Determination of oxygen mass transfer coefficient IKLa) in batch reactor

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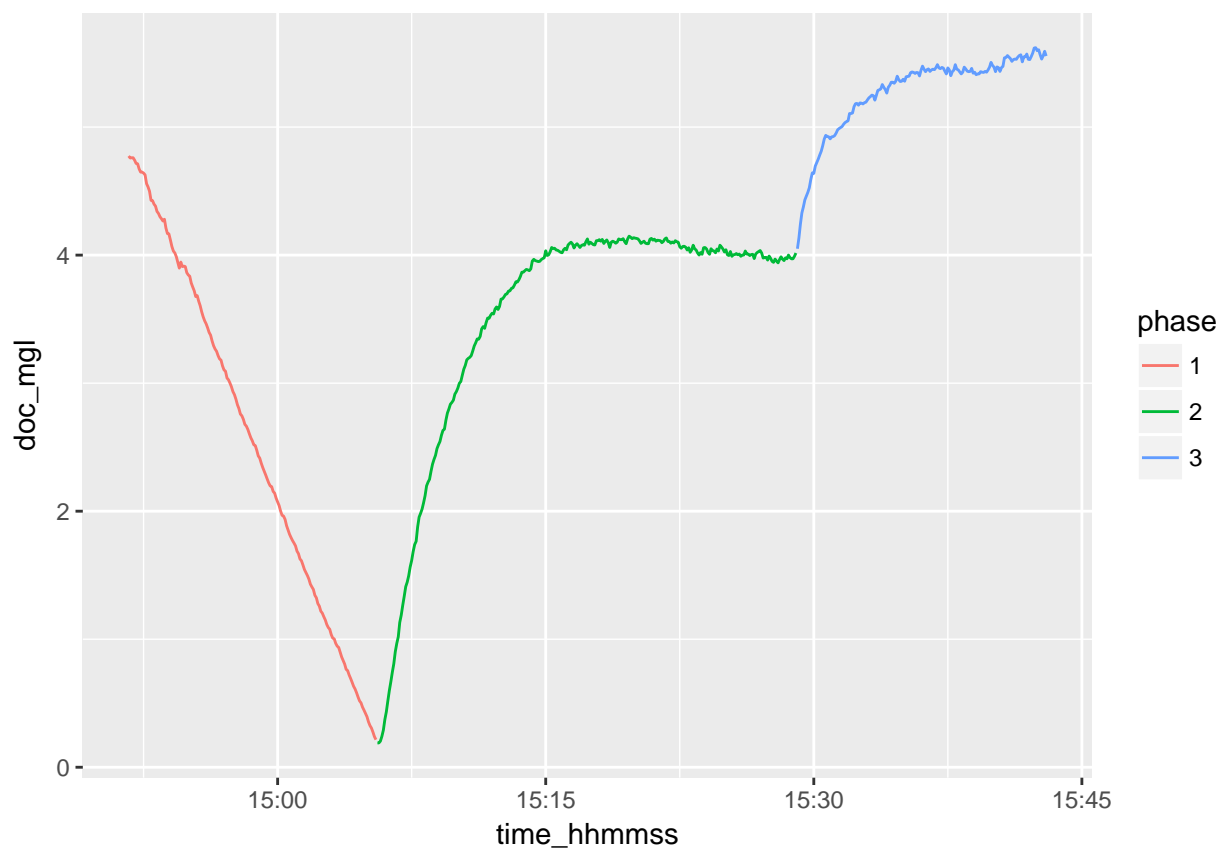**Abstract**

Objectives

Background

Assignment is based on experiment for measuring D.O.

```
## Warning: package 'readxl' was built under R version 3.3.3
```


Procedure

Dissolved Oxygen concentration at equilibrium will be calculated using the Henry's Law. For that purpose: first, determine the barometrice pressure at 2600 [m], given P0, T, R, g, M using the barometric formula:

(1) $P = P0 * e^{\frac{-Mgz}{RT}}$ where:

