygen transfer rate (OTR) using the aeration data during the early start of the rotors and analyzing the oxygen data. By fitting the oxygen data to the formula (2.2, see figure), the  $k_L a_{O_2}$  can be found.

$$OTR (kg_{O_2}/m^3/h) = k_L a_{O_2} T_{Process} \times (C_{O_2}^{Sat T_{Process}} - C_{O_2}^{process}) \quad (2.1)$$

$$k_L a_{O_2} T_{Process} = - \ln (C_{O_2}^{Sat T_{Process}} - C_{O_2}^{time_i process}) \quad (2.2)$$



In the second case the  $k_L a_{O_2}$  can be estimated IF the oxygen level reaches a steady level for several minutes during the aeration phase. The  $k_L a_{O_2}$  is calculated for the whole aerated tank (or for a known aerated section) by calculating the oxygen transfer rate (OTR, g/m<sup>3</sup>/h). The calculation is based on using the steady oxygen reading ( $\bar{C}_{O_2}^{Process}$ ) and the known respiration rate yielding the  $k_L a_{O_2}$  value. The respiration rate,  $q_{O_2} \times X_{Biomass}$ , is linear slope of the oxygen decrease found during the phase immediately after the surface aeration rotors are turned off.

$$k_L a_{O_2} T_{Process} = \frac{q_{O_2} \times X_{Biomass}}{C_{O_2}^{Sat} T_{Process} - \bar{C}_{O_2}^{Process}} \quad (2.3)$$

Oxygen transfer rate in activated sludge:  $OTR = K_L a_{O_2} \times (C_{O_2}^{Sat} - C_{O_2}^i) - q_{O_2} X_{biomass}$   
 At steady state:  $\frac{dC}{dt} = 0$  and  $C_{O_2}^i = \bar{C}_{O_2}$

$$K_L a_{O_2} = \frac{q_{O_2} X_{biomass}}{(C_{O_2}^{Sat} - C_{O_2}^i)} \quad (Y)$$

$q_{O_2}$  and  $O_2$ -mean are from mean over all 14 days.  
 $C^{sat} = 90\%$  of clean water

