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Environmental Modeling in Industrial Application

Models for Supporting Incident Evolution: Release of Dense-than-air Pollutants

a.y. 2016-2017

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INTRODUCTION

Emission of polluting substances can come from:

1) Vehicular traffic
2) Industrial plants
3) Thermo-electric plants
4) Natural sources
5) Accidents

The transport of the polluting substances in atmosphere and their falling on the ground is a primary issue.

We need means to predict the path of the polluting cloud in order to fulfill the required assistance and reclamation operations.

INTRODUCTION

The spatial and temporal distribution of the concentration of the polluting substance can help to quantify:

- The effects on human health (immediate or long-term exposure)
- The effects on the environment

INTRODUCTION
The dense gases

The importance of the problem is very high when dealing with:

- toxic substances (SO2, Cl2 …)
- flammable substances (GPL, propane, buthane …)

The gases released can be denser than air.

- gases with high molecular weight
- gases released in the atmosphere at low temperature

INTRODUCTION
The dense gases

Example: SO_2

Molecular weight (SO_2) = 64 kg/kmol

Molecular weight (air) = 28.9 kg/kmol

Density:

$$\rho(SO2) = [M(SO2)/M(air)]^* \rho(air) = 2.2\ \rho(air)$$

Airborne chemical pollution

- Attention must be paid to:
  - accurately determine the types of pollutants taking into account the modalities of the production process
  - compare the reference concentrations with exposure limit values allowed
  - perform the technical control of concentrations, which must be made exclusively by the source of pollution

Airborne chemical pollution

- Pollutants are gaseous mixtures or aerosols, i.e. suspensions of solid or liquid particles in the air, large enough to remain in suspension for an observable time.

- The following substance types can be individuated:
  - **Gases**, i.e. substances that in reference conditions (temperature 25°C nd atmospheric pressure) are at gaseous state
  - **Vapors,** substances at the gaseous state, which are liquid in reference conditions
  - **Dust or particulate matter** i.e. solid particles with a diameter between 1 and 25 μm
  - **Smokes and fogs**, i.e. solid or liquid particles which generate aerosols by condensation of substances already present in air in the form of gases such particles are in the order of 0.1μm

Airborne chemical pollution

- In general, toxic pollutants can penetrate in the organism through:
  - the respiratory system
  - the skin
  - orally
- The effects of toxic substances may consist in:
  - forms of depression
  - Destruction of tissues
- Such effects can be:
  - immediate
  - protracted
  - posticipated
- The limit values are defined in relation to:
  - Properties of the substances in the environment
  - Results of toxicological tests
  - epidemiological data

Airborne chemical pollution

- An important reference are the tables published and periodically updated by the **American Conference of Governmental Industrial Hygienists** (ACGIH).
- The rules concerning indication of the concentration limit or threshold values TLV (threshold limit value English) are three:
  - **TLV - TWA** (time-weighted average), weighted average value over time, relative to an exposure equivalent to 8 hours a day for 5 days a week;
  - **TLV - C** (limit on the maximum value), which is used for substances with a substantially immediate effect, and expresses a concentration maximum value that should never be exceeded;
  - **TLV - STEL** (short term exposure limit), is a maximum concentration of pollution, it is taken four times a day, with an hour interval between two exposures and, successively, for continuative exposures never longer than 15 minutes

Airborne chemical pollution

- The following indications about TLV can be adopted:
  - If the limit TVL - STEL is identified, this value must not be exceeded by the concentration excursions
  - If the TVL-STEL is not known, the following limits MUST not be exceeded:
    - the TVL-TWA limit in the interval of 8 h
    - 3 times the TLV-TWA value for more than 30 min/day
    - Never, the value of TLV-C

Airborne chemical pollution

- The limits shown in the ACGIH TVL tables refer to the absorption of toxic exclusively through the respiratory tract:
- where it appears the indication "skin" beside the name of a substance, you will have to consider the possibility of dermal absorption of the pollutant.
- In case of substances with independent effect (which, i.e., produce a different effect, or act on different parts of the body) each of them must be checked for :

$$\frac{C_i}{TLV_i} < 1$$

- In case of **substances presenting additive effect** the following condition must be verified:

$$\sum_i \frac{C_i}{TLV_i} < 1$$

- In case of **substances with singular effect**, opportune deepenings are required.

Airborne chemical pollution

- The asphyxiating agents do not have a predetermined limit value for each type, because:
  - the true limiting factor is constituted by the concentration of oxygen in the air, which should be in any case more than 18% in normal volume at atmospheric pressure

  Finally, there are some special categories of substances, on which it is worth reflecting individually:
  - **particulates** annoying but **not fibrogenic** (*non-crystalline amorphous silica*); if the percentage of quartz is less than 1% they do not generate serious damage
  - **fibrogenic particulates** (**quartz**), which provoke the degeneration of pulmonary tissues, becoming
  - **silicates** (**asbestos**), a fundamental component of amiant;
  - **Simple asphyxiating** (e.g. methane - CH_4 – and carbon dioxide - CO_2)
  - **Variable composition substances** as gasoline vapors and fumes from welding requiring specific analyses
  - **carcinogens**

Airborne chemical pollution

- The **experimental measurements** for the determination of the concentration of a pollutant in an environment require the availability of an appropriate instrumentation.

- The **analysis methodologies** employed exploit several principles:
  - for example, it is possible to react the air volumes object of analysis with some substances that change - in a predictable way - the coloring (**Draeger vials** - a specific substance vial is required for each type of pollutant)

Impact on the environment

By law, the Chemical Safety Assessment (CSA) and the compiling of the report on chemical safety (CSR) are mandatory for all the substances emitted in more than 10 tons/year.

All the organisms and ecosystems must be protected: the CSA involves all these environments:

- water
- earth
- atmosphere
- predators at the vertex of the alimentary chain
- micro-organisms

Impact on the environment

The risk evaluation for the environment based on the intrinsic features of the substances, has the aim of:

- The evaluation for the PBT (Persistent, Bio-accumulation and toxic) and vPvB substances
- The definition of the substance classification (e.g. dangerous for the environment)
- The identification of the Preventable No Effect Concentration (PNEC)

Impact on the environment

PBT Criteria:

Persistency

- half life in sea water >60 days
- half life in soft water > 40 days
- half life in marine sediments > 180 days
- half life in soft water sediments > 120 days
- half life in the soil > 120 days

Bio-accumulation

Bio-concentration factor > 2000 – aquatic species

Toxicity

- NOEC < 0.01 mg/l, aquatic organisms
- Carcinogen, mutagen, toxic for reproduction
- other evidences of chronic toxicity

Impact on the environment

vPvB Criteria:

Very persistent substance (vP)

- half life in water >60 days or
- half life in sediments > 180 days
- half life in the soil > 180 days

Very bio-accumulable substances (vB)

Bio-concentration factor > 5000 – aquatic species

Impact on the environment

PNEC determination

PNEC is determined for each environmental compartment on the basis of toxicity data for the compartment organisms (laboratory tests)

Safety factor:

- uncertainty in extrapolating the results of tests on the environment;
- high diversity of the ecosystems, experimental data only for few species;
- sensitivity of the ecosystems higher than that of the single species.

The more numerous are the data and the analyzed species, the lower is the safety factor.

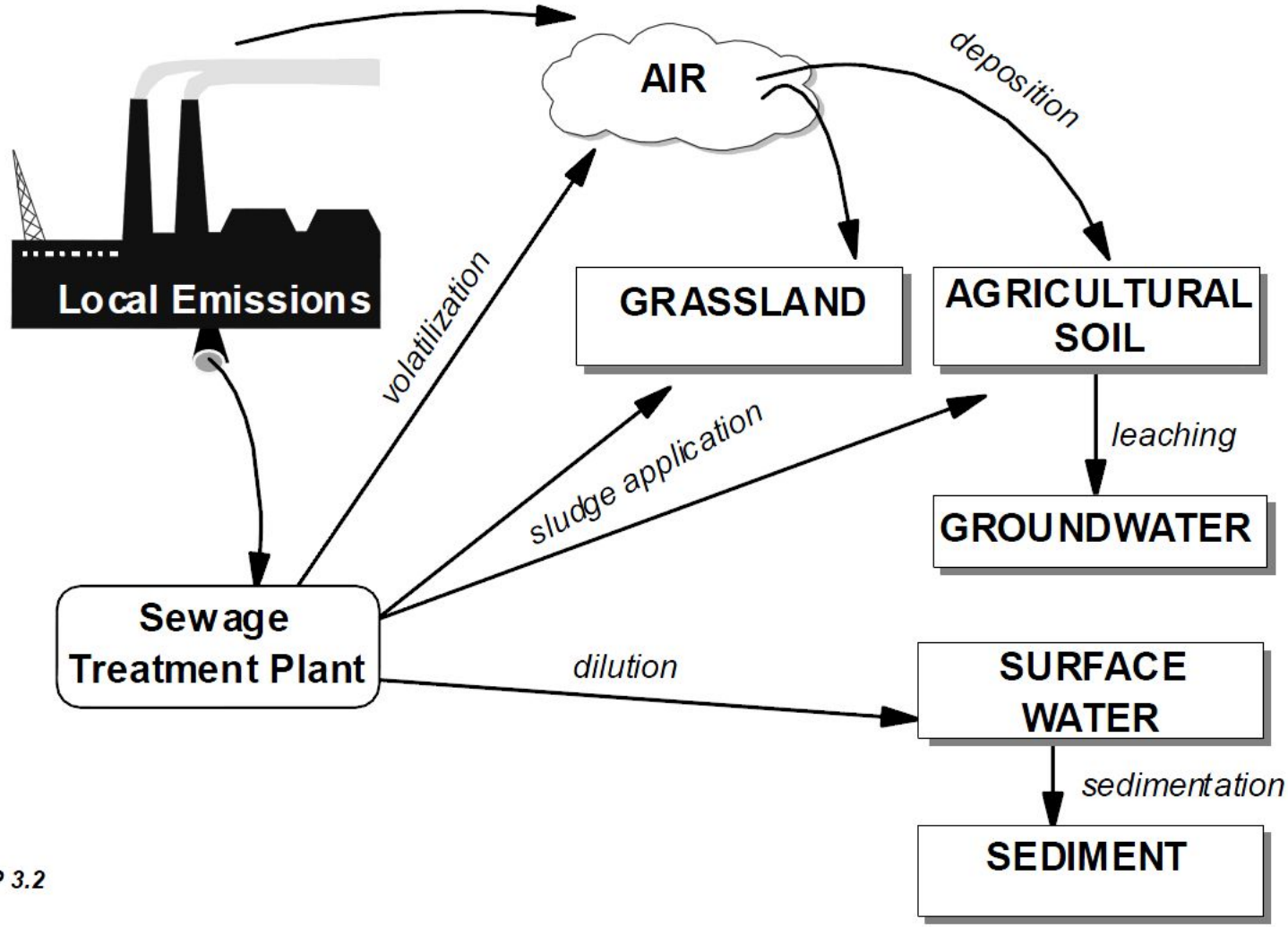
Safety factor higher for the short-term (EC/LC50) tests than the long-term tests.

Impact on the environment

Evaluation of environmental exposure

- Determination of the PEC (Prevented Environmental Concentrations) of the substance for all the compartments exposed.
- Estimation of the emissions in all the phases of the life cycle (production, formulation, industrial use, wastes)
- Characterization of the environmental degradation, reaction, distribution and destiny.
- PEC estimation both for regional and for local scenarios.
- PEC measured or calculated through mathematical models.

Impact on the environment



Fonte RIP 3.2

Impact on the environment

Regional PEC

- Point-shaped releases diffused over a wide area have an effect on a regional scale.
- The regional PEC (stationary) provides also the concentration in the calculation of the local PEC.

Models of regional PEC

- reference area : 200X200 km2, 20 millions inhabitants, 10% production and use of the substance
- The exposure models employed consist in a certain number of homogeneous compartments (box models)
- Evaluations with "multimedia fate models" based on the concept of fugacity (e.g. Mackay).

Impact on the environment

Characterization of the hazard

Comparison between prevented environmental concentrations (PEC) and prevented no effect concentrations (PNEC) for each environmental compartment.

Objectives of protection (earth and water environment)

Local	Regional
$PEClocal_{water}/PNEC_{water}$	$PECregional_{water}/PNEC_{water}$
$PEClocal_{sediment}/PNEC_{sediment}$	$PECregional_{sediment}/PNEC_{sediment}$
$PEClocal_{soil}/PNEC_{soil}$	$PECregional_{agr.soil}/PNEC_{soil}$
$PEC_{stp}/PNEC_{microorganisms}$	
$(0.5 \cdot PEClocal,oral_{fish} + 0.5 \cdot PECregional,oral_{fish})/PNECoral$	
$(0.5 \cdot PEClocal,oral_{worm} + 0.5 \cdot PECregional,oral_{worm})/PNECoral$	

Impact on the environment

Characterization of the hazard

- Hazards adequately controlled if PEC < PNEC.
- If the condition is not satisfied, the evaluation process can be repeated sharpening the information.
- where it is not possible to determine PEC or PNEC, is carried out a qualitative estimation of the negative effects hazards.
- If the PEC/PNEC ratio cannot be further reduced, the substance is a candidate for measures of hazard reduction.

Phenomenology

Phenomenology of the phases of dense gases dispersion:

- Source term;
- Falling and gravitational slumping
- Stratified dispersion
- Turbulent dispersion

Phenomenology

Source term:

- Mass of substance released (puff) or flow rate of the continuous release (plume).
- Nature of the substance released (incondensable gas e.g. **CO2**, vapor e.g. **NH3**, two phase mixture).
- Initial conditions of the cloud (temperature, mass fraction of air in the cloud …)

Phenomenology

Gravitational slumping of the cloud:

The cloud formed by a denser than air release continues to spread for the effect of gravity.

