Assignment #1 Aquasim for BOD_5 measurement

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Note: This is your first assignment which is quite consequent.

The prerequisite is to have fulfilled the basic **(Self-)Training of Aquasim**!

Don't remain alone and stuck if you don't' catch or understand the problem… **Use intensively the Moodle forum** (all together and with teacher assistants)**!**

SHARE TOGETHER and again, write up personally!

For your convenience, **please follow the assignment step by step!**

→ Provide .DOC and .PDF file with your answer with plots and the Aquasim files .AQU (including calculations) you used to solve this assignment (1 .DOC + 1 .PDF +2 .AQU files)

A1. INTRODUCTION - BOD_5 Measurement (design)

The BOD_5 is a biological estimation of the organic content (pollution) in a wastewater sample.

Definition from:
http://en.wikipedia.org/wiki/Biochemical_oxygen_demand

Biochemical oxygen demand or BOD is a chemical procedure for determining the amount of dissolved oxygen needed by aerobic biological organisms in a body of water to break down organic material present in a given water sample at certain temperature over a specific time period. It is not a precise quantitative test, although it is widely used as an indication of the organic quality of water.[1] . It is most commonly expressed in milligrams of oxygen consumed per liter of sample during 5 days of incubation at 20 C and is often used as a robust surrogate of the degree of organic pollution of water.

See also Lecture on COD Balance

By definition, the BOD_5 is given by the O_2 depletion due to the O_2 uptake rate after 5 days of organic pollution biodegradation in a wastewater sample.

In other words, it's the amount of O_2 consumed at 20°C in a S.T.R. - Stirred Tank Reactor in batch mode, during 5 days with known initial conditions:

- dissolved O_2 concentration (**S_O2ini**) is set with the dilution fresh water saturated in O_2 with air
- initial organic content (diluted sample) (**S_Sini**)
- initial biomass (diluted activated sludge) (**X_Hini**)

For these DBO_5 tests are provided:

1. An 0.5 Liter bottle with a magnetic stirrer in a temperature controlled room 20°C.
2. A domestic wastewater sample with a supposed BOD_5 of 300 mg O_2/L (400mg COD/L)
3. An inoculum of fresh activated sludge at 3.5 g TSS/L (1.36*3.5*1000=4760mgCOD/L)

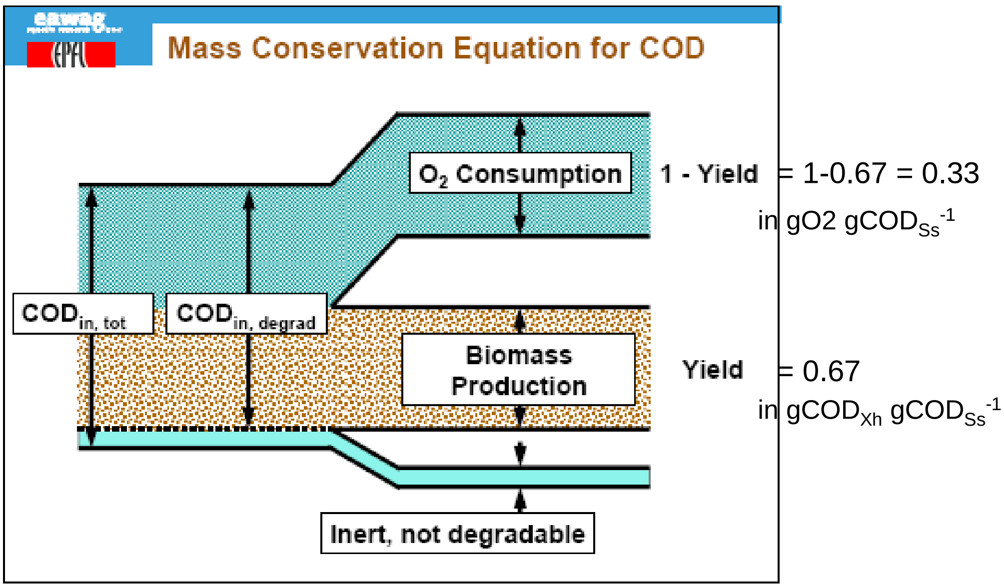
From Lectures about BOD, one can consider the COD balance of a perfectly biodegradable organic matter:

$$- COD_S + BOD + Y_{COD} * COD_S = 0$$

(**Here Y_{COD} = Y_H (see p 24 ofASM1_FinalVersion.pdf** in provided Readings)

