2.6 ATMOSPHERIC DIFFUSION THEORIES

Dispersion of Pollutants:

- Air pollution dispersion is distribution of air pollution into the atmosphere.
- Air pollution is the introduction of particulates, biological molecules, or other harmful materials into Earth's atmosphere, causing disease, death to humans, and damage to other living organisms such as food crops, or the natural or built environment.
- Air pollution may come from anthropogenic or natural sources.
- Dispersion refers to what happens to the pollution during and after its introduction; understanding this may help in identifying and controlling it.
- Air pollution dispersion has become the focus of:
    - ☐ Environmental conservationists
    - ☐ Governmental environmental protection agencies (local, state, province and national) of many countries regarding air pollution control.

Dispersion Modelling

Dispersion is the process of spreading out the emission over a large area thereby reducing the concentration of the pollutants.

- Plume dispersion is in two dimensions
    - ☐ Horizontal
    - ☐ Vertical
- It is assumed that the greatest concentration of the pollutants is on the plume centreline in the direction of the prevailing wind.
- The further the away from the centreline the lower the concentration.

Air Quality Modelling

- Predict pollutant concentrations at various locations around the source.
- Identify source contributions to air quality problems.
- Assess source impacts and design control strategies.

- Predict future pollutant concentrations from sources after implementation of new regulatory programs.
- Mathematical and numerical techniques are used in AQM to simulate the dispersion of air pollutants.

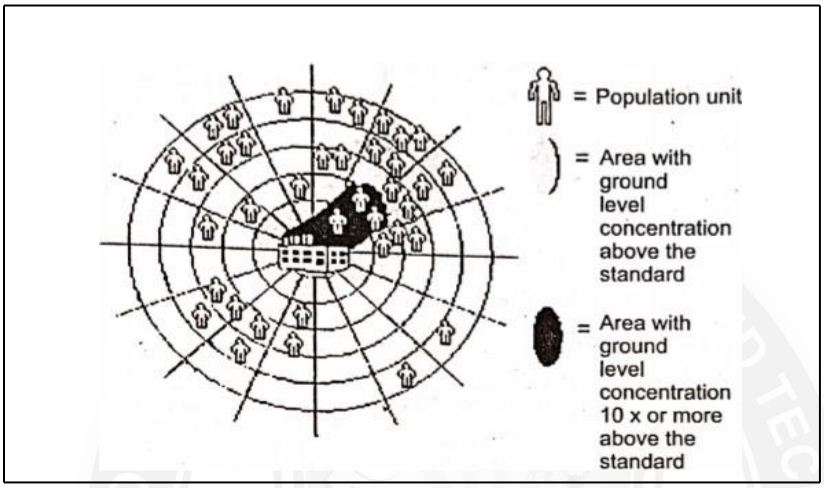

Figure 2.6.1 Areas Surrounding the Site of Release

[Source:https://slideplayer.com/slide/13655520/84/images/95/Areas+Surrounding+the+Site+of+Release.jpg]

- Modelling of the dispersion of pollutants
  - ☐ Toxic and odorous substances
  - ☐ Single or multiple points
  - ☐ Point, area, or volume sources.
- Input data required for Air Quality Modelling
  - ☐ Source characteristics
  - ☐ Meteorological conditions
  - ☐ Site and surrounding conditions.
- Types of Pollutant Sources
  - ☐ Point sources (e.g., stacks or vents)
  - ☐ Area sources (e.g., landfills, ponds, storage piles)
  - ☐ Volume sources (e.g., conveyors, structures with multiple vents)