The mixing with air, particularly at the boundary on an horizontal plane, contributes to the dilution of the polluting cloud.

The size of the cloud continues to increase.

The gravitational slumping phase stops when the spreading of the cloud (for gravity effect) is contrasted by the action of the wind.

Phenomenology

Stratified dispersion:

The cloud concentration reduces further for dilution with air, until its density becomes similar to that of air.

Turbulent dispersion:

The cloud is further dispersed in the atmosphere owing to the turbulence of the wind flow.

PREVISION MODELS

To evaluate and quantify the dispersion of a pollutant emission in the atmosphere, it is very useful to assume a modelling approach.

The main types of models are:

- Stationary Gaussian models
- 3D Lagrangian models (particle models)
- 3D Eulerian models (grid models)

PREVISION MODELS

Gaussian models

These are very simple analytical codes which require a modest metereologic input and limited calculational resources.

They are adapt to simulate stationary situations in space and time, even if a wider application is possible.

The main assumption is that the atmospheric conditions are homogeneous in space and time, for which the concentration of pollutant in a zone is function of the wind speed array.

PREVISION MODELS

3D Lagrangian models

They simulate the dispersion of a pollutant through computational particles displaced in the calculation domain by the motion field and by the local turbulence conditions of the atmosphere

3D Eulerian models

They are based on the numerical integration of balance differential equations for each pollutant, and on the integration of the equations representing the chemical reactions occurring in the atmosphere.

MODELS FOR DENSE GAS RELEASES EVALUATION

Open source models

DEGADIS
SLAB

Proprietary models

AIRTOX
CHARM
FOCUS
SAFEMODE
TRACE

MODELS FOR DENSE GAS RELEASES EVALUATION

DEGADIS

DEGADIS was originally developed for the US Coast Guard to simulate the dispersion of accidental or controlled releases of hazardous liquids or gases in atmosphere.

DEGADIS includes a module for predicting the trajectory and dilution of an elevated dense gas jet.

The concentration/density relation is described using ordered triplets consisting of mole fraction, concentration and mixture density.

DEGADIS contains an internal chemical library that provides the properties of the chemical to be modeled

MODELS FOR DENSE GAS RELEASES EVALUATION

SLAB

SLAB was developed by Lawrence Livermore National Lab to simulate the release of denser than air gases.

SLAB models 4 categories of releases: evaporating pools, vertical jets, horizontal jets and instantaneous releases.

Releases can be treated as transient or steady state, or a combination of both.

SLAB does not contain an internal chemical library, but the user's guide provides the parameters for many substances of interest.

MODELS FOR DENSE GAS RELEASES EVALUATION

AIRTOX

AIRTOX has been developed by ENSR Consulting and Engineering to calculate downwind concentrations from time dependent toxic releases to the atmosphere

Chemical releases are simulated either in jet or in non-jet mode.

AIRTOX is a spreadsheet based model, that utilizes Lotus 123 software.

Chemical properties are provided through the internal database.

MODELS FOR DENSE GAS RELEASES EVALUATION

CHARM

CHARM is a Gaussian puff model created by Radian Corporation to assess the location, extent and concentration of the cloud resulting from the release of a toxic substance.

CHARM includes a chemical database that provides all the necessary chemical parameters of the model.

CHARM is a menu driven system composed of 2 parts: one containing all the screens for data input, the other one performing the calculations.

Model results are provided in a graphical display, providing a snapshot of the cloud passage with time.

MODELS FOR DENSE GAS RELEASES EVALUATION

FOCUS

FOCUS is a hazards analysis software package designed by Quest Consultants Inc. to evaluate transient hazards resulting from accidental or controlled releases of liquids and gases.

FOCUS predicts hazard zones resulting from fires and explosions, and vapor clouds formed from release of toxic and/or flammable materials.

The model provides downwind centerline concentrations as a function of time since release and the lateral distance to three user- specified concentration limits.

The predicted concentrations represent values averaged over the release duration.

MODELS FOR DENSE GAS RELEASES EVALUATION

SAFEMODE

SAFEMODE was developed by Technology and Management Systems Inc.

It is a tool for assessing the potential for acute hazards arising from the accidental release of toxic chemicals.

The user specifies source/release conditions in detail, including container dimensions, chemical name, storage condition, leak geometry and environmental conditions.

Predicted concentrations are displayed graphically as contours.

SAFEMODE has an internal database of more than 100 substances.

MODELS FOR DENSE GAS RELEASES EVALUATION

TRACE

TRACE was developed by EI Dupont De Nemours Company.

TRACE is an interactive menu driven model that allows the user multiple options when developing a release scenario. It contains an extensive chemical library.

The TRACE model output provides information about vapor cloud dynamics, snapshots of concentration isophlets and receptor impacts.

The cloud dynamics section displays various cloud parameters as a function of time after release.

SLAB

INTRODUCTION

SLAB is a computer code that simulates the atmospheric dispersion of denser than air releases.

The last version of SLAB can treat continuous, finite duration and instantaneous release from 4 types of source:

- A ground level evaporating pool,
- An elevated horizontal jet
- A stack (elevated vertical jet)
- A ground based instantaneous release.

The evaporating pool source is assumed to be pure vapor, in accordance with the evaporation process

The other sources can be either pure vapor or a mixture of vapor and liquid

INTRODUCTION

Atmospheric dispersion of the release is calculated by solving the conservation equations of

- Mass
- Momentum
- Energy
- Species

To simplify the solution of the conservation equations, the equations are spatially averaged with the cloud.

INTRODUCTION

The cloud can be modeled as a **steady-state plume** or as a **puff**, as visible in Figures 1 and 2.

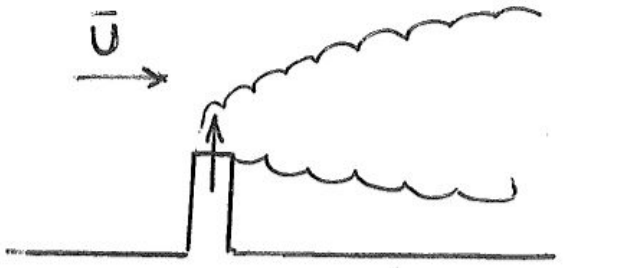


Figure 1: Steady-state plume

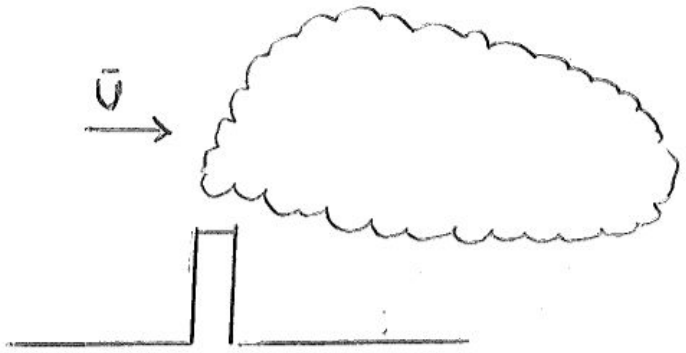


Figure 2: Transient Puff

INTRODUCTION

A continuous release (very long emission duration) is treated as a **plume**.

In the case of a finite duration release, cloud dispersion is initially described using the steady state **plume** mode, and remains in this mode as long as the source is active.

Once the source is shut off, the cloud is treated as a transient **puff** and the subsequent dispersion is calculated using the **puff** mode.

For an instantaneous release (explosion), the transient puff dispersion mode is used for the entire calculation.

INTRODUCTION

Solution of the spatially-averaged conservation equations in either dispersion mode yields the spatially-averaged cloud properties.

To regain the 3D variation of the concentration distribution, are applied particular profile functions of an assumed form and dependence on the calculated cloud dimensions.

INTRODUCTION

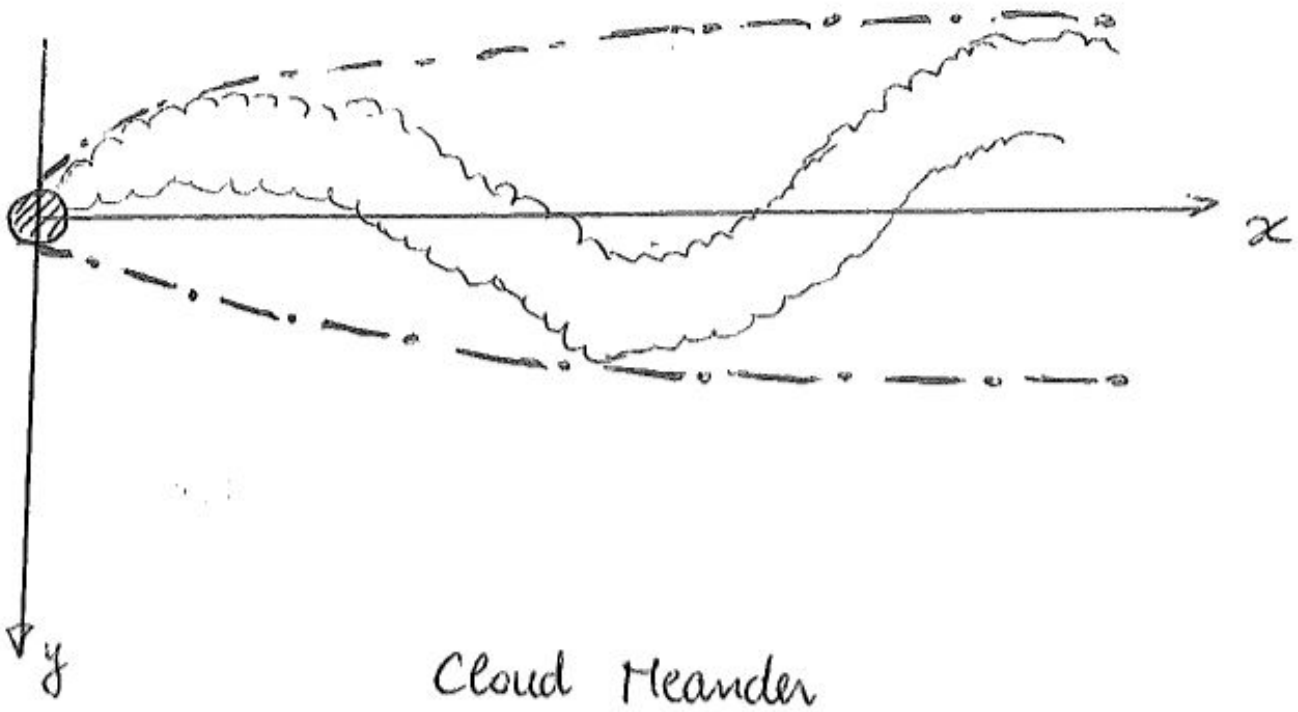
The time averaged concentration is obtained in a two step process:

1) The effect of the cloud meander on the effective width of the cloud is calculated;
2) The concentration is averaged over time using the effective (meander included) width in the concentration profile function.

This calculation yields the final results of the SLAB model, namely, the time averaged concentration in time and space.

MODEL ORGANIZATION

Cloud meander effect



THEORETICAL DESCRIPTION

The atmospheric dispersion of a large denser than air release is affected by phenomena that do not occur in neutrally or positively buoyant trace gas releases:

- Turbulence damping due to stable density stratification of the heavy gas cloud;
- Alteration of the ambient velocity field due to gravity flow and initial source momentum;
- Thermodynamic effects on cloud temperature, buoyancy and turbulence due to liquid droplet formation and evaporation, and ground heating in the case of the release of a superheated or cryogenic liquid

THEORETICAL DESCRIPTION

In combustible gas releases one can be concerned with the instantaneous concentration.

In toxic gas releases, the concern can be about doses over minutes or hours as well as the long term dose.

In order to make meaningful predictions of the size and duration of the hazardous concentration from a dense gas release, all of the significant phenomena need to be included, and the appropriate concentration averaging time needs to be used.

THEORETICAL DESCRIPTION

To meet these requirements, the SLAB model is built upon a theoretical framework that starts with averaged forms of the conservation equations of mass, momentum, energy and species (see figure in the next page).

These equations are used to calculate the spatially-averaged properties of the dispersing cloud and are expressed in two forms, representing two different dispersion modes:

1) Steady state plume
2) Transient puff.

