Lab Report on Smog Modeling

A report submitted in partial fulfillment of requirements for the degree of BE in Chemical Science and Engineering

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1 Introduction

Air pollution is broadly described as a condition that causes human discomfort, sickness, or death, as well as harm to other creatures or the environment, due to the release of specific substances into the atmosphere. It has long been assumed that highly industrialized and/or urbanized towns with topography such as basins and mountains frequently suffer from significant air pollution. Several studies have been conducted on air quality modeling of basins and mountains in different regions of Europe and China to monitor the pollution. Among various approaches, the mole balance as a CSTR approach has been found to be one of the best in some literatures. This study models CO emission in the Los Angeles Basin due to the high number of automobiles and the effect of wind passing through it. The LA Basin, surrounded by high mountains, makes it relatively difficult for the polluted air to pass out of the basin.

This report summarizes the works and objectives based on an unsteady mole balance on the accumulation and depletion of smog in the LA Basin with the CSTR approach adapted from the University of Michigan. The Santa Ana wind is considered as the method of depletion; these are high-velocity winds originating in the Mojave Desert just northeast of Los Angeles. The problem description is explained in the problem statement section of this report.

2 Problem Statement

Adapted from the University of Michigan, the problem is stated as follows:

The Los Angeles basin floor covers approximately 700 square miles (2×10^{10} ft^2) and is almost completely surrounded by mountain ranges. Assuming an inversion height of 2000 feet, the corresponding volume of air in the basin is 4×10^{13} ft^3. Using this system volume, we can model the accumulation and depletion of air pollutants. As a rough first approximation, we treat the Los Angeles basin as a well-mixed container (similar to a CSTR) with no spatial variations in pollutant concentrations. We will simplify the system by considering only carbon monoxide (CO) as the pollutant, assuming its only source is automobile exhaust. On average, we suppose that there are 400,000 cars operating in the basin at any time, each giving off approximately 3000 standard cubic feet of exhaust per hour containing 2% mol carbon monoxide.

We shall perform an unsteady-state mole balance on CO as it is depleted from the basin area by the Santa Ana wind. These winds, originating in the Mojave Desert, flow into the basin through a corridor assumed to be 20 miles wide and 2000 feet high (inversion height), replacing the polluted air that flows out to sea or toward the south. The concentration of CO in the Santa Ana wind entering the basin is 0.08 ppm (2.04×10^{-10} lb mol/ft^3).

The objectives of the study are to calculate:

1. The pound moles of gas in the system for the Los Angeles basin at a temperature of 75°F and a pressure of 1 atm.
2. The rate of smog emitted from all the autos in the basin.
3. The volumetric flow rate of the wind in cubic feet per hour.
4. The molar flow rate of CO being carried by the wind.
5. The equation for unsteady mass balance for the overall system considering the volumetric flow rate throughout the system to be identical, i.e., $v = v_0$.
6. The equation for unsteady mass balance in terms of time.
7. Some cases as explained in further sections.

The initial values of all the parameters for this problem are written with Python code in the Appendix section. Calculations are based on the initial conditions and formulas explained in the methodology section.

3 Methodology

1. The pound moles of CO in the system were calculated by first calculating the volume of the LA Basin, then using the ideal gas constant for 1 lb mol of gas. The value of the gas constant was calculated in $ft^3 \cdot$ atm/lb mol $\cdot$ R. Finally, the number of moles of CO in the basin was calculated.

2. The rate of CO emitted by autos was calculated by first determining the moles of exhaust from the volume of exhaust for all the cars, and then taking the moles of CO to be 2% of the total moles of exhaust.

3. The volumetric flow rate of the wind was provided as the velocity of the wind in ft per hour. The velocity of the wind was multiplied by the cross-sectional area of the wind passing in the basin, and then unit balance was done to get the final flow rate.

4. The equation for unsteady mole balance for the volumetric flow rates entering and leaving the system was derived. The forms of the equations are shown in Equations (1) and (2).

$$F_{\text{in}} - F_{\text{out}} + F_{\text{generation}} = F_{\text{accumulation}} \tag{1}$$

$$F_{\text{CO,S}} - V_0 \cdot C_{\text{CO,out}} + F_{\text{CO,A}} = \frac{dC_{\text{CO}}}{dt} \tag{2}$$

where $F_{\text{CO,S}}$ and $F_{\text{CO,A}}$ represent the flow rate of CO from the wind and from the exhaust of autos respectively.