Thus the BOD_5 is just a fraction of the COD of the sample which corresponds to the O_2 consumption required for biodegradation of a given consumed COD. The rest is assimilated/incorporated by the biomass growth. The BOD_5 measurement is fundamentally a respiration of the biomass and a fraction of the COD consumed depending of Y_{COD} biomass over substrate yield (which depends strongly on the organic matter).

COD balance



From Siegrist H., SIWWTP-09

Ideally, to be a good organic matter measurement of a wastewater sample, a BOD_5 measurement test in a biodegradation agitated flask (batch mode) should respect:

1) **No limitation of available O_2.** At the end of this batch, the O_2 dissolved oxygen concentration shouldn't be below 10 or 20 % of the O_2 saturation. To improve your modeling to avoid an underestimation of the BOD_5 due to oxygen limitation, you can complete the growth process (built during your Aquasim self-training) with an O_2 Switching Function (see p 11 ASM1_FinalVersion.pdf and consider Heterotrophic growth process #1 with $K_{O,H}$ constant p 24).

2) **Full substrate consumption**. As much as possible of the initial substrate loaded into the DBO_5 test bottle, should be consumed by respirometry during these 5 days

Overestimation of the BOD_5 can be due to:

a. The biodegradation/consumption (*Death regeneration*) of the decayed biomass (with implies a second growth (and respiration) of the COD already "anabolised" one time in biomass)

b. or *Endogenic respiration* of the already grown biomass (which is a bias of the estimation of the organic matter measured by BOD_5 test. The respiration of grown biomass on sample organic matter is not respiration of growth on initial organic matter of the sample)

There requirements of good DBO_5 measurement should be fulfilled and these bias should be minimized!

Your duty is using Aquasim batch dynamic simulation to **design the BEST measurement experiment by choosing**:

- The **right INITIAL dilution (i.e. the initial organic load) of the wastewater sample to be measured**
- The **right INITIAL inoculum** (activated sludge) concentration

For this duty, please follow the procedure bellow:

A1.I. **<u>COD Balance preliminary approach</u>**
In first approximation you can use a COD mass balance approximation of the bioprocess occurring in the BOD_5 test flask. This will allow a first estimation of initial substrate organic load that could be poured in the test bottle, which allows the consumption of 90% of the maximum dissolved O_2 (saturation).

A1.II. **<u>Aquasim simulation approach BOD_5 modeling on the basis on ASM1 Heterotrophic growth and decay</u>**
Then using dynamic simulations of the simplified ASM1 modeling in Aquasim (intro_batch.AQU) you would find the best initial values (i.e. experimental conditions) of the BOD5 tests, which will satisfy the above requirements.

This allow you to find by (trials and errors) the 3 states variables S_S, X_H, S_O initial values for the best measurement of the BOD_5 of the given wastewater sample.

B.1. **<u>BOD_5 Test Preparation</u>**
Lastly, from these values you will provide the diluted concentration of each sample, O_2 saturated water and biomass inoculum to fill in the 0.5L BOD_5 flask.

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<u>A1.I. COD Balance preliminary approach (2)</u>

Comes back to "Microbial Stoichiometry (undefined systems)" lecture and consider COD mass balance equation:

$$- COD_S + BOD + Y_{COD} * COD_S = 0$$

$$\rightarrow Y_{COD} = 1 - (BOD / COD_S)$$

$$\rightarrow Y_{H,X} = \text{grown } X/\text{consumed } S = (Y_{COD} * COD_S)/ COD_S = Y_{COD}$$

On a first approach, on the basis of the COD balance, and knowing the **$Y_{COD} = Y_H$ yield (see p 24 ofASM1_FinalVersion.pdf in "Moodle" Readings provided)**.

