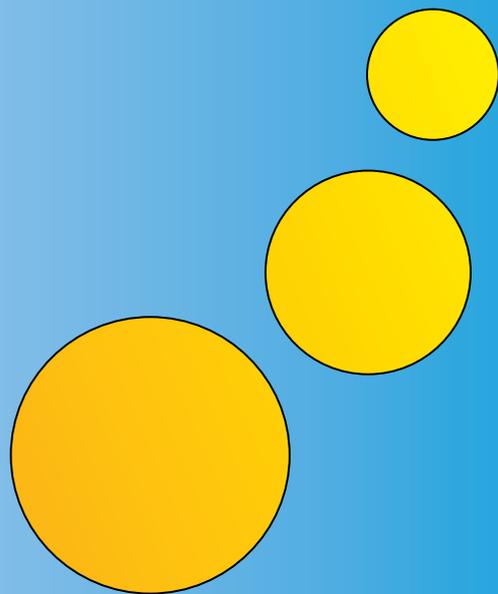
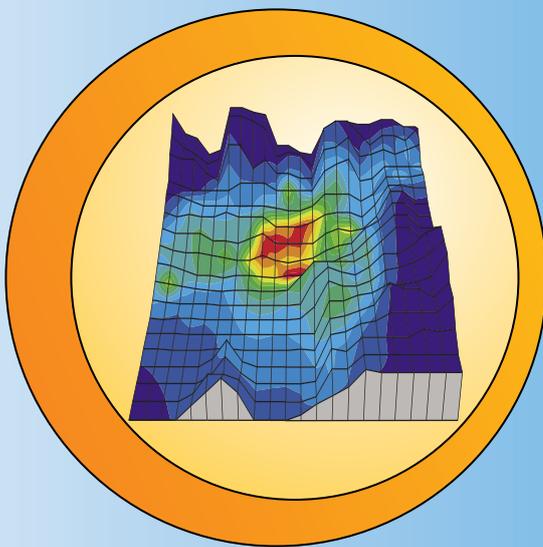


EPISODE – Technical Description



Technical Guide

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**The Urban Air Dispersion
Model EPISODE applied in
AirQUIS₂₀₀₃
Technical Description**

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Sverre Solberg**

Preface

The intention of the present report is to give a detailed description of the urban scale dispersion model EPISODE which is the dispersion model applied in the PC-based Air Quality Information System, AirQUIS₂₀₀₃ (Böhler and Sivertsen, 1998; <http://www.nilu.no/aqm/>).

Contents

	Page
Preface	1
Summary	5
1 Introduction	7
1.1 Overview of the Episode model as applied in AirQUIS ₂₀₀₃	7
1.2 Brief description of the necessary input data for EPISODE	9
1.2.1 Meteorological input	9
1.2.2 Emission input	9
1.2.3 Boundary conditions	10
2 The Meteorological Pre-processor applied in EPISODE	11
2.1 The Profile Method	11
2.2 The Mixing Height	13
2.3 The profile functions for the turbulence parameters (σ_v and σ_w)	14
2.4 Calculation of Stability Classes	15
2.5 The Lagrangian timescale, T_L	15
3 The Eulerian grid model EPISODE	16
3.1 Model equations	16
3.2 The applied sigma coordinate transform	16
3.3 Parameterisations of the eddy diffusivities	18
3.3.1 The horizontal eddy diffusivity, $K^{(H)}$	18
3.3.2 The vertical eddy diffusivity, $K^{(z)}$	18
3.4 Chemistry in the grid model	19
3.4.1 The photo-stationary state assumption	19
3.5 Deposition in the Eulerian grid model	20
3.5.1 Dry deposition	20
3.5.2 Wet deposition	20
3.6 Description of the applied numerical methods	20
3.6.1 Use of timesplitting	20
3.6.2 The horizontal advection	20
3.6.3 The vertical advection	21
3.6.4 The horizontal diffusion	21
3.6.5 The vertical diffusion	21
3.6.6 Calculation of a numerical timestep	21
4 The Subgrid Line Source Model applied in EPISODE	23
4.1 Model description	23
4.1.1 Line Source Model Equations	24
4.1.2 Determination of the dispersion parameters σ_y and σ_z	25
4.1.3 Definition of line source influence zones	27
4.2 Coupling of the subgrid line source model and the Eulerian grid model – mass consistency of the coupled system	29
5 The Point Source Model(s) applied in EPISODE	30
5.1 The Segmented Plume Trajectory Model	30
5.1.1 Overview	30
5.1.2 Input Requirements	31

