

# PHY 555 — Energy and Environment

## PC3 — Carbon Capture & Storage

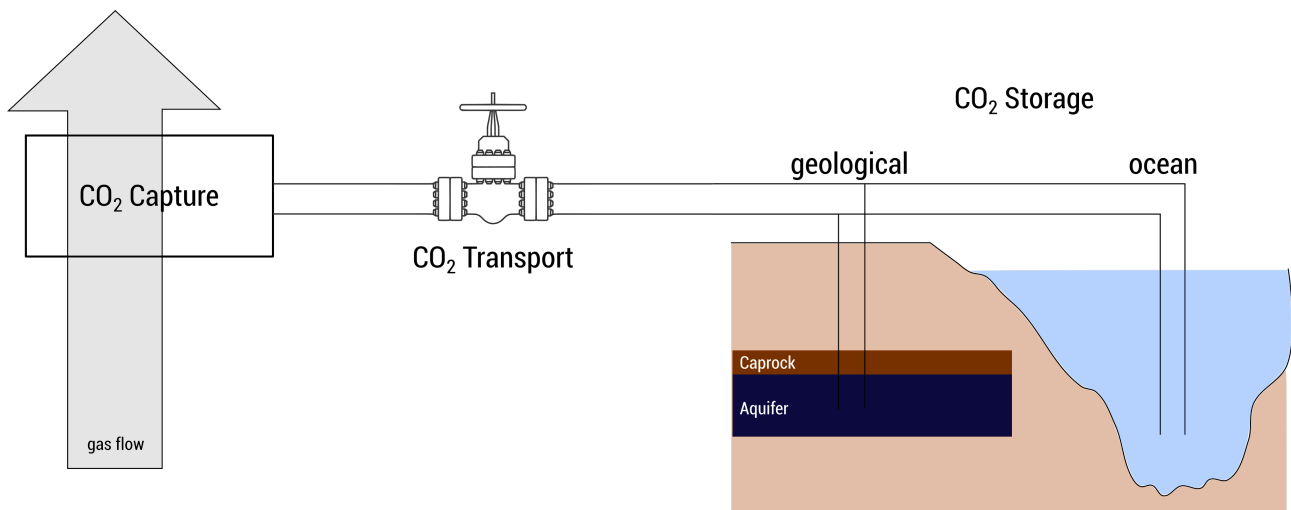
Friday, October 07<sup>th</sup>, 2022

**The exercises marked with a (\*) star are intended for further study and will not be covered in class.**

As the concentration of CO<sub>2</sub> increases in the atmosphere, strategies evolve to attenuate climate change and prevent global warming from reaching values above +2°C as compared to the pre-industrial period. According to the special report of the IPCC on a “Global Warming of 1.5 °C”, it will not be sufficient to reduce emissions, and active CO<sub>2</sub> capture will be mandatory:

“All pathways that limit global warming to 1.5 °C with limited or no overshoot project the use of carbon dioxide removal (CDR) on the order of 100–1000 GtCO<sub>2</sub> over the 21<sup>st</sup> century. CDR would be used to compensate for residual emissions and, in most cases, achieve net negative emissions to return global warming to 1.5 °C following a peak (high confidence).” (IPCC, SR15, SPM (2019)).

Several approaches are considered to achieve CDR. In this problem, we will focus on Carbon Capture and Storage (CCS) and investigate the three main steps of the process: the selective removal of CO<sub>2</sub> from a gas flow, the transportation of liquefied CO<sub>2</sub> and the sequestration of CO<sub>2</sub> either in the ocean or underground.



### 1 Orders of Magnitude

1. Knowing that the atmospheric pressure at sea level is 1 bar (=10<sup>5</sup> Pa), estimate the total mass of the atmosphere.
2. In the pre-industrial period, carbon dioxide represented 280 ppm (parts per million) of the atmosphere composition. Estimate the carbon content of the atmosphere in gigaton of carbon (GtC) not to be confused with GtCO<sub>2</sub>
3. The total anthropic CO<sub>2</sub> emissions until 2018 are estimated to be 2200 GtCO<sub>2</sub>. By the end of 2017, carbon dioxide concentration rose to 405 ppm. Estimate the fraction of carbon from anthropic emissions that has been removed from the atmosphere. Comments?