From this COD mass balance, one can:

1) Rewrite (equilibrate) COD mass balance equation with the **Y_{COD} = Y_H** yield.
2) Rewrite the obtained COD mass balance equation by fixing the maximum BOD (90% of dissolved O2 saturation) which can by consume during the 5 days respiration. (As BOD is known at 90% of O_2 saturation, 1st estimation of COD_S is available. It is a first estimation of **S_Sini** …)

Based on this theoretical COD mass balance calculation, give the amount of biomass produced, substrate consumed and the amount of O_2 consumed. These 3 values are estimations of what could be the initial values for dynamic simulation:

- COD_S → **S_Sini**
- BOD→O2 requirement which should be less than 90% of the maximum Dissolved O2 saturation (9.1mgO_2/L) → **S_O2ini**
- Y_{COD} x COD_S→Final **X_H**

A1.II. Aquasim simulation approach BOD_5 modeling on the basis on ASM1 Heterotrophic growth and decay (5)

This COD balance approach is somewhat not satisfying as it doesn't take into account the biomass decay/endogenic respiration/biomass OR death regeneration phenomenon occurring in the BOD_5 bottle. This phenomenon is rather significant in the BOD_5 test, as measurement lasts for 5 days in batch mode with a quite low the specific growth rate. Use of Aquasim and ASM1 modeling can cope with these phenomena!

You may consider the 2 simplest models you had built during Aquasim Self-Training which differ only on the stoichiometry of the decay process

In both case, use kinetic model parameters and yield coefficients (20°C) from AMS1 IWA Model for Y_H, K_S, $K_{O,H}$", μ^{max}_H, b_H **(see ASM1_FinalVersion.pdf ASM1 document (p24))**

You will have to complete/modify these simplest ASM models (Endogenic respiration AND Death Regeneration)) with a switching function for O_2 for the growth process (see ASM1_FinalVersion.pdf ASM1 document (p11) process#1) to take into account this O_2 limitation.

Endogenic respiration
(presented in the Training MD Aquasim ASM-TUUH and in ASM1_FinalVersion.pdf

Component → i / j Process ↓	1 X_B	2 S_S	3 S_O	Process Rate, ρ_j $[ML^{-3}T^{-1}]$
1 Growth	1	$-\frac{1}{Y}$	$-\frac{1-Y}{Y}$	$\frac{\hat{\mu}S_S}{K_S+S_S}X_B$
2 Decay	−1		−1	bX_B
Observed Conversion Rates $ML^{-3}T^{-1}$				Kinetic Parameters: Maximum specific growth rate: $\hat{\mu}$; Half-velocity constant: K_S; Specific decay rate: b
Stoichiometric Parameters: True growth yield: Y	Biomass $[M(COD)L^{-3}]$	Substrate $[M(COD)L^{-3}]$	Oxygen (negative COD) $[M(-COD)L^{-3}]$	

Death regeneration

Component → i / j Process ↓	1 X_B	2 S_S	3 S_O	Process Rate, ρ_j $[ML^{-3}T^{-1}]$
1 Growth	1	$-\frac{1}{Y}$	$-\frac{1-Y}{Y}$	$\frac{\hat{\mu}S_S}{K_S+S_S}X_B$
2 Decay	−1	1 ←	◯	bX_B
Observed Conversion Rates $ML^{-3}T^{-1}$	$r_i=\sum_j r_{ij}=\sum_j \nu_{ij}\rho_j$			Kinetic Parameters: Maximum specific growth rate: $\hat{\mu}$; Half-velocity constant: K_S; Specific decay rate: b
Stoichiometric Parameters: True growth yield: Y	Biomass $[M(COD)L^{-3}]$	Substrate $[M(COD)L^{-3}]$	Oxygen (negative COD) $[M(-COD)L^{-3}]$	