5.1.3	Stack Downwash	32
5.1.4	Plume Rise Equations.....	32
	5.1.4.1 Neutral-Unstable Conditions.....	32
	5.1.4.2 Stable Conditions	33
5.1.5	Building Effects.....	34
5.1.6	Plume Penetration	35
5.1.7	Topography	35
5.1.8	Advection	36
5.1.9	Dispersion.....	36
5.1.10	Dry Deposition	37
5.1.11	Wet Deposition.....	37
5.2	The puff trajectory model (INPUFF)	38
5.2.1	Overview	38
5.2.2	Input Requirements	41
5.2.3	Stack Downwash	41
5.2.4	(Plume) Rise Equations.....	41
5.2.5	Building Effects.....	41
5.2.6	Penetration.....	41
5.2.7	Topography	41
5.2.8	Advection	41
5.2.9	Dispersion.....	42
	5.2.9.1 Initial dispersion.....	42
	5.2.9.2 Buoyancy induced dispersion	42
	5.2.9.3 Short travel time dispersion	43
	5.2.9.4 Long travel time dispersion scheme.....	44
5.2.10	The effect of the mixing height, h_{mix}	45
5.2.11	Merging of puffs.....	46
5.2.12	Dry deposition and gravitational settling	46
5.2.13	Wet Deposition.....	46
6	References	47
Appendix A Coupling of the subgrid line source model and the Eulerian		
	grid model	51
Appendix A.1	Redistribution of line source emissions in the Eulerian grid model when the line source influence distance is zero.....	53
Appendix A.2	Mass redistribution in the case of infinite influence distances	54
Appendix A.3	Mass redistribution in the case of influence distances with finite lengths.....	55

Summary

The dispersion model EPISODE is an integrated part of the PC-based Air Quality Information System, AirQUIS₂₀₀₃ (Bøhler and Sivertsen, 1998; <http://www.nilu.no/aqm/>). This system has been developed at NILU over the last years. The combined functionalities of emission inventory, numerical modelling, on-line monitoring data collection and statistical assessment methods, within an operable and functional GIS platform, makes AirQUIS₂₀₀₃ an effective tool for air quality management, assessing present day air quality, projecting future air quality and evaluating available abatement options and strategies.

The dispersion model EPISODE (Grønskei et al., 1993; Larssen et al., 1994; Walker et al., 1992, 1999) is an Eulerian grid model with embedded subgrid models for calculations of pollutant concentrations resulting from different types of sources (area-, line- and point sources). EPISODE solves the time dependent advection/-diffusion equation on a 3 dimensional grid. Finite difference numerical methods are applied to integrate the solution forward in time. This part of the model is referred to as the Eulerian grid model. Traditionally EPISODE has been applied for the calculation of airborne species like SO₂, CO, NO_x, NO₂, PM₁₀ and PM_{2.5}.

In addition to the Eulerian grid model, EPISODE also contains different sub-grid models for refined calculations in areas close to important sources.

The sub-grid line source model within the AirQUIS₂₀₀₃ version of EPISODE is based on a standard integrated Gaussian model, HIWAY-2 (Petersen, 1980). This is a model that calculates concentration levels of non-reactive pollutants from road traffic at distances tens to hundreds of meters downwind of the road in relatively uncomplicated terrain. Each lane of traffic is modelled as though it is a straight, continuous, finite length, line source with a uniform emission rate. Air pollution concentrations are found by interpreting the line source as a finite sum of simple Gaussian point-source plumes, and the total line source contribution is then found by integrating (i.e. adding) numerically over the length of the line source.