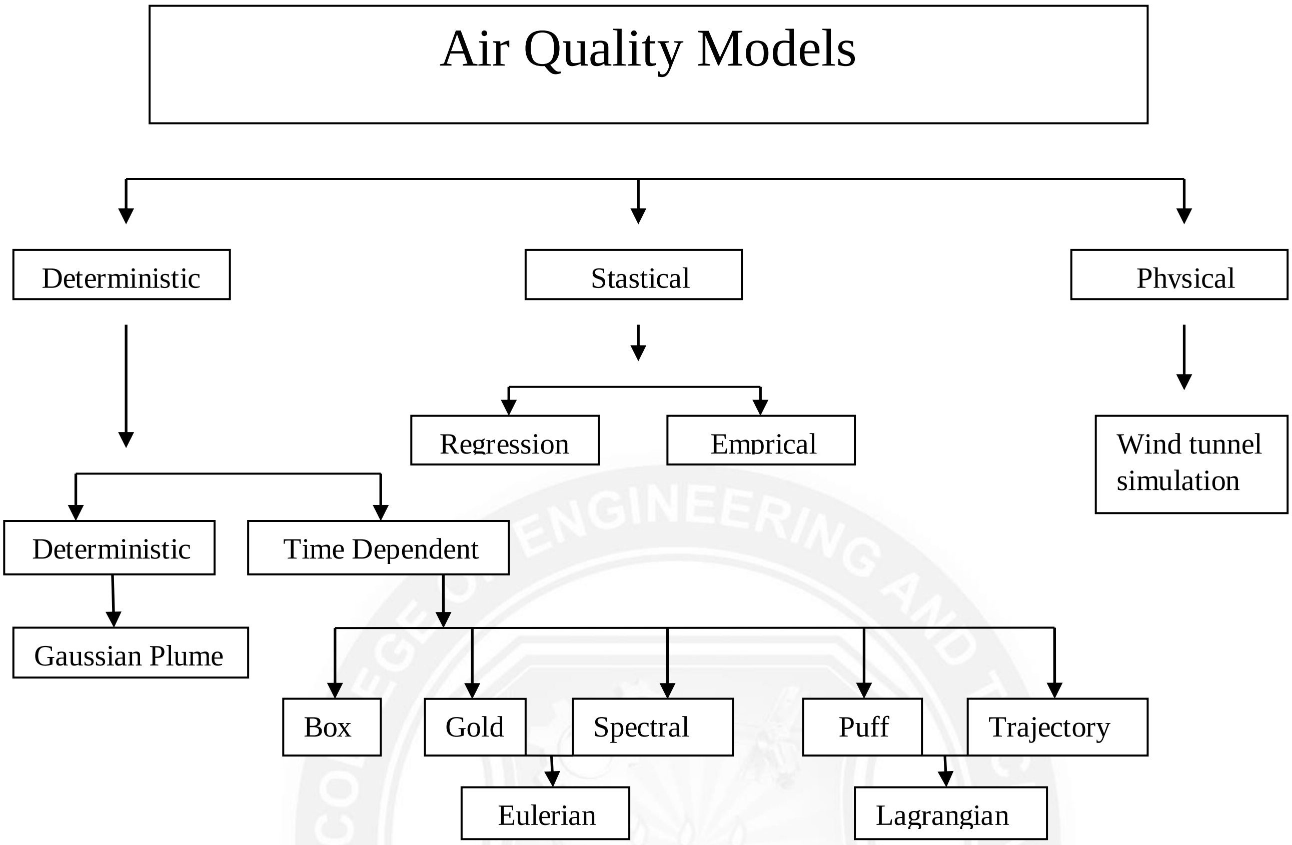

Figure 2.6.2 Classification of Air Quality Models

[Source:https://images.app.goo.gl/hK4D6GWGL7Bj5nqd6]

Factors affecting in Dispersion of Pollutants

- Factors affecting Dispersion of pollutants in the Atmosphere
  - ☐ Source characteristics
  - ☐ Emission rate pollutant
  - ☐ Stack height
  - ☐ Exit velocity of the gas
  - ☐ Exit temperature of the gas
  - ☐ Stack diameter
  - ☐ Meteorological conditions
  - ☐ Wind velocity
  - ☐ Wind direction
  - ☐ Ambient temperature
  - ☐ Atmospheric stability

TYPES OF AIR POLLUTION DISPERSION MODELS

- There are four types of air pollution dispersion models, as well as some hybrids of the five types:
- All the models studied here will be using a general material balance that is (Equation 1):

Accumulation rate = All flow rates in - All flow rates out

+ Creation rate - Destrction rate ...(1)

1. Box Model

- The box model is the simplest of the model types.
- It assumes the air shed (i.e., a given volume of atmospheric air in a geographical region) is in the shape of a box.

