

# CHBE 483 Assignment 2

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The volume of air in the Earth's atmosphere is approximately  $4 \times 10^{18} \text{ m}^3$  at STP (273 K, 1 atm). The  $\text{CO}_2$  concentration in the Earth's atmosphere is 425 ppm(vol/vol). [ppm = part per million]. Consider the following scenario related to  $\text{CO}_2$  emissions for the period 2025 – 2050 (including both 2025 and 2050):

- Fossil fuel combustion generates 37 Gt/year of  $\text{CO}_2$
- Deforestation (e.g., losses in the Amazon delta) contributes on average 2.7 Gt/year of  $\text{CO}_2$
- Oceans absorb approximately 9 Gt/year of  $\text{CO}_2$

Calculate the following:

Note: obtain physico-chemical constants you might need in your calculation from reliable data sources (engineering handbooks, textbooks etc.), indicate the references you used for obtaining the data and specify the simplifying assumptions (if any) you made in your calculations.

a) The total  $\text{CO}_2$  amount in atmosphere (expressed in Gt = gigatonnes) corresponding to the 425 ppm(vol/vol) concentration. [25%]

b) How much  $\text{CO}_2$  must be removed per year (by both natural and technological means) to limit the atmospheric  $\text{CO}_2$  concentration at 435 ppm(vol/vol) in 2050. Comment briefly on the feasibility of achieving this target. What natural and technological options could be utilized? [25%]

c) Convert 435 ppm(vol/vol) to ppm(mass/mass). [25%]

d) What would be the hypothetical  $\text{CO}_2$  concentration in the atmosphere in 2050 (expressed in both ppm(vol/vol) and ppm(mass/mass)) if there would be no additional  $\text{CO}_2$  sink compared to what has been already listed i.e. absorption by oceans. [25%]

**a) The total  $\text{CO}_2$  amount in atmosphere (expressed in Gt = gigatonnes) corresponding to the 425 ppm(vol/vol) concentration. [25%]**

We are given 425 ppm (vol/vol) CO<sub>2</sub> concentration in the atmosphere, and a volume of around  $4 \cdot 10^{18} \text{ m}^3$  of air in the atmosphere. We can take the product of these values to obtain the total volume of CO<sub>2</sub>.

By using these values, we are assuming a constant distribution of CO<sub>2</sub> in the atmosphere, and that the entire atmosphere is at STP, i.e., 298K (~25C) and 1atm.

```
In [43]: co2_volume_concentration = 425e-6 # m^3 CO2 / m^3 air
atmosphere_volume = 4e18 # m^3 air @ STP

co2_volume_in_atmosphere = co2_volume_concentration * atmosphere_volume # m^3 CO2 @
print(f"At STP, there are around {format(co2_volume_in_atmosphere, ".2e")} m^3 of C
```

At STP, there are around  $1.70\text{e}+15 \text{ m}^3$  of CO<sub>2</sub> in the atmosphere

Next, we determine the total mass of atmospheric CO<sub>2</sub>.

To do this, we can apply the ideal gas law:

$$PV = nRT$$

This allows us to determine the number of moles of CO<sub>2</sub>, and we can then use its molar mass to determine the mass of CO<sub>2</sub>.

```
In [44]: # STP conditions
P = 1 # 1 atm (STP pressure)
V = co2_volume_in_atmosphere * 1000 # L CO2 @ STP
# Source: https://en.wikipedia.org/wiki/Gas_constant
R = 0.082057366080960 # Ideal gas constant, L*atm / (mol*K)
T = 293 # STP temperature in Kelvin

n = P * V / (R * T) # moles @ STP

co2_moles_in_atmosphere = n # moles @ STP

print(f"At STP, there are around {format(co2_moles_in_atmosphere, ".2e")} moles of
```

At STP, there are around  $7.07\text{e}+16$  moles of CO<sub>2</sub> in the atmosphere

Finally, we use the tabulated molar masses of Carbon and Oxygen and calculate CO<sub>2</sub>'s molar mass, then multiply by the number of moles to get the total mass of CO<sub>2</sub> in the atmosphere.