Two different types of point-source sub-grid models can be applied within the AirQUIS₂₀₀₃ version of EPISODE. One is based on a segmented plume/trajectory model (Walker et al. 1992), while the other is the puff/trajectory model INPUFF (Petersen and Lavdas, 1986; Knudsen and Hellevik, 1992). In both models the emissions from individual point sources are treated as a temporal sequence of instantaneous releases of a specified pollutant mass. The subsequent position and concentration distribution within each of the plume segments or puffs are then estimated by the models. An option in the segmented plume/trajectory model is that the mass of the individual plume segments can be transferred to the Eulerian grid concentration when the size of the segments become comparable to the grid size. This option is not available in the puff/trajectory model. However, the puff/trajectory model includes functionality for combining neighbouring puffs, i.e. puff merging, thereby controlling the total number of puffs, and thus reducing the computational costs.

The Urban Air Dispersion Model EPISODE applied in AirQUIS2003 Technical Description

1 Introduction

1.1 Overview of the Episode model as applied in AirQUIS₂₀₀₃

The dispersion model EPISODE is an integrated part of the PC-based Air Quality Information System, AirQUIS₂₀₀₃ (Böhler and Sivertsen, 1998; <http://www.nilu.no/aqm/>). This system has been developed at NILU over the last years. The combined functionalities of emission inventory, numerical modelling, on-line monitoring data collection and statistical assessment methods, within an operable and functional GIS platform, makes AirQUIS₂₀₀₃ an effective tool for air quality management, assessing present day air quality and projecting future air quality and evaluating available abatement options and strategies.

The AirQUIS₂₀₀₃ system contains the following modules:

- ❑ *Geographical Module- Geographical Information System (GIS)*
The Geographical Information System (GIS) is used as a platform for integrating the presentation of data from the Measurement Module, Emission Inventory Module and results from model estimates. The Geographical Information System is directly linked to the databases, from which graphical presentations and spatial distributions of stations, emission inventory sources, emissions and consumption data and model results can be presented.
- ❑ *Measurement Module*
The AirQUIS measurement module is designed as a tool for managing air quality and meteorological measurements. The module has a database where the measurements are stored, functionality for managing the database regarding import and export of data, and tools for graphical presentations, statistical calculations and automatic reporting.

 - Automatic Data Acquisition System (ADACS)
 - Measurement database for air quality and meteorological data
 - Statistical and Graphical Presentation Tools
- ❑ *Emission Inventory Module*
This module contains the necessary forms and functionalities for producing a complete and detailed atmospheric emissions inventory for an area.

 - Point source emissions
 - Line source emissions
 - Area source emissions
- ❑ *Models module*
This module contains models for calculating emissions, dispersion and exposure on urban scale:

 - Emission Model,
 - Wind Field Model - *The diagnostic wind field model (MATHEW)*,

- Pollution Dispersion Model - *The urban dispersion model (EPISODE)*,
- Exposure Model - *For stationary population exposure assessments*.

Prior to the dispersion calculations, a mass consistent and topographically modified three-dimensional wind field must be available for the EPISODE model. In the present version of AirQUIS₂₀₀₃ this wind field is calculated by use of the diagnostic MATHEW model (Sherman, 1978; Foster et. al., 1995; Slørdal, 2002b).

If no measured values exists, boundary layer turbulence parameters are estimated in EPISODE by the use of meteorological pre-processor routines (Bøhler, 1996). Important quantities like the surface momentum flux, (τ_0), the surface sensible heat flux, (H_0), the mixing height, (h), and the vertical profile functions of the surface layer wind, temperature and turbulence parameters (σ_v and σ_w) are parameterised by the pre-processor routines. In Section 2 the pre-processor routines presently applied in EPISODE are described more thoroughly.