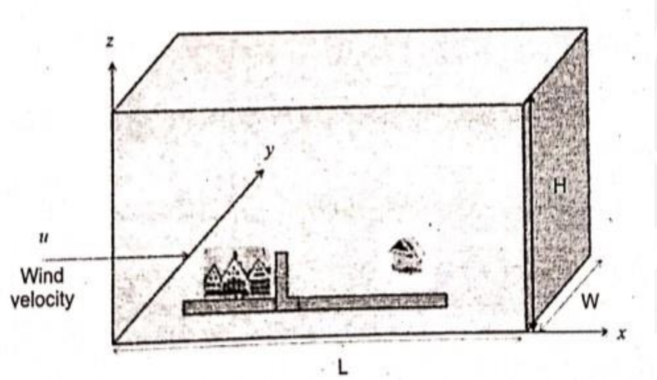

Figure 2.6.3 Rectangular city, showing the symbol of used in the fixed box model

[Source:http://shodor.org/media/content/hpcu/website/resources/xsede14/AirPollutantConcentrationModels]

It also assumes that the air pollutants inside the box are homogeneously distributed and uses that assumption to estimate the average pollutant concentrations anywhere within the air shed.

Although useful, this model is very limited in its ability to accurately predict dispersion of air pollutants over an air shed because the assumption of homogeneous pollutant distribution is much too simple.

- The city is a rectangle with dimension W and L and one side is parallel with wind direction.
- Complete atmospheric turbulence is produced and totals mixing of pollutants up to H and no mixing above this height.
- The turbulence is strong enough in the upwind direction that the pollutant concentration is uniform in the whole volume of air over the city and not higher as downwind side than upwind side.
- The wind blows in x direction with velocity u. This velocity is constant and is independent of time, location or elevation above the ground (steady state condition). We use average u between at the ground and at H.
- The concentration of pollutant entering the city (at x= 0) is constant and is equal to b (background concentration). The units are g/m^3 or $\mu g/m^3$.
- The air pollution rate of the city is Q (g/s). This is usually given as emission rate per unit area, q, $g/s.m^2$. the conversation can be made by

$$Q= qA$$

Where,

A is the area (W x L)

- No pollutant enters or leaves through the top or side of the box.
- The pollutant is long-lived in the atmosphere (destruction rate= 0).

The emission rate is constant and unchanging with time (in steady state condition). With all these assumption, the general mass balance equation is simplified as below (Equation 2):

$$\cancelto{0}{\boxed{\text{Accumulation rate}}} = \boxed{\text{All flow rate in}} - \boxed{\text{All flow rate out}} + \cancelto{0}{\boxed{\text{Creation rate}}} - \cancelto{0}{\boxed{\text{Destruction rate}}} \quad .(2)$$

So, that the equation is simplified as below;

0= (all flow rates in) – (all flow rates out)

There are 2 flow rates. The flow rate of the pollutant into the upwind side is

Flow rate in = (uWH)b = (volume/time) x (mass/volume)

= mass/time

The second flow in is that the pollutant emitted by the city into the lower boundary,

Flow rate in = Q = qWL

According to the assumption, the concentration of entire city is a constant and equal to c.

The flow rate out is:

Flow rate out = (uWH)c

Then, substitute all these equations into equation 2, will ield;

0= (uWHb + QWL –uWHc)

0= [W(uHb + QL – uHc)]

uHc = b+QL/uH ....(3)

This equation is the same as the continuous-stirred-tank reactor (CSTR) model that is widely used in chemical engineering.

2. Gaussian Model

The Gaussian Model is perhaps the oldest (circa 1936) and perhaps the most commonly used model type.

Gaussian plume model is usually called as diffusion model and sometimes dispersion model. Most of diffusion model used Gaussian plume idea which is also a material balance model. In this model, a point source such as a factory smoke stack is selected and the downwind concentration resulting from this point source is calculated.