THEORETICAL DESCRIPTION

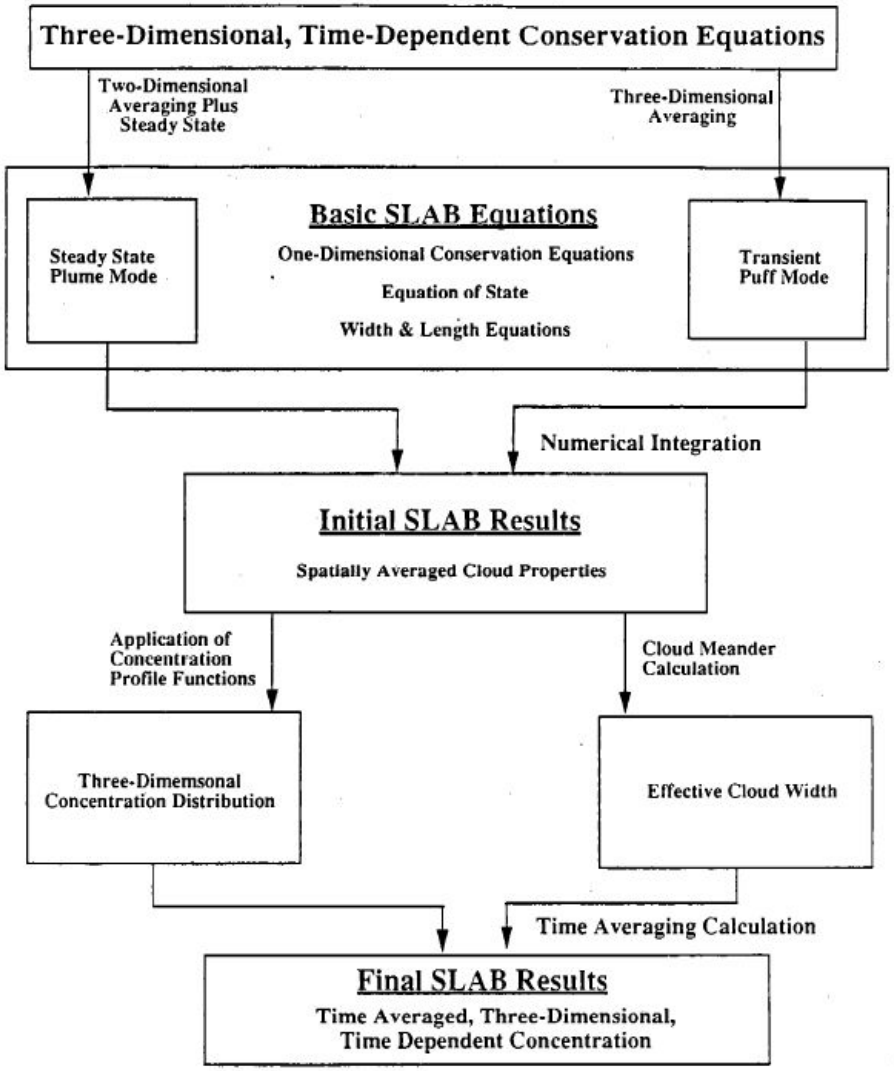


Figure 1. SLAB model concept.

THEORETICAL DESCRIPTION

The conservation equations are different for the two modes, **plume** and **puff**.

The steady state plume form of the equations is obtained by making the steady state assumption (d/dt =0) and by averaging the equations over the cross wind direction (y and z, see figure 3 next page).

The transient puff form of the equations is obtained by averaging the equations over all the three directions (x, y, z).

THEORETICAL DESCRIPTION

Figure 3

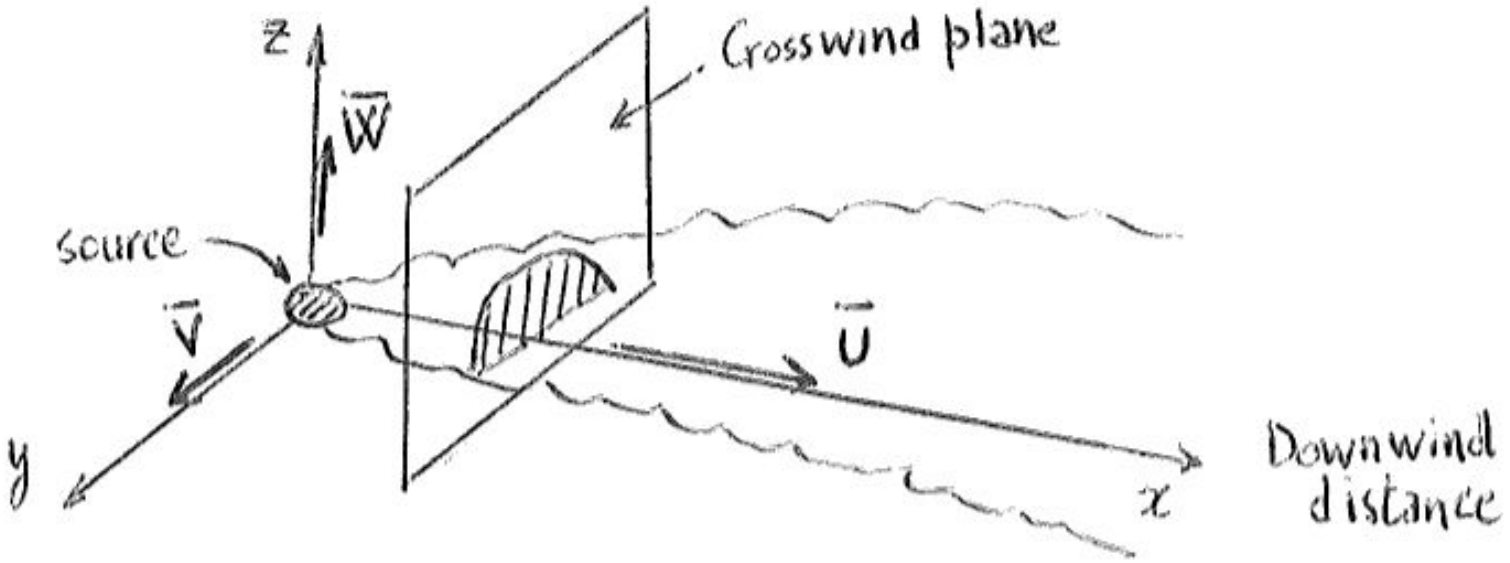


Figure 3: Frame of reference

THEORETICAL DESCRIPTION

The theoretical framework of the SLAB model is completed by the inclusion of the **equation of state** (ideal gas law) and **equations of the growth of cloud dimensions** (plume width in the steady state mode and puff length and width in the transient puff mode)

THEORETICAL DESCRIPTION

To solve the basic set of equations, additional submodels are required.

These submodels describe the dilution of the cloud due to

- The turbulent mixing with surrounding air,
- the formation and evaporation of liquid droplets within the cloud and
- the heating of cold clouds at the ground surface.

THEORETICAL DESCRIPTION

The turbulent mixing with surrounding air, is treated by using the entrainment concept which specifies the rate of air flow into the cloud.

The thermodynamics of liquid droplets within the cloud is modeled by using the local thermodynamic equilibrium approximation.

The size of the liquid droplets is assumed to be sufficiently small so that the transport of the vapor-droplet mixture can be treated as a single fluid.

Ground heating of the cloud is treated by using the radiation boundary condition and a coefficient of surface and heat transfer.

THEORETICAL DESCRIPTION

In the steady state plume mode the conservation equations are averaged over the cross wind plan of the plume, leaving the downwind distance (x) as the single independent variable.

In the transient puff mode the conservation equations are averaged over all three dimensions of the cloud, leaving the downwind travel time (t) of the puff as a single independent variable.

Notice that travel time (t) and downwind distance (x) are related by the downwind cloud velocity (U)

THEORETICAL DESCRIPTION

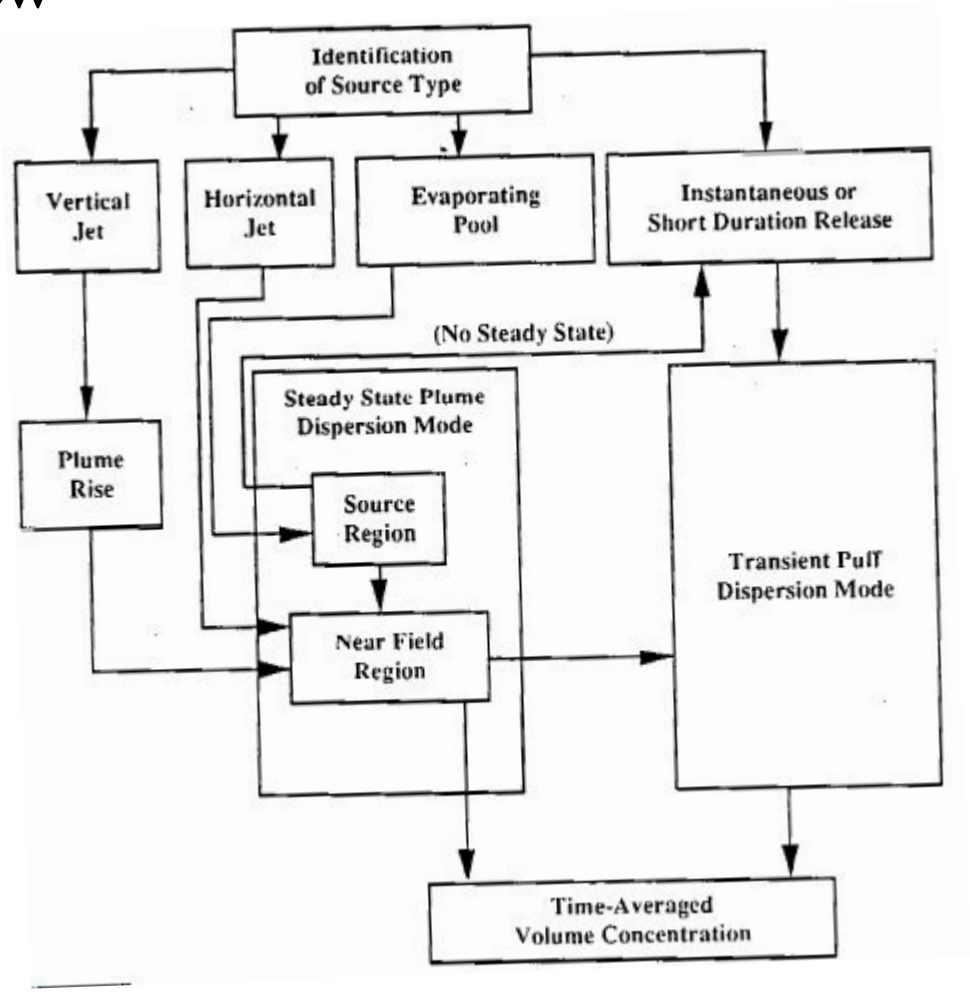
The 3D concentration distribution of the cloud is determined from the average concentration and by using similarity profiles that include the calculated cloud dimensions.

Thus, the code is 1D in both puff and plume modes, but can be seen as quasi 3D, as the cloud dimensions are used to specify the spatial distribution of the cloud.

For most code users, the most important result is the time averaged volume concentration in function of travel time (t), from the source, and as a function of the three spatial dimensions.

MODEL ORGANIZATION

The calculational flow within the SLAB code is reported in Figure below



MODEL ORGANIZATION

There are three stages in a typical simulation:

1) Source identification and initialization for dispersion;
2) Calculation of cloud dispersion;
3) Calculation of the time-averaged concentration

The choice between plume or puff mode depends on the type of source and the duration of the spill.

MODEL ORGANIZATION

Dispersion from an evaporating pool and a horizontal jet both begin in the steady state plume mode.

This mode has two regions:

1) A *source region* where source material is added to the dispersing cloud.
2) A *near-field* region, where no additional source material is added to the cloud but it is still in steady state.

The calculation of evaporating pool begins in the source region and proceeds to the near field region.

The horizontal jet source begins with a pure source emission cloud travelling downwind at a speed equal to the jet exit velocity.

MODEL ORGANIZATION

The situation for the vertical jet is similar to that of the horizontal jet; however, the vertical jet has a plume rise region where the cloud motion is mainly vertical.

Consequently, the plume rise calculation is completed before entering the steady state near field plume dispersion calculation.

MODEL ORGANIZATION

The dispersion calculation for a continuous but limited release of duration t_sd is initially conducted in the steady state plume mode.

In this mode, the downwind distance x is the independent variable and time t is taken to be proportional to the amount of emitted mass within the plume.

Calculation of the plume properties in function of x continues until the emitted mass within the plume, from the upwind edge of the cloud to the downwind distance Xt, is equal to one half of the released mass Qs.

At this downwind location, the dispersion calculation is switched from the plume mode to the puff mode.

MODEL ORGANIZATION

The puff center of mass is set equal to Xt, so that the emitted mass within the puff is equal to the total mass released Qs, with half the mass upwind of Xt and half the mass downwind (see figure 4)

Time t is the single independent variable in the puff mode, and the time of transition from the plume to the puff mode is taken to occur at the end of the release when t = t_sd.

MODEL ORGANIZATION

Figure 4

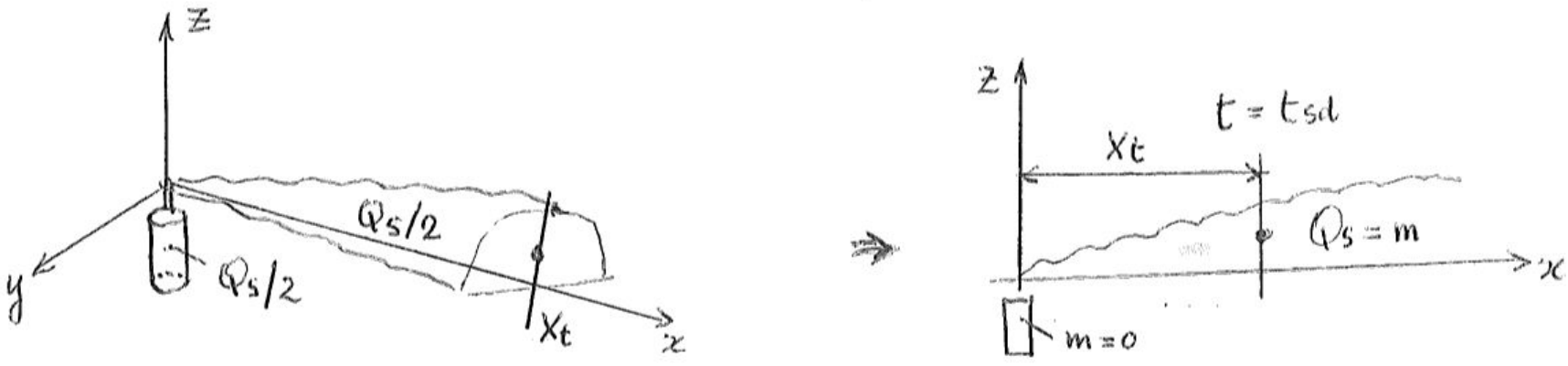


Figure 4 : Center of mass calculation X_t for the puff mode

MODEL ORGANIZATION

An exception to this procedure is taken when an evaporating pool release fails to reach steady state within the source region. (short duration evaporating pool)

This occurs whenever the emitted mass within the source region of the steady state plume is greater than the total released mass Qs.

