# Ocean acidification simulation

## Tutorial for teachers

## 1. Controls and display

### *Brief tutorial on sequential mode*

Sequential mode simulates, one by one, the reactions induced by the presence in the atmosphere of carbon dioxide ($CO_2(g)$, a greenhouse gas), which occur in air and water.

- To **display the next reaction**, click on the **blue play arrow** .
- To **replay** the previous reaction, click on **orange back arrow** .
- To **reset the reactions**, click on **yellow double arrow** .

Reactions can be viewed with or without the corresponding chemical reaction equations. To **view** the chemical equations, activate **Reaction equations**.

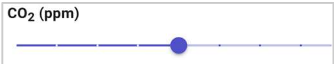
Viewing can be activated during a sequence. The equation corresponding to the current molecule animation is highlighted.

There are six successive reactions, with a round trip of each equilibrium reaction [1,2].

| | | |
|---|---|---|
| *Reaction 1* | *Equilibrium 1 in the direct direction →* | *Dissolution of $CO_2(g)$ in water to become $CO_2(aq)$.* |
| *Reaction 2* | *Equilibrium 2 in the direct direction →* | *Formation of carbonic acid $H_2CO_3$ from $CO_2(aq)$ and $H_2O$.* |
| *Reaction 3* | *Equilibrium 3 in the direct direction →* | *Dissociation of carbonic acid $H_2CO_3$ to form $H^+$ and $HCO_3^-$ ions. Only the first dissociation of carbonic acid is considered in this simulation.* |
| *Reaction 4* | *Equilibrium 3 in the indirect direction ←* | *Formation of carbonic acid $H_2CO_3$ from $H^+$ and $HCO_3^-$ ions.* |
| *Reaction 5* | *Equilibrium 2 in the indirect direction ←* | *Transformation of carbonic acid $H_2CO_3$ to form $CO_2(aq)$ and $H_2O$.* |
| *Reaction 6* | *Equilibrium 1 in the indirect direction ←* | *Transfer of the $CO_2(aq)$ into the air, to become $CO_2(g)$ again.* |

## *Brief tutorial for the continuous mode*

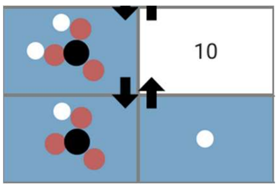
The focus of continuous mode is on understanding the concept of equilibrium and its response to disturbances. All chemical reactions that were detailed in sequential mode are now simulated simultaneously in this mode. Continuous mode simulates the cascade of reactions occurring between the atmosphere and the ocean, triggered by the presence of carbon dioxide ($CO_2(g)$, a greenhouse gas) in the atmosphere.

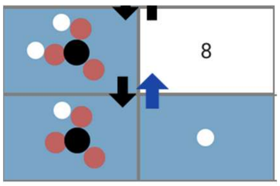
- To start the **animation**, click the **green play arrow**.
- The animation **stops** with a click to the **red stop button**. Note that the stop is not instantaneous; ongoing reactions will continue until the cycle is completed before coming to a halt. Click the **orange arrow** to **reset the reactions** and the **preset $\mathbf{CO_2(g)}$ values**.
- To modify the **amount of carbon dioxide** in the atmosphere of the simulation, you can move the **$\mathbf{CO_2(ppm)}$ slider:** 

to the desired value.
- $CO_2(g)$ molecules appear and disappear directly in the atmospheric section of the simulation, putting the system in a state of imbalance as long as the simulation has not been started with the **green play arrow**.

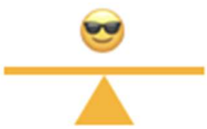
**Three $\mathbf{CO_2(g)}$atmospheric preset values** can be selected below the slider. These correspond to recorded $CO_2(g)$ levels in 1900, in 2015, and to the predicted 2050 value according to the *pessimistic scenario* of the IPCC report. Clicking on one of the presets automatically adjusts the $CO_2(g)$ ppm slider to the corresponding value.

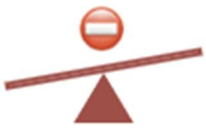
**The table** dynamically displays the number of molecules present in the simulation. Once the simulation starts, these values change as the system moves toward equilibrium, with **blue arrows** indicating the direction of this shift.




On the left, the system is temporarily at equilibrium; on the right, the excess $H^+$ and $HCO_3^-$ is being consumed, and $H_2CO_3$ is being produced.