Standard molar masses are obtained using an abundance-weighted average of different isotopes, so actual mass of CO<sub>2</sub> can vary slightly. We assume this to be negligible.

```
In [45]: # Source: https://iupac.qmul.ac.uk/AtWt/
carbon_molar_mass = 12.011 # g/mol
oxygen_molar_mass = 15.999 # g/mol

co2_molar_mass = carbon_molar_mass + 2 * oxygen_molar_mass # g/mol

print(f"CO2 has a molar mass of {co2_molar_mass} g/mol")
```

CO<sub>2</sub> has a molar mass of 44.009 g/mol

```
In [46]: co2_atmospheric_mass = co2_moles_in_atmosphere * co2_molar_mass # g CO2 @ STP

co2_atmospheric_mass_kg = co2_atmospheric_mass / 1000 # kg CO2 @ STP
co2_atmospheric_mass_gigatonnes = co2_atmospheric_mass_kg / 1000 / 1e9 # Gt CO2 @ STP

print(f"There is approximately {format(co2_atmospheric_mass_kg, ".2e")} kg "
      f"or {co2_atmospheric_mass_gigatonnes:.0f} Gt of CO2 in the atmosphere at STP")
```

There is approximately 3.11e+15 kg or 3112 Gt of CO<sub>2</sub> in the atmosphere at STP

Given our assumptions and that the atmosphere of the air was only specified to one significant figure, we can say that there are around 3000 Gt of CO<sub>2</sub> in the earth's atmosphere.

**b) How much CO<sub>2</sub> must be removed per year (by both natural and technological means) to limit the atmospheric CO<sub>2</sub> concentration at 435 ppm(vol/vol) in 2050. Comment briefly on the feasibility of achieving this target. What natural and technological options could be utilized? [25%]**

I will approach this problem from a mass conservation perspective.

By using the figures provided in this question, we are making a lot of assumptions about the system: we assume emissions and absorption are constant year over year and independent of concentration.

If we are targeting a concentration of 435ppm of CO<sub>2</sub> by 2050, this gives us a "budget" of 10ppm that can be added to the atmosphere in the next 50 years, or 0.2ppm/year.

Rerunning the calculations for part a), we can convert this into an acceptable net change in atmospheric CO<sub>2</sub> mass in Gt/year.

Again, we assume STP everywhere and even distribution of CO<sub>2</sub>.

```
In [47]: co2_ppm_per_year = 0.2
co2_fraction_per_year = co2_ppm_per_year * 1e-6 # m^3 CO2 / m^3 air
co2_volume_per_year = co2_fraction_per_year * atmosphere_volume # m^3/y CO2
co2_moles_per_year = P * co2_volume_per_year / (R * T) # moles/y
co2_mass_per_year_g = co2_moles_per_year * co2_molar_mass # g/y
co2_budget_per_year_gigatonnes = co2_mass_per_year_g / 1000 / 1000 / 1e9 # Gt/y

print(f"CO2 net \"budget\": {co2_budget_per_year_gigatonnes:.5f} Gt/year net allowable")
```

CO<sub>2</sub> net "budget": 0.00146 Gt/year net allowable to reach 435ppm by 2050

The above calculation reveals why net-zero is so important. Even if we allow a slight increase in CO<sub>2</sub>, the current rates of emission greatly exceed the rates which would cause a slow but acceptable increase in CO<sub>2</sub> atmospheric concentration.

Nevertheless, we can use this value in the calculation for the additional CO<sub>2</sub> removal required to reach 435 ppm by 2050.