When this occurs, the steady state calculation is discarded and the entire calculation is restarted in the transient puff mode.

In case of instantaneous source there is also no steady state cloud.

MODEL ORGANIZATION

Completion of the dispersion calculations in either mode, yields the instantaneous spatially averaged cloud properties: mass and volume concentration, density, temperature, downwind velocity, cloud dimensions etc.

The 3D variation of the concentration distribution is accounted for by applying profile functions that are based on the calculated cloud dimensions.

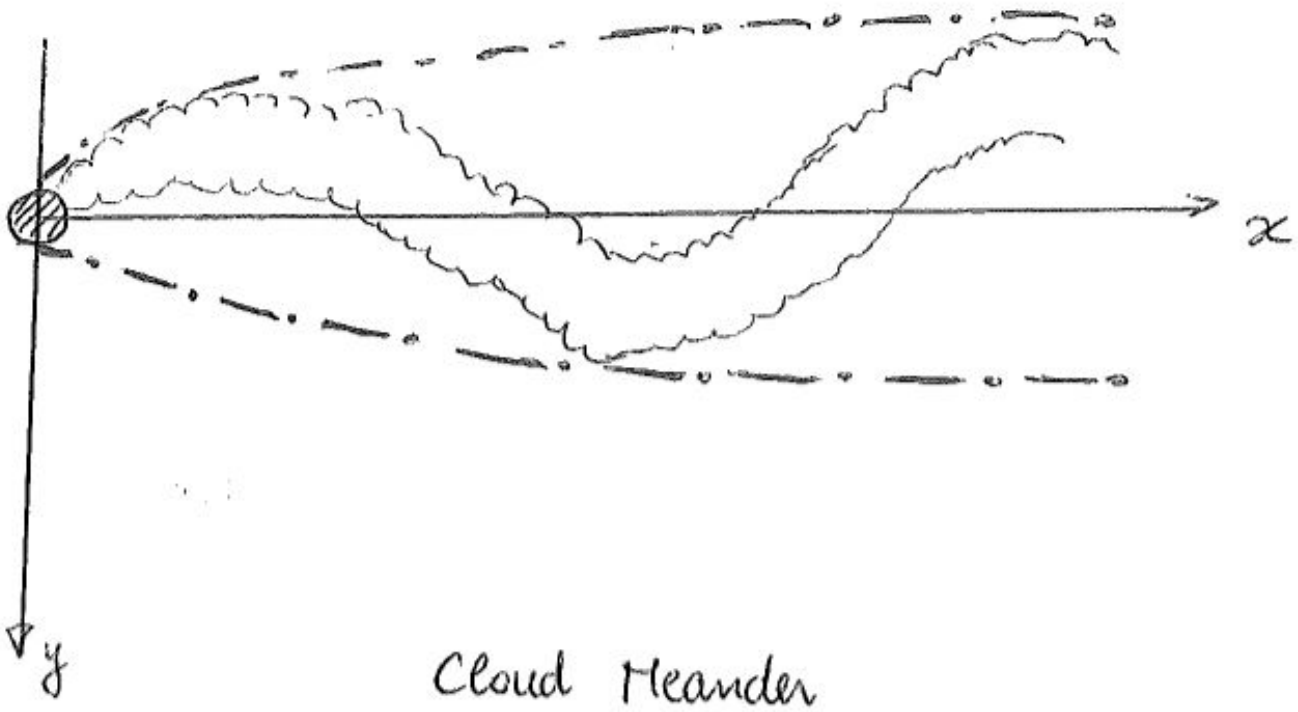
MODEL ORGANIZATION

The calculation of the time-averaged concentration is conducted in 2 steps:

1) The effective cloud width, which includes the increase due to cloud meander, is determined. (N.B.: instantaneous cloud width does not include the effect of cloud meander, which is the non-stationary displacement in the cross-wind direction). The amount of increase in width depends on the duration of averaging time, the duration of release and the instantaneous cloud width
2) The time averaged concentration is calculated from the "new" concentration distribution, which includes the effect of cloud meander in the effective cloud width.

MODEL ORGANIZATION

Cloud meander effect



GOVERNING EQUATIONS
Steady state plume mode

The steady state plume mode of SLAB is based on the steady state crosswind-averaged conservation equations of mass, momentum, energy and species,

It uses the air entrainment concept to account for turbulent mixing of the gas cloud with the surrounding atmosphere, as shown in the figure in the following page.

Species

$$(\rho U B h m)' = \rho_s W_s B_s, \quad \text{where} \quad (\,)' = d(\,)/dz \quad , \tag{1}$$

Mass

$$(\rho U B h)' = \rho_a (V_e h + W_e B) + \rho_s W_s B_s \quad , \tag{2}$$

Energy

$$(\rho U B h C_p T)' = \rho_a (V_e h + W_e B) C_{pa} T_a + \rho_s W_s B_s C_{ps} T_s + f_{pc} + f_t \quad , \tag{3}$$

X-Momentum

$$(\rho U B h U)' = -0.5 \alpha_g g \left[(\rho - \rho_a) B h^2\right]' + \rho_a (V_e h + W_e B) U_a + f_u \quad , \tag{4}$$

Y-Momentum

$$(\rho U B h V_g)' = g(\rho - \rho_a) h^2 + f_{vg} \quad \text{(Grounded Cloud)} \quad , \tag{5a}$$

$$\text{or} \quad V_g = 0 \quad \text{(Lofted Cloud)} \quad , \tag{5b}$$

Z-Momentum

$$(\rho U B h W_c)' = -g(\rho - \rho_a) B h + f_w \quad \text{(Lofted Cloud)} \quad , \tag{6a}$$

$$\text{or} \quad W_c = -V_g \cdot Z_c / B \quad \text{(Grounded Cloud)} \quad , \tag{6b}$$

GOVERNING EQUATIONS
Steady state plume mode

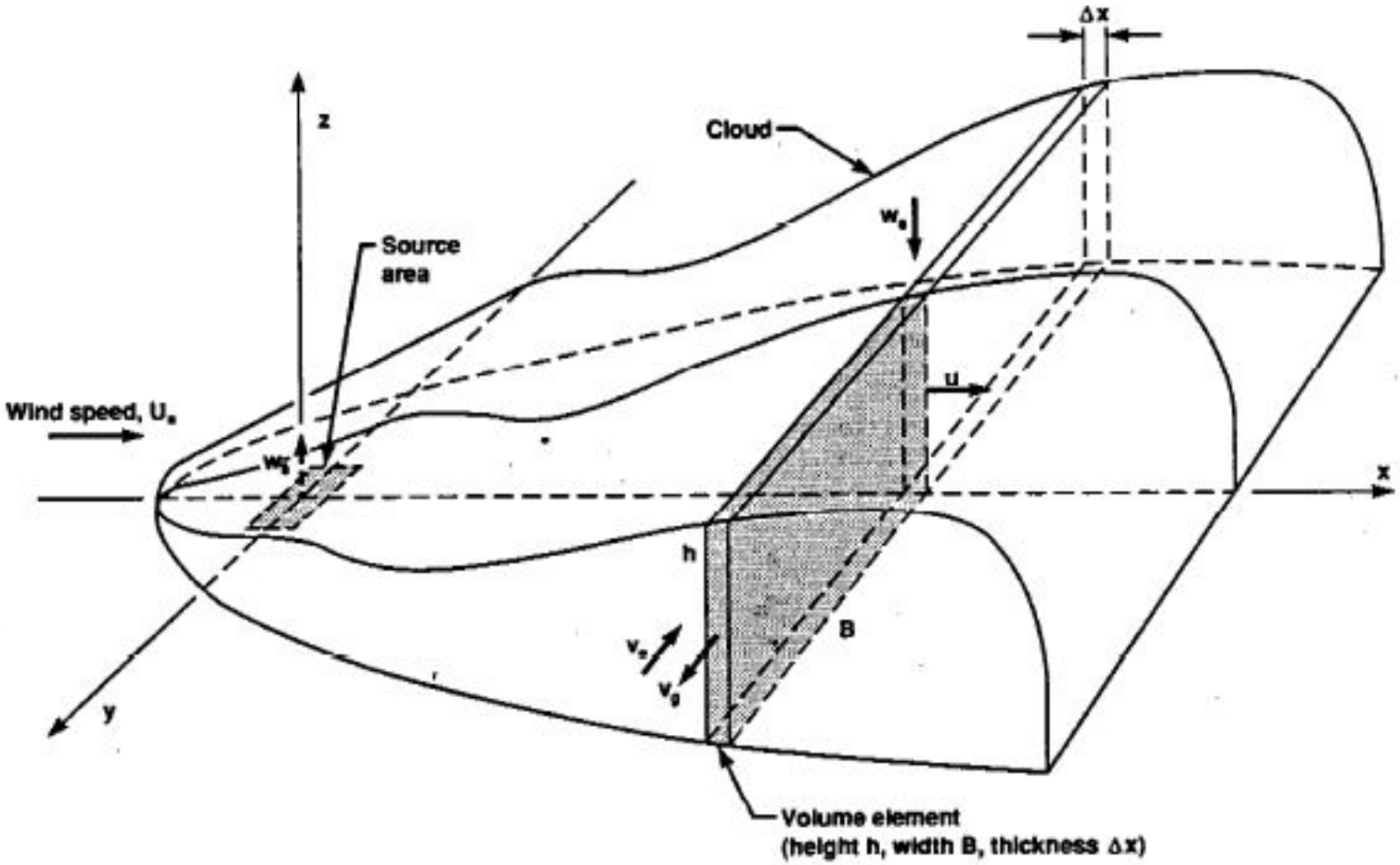
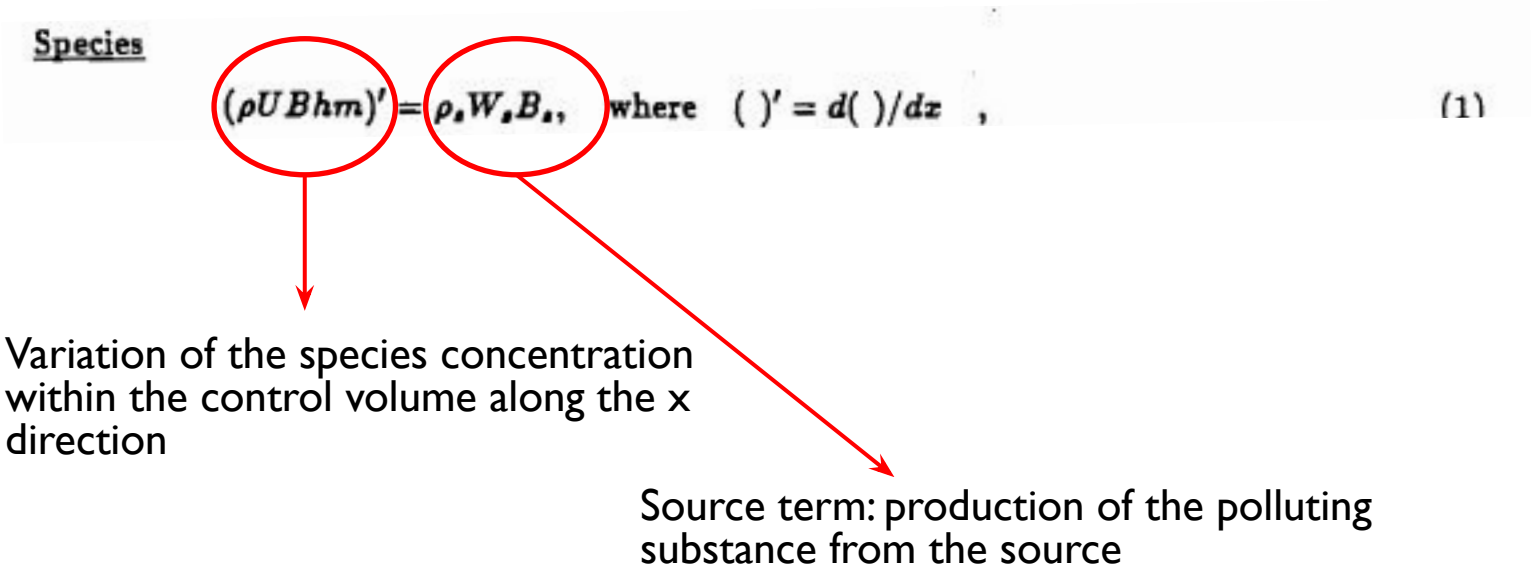


Figure 3. Dispersing heavy gas cloud, as depicted by SLAB in the plume dispersion mode.

