

Determination of oxygen mass transfer coefficient $IKLa$) in batch reactor

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Objectives

Exercise on the statement of a model, programming in AQUASIM, and devising a strategy for parameter fitting. ## Background Assignment is based on experiment for measuring D.O.

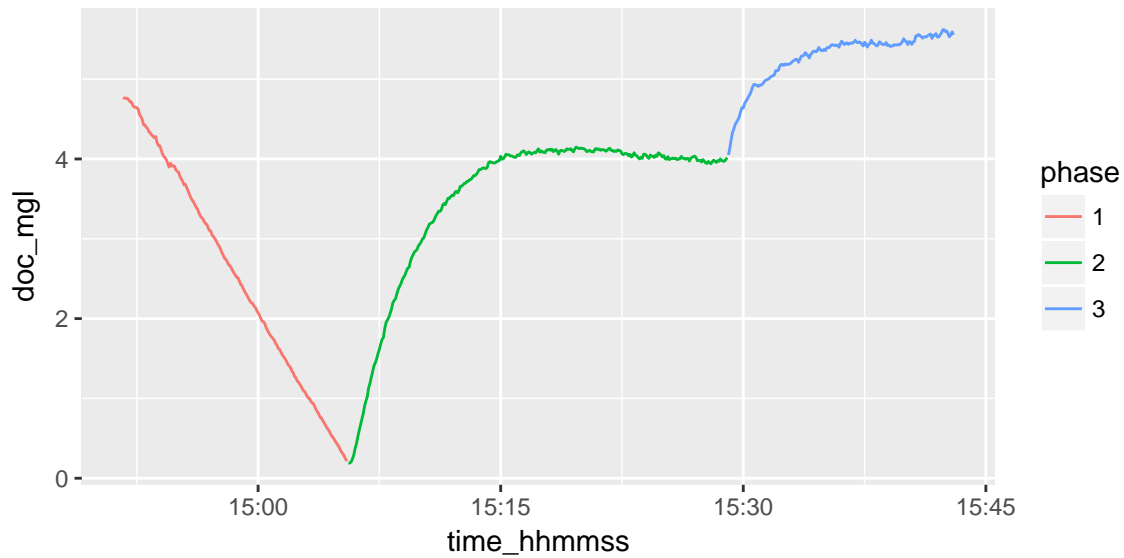


Figure 1: Endogenous respiration- phase I

Procedure

Dissolved Oxygen concentration at equilibrium will be calculated using the Henry's Law. For that purpose: first, determine the barometric pressure at 2600 [m], given P_0 , T , R , g , M using the barometric formula:

(1) $P = P_0 * e^{\frac{-Mgz}{RT}}$ where:

$M = 1,785 * 10^{-3} \text{ [mol]}; P_0 = 101325 \text{ [Pa]}; T = 298,15 \text{ [K]}; R = 8,314 \text{ [J*K/mol]}; g = 9,80 \text{ [m/s}^2\text{]}$

$P = 101325 * \exp\left(-\frac{28,96*10^{-3}*9,8*2600}{8,314*298,15}\right) = 75214 \text{ [Pa]}$

Second, determine dissolve oxygen concentration:

$$SO_{eq} = \frac{P}{K_H}$$

where $P = 75214 \text{ [Pa]}$

$K_H = 78,020 * 10^3 \text{ [Pa*L/mol]}^1$

¹Sanders, R (2015), "Compilation of Henry's Law constants for water as a solvent". Atmos. Chem. Phys 15: 4399-4981

Partial pressure for oxygen is $P_{O_2} = 0,21 * P = 15795$ [Pa]

$$SO_{eq} = \frac{15795 * 32 * 1000}{78,020 * 10^3} = 6.4 \text{ [mg/L]}$$

As substrate is depleted, Biomass undergoes endogenous respiration process in phase 1. As stated in problem definition, OUR is constant.

