Lab Report on Gaussian Dispersion (Puff and Plume) 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

1.1 Transport Models with Reaction

Transport models with reaction incorporate chemical reactions into the dispersion model. These models account for the fact that pollutants can undergo chemical transformations in the atmosphere, which can affect their concentrations and impacts. The general equation for a transport model with reaction is:

$\frac{\partial c}{\partial t} + \nabla \cdot (uc) = \nabla \cdot (K \nabla c) + R$

where:

- c is the concentration
- t is time
- u is the wind velocity vector
- K is the eddy diffusivity tensor
- R is the reaction rate term

The reaction rate term (R) can be complex, depending on the specific chemical reactions involved. These models are more computationally intensive than simple Gaussian plume models but provide a more realistic representation of pollutant behavior in the atmosphere.

1.2 Fixed-Box Model

The Fixed-Box Model is a simplified approach for estimating average air pollutant concentrations within a city. It assumes a rectangular city geometry with one side parallel to a constant wind flow. Pollutants are considered to mix uniformly within a defined "box" height (mixing height, H). The model assumes a constant emission rate (Q or q per unit area) and a background concentration (b) of the pollutant entering the city. Under steady-state conditions, the model is represented by the equation:

$c = b + \frac{qL}{uH}$

where c is the average concentration, L is the length of the city parallel to the wind, and u is the wind speed. Despite its simplifying assumptions, the Fixed-Box Model offers a valuable initial assessment for understanding the relationship between emissions, meteorology, and resulting pollutant concentrations.

1.3 K-Theory (Gradient Transport Theory)

K-theory, also known as gradient transport theory or first-order closure, is an approximation used in turbulence modeling to describe the transport of momentum, heat, and mass in turbulent flows. It assumes that the turbulent fluxes are proportional to the gradients of the mean quantities. In the context of air pollution dispersion, K-theory is used to model the turbulent diffusion of pollutants. The flux of a pollutant is given by:

$J = -K \frac{\partial c}{\partial n}$

where:

- J is the mass flux (mass per unit area per unit time)
- K is the eddy diffusivity (turbulent diffusion coefficient)

- c is the concentration
- n is the distance in the direction of diffusion (x, y, or z)

1.4 Diffusion Model (Gaussian Plume Model)

The Gaussian dispersion model is a widely used mathematical tool for predicting the dispersion of air pollutants released from a point source, such as a smokestack or chimney. It is based on the assumption that the pollutant concentrations follow a Gaussian (normal) distribution in both the horizontal and vertical directions downwind from the source. This model is valuable for assessing the impact of air pollution on the environment and human health, as well as for designing effective emission control strategies.

1.4.1 Gaussian Plume Model Derivation

The Gaussian plume model is derived from the principle of mass conservation, applied to a control volume of air that moves along with the wind. The derivation involves several steps and assumptions:

1. **Material Balance:** The starting point is the general mass balance equation:

   $\frac{dM}{dt} = \dot{M}_{in} - \dot{M}_{out} + \dot{M}_{gen} - \dot{M}_{cons}$

   For a non-reactive pollutant in a steady-state condition, the accumulation ($\frac{dM}{dt}$) and consumption ($\dot{M}_{cons}$) terms are zero.

2. **Turbulent Diffusion:** The model assumes that the primary mechanism for pollutant dispersion is turbulent diffusion, which is approximated using Fick's law of diffusion: $J = -K\frac{\partial c}{\partial n}$

   where:

   - J is the mass flux (mass per unit area per unit time)
   - K is the eddy diffusivity (turbulent diffusion coefficient)
   - c is the concentration
   - n is the distance in the direction of diffusion (x, y, or z)

3. **Coordinate System:** A Cartesian coordinate system is used, with the x-axis aligned with the wind direction, the y-axis perpendicular to the wind direction, and the z-axis vertical.

4. **Gaussian Distribution:** The model assumes that the pollutant concentration follows a Gaussian (normal) distribution in both the y and z directions. This is based on the observation that turbulent diffusion tends to spread pollutants in a bell-shaped pattern.

5. **Gaussian puff equation:** For an instantaneous release of pollutant (a puff), the concentration at a point (x, y, z) downwind from the source is given by:

   $$c(x,y,z) = \frac{Q}{2\pi u\sigma_y\sigma_z}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \tag{1}$$

   where:

   - Q is the mass of pollutant released
   - t is the time since release
   - σ_x, σ_y, σ_z are the dispersion coefficients in the x, y, and z directions, respectively

Dispersion Coefficients: The dispersion coefficients (σ_y and σ_z) are not constant but increase with downwind distance from the source. They depend on atmospheric stability conditions, which are classified into different categories (A-F) based on factors like wind speed and solar radiation. Empirical formulas or graphs are used to estimate the values of σ_y and σ_z for different stability classes and downwind distances.