The dispersion model EPISODE (Grønskei et. al., 1993; Larssen et al., 1994; Walker et al., 1992, 1999) is an Eulerian grid model with embedded subgrid models for calculation of pollutant concentrations resulting from different types of sources (area-, line- and point sources). EPISODE solves the time dependent advection/-diffusion equation on a 3 dimensional grid. Finite difference numerical methods are applied to integrate the solution forward in time. This part of the model is referred to as the Eulerian grid model. Traditionally EPISODE has been applied for the calculation of airborne species such as SO₂, CO, NO_x, NO₂, PM₁₀ and PM_{2.5}. Calculations of NO₂ are based on a simplifying assumption of photochemical equilibrium between NO, NO₂ and O₃ for each time step. Background values of O₃, which enter through the open boundaries of the model domain, are estimated from O₃ measurements at nearby background stations. A detailed description of the Eulerian grid model is given in Section 3 of this report.

In addition to the Eulerian grid model, EPISODE also contains different sub-grid models for refined calculations in areas close to important sources.

The sub-grid line source model within the AirQUIS₂₀₀₃ version of EPISODE is based on a standard integrated Gaussian model, HIWAY-2 (Petersen, 1980). This model calculates concentration levels of non-reactive pollutants from road traffic at distances tens to hundreds of meters downwind of the road in relatively uncomplicated terrain. Each lane of traffic is modelled as though it is a straight, continuous, finite length, line source with a uniform emission rate. Air pollution concentrations are found by interpreting the line source as a finite sum of simple Gaussian point-source plumes, and the total line source contribution is then found by integrating (i.e. adding) numerically over the length of the line source. This sub-grid line source model is described in Section 4.

Two different types of point-source sub-grid models can be applied within the AirQUIS₂₀₀₃ version of EPISODE. One is based on a segmented plume/trajectory model (Walker et al., 1992), while the other is the puff/trajectory model INPUFF (Petersen and Lavdas, 1986; Knudsen and Hellevik, 1992). In both models the emissions from individual point sources are treated as a temporal sequence of

instantaneous releases of a specified pollutant mass. The subsequent position and concentration distribution within each of the plume segments or puffs are then estimated by the models. An option in the segmented plume/trajectory model is that the mass of the individual plume segments can be transferred to the Eulerian grid concentration when the size of the segments become comparable to the grid size. This option is not available in the puff/trajectory model. However, the puff/trajectory model includes functionality for combining neighbouring puffs, i.e. puff merging, thereby controlling the total number of puffs, and thus reducing the computational costs. The subgrid point source models are described further in Section 5.

In recent years EPISODE has been applied in several Norwegian cities, (Slørdal, 2002a; Laupsa and Slørdal, 2002) and in Germany (Wind et al., 2003).

1.2 Brief description of the necessary input data for EPISODE

1.2.1 Meteorological input

The dispersion model requires several meteorological parameters as input. This information has to be specified for each time step either as gridded field values or as spatially homogeneous values. The required parameters are:

- Wind (speed and direction).
- Temperature and atmospheric stability.
- Horizontal and vertical turbulence (σ_v and σ_w) and mixing height.
- Cloud cover, relative humidity and precipitation. (Optional)

Information about the turbulence levels, and thereby the dispersion conditions, are supplied to EPISODE through specification of the standard deviations of horizontal and vertical velocity, i.e. σ_v and σ_w . These quantities are parameterised by the use of a meteorological pre-processor routine (MEPDIM; Böhler, 1996) see Section 2 below.

1.2.2 Emission input

The AirQUIS₂₀₀₃ emission inventory module contains data such as fuel consumption, emission factors, physical description of stacks and processes, traffic load etc. Estimates of hourly emissions of the different air quality components are then calculated by application of the emission model. The emission data are split into three separate categories. These are:

- **Point source emissions:** Includes emissions from industrial plants or large factories.
- **Line source emissions:** Includes all emissions from road traffic. In the calculations only roads with annual daily traffic (ADT) above a user defined limit value are included as line sources. The emission from the roads with lower ADT are treated as area sources.
- **Area source emissions:** Include both stationary sources that are too small to be regarded as point sources as well as road traffic emissions from roads with ADT below a given user defined limit.