GOVERNING EQUATIONS
Steady state plume mode

Conservation of species (only one species of pollutant is considered)



ρ = Density

U=x-velocity

W = z-velocity

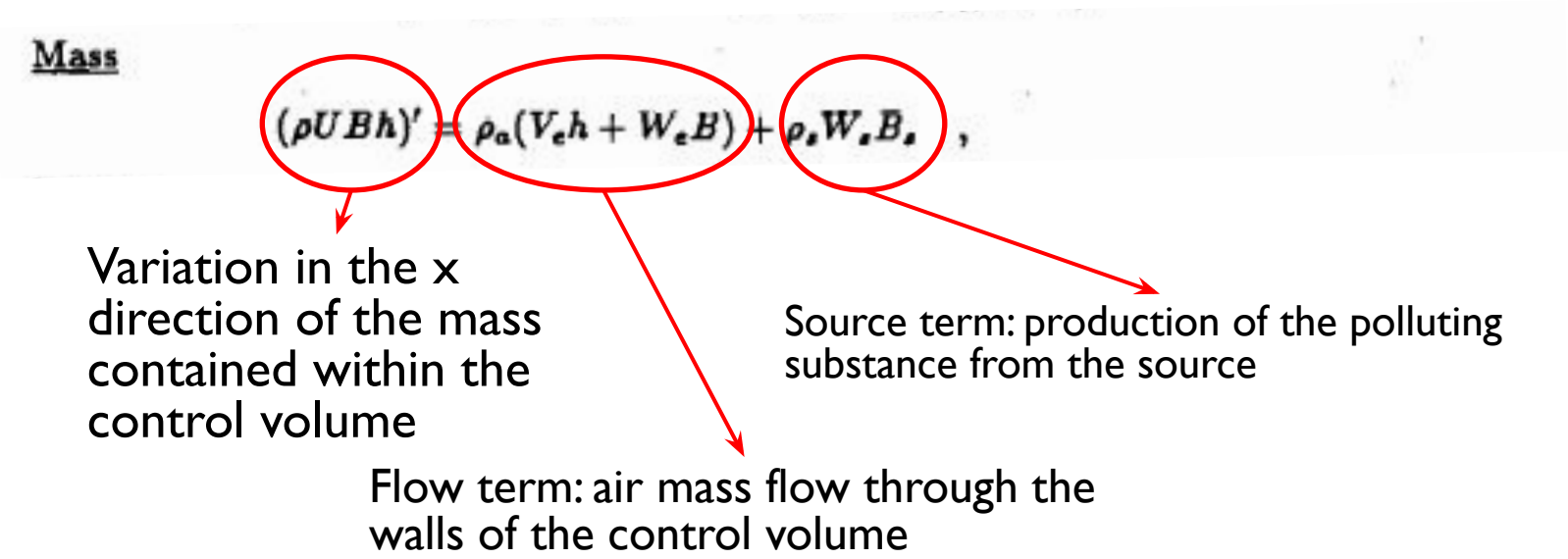
B=width

h = height

s = source

GOVERNING EQUATIONS
Steady state plume mode

Conservation of mass



ρ = Density

U=x-velocity

V = y-velocity, W= z-velocity

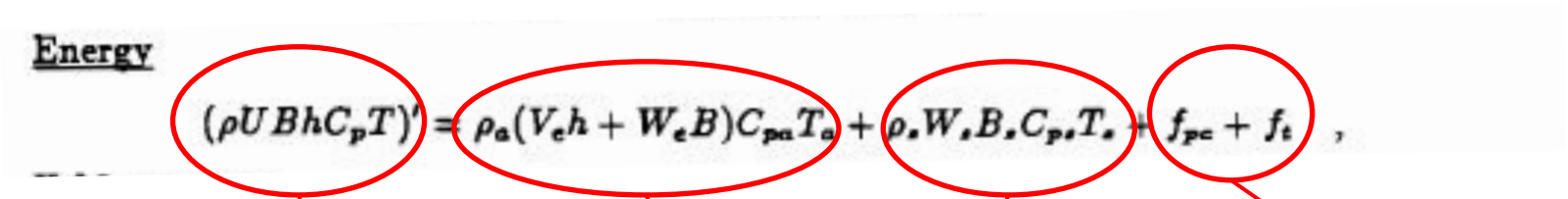
B=width

h = height

s = source , e= external

GOVERNING EQUATIONS
Steady state plume mode

Conservation of energy



Variation in the x direction of the energy content of the control vo

Flow term: energy exchanged through the walls of the control volume by air entering and exiting

Source term: heat from the source

Phase change energy and ground heat flow

Cp = specific heat capacity

T = temperature

a = air

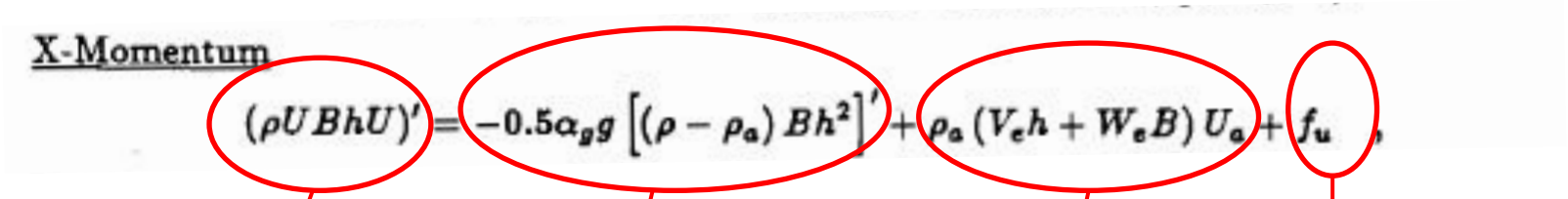
s=source

pc= phase change

t = terrain

GOVERNING EQUATIONS
Steady state plume mode

Conservation of momentum



Variation of the control volume momentum in the x direction

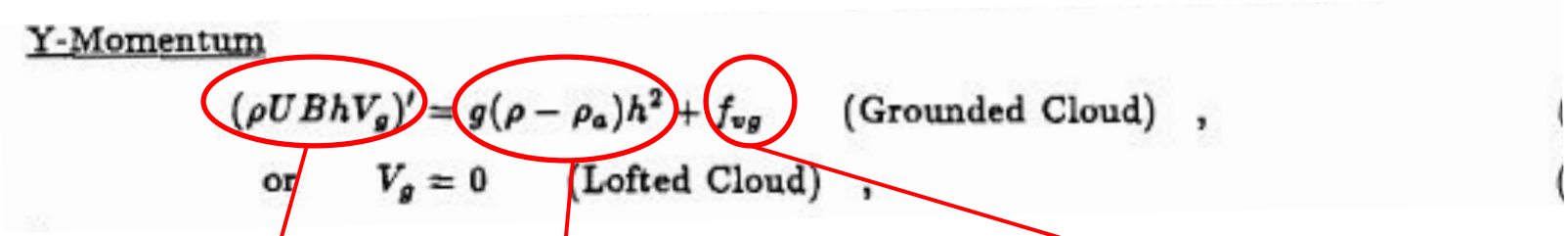
Buoyancy term

Flow of momentum through external walls of the control volume

Downwind friction term

GOVERNING EQUATIONS
Steady state plume mode

Conservation of momentum



Crosswind friction term

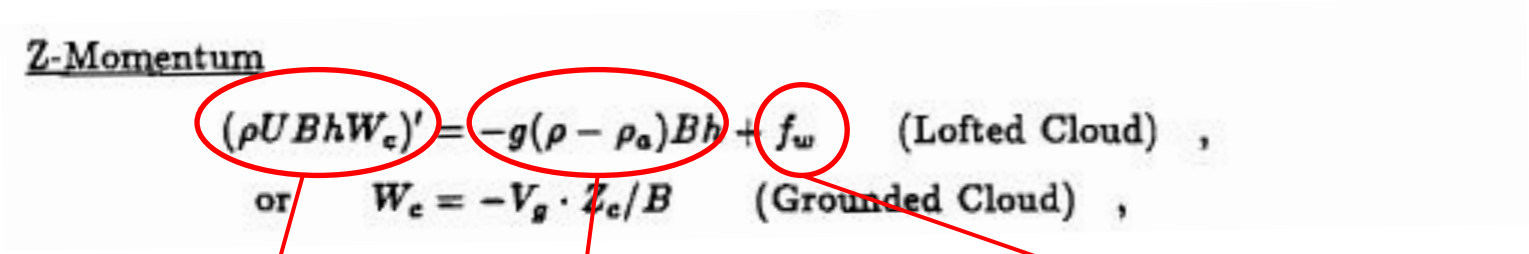
Variation of the control volume momentum in the y direction

Buoyancy term

The equations are different for lofted cloud or grounded cloud

GOVERNING EQUATIONS
Steady state plume mode

Conservation of momentum



Friction term

Variation of the control volume momentum in the z direction

Buoyancy term

GOVERNING EQUATIONS

Steady state plume mode

In a horizontal jet release, the source velocity term Ws = 0 (in the z direction) everywhere. The jet is treated as an elevated area source pointing in the downwind direction with the jet center located at the downwind distance x = 1m and z = hs.

In a vertical jet release the source is treated as an elevated area source pointing upwards with x = y = 0 and z = hs.

The plume rise portion of the cloud dispersion is calculated in a separate submodel .

In the steady state plume region, gravitational falling of the plume occurs if the cloud is denser than air and it is elevated above ground.

GOVERNING EQUATIONS
Steady state plume mode

The solution of the governing equations is divided into two regions for the evaporating pool release. These regions are the source region, where Ws > 0 (vertical jet velocity) and the near field steady state region beyond the source where Ws = 0.

The reason for this separation is that gravity spread of the denser-than-air cloud manifests differently in the two regions.

GOVERNING EQUATIONS
Transient puff mode

The transient puff mode of SLAB is based upon the volume-averaged conservation equations of mass, momentum, energy and species;

As before, it uses the air entrainment concept to account for turbulent mixing of the cloud with the surrounding atmosphere

The cloud is treated as a puff (see next page) and the independent variable is the downwind travel time t of the puff center of mass

GOVERNING EQUATIONS
Transient puff mode

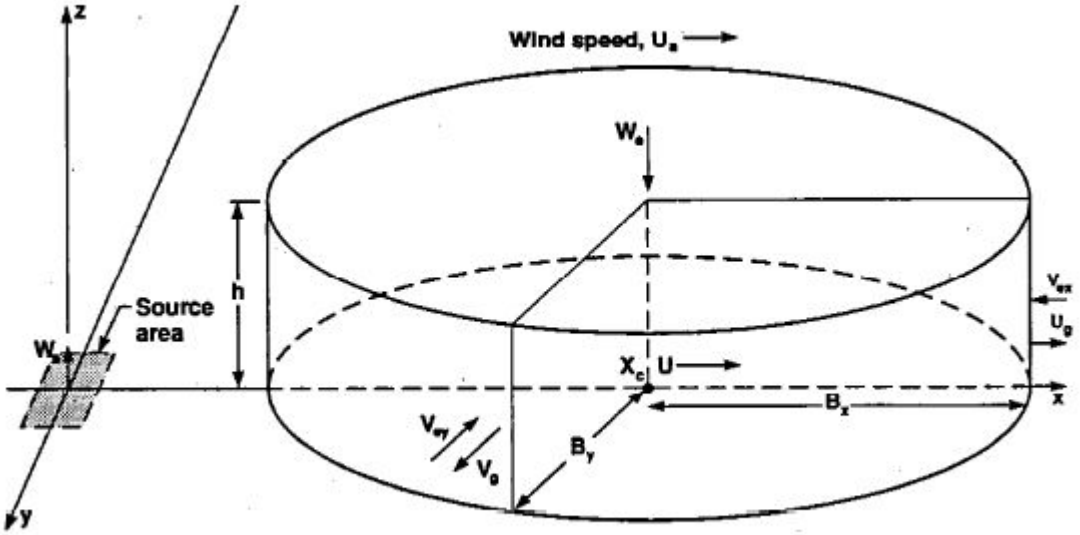


Figure 4. Dispersing heavy gas cloud as depicted by SLAB in the puff dispersion mode.

GOVERNING EQUATIONS
Transient puff mode

Species

$$\left(\rho B_x \dot{B}_y h m\right) = \rho_s W_s B_s^2 \quad , \text{ where } \quad (\dot{}) = d(\ )/dt \quad , \tag{15}$$

Mass

$$\left(\rho B_x \dot{B}_y h\right) = \rho_a \left[\left(V_{cx} B_y + V_{cy} B_y\right) h + W_c B_x B_y\right] + \rho_s W_s B_s^2 \quad , \tag{16}$$

Energy

$$\left(\rho B_x \dot{B}_y h C_p T\right) = \rho_a \left[\left(V_{cx} B_y + V_{cy} B_x\right) h + W_c B_y\right] C_{pa} T_a + \rho_s W_S B_s^2 C_{ps} T_s + B_x \left(f_{pc} + f_t\right) \quad , \tag{17}$$

X-Momentum (Translation)

$$\left(\rho B_x \dot{B}_y h U\right) = \rho_a \left[\left(V_{cx} B_y + V_{cy} B_x\right) h + W_c B_x B_y\right] U_a + B_x f_u \quad , \tag{18}$$

X-Momentum (Gravity Flow)

$$\left(\rho B_x \dot{B}_y h U_g\right) = g\left(\rho - \rho_a\right) h^2 B_x + B_x f_{vg} \qquad \text{(Grounded Cloud)} \quad , \tag{19a}$$

$$\text{or} \qquad U_g = 0 \qquad \text{(Lofted Cloud)} \quad , \tag{19b}$$

Y-Momentum

$$\left(\rho B_x \dot{B}_y h V_g\right) = g\left(\rho - \rho_a\right) h^2 B_y + B_x f_{vg} \qquad \text{(Grounded Cloud)} \quad , \tag{20a}$$

$$\text{or} \qquad V_g = 0 \qquad \text{(Lofted Cloud)} \quad , \tag{20b}$$

Z-Momentum

$$\left(\rho B_x \dot{B}_y h W_c\right) = -g\left(\rho - \rho_a\right) h B_x B_y + B_x f_w \qquad \text{(Lofted Cloud)} \quad , \tag{21a}$$

$$\text{or} \qquad W_c = -\left(V_g / B_y - U_g / B_x\right) Z_c \qquad \text{(Grounded Cloud)} \quad , \tag{21b}$$

Center-of-Mass

$$\dot{X}_c = U - \left(\rho_s W_s B_s^2 X_c / \rho B_x B_y h\right) \quad , \tag{22}$$

Half-width Equations

$$\dot{B}_y = \left(\rho_a / \rho\right) V_{cy} + V_g \quad , \tag{23}$$

$$\dot{b}_y = V_g \cdot b_y / B_y \quad , \tag{24}$$

GOVERNING EQUATIONS
Transient puff mode

The equations for the puff mode differ from those in the plume mode for the fact that the variation of the mass, energy, momentum and species is a variation with time instead of a variation with the x direction.