The equation for time can be derived as:

$$t = \frac{V}{v_0} \ln\left(\frac{(F_{\text{CO,A}} + F_{\text{CO,S}}) - v_0 C_{\text{CO,O}}}{(F_{\text{CO,A}} + F_{\text{CO,S}}) - v_0 C_{\text{CO,f}}}\right) \tag{3}$$

where t represents time, V and v_0 represent volume of the system and volumetric flow rate respectively, and C_{CO} represents the concentration of CO gas with indices o and f meaning initial and final respectively.

5. The time required for the CO level to reach 2 ppm was calculated using the equation for time. The volumetric flow rate at that time was also measured.

6. The concentration with respect to time was plotted to check the influence of time on concentration.

7. Traffic was assumed to be heavier in the mornings and evenings as workers commute to and from downtown LA. The flow of CO into the LA basin was represented by a sine function over a 24-hour period. The equation for the exhaust is given in Equation (4).

$$F_{\text{CO,A}} = a + b \sin\left(\frac{\pi t}{6}\right) \tag{4}$$

where the values of a and b were given as 35000 lb mol/hr and 30000 lb mol/hr respectively.

8. The concentration was then plotted to see the effect of increasing traffic. The numpy sine function was used for the solution. All parameters were kept the same as in initial conditions except for the equation for the exhaust.

3.1 Challenge Problem

9. At the given conditions and equations, the problem was solved in a similar manner, and the concentration of CO in lb mol/m^3 was plotted with respect to time to see the dynamics in different basins.

4 Results and Discussion

The concentration of carbon monoxide decreases exponentially with time. The concentration reaches a steady state at about 10 hours at a value of 0.5 ppm.

4.1 Pound Moles of Air and Carbon Monoxide

Using the ideal gas law:

$$PV = nRT$$

$$1 \cdot 2000 \cdot 1.952 \times 10^{10} = n \cdot 0.7299 \cdot 534.67$$

The number of moles of air in the system (n) = 102426499085.8884 lb mol.

4.2 Molar Flow Rate of Carbon Monoxide Emitted by Cars into the Basin ($F_{\mathbf{CO,auto}}$)

Using the ideal gas law for autos as well, taking basis as 1 hour:

$$PV = nRT$$

$$1 \cdot 1.2 \times 10^{9} = n \cdot 0.7299 \cdot 534.67$$

Number of moles of gas emitted by autos (n) = 3.343×10^4 lb mol/hour. Thus, the rate of emission of carbon monoxide by autos ($F_{\text{CO,auto}}$) is:

$$F_{\text{CO,auto}} = 2\% \text{ of } n = 66827.0451 \text{ lb mol/hour}$$

4.3 Volumetric Flow Rate of Wind

$$v_0 = \text{velocity of wind} \times \text{cross-sectional area of wind passing in the basin}$$

Given the velocity of the wind is 10 mph (52800 ft/hr), and the cross-sectional area is 20 miles wide by 2000 feet high:

$$v_0 = 52800\,\text{ft/hr} \times 20 \times 5280\,\text{ft} \times 2000\,\text{ft}$$

$$v_0 = 1.11776 \times 10^{13}\,\text{ft}^3/\text{hr}$$

4.4 Unsteady State Mole Balance of the Basin by Considering it a CSTR

$$F_{\text{in}} - F_{\text{out}} + F_{\text{generation}} = F_{\text{accumulation}}$$

$$F_{\text{CO,S}} - v_0 \cdot C_{\text{CO}} + F_{\text{CO,A}} = V \cdot \frac{dC_{\text{CO}}}{dt}$$

$$F_{\text{CO,A}} + F_{\text{CO,S}} - v_0 \cdot C_{\text{CO}} = V \cdot \frac{dC_{\text{CO}}}{dt}$$

4.5 Solution of Unsteady State Mole Balance

$$F_{\text{CO,A}} + F_{\text{CO,S}} - v_0 \cdot C_{\text{CO}} = V \cdot \frac{dC_{\text{CO}}}{dt}$$

$$dt = \frac{V}{v_0} \cdot \frac{dC_{\text{CO}}}{F_{\text{CO,A}} + F_{\text{CO,S}} - v_0 \cdot C_{\text{CO}}}$$