The method applied to calculate the PM₁₀ contribution from traffic-induced resuspension takes into account the effect of vehicle composition, traffic speed and, during the winter season, the percentage of vehicles with studded tyres, on each road segment. Since practically no particles are resuspended when the roads are wet, hourly data on relative humidity and precipitation within the modelling area have been included as input to the emission model.

1.2.3 Boundary conditions

The long-range transport contribution of the different species are specified at the open boundaries of the model domain as a constant value for each hour. This value can be user specified or taken from a background measurement station.

2 The Meteorological Pre-processor applied in EPISODE

Below is a short description of the Meteorological Preprocessor for Dispersion Modelling (MEPDIM; Böhler, 1996) which is applied in EPISODE for the parameterization of the surface momentum flux, (τ_0), the surface sensible heat flux, (H_0), the mixing height, (h), and the vertical profile functions of the surface layer wind, temperature and turbulence parameters (σ_v and σ_w). The MEPDIM algorithms are based on the traditional Monin-Obukhov similarity theory, and the theoretical foundation can be found in van Ulden and Holtslag (1985), Holtslag and de Bruin (1988), and Gryning et al. (1987).

MEPDIM contains two alternative methods, the *Profile method* and the *Energy Budget method* (van Ulden and Holtslag, 1985). However, in the present AirQUIS₂₀₀₃ version only the profile method can be applied and therefore only this method is described in the following. The input requirement for this method is summarized in Table 2.1 below.

Table 2.1: Input requirement for the Profile method.

Surface roughness length (z_0)
Wind speed at one height within the surface layer
Air temperature at one height within the surface layer
Vertical temperature difference measured between two heights within the surface layer. The applied heights must be given with the ΔT -value.

2.1 The Profile Method

By applying this method the friction velocity (u_*), the temperature scale (θ_*) and the Monin-Obukhov length (L) are calculated by an iterative procedure. u_* and θ_* are defined, respectively, as:

$$u_* \equiv (\overline{u'w'})_0^{1/2} = (\tau_0/\rho)^{1/2} \quad \text{and} \quad \theta_* \equiv -\frac{(\overline{\theta'w'})_0}{u_*} = -\frac{H_0}{\rho C_p u_*},$$

where τ_0 is the surface momentum flux, H_0 is the surface sensible heat flux, ρ is the air density and C_p is the specific heat at constant pressure. Based on an estimate of the surface roughness, z_0 , measurements of the wind at one height and the temperature difference between two heights, all made within the surface layer (inertial sublayer), u_* , θ_* and L are computed by an iterative solution of the following two profile equations

$$\frac{\kappa \cdot U(z_1)}{u_*} = \ln\left(\frac{z_1}{z_0}\right) - \Psi_M\left(\frac{z_1}{L}\right) + \Psi_M\left(\frac{z_0}{L}\right), \quad (2.1)$$

$$\frac{\kappa \cdot [\theta(z_3) - \theta(z_2)]}{\theta_*} = \ln\left(\frac{z_3}{z_2}\right) - \Psi_H\left(\frac{z_3}{L}\right) + \Psi_H\left(\frac{z_2}{L}\right), \quad (2.2)$$

and the Monin-Obukhov length, defined in the usual way as

$$L \equiv - \frac{(\overline{u'w'})_0^{3/2}}{\kappa \frac{g}{\theta} (\overline{\theta'w'})_0} \equiv \frac{u_*^2}{\kappa \frac{g}{\theta} \theta_*} . \quad (2.3)$$

In these expressions κ is the von Karman constant, with a prescribed value of 0.41. The Monin-Obukhov length, L , is a measure of the buoyant stability of the air, and can be interpreted as the height at which the shear production term of turbulent kinetic energy equals the buoyancy production/loss term. Small positive and negative values of L indicate stable and unstable conditions, respectively. The neutral regime is found for large positive or negative values. This means that the non-dimensional length parameter, $\zeta = z/L$, tends towards zero in the neutral limit. In Table 2.2 the different stability regimes with respect to L are indicated (Seinfeld, 1998).