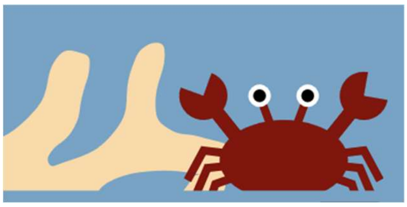


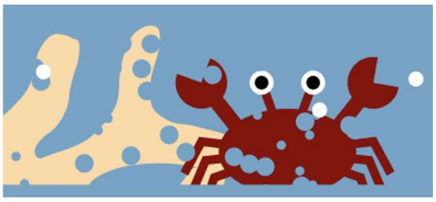
**The scale** icon in the top-right corner of the table indicates whether the system as a whole is at equilibrium or not. A yellow scale with horizontal plates signals that equilibrium has been reached, whereas a red scale with tilted plates indicates the system is out of equilibrium as a whole.

By hovering the pointer over the scale, a short sentence tells students whether or not the system is in equilibrium.

Even after the table values have mostly stabilized, the balance reflects slight fluctuations, illustrating equilibrium as a dynamic phenomenon.

Finally, the toggle switch  at the bottom left of the simulation allows you to display the pH scale, its effect on marine life, and highlights the $H^+$ count in the table to illustrate its connection to the pH value.





On the left, a healthy crab and coral indicate a pH level suitable for marine life. On the right, as the pH decreases, the skeletons of marine organisms deteriorate, represented by a "porous" marine life effect.

Note: It may be relevant to remind students that we are talking about ocean acidification because the pH is becoming more acidic, but in the scenario of a large increase in $CO_2$ in the air it would remain higher than 7, therefore by definition basic.

## 2. For students to discover

Students (who have not all learned what a chemical equilibrium is or yet know the definition of an acid) can first discover the movement of molecular models of chemical species.

By replaying the six reactions with the chemical equations displayed, they will discover the associated equations, and can ask themselves questions about the concept of chemical equilibrium, the meaning of ions and the identity of the acid.

## 3. Modelling and didactic choices

### *Explanation of didactic choices and simplifications in the simulation*

- The simulation represents an enlargement of the air-water interface to distinguish the molecules.
- We have deliberately removed all atmospheric molecules except **Cambria Math** to enhance the visibility of the reactions.
- The scale indicates the equilibrium or disequilibrium of the system as a whole. It cannot therefore be linked to each equilibrium individually.
- For the sake of simplification, the dissociation of $\mathbf{HCO_3^-}$ is omitted, given the number of molecules represented and the very low value of its equilibrium constant.
- The **porosity** depicted in the skeletons of living organisms ($\mathbf{CaCO_3}$) represents structural weakening (see Box 1 for more details).

- In continuous mode, certain molecules remain stationary to reduce visual clutter. Furthermore, we didn't distinguish the movement of gaseous or aqueous molecules.
- The **molecular counts and proportions** (values displayed in the table) are **fictional** in continuous mode, as the actual quantities (calculated using equilibrium constants) would be far too low to be meaningfully represented.
- The three periods 1900, 2015 and 2050 were chosen so that values for atmospheric Cambria Math concentrations could be rounded to the nearest hundred ppm. The value of 300 ppm in 1900 was taken from Chap. 2 (Table 2.1) of the IPCC report (2021) [3]. The value of 400 ppm in 2015 was estimated from the Keeling curve [4] and the value of 500 ppm corresponds to the SSP 2-4.5 projection (intermediate socio-economic pathway representing an average greenhouse gas emission trajectory) according to Chap. 4 of the IPCC report (2021) [3].

### *Calibration of the relationship between atmospheric $CO_2$ concentration and pH*

To determine how pH adjusts when atmospheric $CO_2$ Cambria Math concentration varies over a wide range from 200 ppm to 600 ppm, we took average pH values for four epochs (pre-1900, 1990-2000, 2005-2014 and 2010-2019) measured in seawaters [1, 7, 8, 9, 10]. We then established a linear trend with the corresponding atmospheric $CO_2$ concentration values estimated from the Keeling curve [4], as shown in Fig.1.