Alternatively, OUR can be obtained from linear regression of dissolved oxygen vs time

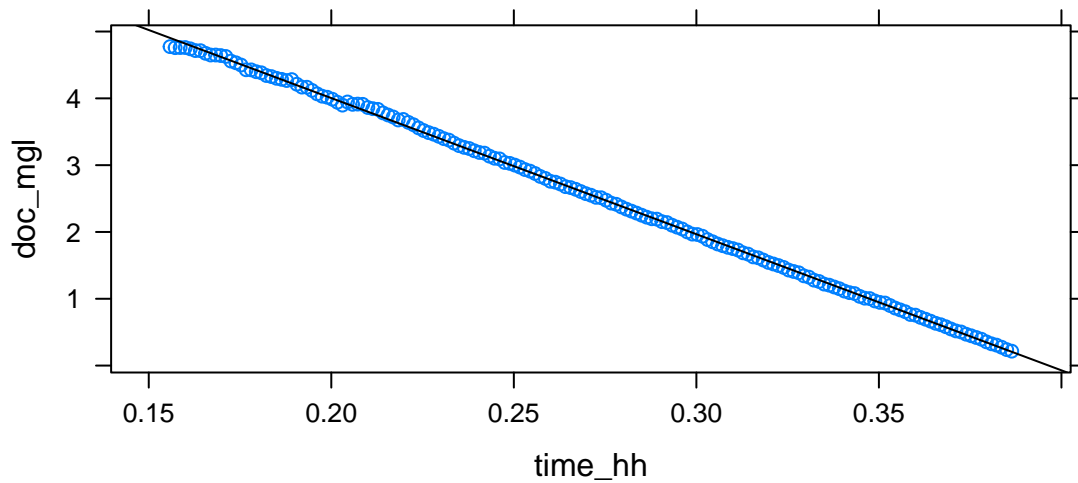
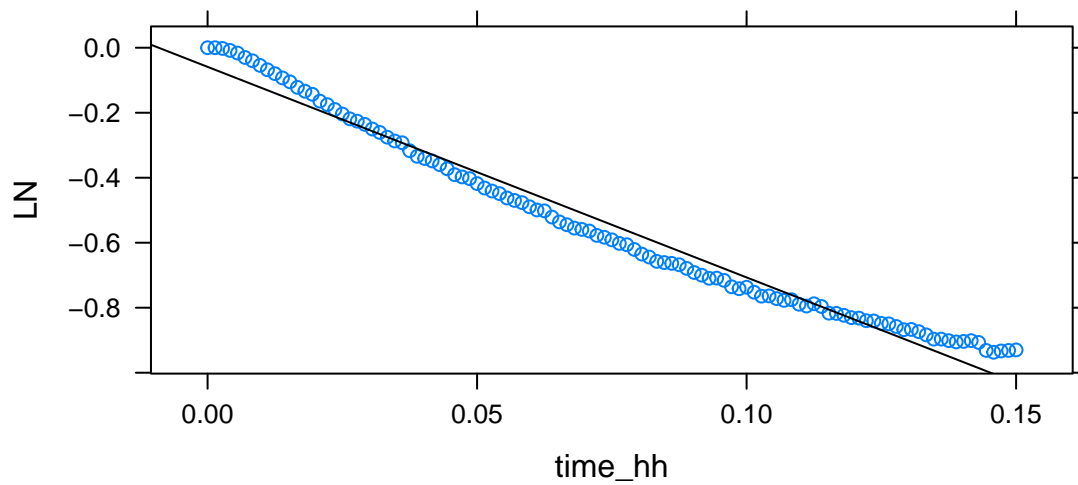


Figure 2: QO2 estimation

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## [1] "OUR_OH0 = -20.3764470549435 [mg/L-h] "
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K_{La} can be obtained directly without need to use AQUASIM, by plotting $\ln(\frac{SO_{eq}-SO}{SO_{eq}-SO_0})$ vs time plus linear regression to obtain the linear slope coefficient as K_{La} with the assumption reactor is modelled as CSTR.



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## [1] "KLa = -6.479 [1/h] "
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Simulation with AQUASIM

State variable are dissolved oxygen concentration in liquid phase(SO) and oxygen concentration in gas phase, both in [mg/L]. For parameter estimation measured SO data is read from a .CSV file.

Process variable is time in [h].

Process are defined as two reactions: $K_{La} * (SO_{sat} - SO)$ for oxygen mass transfer from gas to liquid phase, and $b_X H * X_H$ for endogenous respiration (decay).

Initially, process consisted only of aeration by mean of oxygen transfer reaction rate as defined per $K_{La} * (SO_{sat} - SO)$, where KLa and SO_sat are set to be 6.479 [1/h] and 6.4 [mg/L], respectively as per estimated values calculated above. Reactor volumen is set to be 1,64 [L].Afterwards, endogenous respiration was considered to better fit SO model output to SO measured.

For endogenous respiration (decay) process's reaction rate, b_XH was se to 0.233 [1/h]. As QO2 is constant, initial Biomass concentration XH_0 was estimated by dividing OUR by b_XH: $XH_0 = 85$ [mg/L].