Table 2.2: Stability regimes defined by use of the Monin-Obukhov length L .

L		Stability condition
Small negative	$-100 \text{ m} < L < 0$	Very unstable
Large negative	$-10^5 \text{ m} \leq L \leq -100 \text{ m}$	Unstable
Very large (pos. or neg.)	$ L > 10^5 \text{ m}$	Neutral
Large positive	$10 \text{ m} \leq L \leq 10^5 \text{ m}$	Stable
Small positive	$0 < L < 10 \text{ m}$	Very Stable

The functions, ψ_M and ψ_H in eqs. 2.1 and 2.2 represent the influence of buoyancy, and are therefore often referred to as the stability functions.

For *unstable* conditions the stability function for *momentum*, $\psi_M(\zeta)$, is defined by:

$$\psi_M(\zeta) = 2 \ln \left(\frac{1+x}{2} \right) + \ln \left(\frac{1+x^2}{2} \right) - 2 \tan^{-1}(x) + \frac{\pi}{2} \quad \text{for } \zeta \equiv \frac{z}{L} < 0 \quad (2.4)$$

where:

$$x = (1 - 16\zeta)^{1/4} \quad (2.5)$$

For *stable* conditions, $\psi_M(\zeta)$, is given by (Holtslag and de Bruin, 1988):

$$\psi_M(\zeta) = -0.7\zeta - (0.75\zeta - 10.72)e^{-0.35\zeta} - 10.72 \quad \text{for } 0 \leq \zeta . \quad (2.6)$$

Similarly, for *unstable conditions* the stability function for *heat*, $\psi_H(\zeta)$, is defined by:

$$\psi_H(\zeta) = 2 \ln \left[\frac{1}{2} (1 + x^2) \right] \quad \text{for } \zeta < 0 . \quad (2.7)$$

where (as for momentum)

$$x = (1 - 16\zeta)^{1/4}, \quad (2.8)$$

and for *stable conditions*:

$$\psi_H(\zeta) = \psi_M(\zeta) = -0.7\zeta - (0.75\zeta - 10.72)e^{-0.35\zeta} - 10.72 \quad \text{for } \zeta \geq 0. \quad (2.9)$$

In the present version a maximum of 20 iteration are performed on Eqs. 2.1 to 2.3, and the iteration procedure is ended when the relative change of the Monin-Obukhov length, $|(L^n - L^{n-1}) / L^{n-1}|$, is less than 0.05. Moreover, in order to avoid unrealistically low positive values of L in urban areas under stable situations, the iteration process contains restrictions so that L never get lower than about 20 - 40 m, depending on the surface roughness.

2.2 The Mixing Height

At present only diagnostic expressions are applied in AirQUIS₂₀₀₃ for the estimation of the Atmospheric Boundary Layer (ABL) depth, or the mixing height, h.

For *unstable* and *near neutral* conditions h is estimated from:

$$h = 0.25 \cdot \frac{u_*}{f} \quad \text{for } L < 0 \quad \text{and for } |L| > \frac{u_*}{4|f|} \quad (2.10)$$

where $f = 2\Omega \sin \varphi$ is the Coriolis parameter; Ω being the frequency of the sidereal day ($0.7292 \cdot 10^{-4} \text{ s}^{-1}$), and φ the latitude of the site. It is recommended that the use of (2.11) should be limited to atmospheric conditions that are sufficiently neutral. Van Ulden and Holtslag (1985) give as a practical rule of thumb the requirement that

$$|u_* / fL| < 4, \quad (2.11)$$

which corresponds to $|h/L| < 1$.