4. One of the main natural carbon sink is the Ocean. Assuming that the first  $\sim 100$  m of the Ocean are in chemical equilibrium with the atmosphere and considering the vapour pressure diagram provided in appendix, estimate the concentration in  $\text{g/m}^3$  of  $\text{CO}_2$  dissolved in surface waters. Evaluate the amount of  $\text{CO}_2$ , in  $\text{GtCO}_2$ , currently stored in the surface waters of the Ocean.
5. Comment on the evolution of this storage in the context of climate change.
6. Assuming an overall efficiency of photosynthesis of 0.1%, estimate the net carbon sequestration per hectare and per year by land biomass. What fraction of anthropic emission could be captured by biomass?

## 2 $\text{CO}_2$ Separation

The operation of a coal power plant with carbon capture is illustrated in figure 1. In comparison to classical power plants, carbon capture has the following implications :

- A fraction of the produced heat is used in the separation processes of the exhaust gas (thermochemical or physical absorption), thus reducing the available power and the yield.
- To be transported to the storage location by tanker or pipeline,  $\text{CO}_2$  needs either to be compressed to high pressure (110 bars, corresponding to super-critical state) (HP compressor), or liquefied at a pressure of 20 bars and a temperature of  $-20^\circ\text{C}$  (compressor + liquefier).

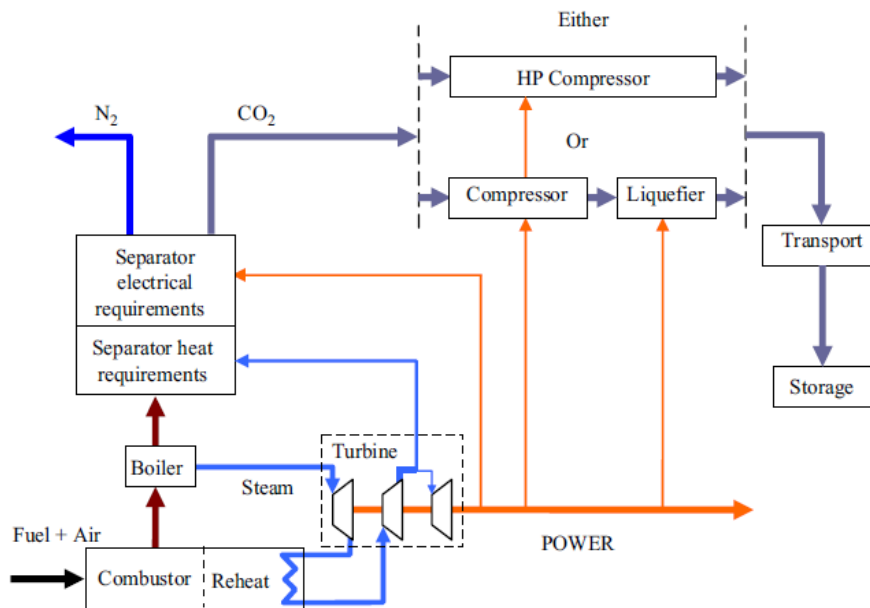


Figure 1 : Operation of a coal power plant with carbon capture (post-combustion)

In this part, we will use the basics laws of thermodynamics to estimate the minimal cost of the separation process, without considering the actual technical process.

1. Consider the inverse operation: an enclosure with two compartments with identical temperature  $T$  and pressure  $P$ , containing initially  $n_1$  moles of gas 1 and  $n_2$  moles of gas 2 respectively. The wall between the compartments is opened, and gases can mix. Estimate the entropy created in the process.
2.  $\text{CO}_2$  separation: Estimate the minimal amount of work required to separate a mixture of  $n_1$  moles of gas 1 and  $n_2$  moles of gas 2 into two separate pure systems at constant temperature  $T$  and pressure  $P$ .