A compartment is defined as a CSRT with aeration and decay process activated. An inflow of air to compartment with no water flow is set with $SG = 203$ [mg/L]. SG is calculated using the Ideal gas law: $SG = PO/RT$ with appropriate units.

Neither diffusive nor adventive link are considered.

Simulation time interval simulation was set to be 0.05 [h] ranging from 0 to 0.3902778 [h].

Simulation run obtained the following output shown in figure 2

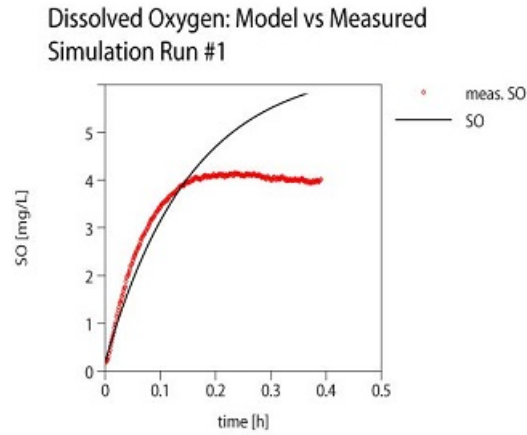


Figure 3: Simulation run #1

Sensitivity Analysis Sensitivity analysis was done for SO_sat, QO2, SO_ini, and KLa. SO showed to increase as SO_sat increases and decreased as KLa increased. A changein QO2 and SO_ini don't change SO as the other parameters did.

The strategy is fitting SO_sat and KLa

The standard error of SO_sat fitting was 0,05.

The standard error for KLa parameter fitting was 0.177

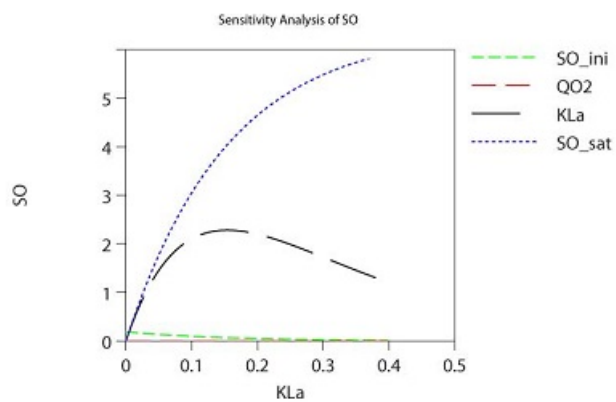


Figure 4: Simulation run #1

Dissolved Oxygen: Model vs Measured
Simulation Run #2: SO_sat parameter fitting

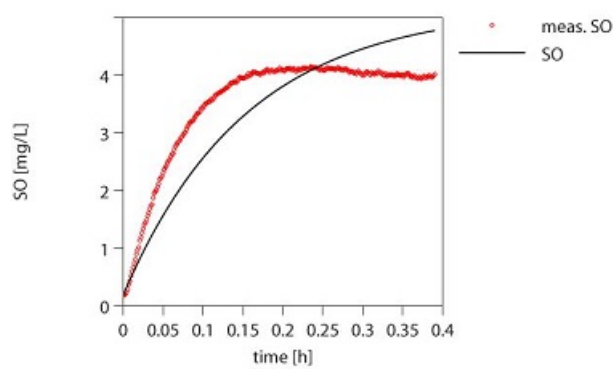


Figure 5: Simulation run #1

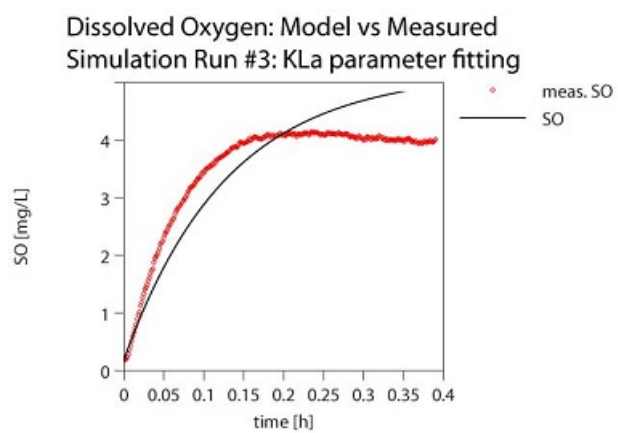


Figure 6: Simulation run #1