As in this Aquasim model file **intro_batch.aqu** you had implemented an oxygen transfer process called “oxygen_trans”, which is not valid for the present purpose. The BOD_5 estimation is a respirometry measurement and where there is NO O_2 transfer, as it occurs in a sealed bottle. Indeed, for this BOD_5 measurement, the amount of O_2 is fixed/provided initially and the bioprocesses occurs in a batch mode in a closed 0.5 L bottle without any O_2 transfer. You could cancel this Aquasim process by many manners:

- Inactivate the O_2 transfer process in the process windows of *the compartment (batch reactor) component windows*
- Delete the process in the *process windows*
- Set the k_La oxygen transfer time constant or set S_O2_Sat constant to Zero

According the 2 approaches (**Endogenic respiration** and **Death regeneration**) you will provide 2 Aquasim simulation files .AQU.

A1.II.a. Mass balance equations and model parameters (3)

To be sure of your understanding provide and write down:

1. The **mass balance equations** for your 3 state variables X_H (X_H), S_S (S_S), S_{O2} (S_O), for the **2 modeling approaches** (i.e. the 3 differential equations for each model – See bioprocesses of ASM1 PDF p 11)
2. A **table of model parameters and kinetic parameters** you will used in yours simulations (See ASM1 PDF Table 5 p 24)

A1.II.b. BOD_5 Simulations (4)

Once, your two (endogenic/death-regeneration) BOD_5 ASM model are ready, on the basis of the COD balance equation, you can compute the theoretical BOD in the effluent (g COD of substrate) according the balance and the Y_{COD}, biomass yield on substrate.

Use as “starting point” the Aquasim model you create during Training MD Aquasim ASM-TUUH, i.e. the Aquasim file **intro_batch.aqu.** You can modify it, according what is explained A1.II.a (above)

From the previous COD mass balance approach A1.I, considering this COD global growth equation in 1L volume, you had obtained a first estimation of the $S_{\_S,\ ini}$ concentration (COD_S substrate to be consumed) and the $X_{\_H,Fin}$ concentration (**Y_{COD} x COD_S** biomass produced). Thus for your 1st Aquasim simulation, you can use these values as initial values:

- $S_{\_S,\ ini}$ for $S_{\_S}$

- $S_{O2,ini}$ = S_O2sat = 9.1 mg/L

- $X_{\_H,ini} = X_{\_H,Fin}$ /100

Probably, your first simulated results will dissatisfy the criteria we mention above… Why?

The COD balance equation is a “theoretical” biomass growth equation rather than a real “observable”. The COD balance, in the Matrix formulation modelling is dependent on the “Endogenic respiration” or “Death regeneration” which have been taken into account in your models.

Note: About the strange behavior of modeling **DBO5 –Endogenic Respiration** (increase of S_S when S_O2 drops to 0! This is an artifact of the Growth rate process calculation in which S_O2 which a state variable which can’t be negative by definition, but which is decreased bellow 0 due to the Decay rate having the stoichiometric coefficient = -1 (this decay process is going on even if S_O2 <=0. To solve the behavior an IF test on S_O2<=0 could be set in the Growth process formula!) (To check the artifact, one can build for plotting, two Formula Variables, Decay and Growth with the same formulas as the two modeled processes). This artifact isn’t observed in the modeling **DBO5 _Lyse** (Death Regeneration) in which lysed biomass becomes new substrate S_S. In fact the dynamic of the 1st modeling is only valid when S_O2 stay above zero along the simulation!

By changing $S_{\_S,\,ini}$ and $X_{\_H,ini}$ with trials and errors, try to find YOUR best BOD_5 initial conditions.