This is because in the puff mode the system is no more stationary, but it proceeds forward in the space changing its position and its volume with time.

Equation 22 in fact describes the position of the cloud center of mass in function of its geometry and of the source term.

GOVERNING EQUATIONS
Transition from plume to puff mode

The puff dispersion mode can be entered:

at the beginning of a simulation by specifying an instantaneous or short duration evaporating pool source;

Or in the middle of a simulation after the release is completed and the steady state period is over.

In the latter case there is a transition in the calculation of the spacially-averaged cloud properties from the steady state plume equations to the transient puff equations.

In the plume mode the equations are averaged over the crosswind plane of the cloud

In the puff mode they are averaged over the cloud volume.

GOVERNING EQUATIONS
Transition from plume to puff mode

To begin the puff mode calculation it is necessary to define the time of this transition and the cloud length and the center of mass at this time.

The transition time is taken to occur at the end of the release, when t = t_sd.

The downwind location of the cloud center of mass Xc(t_sd) is obtained by calculating the total mass of the released material within the cloud as a function of downwind distance. The cloud center of mass is taken to be the downwind location at which the mass of released material from the upwind edge to the center of mass is equal to ½ of the total amount of material released.

GOVERNING EQUATIONS

Cloud length and time dependence in the plume mode

The approach taken in the previous section for the calculation of the cloud center of mass and half length at the transition plume-puff can be extended to a calculation of the properties for any time during the release, $0<t<t_{sd}$.

The cloud center of mass is defined as the downwind distance at which the mass of released material from the upwind edge to the center of mass is equal to ½ the material released during time t.

GOVERNING EQUATIONS
Solution of the dispersion equations

The basic model equations can be solved by direct numerical integration of the equations as given in the previous subsections.

However, analytic solutions to some of these equations can be obtained by rearranging the equations and defining new variables.

This approach is used in SLAB since it presumably will provide more accurate results.

GOVERNING EQUATIONS
Ambient velocity profile

The ambient wind velocity profile is derived from the following assumed gradient:

$$\frac{dU_a}{dz} = \frac{U_{a*}}{kz} \cdot \Phi_m(z/L) \cdot g(z/H)$$

Where Ua is the ambient wind velocity, Ua* the ambient friction velocity, k=0.41, z is height L is length, H is the height of the mixing layer.

Φm is the momentum function and g(z/H) is a mixing layer function

These velocity profiles are used in the previous equations.

GOVERNING EQUATIONS
Entrainment rates

The vertical entrainment rate includes the effects of surface friction, differential motion between air and cloud, thermal convection due to ground heating, damping of air-cloud mixing due to stable density stratification within the cloud.

The formula used in SLAB is based on experimental data from several sources.

GOVERNING EQUATIONS
Heat and momentum flux terms

The flux terms are adapted from Zeman (1982).

The thermal flux at ground is given by

$$f_t = \rho \cdot B \cdot V_H \cdot C_p \cdot (T_g - T)$$

The downwind velocity flux is defined to be

$$f_u = -\rho \cdot B \cdot \left\{ C_f^2 \cdot \left[(U - \delta U)^2 - \overline{U}_a^2 \right] + C_g \cdot \delta U^2 \right\}$$

The crosswind velocity flux is also composed of a ground friction term and is defined as

$$f_v = -0.25\rho \cdot B \left[C_f^2 + C_g \cdot (\rho_a/\rho)^2 \right] V_g^2 \quad .$$

GOVERNING EQUATIONS
Thermodynamic model

Liquid droplets formation and evaporation is governed by an equilibrium thermodynamic model in SLAB.

Two species are allowed to form droplets: the ambient water vapor that enters the cloud and the released emission within the cloud.

The governing equations are:

- the mass conservation equation for the released material
- additional mass conservation equations for the dry air, total water and the liquid-vapor fractions of water and emission
- the energy conservation
- the equation of state for a liquid droplet-vapor mixture
- the equilibrium condition that controls the liquid-vapor ratio for each species.

GOVERNING EQUATIONS
Plume rise

The plume from a vertical jet or stack release initially rises until a maximum plume height is attained.

In SLAB the plume rise region is obtained from the results of wind tunnel and field experiments.

Three types of jet are considered:

- denser than air jets ($\rho s > \rho a$)
- momentum jets ($\rho s = \rho a$)
- buoyant jets ($\rho s < \rho a$)

TIME AVERAGED CONCENTRATIONS

All of the SLAB results (concentration, cloud width …) represent ensemble averages.

An ensemble average is an average over numerous experiments under the same conditions.

In a dispersion experiment these conditions are the spill terrain, and meteorological conditions.

Since the model predicted concentration is an ensemble average, it may be greater than or less than the measured concentration.

The situation is depicted in the next page, where the instantaneous concentration at time t and downwind distance x is compared with the ensemble average.

TIME AVERAGED CONCENTRATIONS

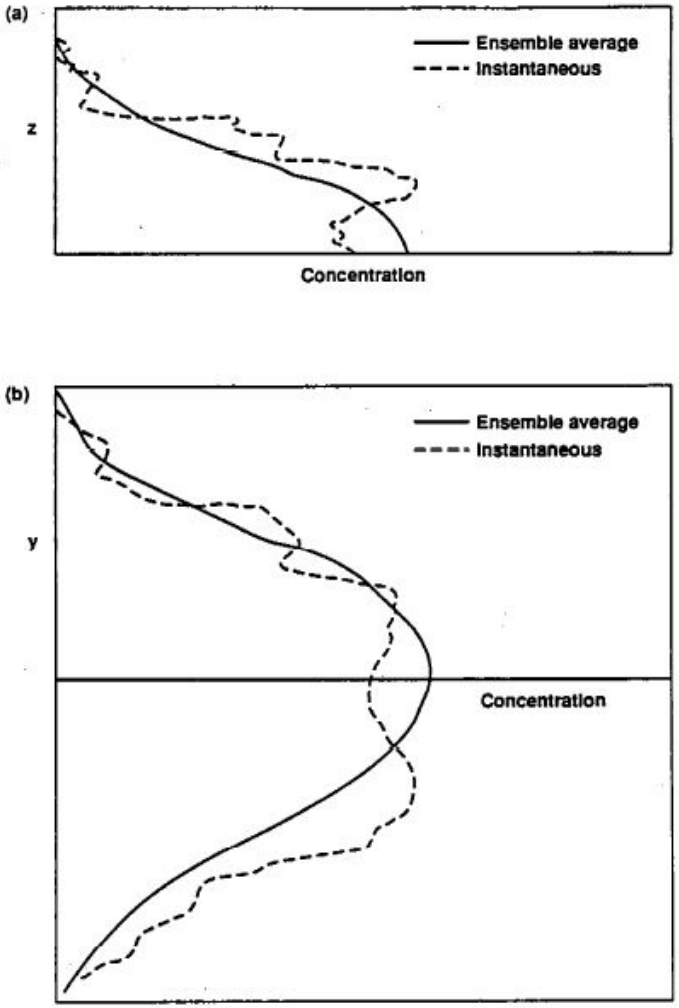


Figure 8. Comparison of the instantaneous concentration at time t with the ensemble average; (a) vertical profile and (b) horizontal profile.

TIME AVERAGED CONCENTRATIONS

in addition to the ensemble average, SLAB uses two other average types:

- **Spatial averages** which are used in the dispersion equations to simplify them.
- **Time averages** which are averages taken at a particular location (x,y,z) over a duration of time t_av, called concentration averaging time.

The reason for time averaging is that safety levels for hazardous chemicals are generally expressed as a maximum allowable average concentration level for a given time exposure.

In SLAB the concentration averaging time is an input data.

Cloud meander

Cloud meander is the random oscillation of the cloud centerline about the mean wind direction as shown in the next image.

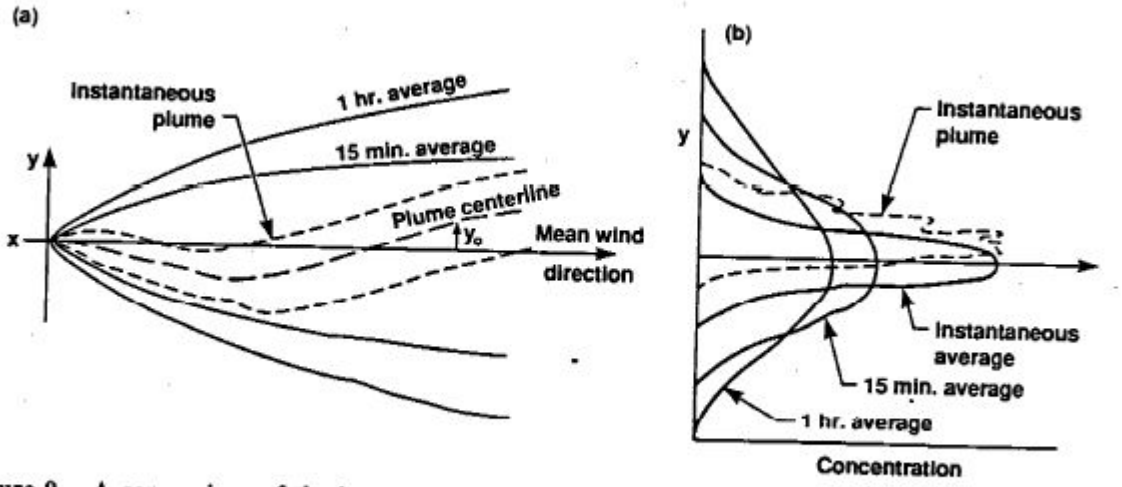


Figure 9. A comparison of the instantaneous plume with several time averages; (a) the plume as observed from above and (b) the crosswind concentration distribution.

Cloud meander

When the cloud concentration os averaged over time, the effective width of the cloud appears to be wider due to the wandering of the cloud centerline.

In addition, the mean cloud concentration decreases in the region about the mean centerline.

Empirically, it has been found that the effective width of the cloud increases as the concentration averaging time is increased (see figure in previous page)

Cloud meander

In SLAB code solution to the dispersion equations, the cloud meander is ignored and the cloud is assumed to travel in a straight line.

Consequently, in terms of time averaging, these results are the "instantaneous" average obtained in absence of cloud meander.

To include the effects of cloud meander the "instantaneous" average cloud needs to be modified to include the cloud width due to the displacement y0 (see figure) of the meandering cloud centerline about the mean wind direction.

Time averaged volume concentration

With the determination of the effective cloud half width for the concentration averaging time t_av, the calculation of the time-averaged cloud properties is easily accomplished.

In SLAB, the only calculated time-averaged property is the volume concentration expressed as the volume fraction with values from 0 to 1.

The time averaged volume concentration C_tav is obtained by averaging the cloud volume concentration C(x,y,z,t) including meander effects.

$$C_{tav} = \frac{1}{t_{av}} \int_{t_{pk}-\frac{1}{2}\cdot t_{av}}^{t_{pk}+\frac{1}{2}\cdot t_{av}} dt \cdot C(x,y,z,t) \quad ,$$

Where t_pk is the time of peak concentration.

SLAB
User's guide

General information

SLAB is implemented in the Fortran 77 language.

SLAB operates by acquiring an input data file named INPUT containing the input parameters.

A SLAB problem may consist of a single run or several runs where metereologic conditions can vary while the remainder of the spill scenario is the same.

SLAB produces as output a file named PREDICT containing the output from a single problem which may include one or more SLAB runs.

Input file

There are 30 possible input parameters required to run in SLAB.

Such parameters include the source type, source properties, spill properties, field properties, meteorological parameters and a numerical substep parameter.

These input parameters define uniquely the problem.

The table in the next page lists the input parameters.

Input file

Table 1. Definition of input variables.