For *stable* conditions the following diagnostic expression is used in MEPDIM (Zilitinkevich, 1972):

$$h_{\text{mix}} = 0.4 \sqrt{\frac{u_* L}{f}} \quad \text{for } 0 \leq L \leq \frac{u_*}{4|f|} \quad (2.12)$$

Van Ulden and Holtslag (1985) state that the use of Eq. (2.12) offers problems at high wind speeds and low θ_* values, because L may become quite large. Therefore in practice h is limited by its neutral value (2.10) in cases for which (2.12) gives higher values than (2.10).

The expressions (2.10) and (2.12) have only been validated at mid-latitude sites. For applications closer to the equator, where the Coriolis parameter decreases towards zero, expressions such as (2.10) and (2.12) obviously will fail. This problem is avoided simply by defining a minimum value of $1 \cdot 10^{-5} \text{ s}^{-1}$ for the Coriolis parameter (the value at a latitude of about 20°). Nevertheless, for application at latitudes less than 20° , mixing height estimates from expressions such as eqs. (2.10) and (2.12) should be treated with caution.

2.3 The profile functions for the turbulence parameters (σ_v and σ_w)

MEPDIM calculates σ_v and σ_w as functions of the height above the ground, z , the mixing height, h , the friction velocity, u_* , and the Monin-Obukhov length, L . The applied formulas are specified in the following.

For *unstable conditions*, i.e. for $L < 0$:

For $z < h$:

$$\sigma_v(z) = u_* \left[0.35 \cdot \left(-\frac{h}{\kappa L} \right)^{2/3} + \left(2 - \frac{z}{h} \right) \right]^{1/2} \quad (2.13.a)$$

$$\sigma_w(z) = u_* \left[1.5 \cdot \left(-\frac{z}{\kappa L} \right)^{2/3} \cdot e^{-2z/h} + \left(1.7 - \frac{z}{h} \right) \right]^{1/2} \quad (2.14.a)$$

and for $z \geq h$:

$$\sigma_v(z) = u_* \left[0.35 \cdot \left(-\frac{h}{\kappa L} \right)^{2/3} + 1 \right]^{1/2} \quad (2.13.b)$$

$$\sigma_w(z) = u_* \left[1.5 \cdot \left(-\frac{z}{\kappa L} \right)^{2/3} \cdot e^{-2} + 0.7 \right]^{1/2} \quad (2.14.b)$$

where a value of 0.41 is applied for the von Karman constant, κ . Eqs. (2.13) and (2.14) were recommended by Gryning et al. (1987) and they are based on an empirical model by Brost et al. (1982). Equation (2.13) is also based on Caughey (1982). Equation (2.14) have been tested by Irwin and Paumier (1990, CONDORS experiment). Note that the expressions valid above the mixing height simply are found by replacing z/h by 1 in (2.13a) and (2.14a).

For *stable conditions*, i.e. for $L \geq 0$:

For $z < h$:

$$\sigma_v(z) = u_* \left[2 \cdot \left(1 - \frac{z}{h} \right) \right]^{1/2} \quad (2.15.a)$$

$$\sigma_w(z) = u_* \left[1.7 \cdot \left(1 - \frac{z}{h} \right)^{3/2} \right]^{1/2} \quad (2.16.a)$$

and for $z \geq h$:

$$\sigma_v(z) = 0 \quad (2.15.b)$$

$$\sigma_w(z) = 0 \quad (2.16.b)$$

Equations (2.15) and (2.16) are based on Nieuwstadt (1984), and are also recommended by Gryning et al. (1987). Again (2.15.b) and (2.16.b) is the limiting value of (2.15.a) and (2.16.a) when $z \rightarrow h$.

2.4 Calculation of Stability Classes

In the determination of dispersion parameters in the Subgrid Line Source model (Section 4) and in the Subgrid Point Source models (Section 5), a stability classification is required. In EPISODE this classification is computed as part of the meteorological preprocessing.

The stability classification is made solely on the basis of the measurement of a temperature difference, ΔT , between two heights in the surface layer. Normally this temperature difference is taken between the heights of 10 m and 2 m above ground. However, the ΔT -value can alternatively be estimated between 25 m and 8 m, or between 36 m and 10 m. The ΔT -value is given in °C (or °K).

