Determination of oxygen mass transfer coefficient IKLa) in batch reactor

Rafael Ventura

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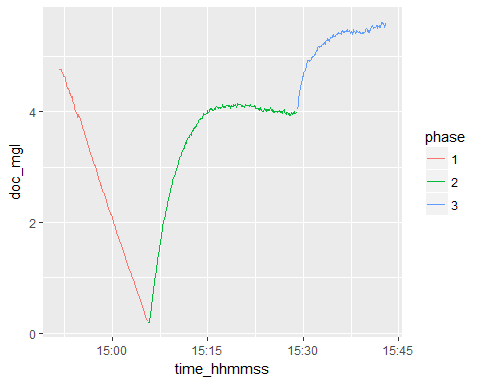
## Abstract

## 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. where:

[mol]; [Pa]; [K]; [J\*K/mol]; [m/s^2]

[Pa]

Second, determine dissolve oxygen concentration:

where [Pa]

[Pa\*L/mol] [[1]](#footnote-26)

Partial pressure for oxygen is [Pa]

[mg/L]

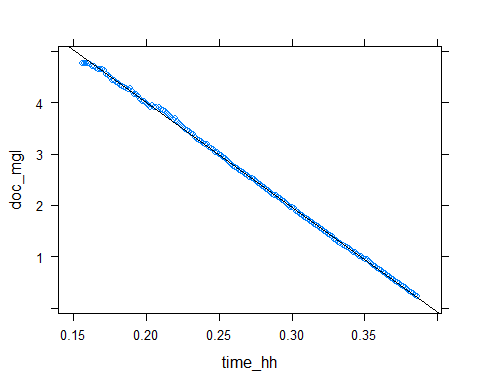
As substrate is depleted, Biomass undergoes endogenous respiration process in phase 1. As stated in problem definition, OUR is constant and it is calculated by mean of the following expression:

[mg/L-h]

## [1] "OUR\_OHO = 19.77 [mg/L-h] "

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

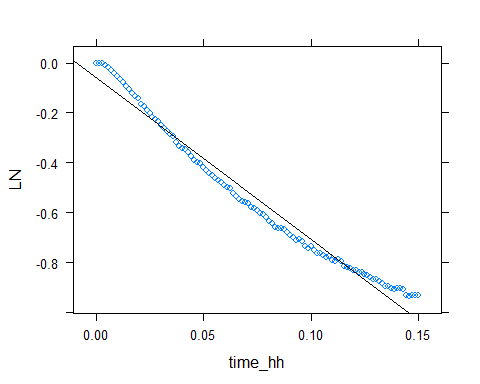
##   
## Call:  
## lm(formula = doc\_mgl ~ time\_hh, data = p1\_dataset)  
##   
## Coefficients:  
## (Intercept) time\_hh   
## 8.079 -20.376



## [1] "OUR\_OHO = -20.3764470549435 [mg/L-h] "

can obtained directly without need to use AQUASIM, by plotting vs time plus linear regression to obtain the linear slope coefficient as 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 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: for oxygen mass transfer from gas to liquid phase, and for endogenous respiration (decay).

Initially, process consisted only of airation by mean of oxygen transfer reaction rate as defined per , 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 airation 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: 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].

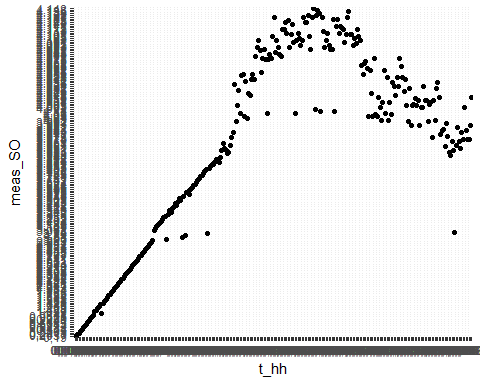
Simulation run obtained the following output shown in figure 2 Simulation run #1

## Discussion

Data from simulation is shown in figure

## Warning: package 'readr' was built under R version 3.3.3

## Parsed with column specification:  
## cols(  
## t\_hh = col\_character(),  
## meas\_SO = col\_character(),  
## t\_hh\_1 = col\_character(),  
## SO = col\_character()  
## )



## Conclussions

1. Sanders, R (2015), "Compilation of Henry's Law constants for water as a solvent". Atmos. Chem. Phys 15: 4399-4981 [↑](#footnote-ref-26)