- It assumes that the air pollutant dispersion has a Gaussian distribution, meaning that the pollutant distribution has a normal probability distribution.
- Gaussian models are most often used for predicting the dispersion of continuous buoyant air pollutant distribution has a normal probability distribution.
- Gaussian models may also be used for predicting the dispersion of non-continuous air pollution plume (called puff models).
- The primary algorithm used in Gaussian modelling is the Generalized Dispersion Equation for a Continuous Point-Source Plume.

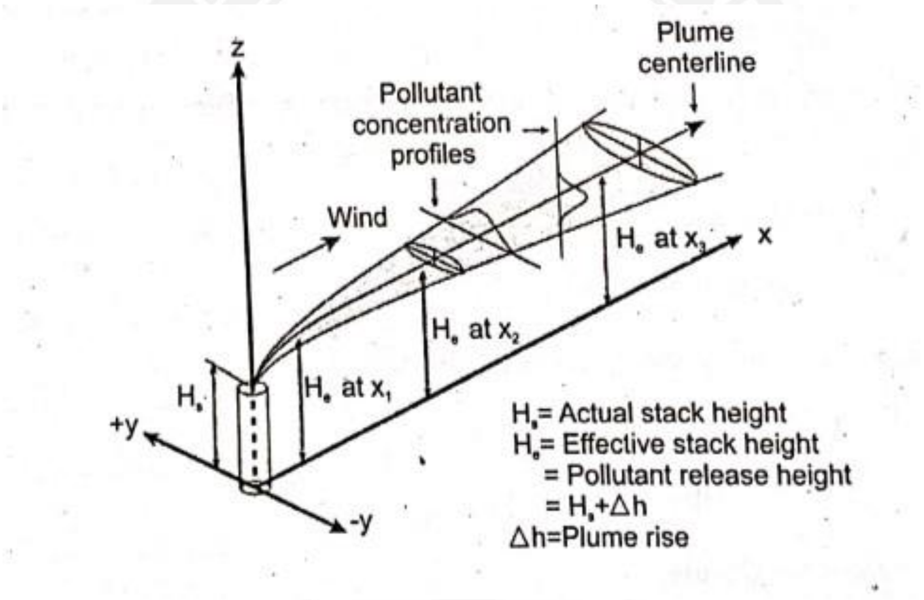

Fig 2.6.4 Co-ordinate system and nomenclature for Gaussian Plume

[Source:https://en.wikipedia.org/wiki/File:Gaussian_Plume_(SVG).svg]

Where,

C = Downwind concentration

Q = Pollution source emission rate

u = Average wind speed

σy = y direction plume standard deviation

σz = z direction plume standard deviation

x = Position in the x direction or downwind direction

y = Position in the y direction

z = Position in the z direction

H = Effective stack height

From the figure , the origin of the coordinate system is placed at the base of the smokestack with the x axis aligned in the downwind direction.

- The contaminated gas stream or plume rising from the smoke stack (Δh) and then travel in x direction and spread in the y and z direction as it travels.
- The plumes normally rise higher above the smoke stack because they are emitted at higher temperature than atmosphere and with vertical velocity.

For the calculations, the plume is assumed to be emitted at coordinate.

(0, 0, H)

Where,

H is effective stack height which is the summation of the physical stack height and plume rise

(h + Δh).

The smoke emitted at the point source is assumed to be a non- buoyant pollutant ar emission rate Q(g/s) and blows in x direction with velocity u that independent of time, elevation or location.

The problem is to compute the concentration due to this source at any point (x, y, z) for x>0.

If the molecular diffusion alone were causing the plume to mix with the surrounding air, the plume will spread slowly as a thin steak moving straight down the sky.