$M = 1,785 * 10^2 0$ [mol]; $P0 = 101325$ [Pa]; $T = 298, 15$ [K]; $R = 3,314$ [J*K/mol]; $g = 9,80$ [m/s^2]

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

Second, determine dissolve oxygen concentration:

$SO_eq = \frac{P}{K_H}$

where $P = 75214$ [Pa]

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

Partial pressure for oxygen is $P_{O2} = 0,21 * P = 15795$ [Pa]

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

As substrate is depleted, Biomass undergoes endogenous respiration process in phase 1. As stated in problem definition, OUR is constant and it is calculated by mean of the following expression:

$OUR = -\frac{DO_{end-of-phase1}-DO_{t0}}{t_{end-of-phase1}-t_0}$ [mg/L-h]

```
## [1] "OUR_OHO =  19.77  [mg/L-h] "
```

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

```
##
## Call:
## lm(formula = doc_mgl ~ time_hh, data = p1_dataset)
##
## Coefficients:
## (Intercept)      time_hh
##       8.079      -20.376
```
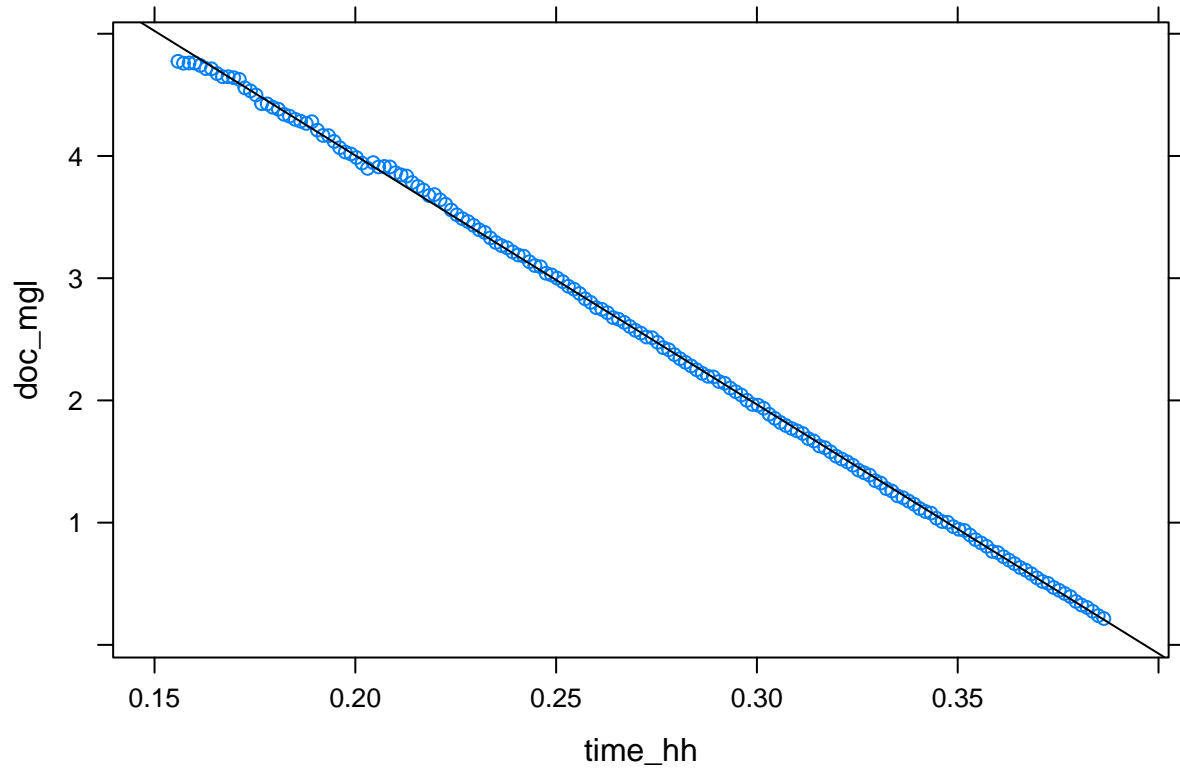
[1]Sanders, R (2015), "Compilation of Henry's Law constants for water as a solvent". Atmos. Chem. Phys 15: 4399-4981

```
## [1] "OUR_OHO =  -20.3764470549435  [mg/L-h] "
```