3. Consider a gas containing a molar fraction  $x$  of  $\text{CO}_2$ . In the low concentration regime ( $x \ll 1$ ), show that the minimal energy  $W$  required to extract 1 mole of  $\text{CO}_2$  from such a gas can be written as:  $W_{1\text{molCO}_2} = -RT(\log x - 1)$
4. Direct Air Capture consists of capturing  $\text{CO}_2$  from the ambient atmosphere: Using previous results, evaluate in kWh the minimal energy  $W_0$  required per kilogram of captured  $\text{CO}_2$  from ambient air.
5. Rather than Direct Air Capture, it is also possible to capture  $\text{CO}_2$  in the exhaust gases of a combustion process. Consider for instance a combustion process under atmospheric conditions, assuming every oxygen molecule reacts with a carbon atom to form a  $\text{CO}_2$  molecule. Using previous results, estimate the energy required to isolate one kilogram of  $\text{CO}_2$ . Comment this result.
6. In the oxy-combustion process, oxygen is separated from nitrogen by cryogenic processes before combustion from the coal, and then the coal is burned in pure  $\text{O}_2$  (or in a mixture of  $\text{O}_2$  and  $\text{CO}_2$  taken from the exhaust gas). What are the advantages and drawbacks of this process?

7. Real processes for  $\text{CO}_2$  capture require much more work than the thermodynamic limit evaluated in the previous question (Figure 2). We denote  $\eta$  the ratio between the thermodynamic limit  $W_0$  and the quantity of energy actually required to extract a kilogram of  $\text{CO}_2$ . Furthermore, the energy used to capture the  $\text{CO}_2$  might produce emission itself, which have to be taken into account in the balance. Considering that this energy is provided by a power source emitting  $I$  tons of  $\text{CO}_2$  per kWh, estimate the energy cost per net kilogram of captured  $\text{CO}_2$ .

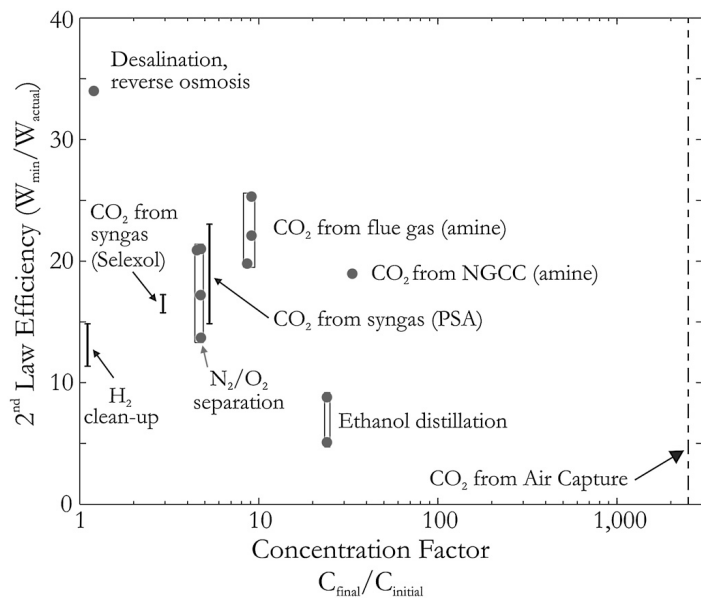


Figure 2: Empirical relationship between the concentration factor of industrial processes vs. the achieved efficiency of those processes. Kurt Zenz House, 2011

### 3 Transport

1. Adiabatic compression of  $\text{CO}_2$ : Estimate the minimum work for the adiabatic compression of a perfect gas from a pressure  $P_1$  to a pressure  $P_2$ . For each of the two processes (110 and 20 bars), estimate the compression work per unit of mass of  $\text{CO}_2$ .
2. Liquefaction of  $\text{CO}_2$ . Latent heat of liquefaction of  $\text{CO}_2$  is 300kJ/kg. Assuming that after the separation process, the gas is at atmospheric temperature and pressure, what is the required work to liquefy  $\text{CO}_2$  at  $-20^\circ\text{C}$  ?
3. Global analysis: Let's consider a coal power plant, using standard coal grade (80 % carbon, calorific content 36MJ/kg) with carbon removal from the exhaust. Estimate the overall energetic cost, and the corresponding yield loss for  $\eta=1$  (theoretical thermodynamical limit) and  $\eta=0.05$  (current state of the art).