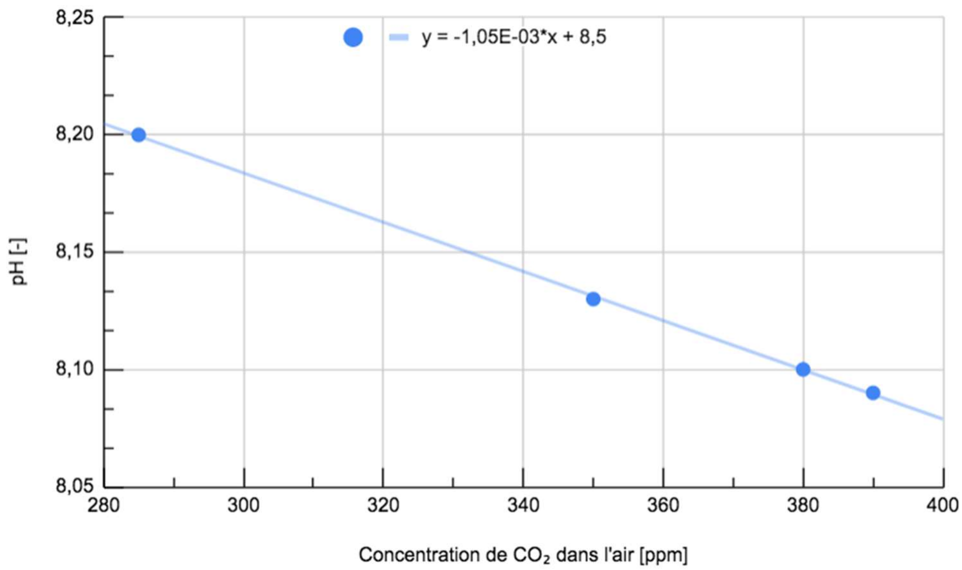



**Fig. 1 :** Linear relationship between pH values and atmospheric $CO_2$ concentration

This linear relationship is consistent with the linear regression of the pH time series obtained in northern Hawaii over the shorter period 1990-2008, during which the atmospheric $CO_2$ concentration can also be linearized [2].

**Box 1. Effects on Corals (and Other Calcium-Containing Organisms)**

Chemically, an acid such as carbonic acid ($\mathbf{H_2CO_3}$) reacts with calcium carbonate ($\mathbf{CaCO_3}$) in what is known as a **neutralization reaction** [1,2].

Many marine organisms are partially composed of calcium carbonate, for instance, corals, as well as the shells and exoskeletons of molluscs and crustaceans. As a result, they are affected by the **decreasing pH of the oceans**, though not always as immediately as the simulation suggests. The increase in $\mathbf{H^+}$ **concentration in seawater** occurs very gradually, meaning that the primary impact of these reactions is on developing marine life. The rising acidity prevents young organisms from effectively incorporating the calcium necessary for building their shells or skeletons. Consequently, **new generations of marine organisms will have weaker, more fragile exoskeletons compared to those of past centuries**, making them less resilient and more vulnerable [5].

Coral bleaching, widely documented in alarming photographs and reports, is also linked to **climate change**, though in a more direct manner. In this case, it is the **rising ocean temperature**, caused by increased greenhouse gas concentrations such as atmospheric $CO_2$, that triggers the bleaching effect [6].

## References


[1] S. Barker & A. Ridgwell (2012), *Ocean acidification*, Nature Ed. Knowledge

[2] Feely, R. et al. (2021), *An international observational network for ocean acidification*, Proceedings of Ocean Obs.

[3] GIEC (2021). *Climate change 2021: the physical science basis*, Contribution of working group I to the sixth assessment report of the intergovernmental panel on climate change

[4] Scripps Institution of Oceanography, *the Keeling curve*

[5] NOAA (National Oceanic and Atmospheric Administration USA) – *Understanding Ocean & Coastal Acidification : For Teachers*

[6] NOAA (National Oceanic and Atmospheric Administration USA) – *Investigating Coral Bleaching : For Teachers*

[7] European Environ Agency, *Decline in ocean pH measured Aloha station and yearly mean surface seawater pH reported on a global scale* (adapted from Dore, J.E., R. Lukas, D.W. Sadler, M.J. Church, and D.M. Karl. 2009. Physical and biogeochemical modulation of ocean acidification in the central North Pacific. Proc Natl Acad Sci USA 106:12235-12240)

[8] United States Environmental Protection Agency, *Understanding the Science of Ocean and Coastal Acidification*

[9] Encyclopédie Universalis Éducation Avancé, *Acidification des océans*, Paul Tréguier

[10] Ministère de la transition écologique et de la cohésion des territoires, *Réchauffement et acidification des océans*