1.5 Advection-Dispersion-Reaction (ADR)

The Advection-Dispersion-Reaction (ADR) equation is a fundamental model in environmental science and engineering, used to describe the transport and fate of pollutants in air, water, or soil. It combines three key processes:

- **Advection:** The transport of pollutants due to the bulk movement of the fluid (e.g., wind or water currents).
- **Dispersion:** The spreading of pollutants due to random mixing processes, such as turbulence or molecular diffusion.
- **Reaction:** The transformation of pollutants through chemical or biological reactions.

The ADR equation is a partial differential equation that describes how the concentration of a pollutant changes over time and space due to these three processes. It is a powerful tool for understanding and predicting the behavior of pollutants in the environment, and it is used in a wide range of applications, including air quality modeling, water quality modeling, and risk assessment.

1.5.1 Mathematical Representation

The general form of the ADR equation in one dimension is:

$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}(D\frac{\partial c}{\partial x}) - v\frac{\partial c}{\partial x} - \lambda c$

where:

- c is the concentration of the pollutant
- t is time
- x is the spatial coordinate
- D is the dispersion coefficient
- v is the advection velocity
- λ is the first-order reaction rate constant

The first term on the right-hand side of the equation represents dispersion, the second term represents advection, and the third term represents reaction. The specific form of the equation can vary depending on the number of dimensions considered (1D, 2D, or 3D) and the complexity of the reaction processes involved.

1.5.2 One-, Two-, and Three-Dimensional Spreading

The ADR equation is regularly applied to pollutant spreading in one, two, or three dimensions. The resulting concentrations calculated for one-, two-, and three-dimensional spreading are:

- $c(x,t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-vt)^2}{4Dt} - \lambda t\right)$ for one dimension
- $c(x,y,t) = \frac{M}{4\pi t\sqrt{D_x D_y}} \exp\left(-\frac{1}{4t}\left(\frac{(x-vt)^2}{D_x} + \frac{y^2}{D_y}\right) - \lambda t\right)$ for two dimensions
- $c(x,y,z,t) = \frac{M}{(4\pi t)^{3/2}\sqrt{D_x D_y D_z}} \exp\left(-\frac{1}{4t}\left(\frac{(x-vt)^2}{D_x} + \frac{y^2}{D_y} + \frac{z^2}{D_z}\right) - \lambda t\right)$ for three dimensions

2 Objectives

The objectives of the modeling are as follows: - Demonstrate the Gaussian plume model's application in estimating pollutant dispersion from a point source. - Analyze factors influencing pollutant dispersion, such as wind speed and emission rate. - Introduce the mathematical representation of the ADR equation in one dimension, including the meaning of each parameter.

3 Applications

- **Environmental Impact Assessment:** Predicting the dispersion of pollutants from chemical plants and industrial processes to assess their impact on air quality and human health.
- **Risk Assessment and Emergency Response:** Estimating the spread of hazardous chemical releases to develop evacuation plans and safety measures for workers and communities.
- **Process Design and Optimization:** Incorporating the model into the design of chemical processes to minimize pollutant emissions and ensure regulatory compliance.
- **Monitoring and Validation:** Using the model in conjunction with air quality data to validate its predictions and improve its accuracy for decision-making.

4 Results and Discussion

In the following section, we present the results obtained from our simulations and discuss their significance. These findings will provide insights into the behavior of the modeled systems and inform subsequent analyses.

4.0.1 Problem:

A factory emits 20 g/s of SO2 at height H. The wind speed is 3 m/s. At a distance of 1 km downwind, the values of (σ_y) and (σ_z) are 30 m and 20 m, respectively. What are the SO2 concentrations at the centerline of the plume, and at a point 60 meters to the side of and 20 meters below the centerline?

4.0.2 Analytical Solution:

The centerline values are those for which $y = 0$ and $z = H$, so both of the terms in the exponential are zero. Since $e^0 = 1$, the exponential term is unity. At the centerline:

$c = \frac{20\,\mathrm{g/s}}{(2\pi)(3\,\mathrm{m/s})(30\,\mathrm{m})(20\,\mathrm{m})} = 0.00177\,\mathrm{g/m^3} = 1770\,\mu\mathrm{g/m^3}$

At the point away from the centerline, we must multiply the preceding expression by

$\exp\left(-\frac{1}{2}\left[\frac{60\,\mathrm{m}}{30\,\mathrm{m}}\right]^2 + \left[\frac{-20\,\mathrm{m}}{20\,\mathrm{m}}\right]^2\right) = \exp(-2.5) = 0.0818$

so

$c = (1770\,\mu\mathrm{g/m^3}) \times 0.0818 = 145\,\mu\mathrm{g/m^3}$

This model assumes that pollutants are normally distributed in both the horizontal and vertical directions, with the concentration decreasing as distance from the centerline increases.