Source Type and Numerical Substep Parameter

—IDSPL Spill source type
- 1—evaporating pool release
- 2—horizontal jet release
- 3—vertical jet or stack release
- 4—instantaneous or short duration evaporating pool release

—NCALC Numerical substep parameter

Source Properties

—WMS Molecular weight of source material (KG)
—CPS Vapor heat capacity at constant pressure (J/KG-°K)
—TBP Boiling point temperature (°K).
—CMEDO Initial liquid mass fraction
—DHE Heat of vaporization (J/KG)
—CPSL Liquid heat capacity (J/KG-°K)
—RHOSL Liquid density of source material (KG/M3)
—SPB Saturation pressure constant (Default: SPB = −1.0)
—SPC Saturation pressure constant (Default: SPC = 0.0)

Spill Parameters

—TS Temperature of source material (°K)
—QS Mass source rate (KG/S)
—AS Source area (M2)
—TSD Continuous source duration (S)
—QTIS Instantaneous source mass (KG)
—HS Source height (M)

Field Parameters

—TAV Concentration averaging time (S)
—XFFM Maximum downwind distance (M)
—ZP(I) Heights of concentration calculation (M); I = 1, 4

Meteorological Parameters

—ZO Surface roughness height (M)
—ZA Ambient measurement height (M)
—UA Ambient wind speed (M/S)
—TA Ambient temperature (°K)
—RH Relative humidity (percent)
—STAB Stability class values

Class	Value	Description
A-F	1.0–6.0	Unstable-Stable
Default	0.0	Input "ALA" for stability

Source type and numerical substep parameter

IDSPL – Spill source type

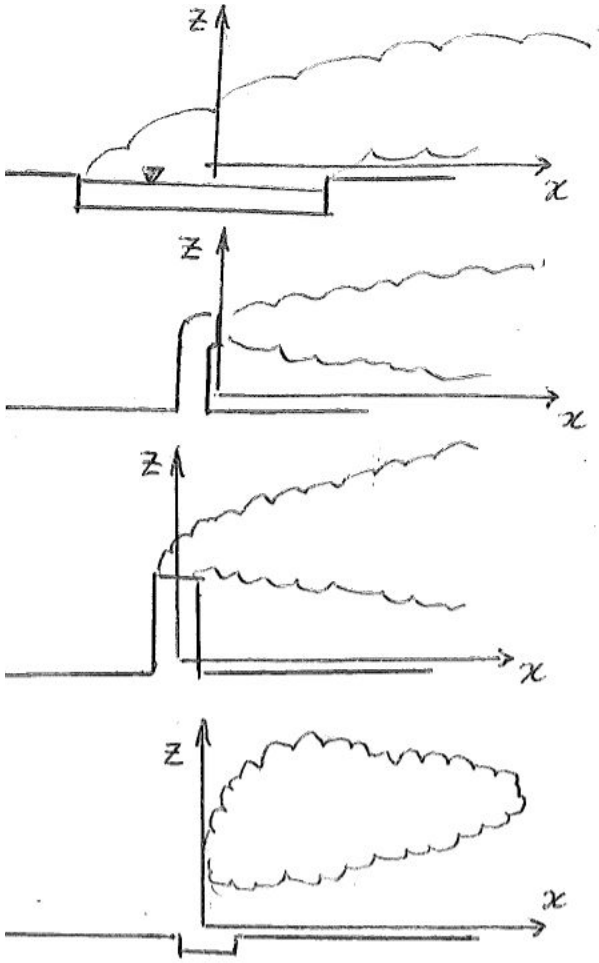
SLAB has 4 types of sources identified by the integer 1 – 4.

1) Evaporating pool release
2) Horizontal jet release
3) Vertical jet or stack release
4) Instantaneous or short duration evaporating pool release

These 4 kinds of sources are schematized in the next figure 5.

Source type and numerical substep parameter

Figure 5



1- Evaporating pool

2- Horizontal jet

3- Vertical jet

4- Instantaneous or short duration evaporating pool release

Figure 5: types of sources

Source type and numerical substep parameter

The **evaporating pool** is a ground level area source of finite duration TSD. The source is located at the axes origin.

When the spill duration is short enough a steady state plume will not form.

In this case the code automatically stops and redefines the source type to "short duration evaporating pool release (IDSPL = 4).

The **horizontal jet** release is an area source with jet center located at x=1, y=0, z=HS.

The initial mass fraction is 1.0 with the initial liquid mass fraction specified by the input parameter CMEDO.

The initial vapor mass fraction is thus 1 – CMEDO.

Source type and numerical substep parameter

The **vertical jet** release is an area source with source plane parallel to the ground and source velocity pointing upward.

The same considerations as the horizontal jet can be done for the mass fraction.

The **instantaneous or short duration evaporating pool** release is a combination of two sources: an instantaneous volume source with a total mass given by the parameter QTIS and a short duration, ground level area source with a source rate and a spill duration given by the input parameters QS and TSD respectively.

When an instantaneous volume release is simulated, QTIS is specified and QS and TSD are set to zero.

Source type and numerical substep parameter

In SLAB the pressure within the cloud is always 101325 Pa. If an explosion is to be simulated the SLAB calculation begins after the source is fully expanded to atmospheric pressure.

It is recommended that an evaporating pool release of any finite duration be run in the source type parameter with IDSPL = 1.

If the steady state cloud is not achieved, the code will turn automatically into IDSPL = 4.

Source type and numerical substep parameter

The parameter NCALC is an integer substep multiplier that specifies the number of calculation sub-steps performed during the integration of the conservation equations.

A value of NCALC=1 is generally recommended to provide computational stability and sufficient numerical accuracy

However, if stability problems rise, the value of NCALC can be increased.

Source properties

WMS = molecular weight of the source material [kg]

CPS = vapor heat capacity at constant pressure [J/kgK]

TBP = boiling point temperature of source material [K]

CMEDO = Initial liquid mass fraction

The emission is assumed to be the pure substance with a fraction CMEDO in liquid phase in the form of liquid droplets; the remainder (1 – CMEDO) is in the vapor phase.

Source properties

DHE = heat of vaporization at the boiling point temperature[J/kg]

CPSL = liquid specific heat of the source material[J/kgK]

RHOSL = liquid density of source material [kg/m3]

SBP-SPC = saturation pressure constants

The saturation pressure constants are used in the following formula for the saturation pressure

$$P_{SAT} = P_A \cdot \exp\left[\mathrm{SPA} - \mathrm{SPB}/(\mathrm{T} + \mathrm{SPC})\right]$$

Where PA is ambient pressure and T the local temperature.

Source properties

Some examples of substances are here provided

Table 2. Material properties in SI units for use in the SLAB code (see text for definition of parameters).

Name	Formula	WMS (kg)	CPS (J/kg-°K)	TBP (°K)	DHE (J/kg)	CPSL (J/kg-°K)	RHOSL (kg/m^3)	SPB —	SPC °K	γ —
Methane	CH_4	.016043	2240.	111.66	509880.	3349.	424.1	597.84	−7.16	1.305
Ethane	C_2H_6	.030070	1774.	184.52	489360.	—	546.5	1511.42	−17.16	1.192
Vinyl Cloride	C_2H_3Cl	.062499	857.7	259.35	357290.	1255.	972.	1803.85	−43.15	—
Ethylene Oxide	C_2H_4O	.044054	1121.	283.66	579450.	1954.	872.	2507.61	−29.01	—
Propylene	C_3H_6	.042081	1482.	225.45	437680.	2176.	513.9	1807.55	−26.15	1.154
Propane	C_3H_8	.044097	1678.	231.09	425740.	2520.	500.5	1872.46	−25.16	1.142
Phosgene	$COCl_2$	.098916	583.3	280.71	246680.	1017.	1371.4	2167.33	−43.15	—
Chlorine	Cl_2	.070906	498.1	239.10	287340.	926.3	1574.	1978.34	−27.01	1.308
Hydrogen Cyanide	HCN	.027026	1444.	298.85	933000.	2608.	679.7	2585.80	−37.15	1.31
Hydrogen Fluoride	HF	.020006	1450.	292.67	373200.	2528.	957.	3404.51	+15.06	—
Hydrogen Sulfide	H_2S	.034076	1004.	212.81	547980.	2010.	960.	1768.71	−26.06	1.33
Ammonia	NH_3	.017031	2170.	239.72	1370840.	4294.	682.8	2132.52	−32.98	1.307
Nitrogen Tetroxide	N_2O_4	.092011	796.5	294.30	414250.	1540.	1446.9	4141.29	+3.65	—
Sulfur Dioxide	SO_2	.064063	622.6	263.13	386500.	1331.	1462.	2302.35	−35.97	1.29

Spill parameters

TS = temperature of the source material

When the release is an evaporating pool, the source temperature is the boiling point temperature TBP.

When the release is instantaneous (IDSPL=4) and the source is the result of an explosion, TS is the temperature of the material after it has fully expanded.

For a pressurized jet release (IDSPL=2 or 3), TS is the temperature of the material after it has fully expanded.

The source temperature is then given by the formula

$$TS = (1/\gamma) \cdot [1 + (\gamma - 1) \cdot (P_a/P_{st})] \cdot T_{st}$$

GAMMA = Cp/Cv

Pst and Tst the storage pressure and temperatures

Spill parameters

QS = mass source rate [kg/s]4

For an instantaneous release, the QS value should be set to zero.

AS = source area [m2]

If AS is not known, it can be calculated through the mass continuity equation:

$$AS = \frac{QS}{RHOS \cdot WS}$$

Spill parameters

TSD = continuous source duration [s]

This parameter specifies the duration of the release from an evaporating pool, (IDSPL=1 or 4) or jet (IDSPL = 2 or 3) source.

When an instantaneous release is to be simulated, TSD =0.

QTIS = instantaneous source mass [kg]

This is the total mass of the instantaneous release. For an evaporating pool or jet should be equal to zero.

HS = source height [m]

For a pool, HS=0

For horizontal jet is the height at jet center

For an instantaneous release, the source area AS multiplied by the height HS is equal to the total volume released.

Field parameters

TAV = concentration averaging time [s]

The concentration averaging time is the appropriate averaging time for the safety standard of interest. E.G. if the safety standard of interest for a particular material is a maximum average concentration of 100 ppm for a 1h exposure, then TAV=3600 s.

Care should be taken when TAV is greater than the cloud duration TCD. In this case the average concentration will be reduced since the puff is relatively short and the observer is exposed to the material for only a fraction of the concentration averaging time.

In this case, a more meaningful TAV value to use might be one that is less or equal to the cloud duration.

Field parameters

XFFM=maximum downwind distance [m]

This is the maximum downwind (x) distance for which the user is interested in knowing the cloud concentration.

In steady state plume mode, the simulation is conducted to a downwind distance equal to XFFM. However, in the transient puff dispersion mode, time is the independent variable rather than distance.

Then, in puff mode the simulation is conducted to a downwind distance a bit larger than XFFM.

ZP(I), I=1,4 = heights of concentration calculation

There are a maximum of 4 heights at which the concentration is calculated as a function of downwind distance.

Meteo parameters

ZO = surface roughness height [m]

Is generally estimated in two ways:

The first method is to extrapolate measured ambient velocity profile data under neutral stability conditions. This can be done by a least square fit to determine the friction velocity U0 and surface roughness height ZO.

The second method uses values of ZO that have been empirically determined for various ground surface conditions, as listed in the table below

Table 3. Typical values of surface roughness.

Type of surface	Surface roughness, Z_o (cm)
Smooth mud flats; ice	0.001
Smooth snow	0.005
Smooth sea	0.02
Level desert	0.03
Snow surface; lawn to 1 cm high	0.1
Lawn, grass to 5 cm	1–2
Lawn, grass to 60 cm	4–9
Fully grown root crops	14

Meteo parameters

ZA = ambient measurement height [m]

This is the height at which ambient windspeed is measured. This height should be much larger than ZO.

UA = ambient wind speed [m/s]

TA = ambient temperature [K]

RH = relative humidity [%]

Meteo parameters

STAB = stability class values

The whole numbers from 1 to 6 are used in the code to describe the ambient atmospheric stability using the standard Pasquill-Gifford stability scheme, as shown in the table below.

Table 4. Atmospheric stability scheme.

Class	Value	Description
A	1.0	Very unstable
B	2.0	Unstable
C	3.0	Slightly unstable
D	4.0	Neutral
E	5.0	Slightly stable
F	6.0	Stable
Default	0.0	Input "ALA" for stability

Meteo parameters

The classes of atmospheric stability are an method of classification of the atmospheric stability, i.e. they are a method for classifying the atmospheric turbulence.

The atmospheric turbulence is subdivided into 6 classes from A to F, where A is the most unstable and F is the most stable.

Stability class	Definition
A	Very unstable
B	Unstable
C	Slightly unstable
D	Neutral
E	Slightly stable
F	Stable

Surface wind speed	**Solar radiation intensity**			**Clouds in the night**	
m/s	Strong	Moderate	Light	> 50%	< 50%
<2	A	A - B	B	E	F
2-3	A - B	B	C	E	F
3-5	B	B - C	C	D	E
5-6	C	C - D	D	D	D
>6	C	D	D	D	D

Meteo parameters

ALA = inverse Monin-Obukhov length [1/m]

This is a stability parameter used to describe the vertical profile of ambient wind speed and the vertical turbulent diffusivity.

This option for describing atmospheric stability is activated by setting STAB=0.0. ALA is an input parameter only when STAB=0.0. Inclusion of ALA when STAB is not zero results in an error.

Meteo parameters

The Obukhov length is used to describe the effects of buoyancy on turbulent flows, particularly in the lower tenth of the atmospheric boundary layer.

The Obukhov length is defined by:

$$L = -\frac{u_*^3 \bar{\theta}_v}{kg(\overline{w'\theta'_v})_s}$$

Where

u* is the frictional velocity;

$\bar{\theta}_v$ is the mean virtual potential temperature;

$(\overline{w'\theta'_v})_s$ is the surface virtual potential temperature flux;

k is the Von Karman constant.

Input file closure

After the code has read the input and executed a run, it returns to the start of the code looking for an additional value of ZO (surface roughness height) .

If an additional value of ZO is specified, the code will look for the remaining meteo input parameters (ZA, UA, TA, RH, STAB, ALA) and executes an additional run with the new metrologicla inputs.

In this way multiple runs can be made with the same source, but different meteo conditions.

When the code looks for an additional value of ZO and finds a value minor than zero, it terminates the problem.

Thus the problem is terminated by including an additional input parameter with the value -1.

CALCULATIONAL FLOW

A SLAB model simulation can be viewed as occurring in three sequential phases: initialization, sequential calculation and time averaged concentration calculation.

The calculational flow starting with the identified source type and ending with the calculation of the time averaged concentration as shown in the figure below.