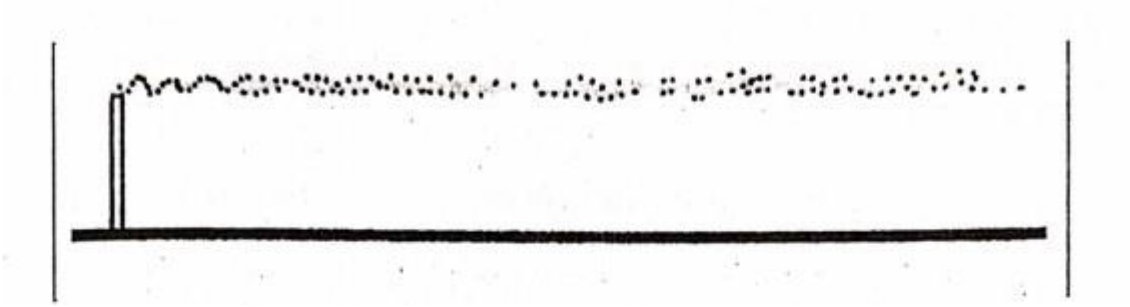

Figure 2.6.5 Time exposure of a visible plume

[Source:http://shodor.org/media/content/hpcu/website/resources/xsede14/AirPollutantConcentrationModels]

- The spread of the plume does not depend on molecular diffusion only.
- The main cause of the spreading is the large scale turbulent mixing that exists in atmosphere.
- The twisting behaviour is caused by the turbulent motion of the atmosphere that is superimposed on the plume's large scale linear motion caused by horizontal wind.
- This turbulent motion is random in nature; a snapshot taken after a few minutes after the first will show different snapshot in different places.
- Time averages the variation and thus the concentration will appear quit uniform and symmetrical.

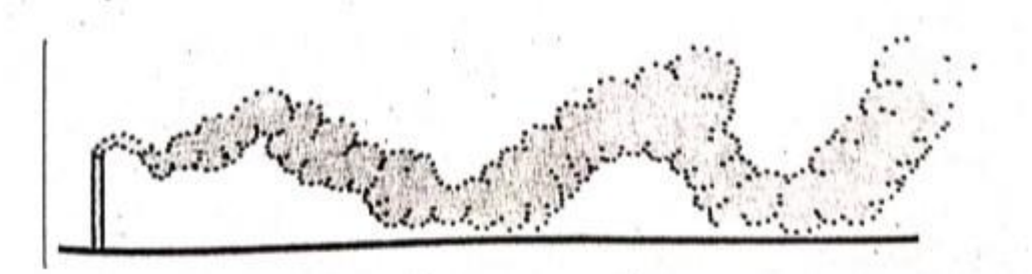

Figure 2.6.6 Snapshot of a visible plume

[Source:http://shodor.org/media/content/hpcu/website/resources/xsede14/AirPollutantConcentrationModels]

(i)Gaussian Plume Derivation

Discovering on how the air expands by turbulent mixing, we need to perform material balance around some small cube of space near the centre of the plume. Assume that neither material is created nor destroyed in the atmosphere:

$$\boxed{\text{Accumulation rate}} = \boxed{\text{All flow rates in}} - \boxed{\text{All flow rates out}}$$

$$+ \cancelto{0}{\boxed{\text{Creation rate}}} - \cancelto{0}{\boxed{\text{Destruction rate}}} \qquad ...(4)$$

Accumulation rate = (all flow rates in) – (all flow rates out)

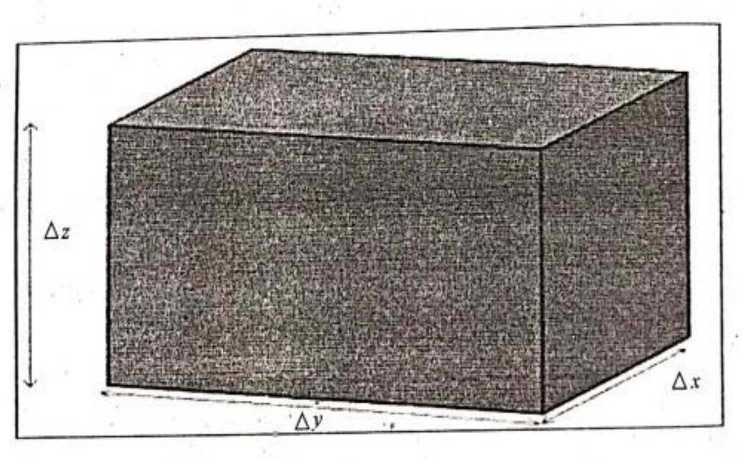

Figure 2.6.7 Dimension of cube used for material balance

[Source:http://shodor.org/media/content/hpcu/website/resources/xsede14/AirPollutantConcentrationModels]