This [NASA visualization](#) helped me understand the real-life dynamics of the atmosphere's CO2 balance.

```
In [48]: fossil_fuel_emissions = 37 # Gt/y CO2 added
deforestation_emissions = 2.7 # Gt/y CO2 added
ocean_absorbtion = 9 # Gt/y CO2 removed
co2_budget = co2_budget_per_year_gigatonnes # Gt/y, can be subtracted as we are "at budget"
# The co2 budget turns out to be negligible in this calculation

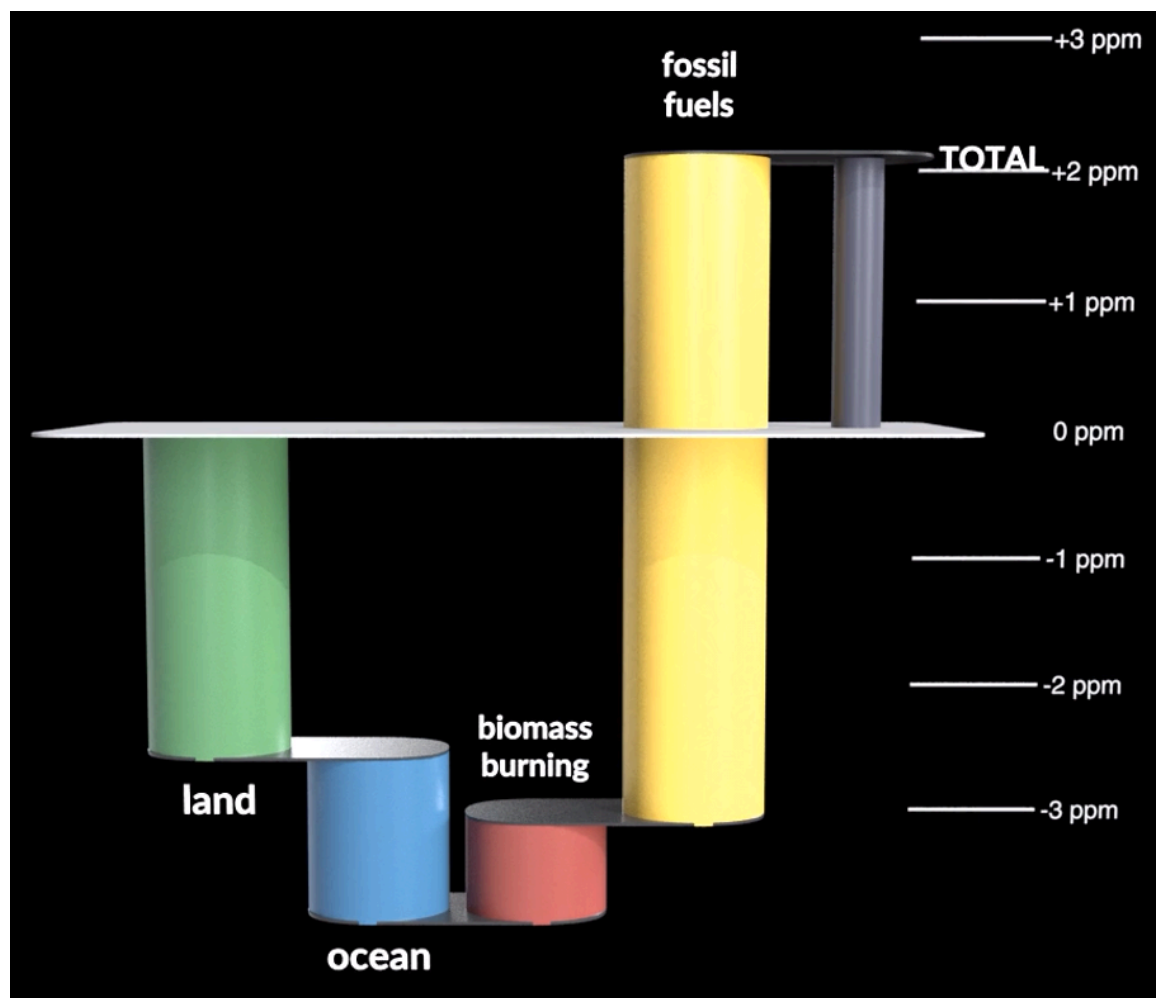
co2_removal_required = fossil_fuel_emissions + deforestation_emissions - ocean_absorbtion

print(f"{co2_removal_required:.2f} gigatonnes per year of CO2 must be removed to reach 435 ppm by 2050.")
```

30.70 gigatonnes per year of CO2 must be removed to reach a concentration of 435 ppm by 2050.

As shown above, the earth needs to absorb 30.7 Gt/year of CO2 if we want to reach 435 ppm CO2 by 2050.

In the Nasa visualization linked above, I found this graphic showing carbon sinks and sources in 2021 that helped me understand the atmosphere's CO2 balance.



Clearly, the largest carbon sink that we have today that is making it so that we do not have a *net* 40 Gt/y increase in CO<sub>2</sub> is the category marked as "land". This includes peatlands, forests, and all the biomass which absorbs CO<sub>2</sub> via photosynthesis. I'm not sure if polar ice would be considered under the ocean or land category.

The action that could be taken by humans to keep CO<sub>2</sub> emissions balanced with absorption are threefold:

1. Protect CO<sub>2</sub>-absorbing biological systems and replant / restore damaged ecosystems
2. Reduce fossil fuel emissions by improving efficiency of systems, using renewable energies and limiting consumption
3. Remove CO<sub>2</sub> from the air via carbon capture, either at point-source emissions or using Direct Air Capture

I feel strongly that these options are not of equal importance. While a combination of all these techniques will be necessary, some will be much more effective than others: It is much easier to reduce CO<sub>2</sub> emissions than to remove CO<sub>2</sub> after it has been emitted. Ceasing the most environmentally damaging human practices as soon as possible should be our top priority for climate action.

Reaching this climate goal is technologically feasible. However, doing so would likely require significant economic and societal changes - a global perspective shift around consumption and costs of CO<sub>2</sub> emission. Societally and politically, reaching such a climate goal extremely difficult. The negative externality caused by CO<sub>2</sub> emission is borne by everyone in the world, whereas only a single party benefits from the use of a fossil fuel. Presently, individuals and companies are not subject to economic conditions which incentivize them to limit their CO<sub>2</sub> emissions to what is strictly necessary, and changing this fact will be extremely difficult on a global scale.

