Case study 1

1. We are conducting an experiment in our Lab during 7 days, and we have recorded pH and total alkalinity during Day 1, 3 and 7. This experiment is focused in evaluate the effect of ocean acidification on the physiological traits of the copepod *Acartia tonsa*. We have considered two different levels of pCO_2, 400 and 1200 µatm. We need to check if the pCO_2 and Ω levels are in agreement with our experimental setup.

    Our lab assistant measured pH$_T$ at 25ºC and TA. Please, consider the following data and compare the pCO_2 calculated with the theoretical level we considered in our experimental setup.

Temperature pH measurement: 25ºC
Experimental temperature: 14ºC

Consider:
K1, K2 from Mehrbach et al. 1973 refit by Dickson and Millero 1987
KHSO4 constant: Dickson
Boron constant: Lee et al. 2010

Day	Phosphate	Silicates
1	0,34	7,88
3	0,32	5,67
7	0,31	10,23

	Low pCO_2			High pCO_2		
Day	Salinity	TA	pH (25ºC)	Salinity	TA	pH (25ºC)
1	34,2	2376,33	7,895	34,2	2376,21	7,552
3	34,1	2326,24	7,888	34,1	2325,14	7,546
7	32,0	1800,34	7,945	32,0	1799,21	7,645

Case Study 2

2. Next week we will start an experiment focused on the impact of Ocean Acidification on mussel physiology. With this purpose we will consider two pCO_2 levels, 450 and 1000 μatm, and incubation temperature of 12ºC.
We have been conducting measurements of Total Alkalinity in the incubation water collected on the coast of Ensenada, and we found a mean TA of 2250 $\mu M\ kg^{-1}$ at a salinity of 33.5 psu. Based on this information;

¿Which levels of $pH_{25ºC}$ we need to setup our lab mesocosm for an experiment to **Low** and **High** pCO_2 condition (450 and 1000 μatm)?
Note: Our last bottle of seawater buffer is finished, and therefore we will estimate pH_{NBS}

Consider:
K1, K2 from Mehrbach et al. 1973 refit by Dickson and Millero 1987
KHSO4 constant: Dickson
Boron constant: Lee et al. 2010

Case study 3

3. A colleague is interested in characterize the carbonate system in the intertidal zone of a remote area (DIC, pCO_2) (1 m depth) along the Mexican coast, and he don't have a good temperature/salinity sensor for characterizing $pH_{In-Situ}$; and his temperature/salinity sensor has an error of about **+/– 1.5 ºC y +/– 0.5 PSU**, respectively. He also doesn't have any sample for estimate phosphate and silicate concentration in this sampling site.

    Our colleague estimated **pH at 25ºC**, and he used seawater buffer. Measurements of **A_T** were conducted in a laboratory with **ca. 2 µmoles kg^{-1}** precision. ¿Which is the potential error associated to this error in temperature and salinity measurements, and if we do not consider the contribution of P and Si to alkalinity?

Situation	Temperature (ºC)	Salinity (PSU)	pH$_{In}$	A$_T$ (µmoles kg^{-1})	PO$_4$ (µM)	Si(OH)$_4$ (µM)
Control (ideal)	10.25	34.52	7.892	2356	0.54	3.54
−1.5 ºC temperature c/P and Si	9.75	34.52	7.892	2356	0.54	3.54
−0.5 PSU salinity c/P and Si	10.25	34.02	7.892	2356	0.54	3.54
−1.5 ºC temperature Without/P and Si	9.75	34.52	7.892	2356		
−0.5 PSU salinity without/P and Si	10.25	34.02	7.892	2356		

Guidelines for reporting ocean acidification data in scientific journals

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This document was prepared in the framework of the data management activity of the Ocean Acidification International Coordination Centre of the International Atomic Energy Agency (OA-ICC; www.iaea.org/ocean-acidification). Please contact the first author (gattuso@obs-vlfr.fr) in case of any error or omission. It is primarily based on Dickson *et al.* (2007), Dickson (2010), Nisumaa *et al.* (2010), Pesant *et al.* (2010), Pörtner *et al.* (2010) and Orr *et al.* (2015).

To ensure reproducibility, it is critical to report at least two variables of the carbonate system of seawater as well as salinity, temperature, and the hydrostatic pressure (if the measurements were not performed at atmospheric pressure). In addition, authors should report concentrations of total dissolved inorganic phosphorus as well as total dissolved inorganic silicon (in $\mu mol\ kg^{-1}$) whenever possible. Furthermore,

- Authors should carefully report how the parameters were measured and, if applicable, which protocol they followed.

- The use of Certified Reference Materials, source, and batch numbers must be mentioned

- At least two of the following carbonate system parameters should be measured and reported (note the preferred acronyms and units):

    - Dissolved inorganic carbon (C_T; $\mu mol\ kg^{-1}$)
    - Total alkalinity (A_T; $\mu mol\ kg^{-1}$)
    - pH (it is critical to mention its scale; see below)
    - Partial pressure of carbon dioxide (pCO_2; μatm)
    - Fugacity of carbon dioxide (fCO_2; μatm)
    - Carbonate ion concentration (CO_3^{2-}; $\mu mol\ kg^{-1}$)

- The pH scale (NBS, free, total, or seawater) must be mentioned prominently in the manuscript.

- If more than one pH scale is used in a given manuscript, the pH should always be given with the associated scale as a subscript:

  - on the National Bureau of Standards scale (pH_{NBS})
  - on the seawater scale (pH_{SWS})
  - on the free scale (pH_F)
  - on the total scale (pH_T)

- The temperature at the time of sampling and at the time of measurement should both be mentioned, if they differ.

- Salinity is needed (note that it is unitless)
- The formulations used to calculate the following variables should be mentioned:

  - Concentrations of total boron
  - CO_2 solubility (K_0)
  - Dissociation constants of carbonic acid (K_1 and K_2), boric acid (K_b), water (K_w), phosphoric acid (K_{p1}, K_{p2}, K_{p3}), silicic acid (K_{si}), hydrogen fluoride (K_f), and bisulfate (K_s)
  - Solubility products of calcite (K_{spc}) and aragonite (K_{spa})

- The software package used to calculate the carbonate chemistry, along with its version number, and any associated options must all be mentioned.

- Average reproducibility of the performed measurements (with number of measurements) should be mentioned.

- Finally, it is strongly recommended that the chemistry and biological data are either archived in an on-line database (preferred) or provided along with the paper as supplementary information.