The accumulation rate is the time derivative of the amount contained that is concentration and volume. But the volume of the cubes is not changing with time:

Dispersion = Advection (Transport) + Dilution

= Advection + Diffusion

$$(\partial C/\partial t) = -\partial/\partial x(u^{-}C)\nabla t + K_i(\partial^2 C/\partial t^2)$$

$$(\partial C/\partial t) = \bar{U}\nabla C - \nabla \bar{F}_t + Q + R$$

Where,

$$\bar{F}_t = [\overline{u'C'}\ ,\ \overline{v'C'}\ ,\ \overline{w'C'}]$$

Where,

C = pollutant concentration

t = time

= wind vector

Q = source term

R = removal term

= turbulent flux of pollutants

The deterministic based air quality model is developed by relating the rate of change of pollutant concentration in terms of average wind and turbulent diffusion which, in turn, is derived from the mass conversation principle.

$$\frac{\partial C}{\partial t} = -\left(u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z}\right) + \frac{\partial}{\partial x}K_H\frac{\partial C}{\partial x} + \frac{\partial}{\partial y}K_H\frac{\partial C}{\partial y} + \frac{\partial}{\partial z}K_z\frac{\partial C}{\partial z} + Q + R$$

Where,

C = pollutant concentration

t = time

x, y, z = position of the receptor relative to the source

u, v, w = wind speed coordinate in x, y and z direction

Kx, Ky, Kz = coefficients of turbulent diffusion in x, y and z direction

Q = source strength

R = sink (changes caused by chemical reaction)

- The above diffusion equation is derived in several ways under different set of assumptions for development of air quality models.
- Gaussian model is one of the mostly used air quality model based on 'deterministic principle'.

$$C(x,y,z)=\frac{Q}{u\sigma_y\sigma_z 2\pi}e^{-\left(y^2/2\sigma_y^2\right)}\left[e^{-\left((z_r+H_e)^2/2\sigma_z^2\right)}+e^{-\left((z_r-H_e)^2/2\sigma_z^2\right)}\right]$$

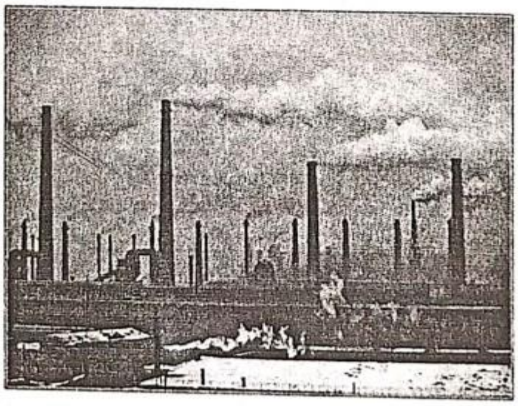

Figure 2.6.8 Gaussian plume Dispersion model

[Source:http://shodor.org/media/content/hpcu/website/resources/xsede14/AirPollutantConcentrationModels]

- The basic approach for development of deterministic vehicular pollution (line source) model is the coordinate transformation between wind coordinate system (X_1, Y_1, Z_1) and line source coordinate system (X, Y, Z).