Integrating from $t = 0$ to t and $C_{\text{CO}} = C_{\text{CO,O}}$ to $C_{\text{CO,f}}$:

$$\int_0^t dt = \frac{V}{v_0} \int_{C_{\text{CO,O}}}^{C_{\text{CO,f}}} \frac{dC_{\text{CO}}}{F_{\text{CO,A}} + F_{\text{CO,S}} - v_0 \cdot C_{\text{CO}}}$$

$$t = \frac{V}{v_0} \ln\left(\frac{F_{\text{CO,A}} + F_{\text{CO,S}} - v_0 \cdot C_{\text{CO,O}}}{F_{\text{CO,A}} + F_{\text{CO,S}} - v_0 \cdot C_{\text{CO,f}}}\right)$$

4.6 Time Taken for the Concentration to Reach 2 ppm from 8 ppm

Using the equation for time:

$$t = \frac{V}{v_0} \ln\left(\frac{F_{\text{CO,A}} + F_{\text{CO,S}} - v_0 \cdot C_{\text{CO,O}}}{F_{\text{CO,A}} + F_{\text{CO,S}} - v_0 \cdot C_{\text{CO,f}}}\right)$$

Substituting the values gives $t = 6.86$ hours.

The sinusoidal variation in traffic yields:

$$F_{\text{CO,A}} = 35000 + 30000 \sin\left(\frac{\pi t}{6}\right)$$

The concentration can be seen increasing and decreasing over the first 24 hours, increasing when traffic is heavy and decreasing in between.

5 Challenge Problem

Problem Statement: The South Coast Air Basin (SoCAB) includes the non-desert regions of four counties: Los Angeles, Orange, Riverside, and San Bernardino. The total area in the SoCAB amounts to 13,350 mi^2, with one half pertaining to L.A. and the other half to the remaining three counties. Riverside includes 60% of this half, while Orange and San Bernardino account for 20% each. Los Angeles, Orange, and Riverside line up along the Pacific Coast, forming three individual systems (CSTRs) in a sequential series once the Santa Ana wind blows from the northwest to the southeastern part of the Coast.

The total population in the South Coast Air Basin amounts to 15 million residents, who own 12 million vehicles. Out of this total, 90% commute to work, averaging 10.8 million cars daily. Assuming that L.A. holds 55% of those vehicles, Orange 25%, and Riverside 20%, and that the carbon monoxide emitted per vehicle in these areas was found to be 2.5 ppm, 1.8 ppm, and 2.2 ppm respectively, we modeled the CSTR system over 72 hours to analyze CO accumulation.

6 Conclusion

The problem was successfully simulated using the CSTR approach along with the CSTR problem. The conclusions in bullet points are:

1. All the values from the given parameters were calculated theoretically and using Python.
2. The models were successfully simulated using the CSTR approach.

3. The concentration of carbon monoxide was found to be decreasing exponentially with time. The concentration reaches steady state at about 10 hours at a value of 0.5 ppm.
4. The concentration was found fluctuating for the varying traffic with sinusoidal variation with respect to time.
5. In the case of the challenging problem, the concentration of all three sub-systems was found to be decreasing with respect to time.

Both the systems were successfully simulated using the CSTR approach. The CSTR approach could be promising in air quality modeling if all the parameters are properly considered.

Appendix 1 LA Basin Modelling

In [2]:
```
from scipy.integrate import odeint
import matplotlib.pyplot as plt
import numpy as np
```

Initial Conditions

In [3]:
```
Auto = 400000        #number of automobiles
Exhaust = 3000       #ft cube per hr per auto
C_CO=2               #mol%
T=75+460             #degree R
P = 1                #atm
Area = 2e10          #sq ft
Height = 2000        #ft
```

In [4]:
```
#Exhaust = 35000+30000*np.sin(np.pi*t/6)
```

Basin

Volume of Basin

In [5]:
```
volume = Area*Height #ft cube
volume
```

Out[5]:
```
40000000000000.0
```

Number of moles of CO in basin

In [6]:
```
n = P*volume/(0.7302*T)         #gas constant, R=0.7302 ft^3.atm/(lb mol. R)
n                               #lb mol
```

Out[6]:
```
102391612079.13849
```

Exhaust

Molar flowrate from exhaust

In [7]:
```
n_exhaust = P*Exhaust/(T*0.7302)
n_exhaust                      #lb mol
```

Out[7]:
```
7.679370905935386
```

Number of moles of CO in exhaust

In [8]:
```
n_CO = 0.02*n_exhaust    #lb moles of CO in exhaust
n_CO
```

Out[8]:
```
0.1535874181187077
```

Previously the mole CO was for one auto, now for all the 400000 auto

In [9]:
```
F_CO_auto = n_CO*Auto      #in lb moles per hr
F_CO_auto
```

Out[9]:
```
61434.96724748309
```

Out[9]:

Wind Blows

Velocity and volumetric flowrate of wind entring

In [10]:
```
v_wind = 15*5280                          #velocity of wind, ft/hr (as given in solution)
F_wind = 20*5280*v_wind*2000
F_wind                                    #volumetric flowrate, ft^3/hr
```

Out[10]:
```
16727040000000
```

Molar conentration of CO in entring wind

In [11]:
```
F_CO_wind = F_wind*2.04e-10       #in lb mol per hr
F_CO_wind
```

Out[11]:
```
3412.31616
```

Total CO Emission

Moles of CO in total

In [12]:
```
F_CO_total = F_CO_auto+F_CO_wind      #in lb mol per hr
F_CO_total
```

Out[12]:
```
64847.28340748309
```

Volume of CO in the basin after wind enters

In [13]:
```
Volume_CO = F_CO_total*0.7302*T/P      #volume of CO coming out in ft cube per
Volume_CO
```

Out[13]:
```
25333045.194117118
```

Mole Balance

$$F_{in} - F_{out} + F_{generation} = F_{accumulation}$$

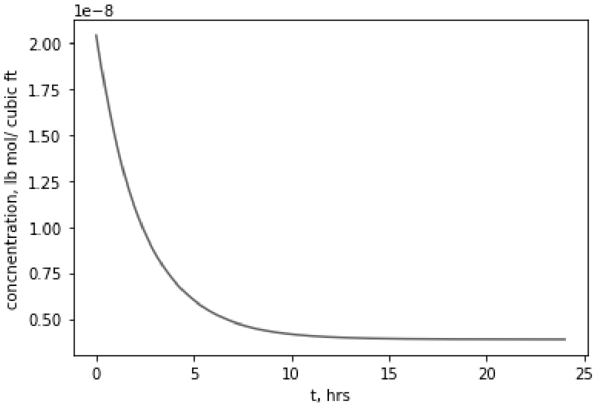
$$F_{CO,wind} - V_0 * C_{CO,out} + F_{CO,autos} = \frac{dC_{CO}}{dt}$$

at given conditions

In [21]:
```
v0=1.67e13    #total volumetric flowrate (sum of volumetric flowrate of car and wind)
V=4e13       #volume of system
def dCOdt(x,t):
    return np.array([(F_CO_wind+F_CO_auto-(v0*x[0]))/V])
t = np.linspace(0,24,200)
C_CO = 2.04e-8
C_CO,infodict = odeint(dCOdt,C_CO,t,full_output=True)
print(infodict['message'])
plt.xlabel('t, hrs')
plt.ylabel('concnentration, lb mol/ cubic ft')
```

```
plt.plot(t, C_CO)
plt.show()
```

```
Integration successful.
```

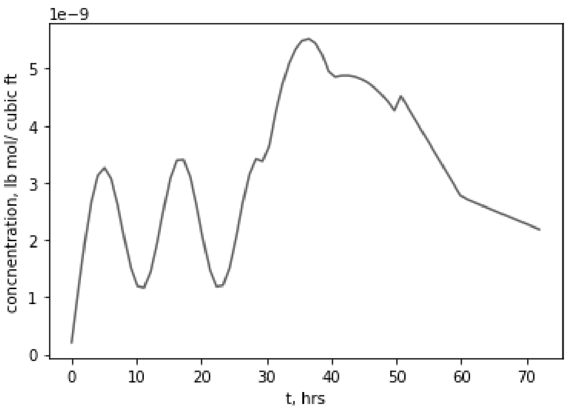


when the traffic is considered varying with sine fuction with respect to time

In [38]:

```
vo = 16728240000000                    #total volumetric flowrate (sum of volumetric flowrate of car and wind)
V = 4e13                               #volume of system
def dCo_dt(x,t):
    a=35000
    b=30000
    return np.array([(a+(b*np.sin((np.pi*t)/6))+F_CO_wind-(vo*x[0]))/V])
t=np.linspace(0,72,72)
C_CO=np.array([2.04e-10])
Co, infodict=odeint(dCo_dt,C_CO,t,full_output=True)
print(infodict['message'])
plt.xlabel('t, hrs')
plt.ylabel('concnentration, lb mol/ cubic ft')
plt.plot(t,Co)
plt.show()
```

```
Integration successful.
```



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Appendix 2 Challenging Problem Modelling

In [2]:

```
import sympy as sp
import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import odeint
from scipy import *
```