## 4 Submarine Liquid Storage (\*)

Several options are considered for CO<sub>2</sub> storage: depleted oil or gas well reservoirs, deep aquifers or deep ocean. It is of prime importance to ensure that the trapped CO<sub>2</sub> cannot be released again in the environment, because CO<sub>2</sub> is more dense than air and can be lethal in moderate concentrations.

1. The total volume of the oceans is 1 370 millions of cubic kilometres. If one dissolves CO<sub>2</sub> in the full column of water instead of the first 100 m as in question 1.4, what fraction of human production could be stored?

T (°C)	0	25	80
pK1	6,58	6,37	6,32
pK2	10,63	10,33	10,12

2. Figure 3 gives the boiling curve of CO<sub>2</sub> as function of pressure. Can liquid storage on the ocean floor be envisaged? If yes, below which depth? (Liquid water is barely compressible, its density varies between 1020 kg/m<sup>3</sup> at the surface and 1050 kg/m<sup>3</sup> on the ocean floor). Density of liquid carbon dioxide is given in figure 4).

Tableau 1 : Equilibrium constant of carbonate and bicarbonate ions

## 5 Ocean Acidification (\*)

1. The solubility of CO<sub>2</sub> computed above is underestimated because of the existing chemical reaction leading to the formation of carbonic acid :



(H<sub>2</sub>CO<sub>3</sub> is the hydrated form of dissolved CO<sub>2</sub>, in equilibrium with atmospheric CO<sub>2</sub>). The chemical equilibrium constants are given in table 1.

Compute the total solubility of CO<sub>2</sub> as function of pH. How does it vary with temperature?

### Data

#### Gaseous CO<sub>2</sub> :

Calorific capacity:  $C_p = 37,1 \text{ J mol}^{-1} \text{ K}^{-1}$

$C_v = 28,8 \text{ J mol}^{-1} \text{ K}^{-1}$

Adiabatic index:  $\gamma = C_p / C_v = 1,29$

Boiling latent heat:  $L_f = 330 \text{ kJ kg}^{-1}$  at  $-20^\circ \text{C}$

Molar mass:  $44 \text{ g mol}^{-1}$

#### Coal :

Carbon content: 80%

Higher heating value:  $h_v = 36 \text{ MJ kg}^{-1}$

#### Storage Processes :

– Process 1 : compression to 110 bars (supercritical CO<sub>2</sub>), ambient temperature