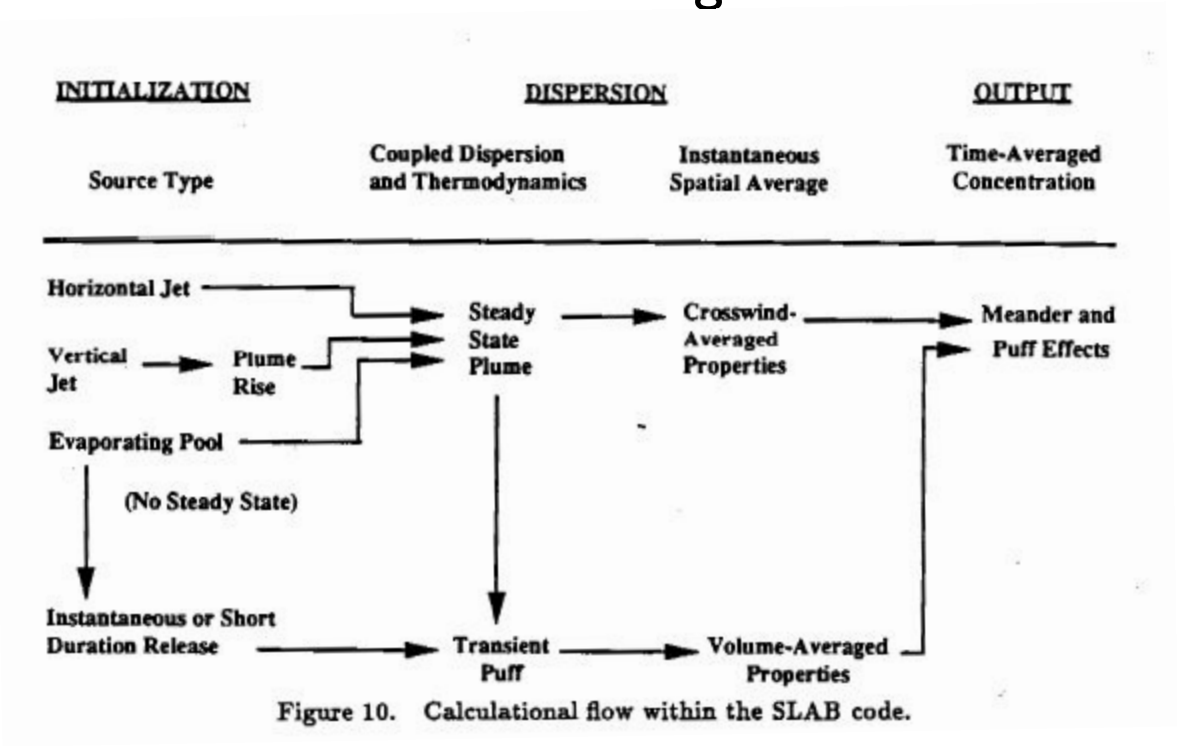


Figure 10. Calculational flow within the SLAB code.

CALCULATIONAL FLOW
Initialization

The initialization begins with the specification of the source type.

There is one case where the code overrides the specified source type, that is when "evaporating pool" is specified and the release duration is so short that a steady state cloud is not reached. In this case, the source type is switched to "instantaneous or short duration release".

CALCULATIONAL FLOW
Dispersion calculation

The dispersion phase contains the bulk of the calculation. It is here that the conservation and thermodynamic equations are solved, yielding the instantaneous (no meander) spacially averaged properties in function of downwind distance.

There are two dispersion modes: plume and puff., of which a sketch is given in the picture below

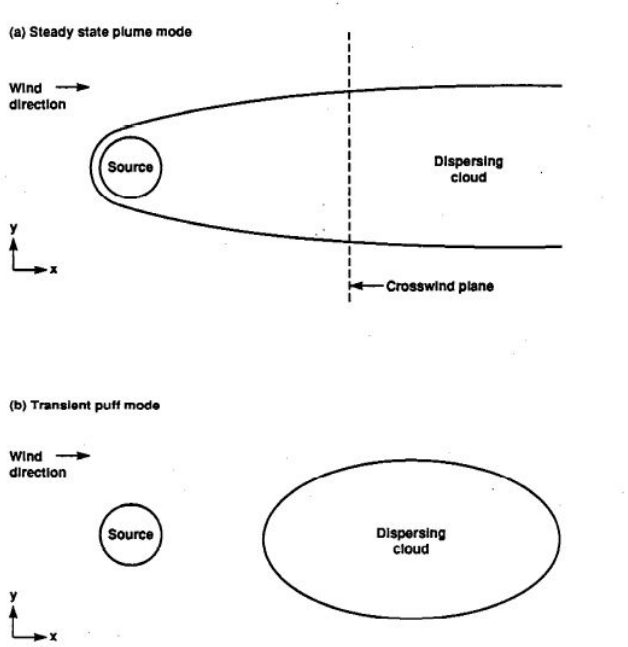


Figure 11. A dispersing cloud in the (a) steady state plume mode and the (b) transient puff mode.

CALCULATIONAL FLOW
Dispersion calculation

The steady state plume mode is used for the finite duration releases until the end of the release.

After the release is over, the transient puff mode is used for the remainder of the simulation.

The transient puff mode is also used in the case of an instantaneous release or when the release is so short that a steady state is not reached.

These two models represent two different forms of the conservation equations.

CALCULATIONAL FLOW
Dispersion calculation

In the steady state plume mode the conservation equations are spatially averaged over the cross-wind plane of the cloud, as visible in the picture at page 78.

Consequently, the resulting cloud properties are also spatially averaged over the crosswind plane.

Thus, the relation between concentration C(x,y,z) and the cross averaged concentration C(x) is given by:

$$\overline{C}(x) = \frac{1}{2Bh} \int_0^{\infty} dz \int_{-\infty}^{\infty} dy \; C(x,y,z)$$

Where B an height.

The crosswind averaged concentration is not expressed as a function of time since the plume is considered in steady state.

CALCULATIONAL FLOW
Dispersion calculation

In the transient puff mode the conservation equations are averaged over the entire volume of the cloud.

Consequently, the solution yields volume-averaged properties.

So, the relationship between the concentration C(x,y,z,t) and the volume-averaged concentration C(t) is given by:

$$\overline{C}(t) = \frac{1}{4BB_x h} \int_o^\infty dx \int_{-\infty}^\infty dy \int_{-\infty}^\infty dx \; C(x,y,z,t)$$

Where B, Bx and h are the cloud half width, half length and half height.

These parameters and the cloud center of mass are calculated along with the solution of the conservation equations.

CALCULATIONAL FLOW
Dispersion calculation

In the transient puff mode the conservation equations are averaged over the entire volume of the cloud.

Consequently, the solution yields volume-averaged properties.

So, the relationship between the concentration C(x,y,z,t) and the volume-averaged concentration C(t) is given by:

$$\overline{C}(t) = \frac{1}{4BB_x h} \int_o^\infty dx \int_{-\infty}^\infty dy \int_{-\infty}^\infty dx \; C(x,y,z,t)$$

Where B, Bx and h are the cloud half width, half length and half height.

These parameters and the cloud center of mass are calculated along with the solution of the conservation equations.

CALCULATIONAL FLOW
Time averaged concentration calculation

After the spatially-averaged cloud properties are calculated at all downwind distances, the code calculates the time averaged concentration.

In SLAB, the concentration is expressed as the volume fraction, ranging from 0 to 1.

The time-averaged volume fraction C_tav(x,y,z,t) is calculated by the spatially averaged volume fraction C(Xc,t) and the cloud height, width and length parameters.

To do this, the concentration distribution about the center of mass Xc must be assumed since C(Xc,t) does not contain this information.

SLAB uses profile distribution functions, which are functions of the calculated half width, half length and height of the cloud.

CALCULATIONAL FLOW
Time averaged concentration calculation

The calculation of the time averaged volume fraction C_tav(x,y,z,t) from the volume fraction C(x-Xc,y,z,t), involves two steps:

1) The calculation of the cloud half-width
2) The calculation of the time averaged volume fraction

The effects of the cloud meander is to increase the width of the cloud, reducing the average concentration observed in the cloud centerline region.

The longer the averaging time, the more meander can occur and the greater the increase in the effective width.

CALCULATIONAL FLOW
Time averaged concentration calculation

The time available for cloud meander at the downwind location x cannot be longer than the duration of the exposure to the cloud at the same location.

Thus, the time available for cloud meander is assumed to be equal to the concentration averaging time t_av with a maximum value equal to the cloud duration t_cd.

As a result, the cloud effective width increases monotonically with the concentration averaging time t_av until some maximum value is reached that is dependent on the length of the cloud.

With the calculation of the cloud effective half width, the time averaged volume fraction can now be determined.

The calculation of the time averaged volume fraction concludes the SLAB run.

OUTPUT FILE

The output file contains several types of information which can be grouped in 3 categories:

1) Problem description
2) Instantaneous spatially averaged cloud properties
3) Time averaged volume fraction

These categories correspond to the three sequential phases (initialization, dispersion calculation and time-averaged concentration calculation) of the SLAB code calculation.

OUTPUT FILE
Problem description

The Problem description output lists the various input parameters used by the code and thereby defines the problem to be solved.

The first group is the problem input parameter values as specified by the user.

Some input parameters (IDSPL, SPB, SPC, TS and STAB) may be changed by the code in order to be consistent with SLAB model assumptions.

OUTPUT FILE

Instantaneous spatially averaged cloud properties

The instantaneous spatially averaged cloud properties output gives the results of the dispersion calculation phase of the simulation.

These results are intermediate results in that they are the solution of the spatially averaged (plume or pluff) conservation equations, the equation of state and the length and width equations.

However they do not include the effects of cloud meander time averaging.

OUTPUT FILE

Instantaneous spatially averaged cloud properties

The table below lists the instantaneous spatially averaged parameters and identifies their units. These parameters are listed in the output in function of the x coordinate.

Table 6. Definition of the instantaneous spatially-averaged cloud parameters.

[In the steady state dispersion mode, spatial averaging is over the crosswind plane of the cloud. In the puff dispersion mode, spatial averaging is over the entire volume of the cloud.]

—X	Downwind distance (M)
—ZC	Profile center height (M)
—H	Cloud height (M)
—BB	Cloud half-width (M)
—B	Half-width parameter (M)
—BBX	Cloud half-length (M)
—BX	Half-length parameter (M)
—CV	Volume fraction of emission
—RHO	Density (KG/M3)
—T	Temperature (°K)
—U	Downwind cloud velocity (M/S)
—UA	Height-averaged ambient wind speed (M/S)
—CM	Mass fraction of emission
—CMV	Mass fraction of emission vapor
—CMDA	Mass fraction of dry air
—CMW	Mass fraction of water
—CMWV	Mass fraction of water vapor
—WC	Gravity flow velocity, Z-direction (M/S)
—VG	Gravity flow velocity, Y-direction (M/S)
—UG	Gravity flow velocity, X-direction (M/S)
—W	Vertical entrainment velocity (M/S)
—V	Crosswind horizontal entrainment velocity (M/S)
—VX	Downwind horizontal entrainment velocity (M/S)

OUTPUT FILE

Instantaneous spatially averaged cloud properties

The cloud properties listed before, are described as "instantaneous" and "spatially" averaged properties.

All of the SLAB results are ensemble average values: they represent the average taken over numerous trials under the same conditions.

In addition, these ensemble average values can be averaged over time and space.

The term "instantaneous" refers to the time averaging and indicates that the duration of the time period over which the average is taken is essentially zero.

Thus the effects of cloud meander are assumed to be absent in the "instantaneous" average.

OUTPUT FILE

Instantaneous spatially averaged cloud properties

The "spatial" averaging in SLAB is of 2 types: cross-wind and volume average.

The choice of the spatial average depends on the dispersion mode (plume or puff).

When a finite duration release is simulated, a transition occurs in the dispersion calculation as the code switches from the plume to the puff mode, with the transition occurring at the end of the release, t = TSD.

Since there is no discontinuity in the actual dispersion of the cloud at this time, the code predicted values should also maintain this continuity.

This is done in SLAB by the definition of the cloud half length at the time of the transition in the dispersion mode calculation.

OUTPUT FILE
Time averaged volume fraction

In SLAB the time averaged concentration is expressed as the time averaged volume fraction with values ranging from 0 to 1.

This is easily turned into ppm concentration multiplying by one million.

The time average volume concentration output is is presented under 3 sub titles:

1) Concentration contour parameters
2) Concentration in the Z = ZP(I) plane (height of concentration calculation)
3) Maximum centerline concentration

All of these results are presented from the point of view of an observer located at the downwind distance x, crosswind distance y and height z above the ground.

OUTPUT FILE
Time averaged volume fraction

The concentration contour parameters output lists a number of parameters from which the time-averaged volume concentration at any downwind location and time within the problem domain can be calculated.

OUTPUT FILE
Time averaged volume fraction

The concentration in the Z=ZP(I) plane gives the the time averaged volume concentration in the horizontal plane at the height ZP(I) above ground.

Up to four planes can be selected by the user, all of which are specified in the input.

In the output, concentration is listed in function of downwind distance x.

At each downwind distance, the time of maximum concentration, cloud duration and effective cloud half-width is given.

OUTPUT FILE
Time averaged volume fraction

The final result is the maximum centerline concentration.

Here the maximum time averaged volume concentration along the cloud centerline is given as a function of the downwind distance x and the height Z_pk at which the maximum occurs.

Generally, Z_pk = 0 except when the source is elevated or the cloud becomes positively buoyant and begins to loft.

In the output, at each specified downwind location, the code lists the height at which the maximum occurs, the maximum time averaged volume concentration expressed as a volume fraction from 0 to 1, the time of maximum concentration and the cloud duration.

CONCLUDING REMARKS

Two cautions are given regarding the use of SLAB predicted values of the time-averaged concentration.

1) The comparison of the model predictions with safety standards for a hazardous material
2) The comparison of model prediction with actual experiments.

Safety standards are given as a maximum average concentration for a specified exposure duration.