To help you, to find the initial simulation conditions that will allow the best BOD_5 measurement, a non-subjective criterion is to calculate, for each simulation, the observed Y_{COD} yield at the end of the simulation (i.e. the BOD_5 measurement). Remembering:

$$- COD_S + BOD + Y_{COD} * COD_S = 0$$

$$\rightarrow Y_{COD} = 1- (BOD / COD_S)$$

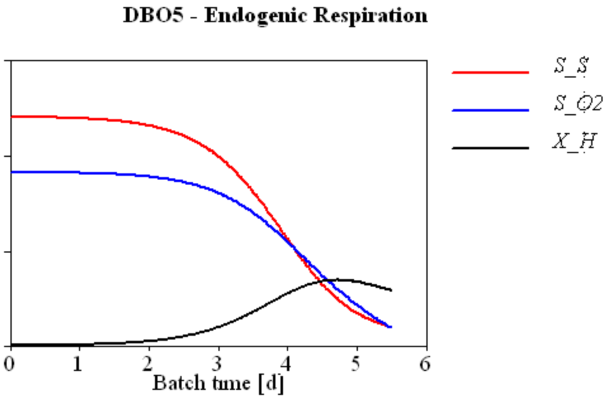
Thus, from simulation:

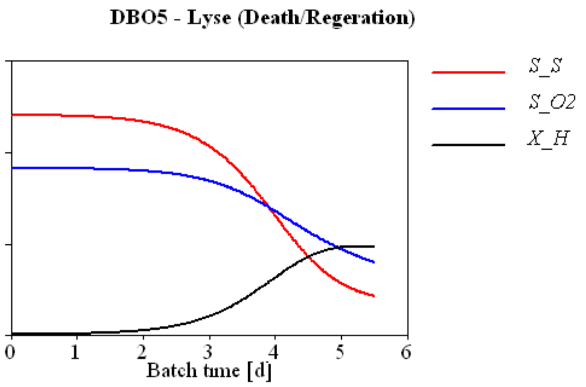
- CODs ≈ Δ S_S
- BOD ≈ Δ S_O2
- $Y_{COD,obs}$ = 1- (Δ S_O/Δ S_S)

This $Y_{COD.Obs}$ estimation should be as closest as possible to the theoretical Y_{COD} of COD mass balance equation, see A1.I.).

In others words, try to find the best simulation conditions, which compute the least "biased" (due to Endogenic respiration or Death/Regeneration) simulation of the BOD5 measurement, trying to be closest to the Theoretical COD mass balance.

By trials and errors you may find YOUR good compromise dynamic behaviors which can look like the figures below:





Auto Checking: To check the effect of "Endogenic respiration" or "Lyse – Death/Regeneration" you can invalidate them in your 2 modellings, and check that you will retrieve a theoretical COD mass balance growth… ;-)))

B.1 BOD_5 Test Preparation (3)

Using your best initial simulated values ($S_{\_S,\,ini}$, $S_{O2,ini}$, $X_{\_H,ini}$) setup your experiment in the 0.5L bottle to measure the BOD_5. Calculate the dilution required from the wastewater sample and the required activated sludge inoculum, that respect your choice to do the best BOD_5 measurement (i.e. (i) wastewater sample volume, (ii) activated sludge biomass inoculum volume and (iii) saturated O_2 fresh water for dilution).

Note: Dilution formula mass conservation with dilution

$$C1.V1 = C2.V2 \quad [mgCOD.L^{-1}.\,L = mg\ COD]$$

May be a comment of these calculations?

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Note: In fact in Standard Methods DBO_5 measurement protocol, the amount of S_S (organic pollution to be measured) and S_O2, are not fixed as here. The standard protocol, fixe the S_S and S_O2 proportion by the ration of two volumes, the sample non diluted volume, which implies a gas phase volume complement to the 0.5L of the bottle. This allows two benefits: 1) as there is much more O_2 in air (21%) than in air saturated water, the amount of COD_S to be measured could be more important 2) the measurable gas phase depletion would be greater for more accuracy. This could be modeled using gas transfer phenomenon, but it couldn't be proposed here, as you will learn it, later in the course.