### c) Convert 435 ppm(vol/vol) to ppm(mass/mass). [25%]

In order to answer this question we need to know the volume densities of both CO<sub>2</sub> and air.

```
In [49]: co2_ppm_vol = 435
co2_frac_vol = co2_ppm_vol * 1e-6 # L CO2 / L AIR

# Ideal gas Law: n/V = P/(RT) @ STP
gas_moles_per_liter = P / (R * T) # mol / L

co2_mass_per_liter = gas_moles_per_liter * co2_molar_mass # g / L
# Source: https://www.engineeringtoolbox.com/air-density-specific-weight-d_600.html
air_mass_per_liter = 1.204 # g / L

print(f"CO2 density @ STP: {co2_mass_per_liter:.2f} g/L")
print(f"Air density @ STP: {air_mass_per_liter:.2f} g/L")
```

CO<sub>2</sub> density @ STP: 1.83 g/L

Air density @ STP: 1.20 g/L

We get our converted mass-ppm value with some unit conversion magic. While the volumetric ppm is technically dimensionless, we can think of it as L CO<sub>2</sub> / L AIR. We then multiply by CO<sub>2</sub> density, which has units of g CO<sub>2</sub> / L CO<sub>2</sub>, and divide by air density which has units of g AIR / L air.

After we cancel out the units, we get:

$$\frac{\text{L CO}_2}{\text{L air}} \frac{\text{g CO}_2}{\text{L CO}_2} \left( \frac{\text{g air}}{\text{L air}} \right)^{-1} = \frac{\text{g CO}_2}{\text{g air}}$$

```
In [50]: co2_frac_mass = co2_frac_vol * co2_mass_per_liter / air_mass_per_liter
co2_ppm_mass = co2_frac_mass * 1e6

print(f"{co2_ppm_vol} ppm (vol/vol) of CO2 in air at STP is equivalent to {co2_ppm_
435 ppm (vol/vol) of CO2 in air at STP is equivalent to 661.3 ppm (mass/mass)
```

**d) What would be the hypothetical CO<sub>2</sub> concentration in the atmosphere in 2050 (expressed in both ppm(vol/vol) and ppm(mass/mass)) if there would be no additional CO<sub>2</sub> sink compared to what has been already listed i.e. absorption by oceans. [25%]**

To compute the added mass of CO<sub>2</sub>, we simply compute the estimated yearly net increase in CO<sub>2</sub> mass per year and multiply by the time until 2050.

```
In [51]: net_co2_mass_annual = fossil_fuel_emissions + deforestation_emissions - ocean_absor
this_year = 2025 # years
years_until_2050 = 2050 - this_year # years

est_added_co2_mass = net_co2_mass_annual * years_until_2050 # Gt CO2

print(f"By 2050, if there is no additional CO2 sink than the ocean (the only sink l
```

By 2050, if there is no additional CO<sub>2</sub> sink than the ocean (the only sink listed), we would add 768 Gt CO<sub>2</sub> to the atmosphere.

Next, we convert the mass to a ppm (vol/vol) value.

```
In [52]: grams_per_gigatonne = 1e15
est_added_co2_moles = (est_added_co2_mass * grams_per_gigatonne) / co2_molar_mass #
est_added_co2_volume = est_added_co2_moles * R * T / P # L

l_per_m3 = 1000
est_added_co2_frac = (est_added_co2_volume / l_per_m3) / atmosphere_volume # (vol/v
est_added_co2_ppm = est_added_co2_frac * 1e6 # ppm (vol/vol)
est_2050_co2_ppm_vol = 425 + est_added_co2_ppm # ppm (vol/vol)

print(f"{est_added_co2_mass:.0f} Gt over {years_until_2050} years results in an add
print(f"CO2 ppm (vol/vol) by 2050, assuming the ocean is the only sink: {est_2050_c
```

768 Gt over 25 years results in an added 104.8 ppm (vol/vol) to the atmosphere's CO<sub>2</sub> concentration

CO<sub>2</sub> ppm (vol/vol) by 2050, assuming the ocean is the only sink: 529.8

Finally, we multiply by the same terms as in part c) to convert to a (mass/mass) ppm. This time I leave the value as a ppm instead of converting it to a fraction because it cancels out when we convert back to a ppm later.

```
In [53]: est_2050_co2_ppm_mass = est_2050_co2_ppm_vol * co2_mass_per_liter / air_mass_per_li
print(f"CO2 ppm (mass/mass) by 2050, assuming the ocean is the only sink: {est_2050
CO2 ppm (mass/mass) by 2050, assuming the ocean is the only sink: 805.5
```