In [3]:

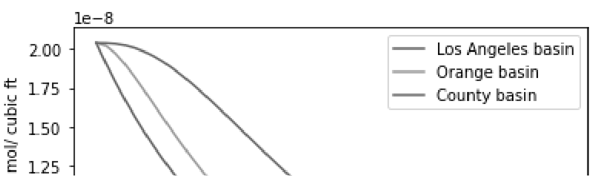
```
def challenge(z,t):
      A =  372176640000  #Total area of South CA Basin (ft2)
      Cars = 10.8E6 #Total number of vehicles in SoCAB
      A1 =  A*.5  #Area of Los Angeles
      A2 =  A*.5*.2  #Area of Orange County
      A3 =  A*.5*.6  #Area of Riverside County
      Cars1 =  Cars*.55  #Number of cars in LA
      Cars2 =  Cars*.25  #Number of cars in Orange
      Cars3 =  Cars*.20  #Number of cars in Riverside
      H =  2000  #Height of Basin (ft)
      V1 =  A1*H  #
      V2 =  A2*H  #
      V3 =  A3*H  #
      Cars1ppm =  2.5  #
      Cars2ppm =  1.8  #
      Cars3ppm =  2.2  #
      TBasin =  534.7  #Rankine
      PBasin =  1  #atm
      R =  0.7302  #ft3*atm/lbmol*R
      vwind =  79200  #ft/h wind velocity
      corridor =  105600*2000  #ft2 wind corridor
      vemissions =  3000  #ft3/h STD vehicular emissions
      Temissions =  491.67
      n1 =  PBasin*V1/(R*TBasin)  #lbmol of air in Vx
      n2 =  PBasin*V2/(R*TBasin)  #lbmol of air in Vx
      n3 =  PBasin*V3/(R*TBasin)  #
      ncars1 =  PBasin*vemissions/(R*Temissions)*Cars1  #lbmol gas emissions from Cars-x
      ncars2 =  PBasin*vemissions/(R*Temissions)*Cars2  #
      ncars3 =  PBasin*vemissions/(R*Temissions)*Cars3  #
      COcars1 =  Cars1ppm/1000000*ncars1  #lbmol CO emissions from cars
      COcars2 =  Cars2ppm/1000000*ncars2  #
      COcars3 =  Cars3ppm/1000000*ncars3  #
      Qo =  vwind*corridor  #vo
      Q1 =  Qo+vemissions*Cars1  #
      Q2 =  Q1+vemissions*Cars2  #
      Q3 =  Q2+vemissions*Cars3  #
      COo =  .08  #ppm
      COwind0 =  2.04E-10  #lbmol CO / ft3
      COs0 =  COwind0*Qo  #lbmol CO in wind
      A=z[0]
      B=z[1]
      C=z[2]
      COs1 = A*Q1
      COs2 = B*Q2
      CO1ppm =A*1000000*V1/n1
      CO2ppm =B*1000000*V2/n2
      CO3ppm =C*1000000*V3/n3
      dCO1dt=(COcars1 + COs0 - Q1*A)/V1
      dCO2dt=(COcars2 + COs1 - Q2*B)/V2
      dCO3dt=(COcars3 + COs2 - Q3*C)/V3
      return(dCO1dt,dCO2dt,dCO3dt)
```

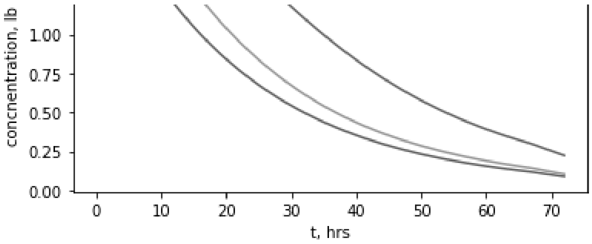
In [6]:

```
t=np.linspace(0,72,50)  #500 points between 0 and 2500
zo=[2.04E-8,2.04E-8,2.04E-8]        #Initializing values
z=odeint(challenge,zo,t)       #solving ODE
A=z[:,0]
B=z[:,1]
C=z[:,2]
plt.plot(t,A,label="Los Angeles basin")
plt.plot(t,B,label="Orange basin")
plt.plot(t,C,label="County basin")
plt.xlabel('t, hrs')
plt.ylabel('concnentration, lb mol/ cubic ft')
plt.legend()
```

Out[6]:

```
<matplotlib.legend.Legend at 0x1d40dbb37f0>
```





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