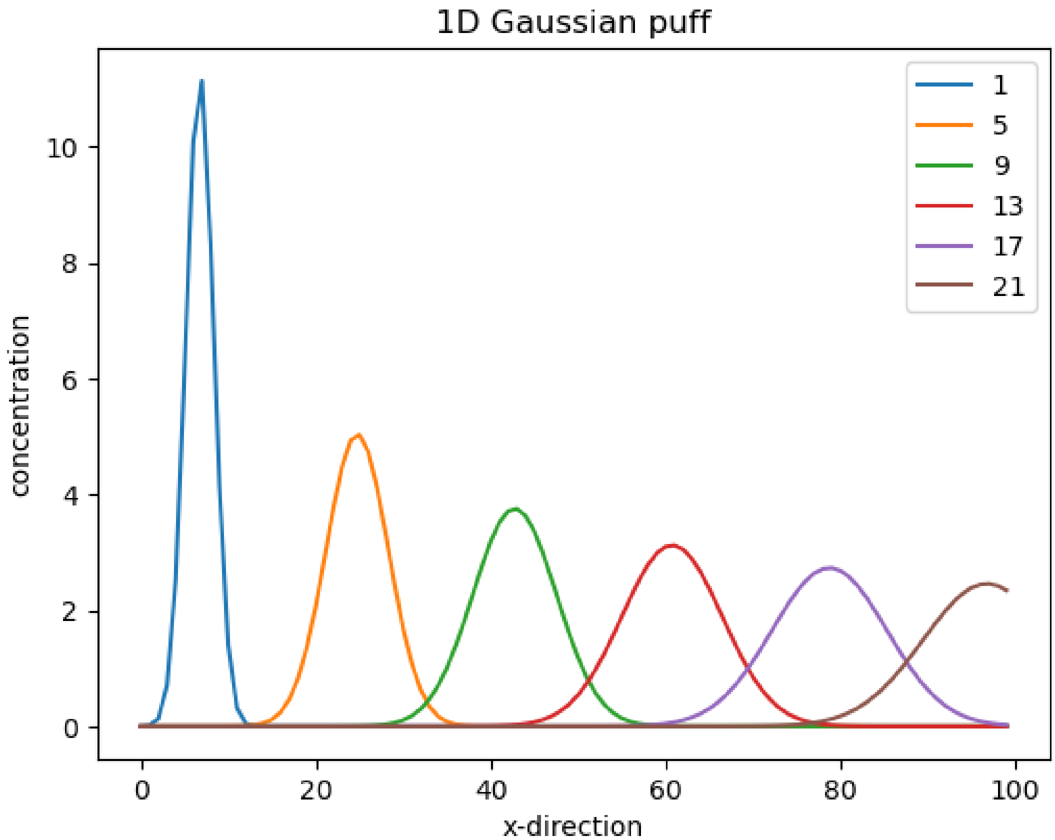
Centerline Concentration: The SO2 concentration at the centerline of the plume, 1 km downwind from the factory, is 1770 µg/m³. This is the highest concentration expected at this distance, as the plume is most concentrated along its centerline.

Off-Centerline Concentration: The concentration at a point 60 meters to the side and 20 meters below the centerline is significantly lower, at 145 µg/m³. This decrease is due to the dispersion of the pollutant in the horizontal and vertical directions.

4.0.3 Problem:

- Dx = 0.000625 # diffusivity
- v = 0.1 # velocity
- M = 1 # mass
- xmin = -0.05
- xmax = 2.15 # x-axis interval
- t = range(1,24,4) # time

[10]:
```
import numpy as np
import matplotlib.pylab as plt
Dx = 0.000625 # diffusivity
v = 0.1 # velocity
M = 1 # mass
xmin = -0.05
xmax = 2.15 # x-axis interval
t = range(1,24,4) # time
x = np.linspace(xmin,xmax,100)
ctot = []
for i in t:
 xx = x - v*i
 c = (M/np.sqrt(4*np.pi*Dx*i))*np.exp(-(xx*xx)/(4*Dx*i))
 #print(i,c)
 ctot.append(c)
 plt.plot(c,label=str(i))
plt.xlabel('x-direction')
plt.ylabel('concentration')
plt.title('1D Gaussian puff')
plt.legend()
plt.show()
```



The plot illustrates how the concentration distribution of a Gaussian puff evolves over time in one dimension. As time progresses, the puff spreads out due to diffusion, resulting in a broader distribution. The maximum concentration decreases over time due to dispersion, as the pollutant is spreading out over a larger area. The shape of the concentration profile becomes flatter and more spread out as time increases. The legend indicates the progression of time, with each curve representing the concentration profile at a specific time point.

5 Conclusion

The Gaussian plume model successfully predicted the dispersion of SO2 emissions from a factory, demonstrating its effectiveness in air quality modeling. The model's ability to estimate pollutant concentrations at various locations is crucial for environmental impact assessment and risk management. Understanding the factors influencing pollutant dispersion allows for the optimization of industrial processes and emission control strategies. By accurately predicting pollution levels, the Gaussian plume model contributes to informed decision-making in environmental protection and public health.