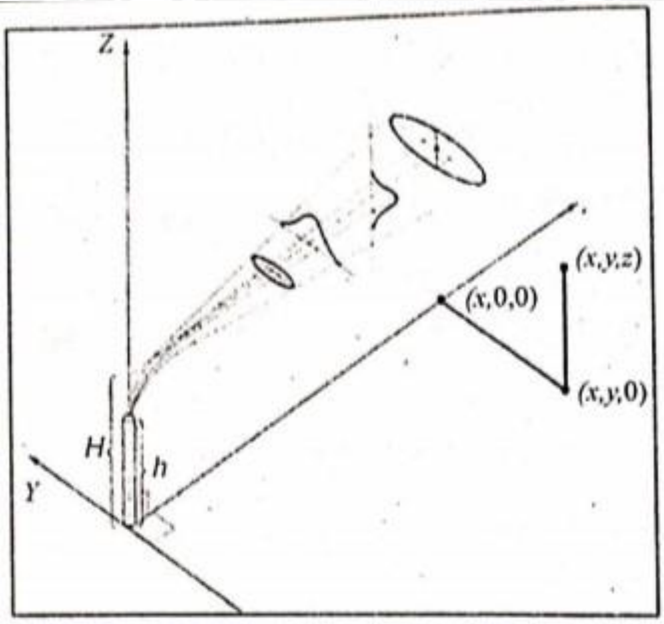

Figure 2.6.9 Line co-ordinate system

[Source:http://shodor.org/media/content/hpcu/website/resources/xsede14/AirPollutantConcentrationModels]

- A hypothetical line source is assumed to exist along Y_1 that makes the wind direction perpendicular to it (fig). the concentration at receptor is given by Csanady (1972):

$$C = \frac{Q_L}{2\pi\sigma'_y\,\sigma'_z\,\bar{u}}\left[\exp\left\{-\frac{1}{2}\left(\frac{z-H}{\sigma'_z}\right)^2\right\}+\exp\left\{-\frac{1}{2}\left(\frac{z-H}{\sigma'_z}\right)^2\right\}\right]$$
$$x\int_{-\frac{1}{2}}^{\frac{1}{2}}\exp\left[-\frac{1}{2}\left(\frac{Y_1'-Y_1}{\sigma'_y}\right)^2\right]dY_1'$$

(ii)Gaussian plume Dispersion model: Assumptions

- Steady state conditions, which imply that the rate of emission from the point source is constant.
- Homogeneous flow, which implies that the wind speed is constant both in time and with height (wind direction shear is not considered).
- Pollutant is conservative and no gravity fallout.
- Perfect reflection of the plume at the underlying surface, i.e. no ground absorption.
- The turbulent diffusion in the x-direction is neglected relative to advection in the transport direction, which implies that the model should be applied for average wind speeds of more than 1 m/s (> 1 m/s).
- The coordinate system is directed with its x-axis into the direction of the flow and v (lateral) and w (vertical) components of the time averaged wind vector are set to zero.
- The terrain underlying the plume is flat.
- All variables are ensemble averaged, which implies long-term averaging with stationary conditions.

Advantages

- Produce results that match closely with experimental data
- Incorporate turbulence in an ad-hoc manner
- Simple in their mathematics
- Quicker than numerical models

- ❖ Do not require super computers

Disadvantages

- ❖ Not suitable if the pollutant is reactive in nature
- ❖ Fails to incorporate turbulence in comprehensive sense
- ❖ Unable to predict concentrations beyond radius of approximately 20 Km
- ❖ For greater distances, wind vibrations, mixing depths and temporal variations become predominant.

3. Lagrangian Model

- ➢ A Lagrangian dispersion model mathematically follows pollution plume parcels (also called particles) as the parcels move in the atmosphere and they model the motion of the parcels as a random walk process.
- ➢ The Lagrangian model then calculates the air pollution dispersion by computing the statistics of the trajectories of a large number of the pollution plume parcels.
- ➢ A Lagrangian model uses a moving frame of reference as the parcels move from their initial location.
- ➢ It is said that an observer of a Lgrangian model follows along with the plume.

4. Eulerian Model

An Eulerian dispersions model is similar to a Lagrangian model in that it also tracks the movement of a large number of pollution plume parcels as they move from their initial location.

- ➢ The most important difference between the two models is that the Eulerian model uses a fixed three-dimensional Cartesian grid as a frame of reference rather than a moving frame of reference.
- ➢ It is said that an observer of an Eulerian model watches the plume go by.

