ATM 505 Problem Set for Atmospheric Chemistry Module

Feb. 20, 2023

Due Feb. 27, 2022

100 points

**Basic information of concentration**

**1.** (10 points total, 5 for each of part) **Concentration air mass concentration**

The ideal gas law can be written as

pV = NRT (1)

with p = pressure in atmospheres (atm)

V = volume in liters (L)

N = number of moles (mole or mol)

T = temperature in degrees K (°K)

R = Gas Constant = 0.08206 L atm mol-1 °K-1 (when using these units)

The number density (or concentration) of air (in molecules cm-3 or molecular cm-3) is

na = (AV×N)/V × (1 L/1000 cm3) = (AV×N)/1000V (2)

where Av is Avogadro’s number = 6.023x1023 molecular mol-1.

Solving each of the above relations for N/V and combining yields

N/V = p/(R×T) (3)

N/V = 1000na/Av  (4)

na = (Av×p)/(1000×R×T) (5)

Use the above relations to calculate the following.

a) Calculate na for surface conditions of p = 1 atm and T = 298 °K.

b) Calculate na for conditions representative of an altitude of 25 km in the middle stratosphere, p = 0.025 atm and T = 220 °K.

**2.** (10 points total, 5 for each of part) **Concentrations vs. Mixing Ratios**

Based on the conversion equation given in Page 8 Lecture 1, as shown below:

Mixing ratio of i in ppm Concentration of i in μg m-3

where T is the temperature with unite in K, ρ is the pressure in P, Mi is the molecular weight of the species. (Note: only put the number into this equation for calculating).

Use the above question to make the below conversion:

a) The Chinese national ozone air quality standard is a daily maximum 8-hour average greater than 160 μg m-3. Calculate the Chinese ozone standard in **ppb** for surface conditions of ρ = 1 atm and T = 298 °K. (1 atm =101325 Pa, Mo3=48 µg mol-1, 1 ppm=1000 ppb).

b) The highest ozone concentration can be over 130 ppb in the south shore Long Island for summer surface conditions of ρ = 1 atm and T= 303°K. Converse to a concentration of μg m-3.

**Stratospheric Chemistry**

**3.** (10 points) The set of Chapman mechanisms does not give a good representation of the magnitude of the ozone burden and concentrations in the stratosphere. (1) Are the predicted concentrations too high or too low (compared to observations)? (2) What is needed to improve the agreement between predictions and observations?

**Tropospheric Gas Phase Chemistry**

**4.** The trace gas (i.e., NO2, HCHO) column concentrations measured by the satellite (i.e., OMI) have been currently used to estimate the pollution regime. Use the data obtained from **Giovanni**: <https://giovanni.gsfc.nasa.gov/giovanni/> to finish the following questions (55 points):

(1) List the location of your hometown. Set a square region with a range of 1°C covering your hometown, which will be used in Giovanni. (example: my hometown. Qingzhou, China. [118 36 119 37]) (5 points)

(2) Calculate the summer averaged value for NO2 from OMI of each year- 2005, 2010, 2015, and 2019. Description of its variation trends. (10 points, summer: June, July and Aug)

(3) Calculate the summer averaged value for HCHO from OMI of each year- 2005, 2010, 2015, and 2019. Description of its variation trends. (10 points)

(4) Calculate the summer value of HCHOaveraged /NO2averaged of each year- 2005, 2010, 2015, and 2019. What was the Ozone production regime (NOx-limited or VOC limited) for each year? What was its variation trend? (Using a value of 3.5 as a dividing point, a value over 3.5 belongs to NOx-limited, and a value below 3.5 belong to VOC-limited). (20 points)

(5) If the NO2 emission is keeping drop for your hometown, explain the possible variation trend of the ozone concentration. (10 points).

**Aqueous Atmospheric Chemistry**

5. (15 points, 5 points for each) Nitrous acid (HONO or HNO2) is a weak acid like H2CO3 or H2SO3. The equations that govern its dissolution and dissociation are

HONO(g) ⇄ HONO(aq) HHONO(298K) = 49 M atm-1 ∆H = -9.5 kcal/mole

HONO(aq) ⇄ H+ + NO2- Ka(298K) = 5.1x10-4 M ∆H = 2.5 kcal/mole

1. Write an expression for the effective Henry’s Law for [N(III)] – the sum of [HONO(aq)] and [NO2-]. (That is, [N(III)] = [HONO(aq)] + [NO2-]. Your answer will be a function of [H+].)
2. Compute the value for this effective Henry’s Law coefficient at pH = 5 and T = 298 K.
3. If [NO2-] = 1x10-7 M, pH = 4, and T = 298 K, what is pHONO? (That is, find the gas phase partial pressure of HONO.)