K_{La} can 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.

```
##
## Call:
## lm(formula = LN ~ time_hh, data = p2_dataset_lm)
##
## Coefficients:
## (Intercept)      time_hh
##    -0.05884     -6.47921
```
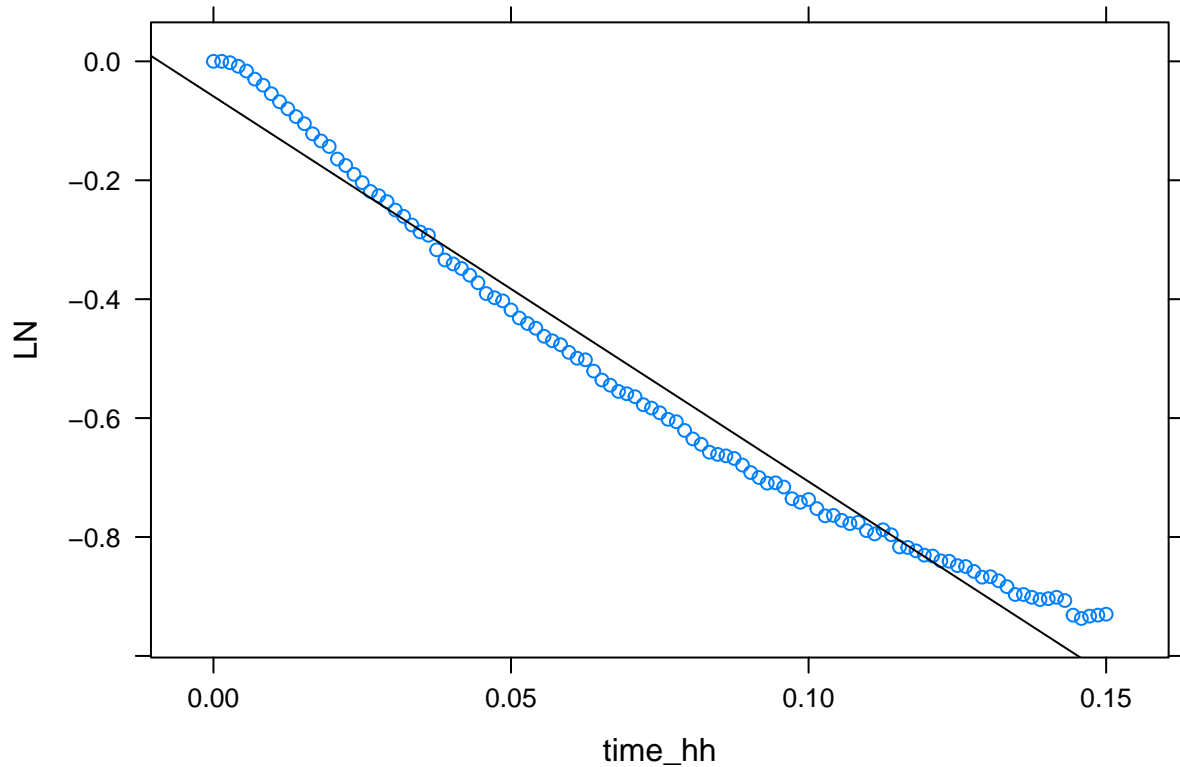
```
## [1] "KLa =  -6.479  [1/h] "
```

Simulation with AQUASIM

State variable is dissolved oxygen concentration (SO) in [mg/L], read from a .CSV file.

Process variable is time in [h].

Process is defined as reaction in CSTR

Reaction rate is defined as $K_{La} * (SO_{sat} - SO)$, where KLa and SOsat 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].

Neither diffusive nor adventive link are considered.

Time interval simulation is set to be 0.10 [h] from 0 to 0.3902778.

Simulation is run obtaining the following output shown in figure 2

Discussion

Conclussions