– Process 2 : compression to 20 bars, liquefaction at  $-20^\circ \text{C}$

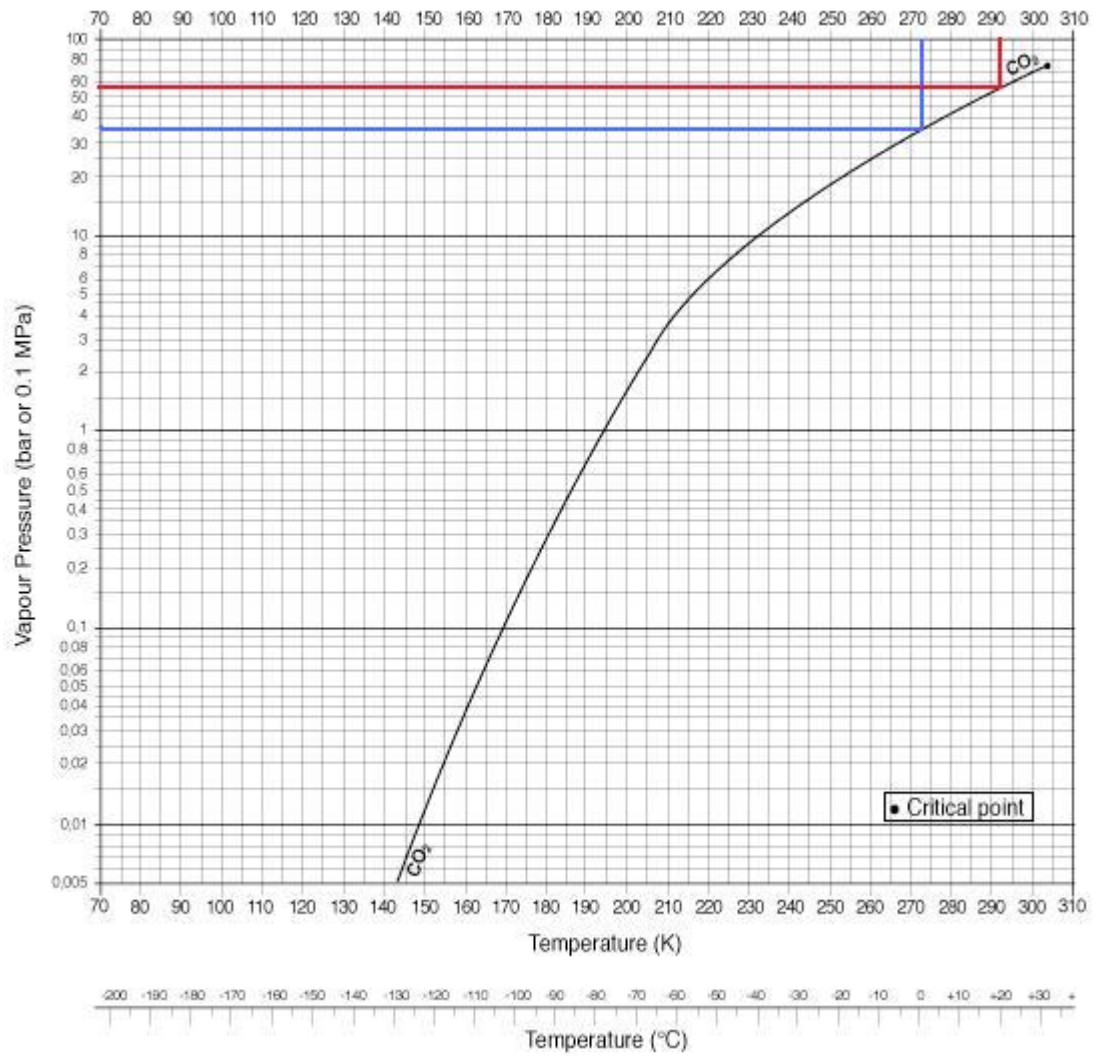


Figure 3 : Boiling curve of carbon dioxide

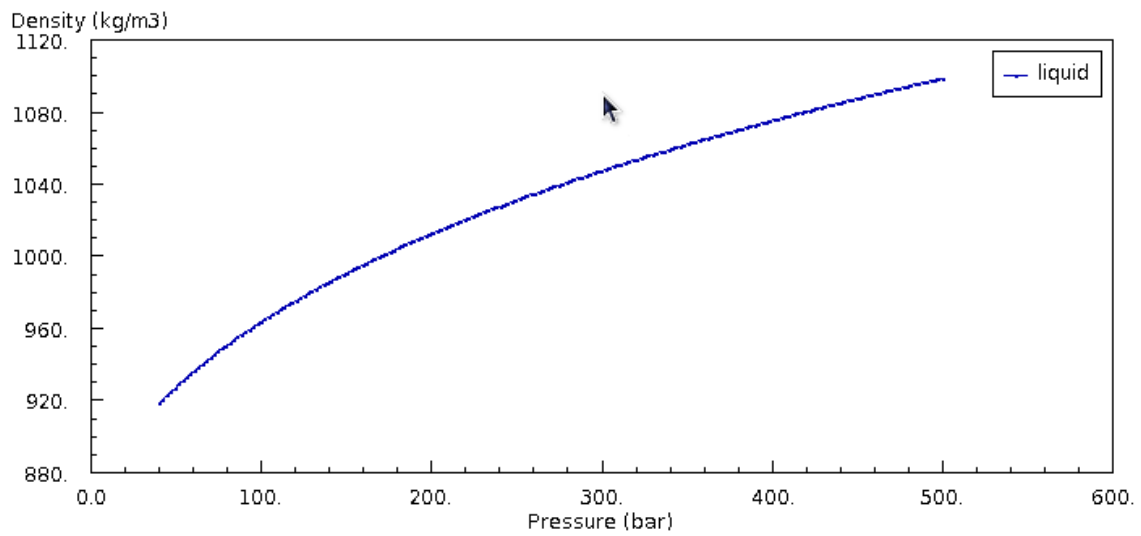


Figure 4 : Density of carbon dioxide as function of pressure at 275K. Source NIST (<http://webbook.nist.gov/>)