APPLICATIONS OF DISPERSION MODELLING

The application of dispersion modelling is given below.

- ☐ Air shed modelling
- ☐ Roadway emissions modelling
- ☐ Modelling coastal fumigation
- ☐ Visibility modelling
- ☐ Dispersion modelling on larger scales
  - The regional scale
  - Long-range transport
- ☐ Salt and steam effects: cooling towers

EXAMPLE FOR MODELLING

Prognostic meteorological models Prognostic models ate driven by large-scale synoptic analyses and numerically solve the equations if atmospheric dynamics to determine local meteorological conditions.

1. RAMS and MM5

- RAMS is most commonly used prognostic meteorological model in New Zealand (Wratt et al., 2001), followed by MM5, ARPS, and (more recently) TAPM, RAMS and MM5.
- RAMS and MM5 are three-dimensional, non-hydrostatic prognostic mesoscale models.

MM5 is the fifth-generation NCAR/Penn State Mesoscale model. The model includes a multiple nesting capability, non-hydrostatic dynamics and four-dimensional data assimilation (Dudhia et al., 1999). MM5 is free to users, while RAMS is subjected to licensing costs.

Both models enjoy widespread use throughout the world, are well supported, continually under development, have been used in many studies, and appear regularly in the scientific literature.

Advantages

- ❖ Have the ability to assimilate local meteorological data.

- Have realistic dynamical and physical formulations, suitable for simulations in New Zealand’s complex environment.
- Can produce realistic meteorological fields in data-sparse regions.
- Are flexible enough to couple output meteorological fields to the dispersion model runs at any resolution (e.g. RAMS coupled to HYPACT).

Disadvantages

- Have relatively high computational demands
- Require a large amount of user knowledge and expertise to produce reliable and convincing results
- Do not themselves include dispersion models, and the associated dispersion models do not necessarily comprise all of the features required for regulatory assessments (e.g. building effects).

2.TAPM

At present, most prognostic models require significant computer resources to run. They also describe a comprehensive collection of meteorological phenomena and are widely used in meteorological research.

However, some features that contribute significantly to the computational cost of mesoscale modelling are not important for air quality simulations, such as gravity waves and complicated microphysical processes.

Careful formulation of the model dynamics so as to omit or filter out these features can increase the run speed, enabling longer runs to be contemplated for regulatory applications. This has been done with the CSIRO’s TAPM.

- TAPM is a PC-based three-dimensional prognostic meteorological modelling system, including various dispersion modules.

TAPM has a GUI that allows the user to set up and run the model under the Windows operating system.

It connects to databases of terrain, vegetation, soil type, sea surface temperature and synoptic-scale meteorological analyses for Australia and New Zealand, as well as most regions throughout the world.

- TAPM is driven by six-hourly synoptic analyses at approximately 75 km resolution.
- This database is derived from LAPS analysis data from the Bureau of Meteorology.

Advantages

- It is easy to use and completely self-contained, with good visualization of model results.
- The model output is easy to convert for input into other models, such as CALMET, AUSPLUME, DISPMOD and ISCST3.
- As for any prognostic model, it requires no local data to run, although it has the ability to assimilate local surface meteorological data.
- It is designed to run on a modern personal computer.
- Describes the effects of point, line and volume sources, simulates the effects of buildings on dispersion, and simulates chemical reactions between pollutants.
- Resolution of the pollution dispersion models can be higher than that of the meteorological model- and will usually need to be for regulatory assessments.

Disadvantages

- Although easy to use, a high level of understanding of boundary-layer meteorology and pollution dispersion is needed, as with all prognostic model systems, to produce meaningful results.
- The maximum horizontal resolution of the meteorological model component of TAPM is of the order of a 1 km grid-size.
- If meteorological features are expected, or geographical forcing is present at smaller scales, then the user should take care.

- Although assimilation of meteorological data is possible, care must be taken to ensure that the meteorological data are representative of the scales modelled by the meteorological model.