The classification is defined as follows:

$$\begin{aligned} < \Delta T \leq -0.5 &\Leftrightarrow \text{Stability Class 1: Unstable conditions} & (2.17.a) \\ -0.5 < \Delta T \leq 0.0 &\Leftrightarrow \text{Stability Class 2: Neutral conditions} & (2.17.b) \\ 0.0 < \Delta T \leq 0.5 &\Leftrightarrow \text{Stability Class 3: Moderately stable conditions} & (2.17.c) \\ 0.5 < \Delta T &\Leftrightarrow \text{Stability Class 4: Stable conditions} & (2.17.d) \end{aligned}$$

2.5 The Lagrangian timescale, T_L

The Lagrangian time scale is applied in the parameterisations of the dispersion parameters (σ_y , σ_z) in the point source model. The parameterisation of this quantity is based on the expressions of Venkatram et al. (1984). Thus, for emission heights at or below the mixing height, the gradient of the potential temperature is calculated according to:

$$\frac{d\theta}{dz} = \frac{dT}{dz} + 0.01 \quad (2.18)$$

For emission heights above the mixing height $d\theta/dz$ is preset to: $\frac{d\theta}{dz} = 0.003$.

This gradient is then used to calculate the Brunt-Vaiasala frequency

$$N^2 = \frac{g}{T_0} \frac{d\theta}{dz} \quad \text{for positive values of } d\theta/dz. \quad (2.19)$$

where T_0 is the surface layer reference temperature in degrees Kelvin. For zero or negative values of $d\theta/dz$ the Brunt-Vaiasala frequency is set equal to zero. Finally, the Lagrangian time scale is calculated according to:

$$T_L = \frac{l_n}{\sigma_w} \quad \text{when } N = 0. \quad (2.20)$$

and

$$T_L = \frac{l_s l_n}{(l_s + l_n) \sigma_w} \quad \text{when } N > 0. \quad (2.21)$$

where: $l_n = \alpha z$; $\alpha = 0.36$ and $l_s = \frac{\gamma^2 \sigma_w}{N}$; ($\gamma^2 = 0.27$).

3 The Eulerian grid model EPISODE

3.1 Model equations

The advection/diffusion equation(s) that are solved in EPISODE are given by

$$\begin{aligned} \frac{\partial c_i}{\partial t} + \frac{\partial}{\partial x}(uc_i) + \frac{\partial}{\partial y}(vc_i) + \frac{\partial}{\partial z}(wc_i) = \frac{\partial}{\partial x} \left(K^{(H)} \frac{\partial c_i}{\partial x} \right) + \\ \frac{\partial}{\partial y} \left(K^{(H)} \frac{\partial c_i}{\partial y} \right) + \frac{\partial}{\partial z} \left(K^{(z)} \frac{\partial c_i}{\partial z} \right) + R_i - S_i \end{aligned} \quad (3.1)$$

Here c_i is the mass concentration of the species considered; u , v and w are the three components of the wind vector; $K^{(H)}$ and $K^{(z)}$ are the horizontal and vertical eddy diffusivities, respectively, R_i is the source terms, and S_i the sinks. Note that all of the above variables are averaged (or mean) values. As seen in (3.1) the terms describing the turbulent diffusion are represented according to the mixing length theory (or K-theory). One should bear in mind that K-theory is only valid as long as the reaction processes are slow compared with the turbulent transport, and the characteristic length scales and timescales for changes in the (mean) concentration field are large compared with the corresponding scales for turbulent transport (Seinfeld and Pandis, 1998; pp. 885-889).

In addition the wind velocity field applied in (3.1), is required to be mass consistent, which in the urban scale EPISODE model is approximated by demanding the wind flow to be divergence-free, i.e.

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad (3.2)$$

Eq. (3.2) is the continuity (mass conservation) equation for an incompressible atmosphere, and this is a reasonable approximation for layers close to the Earth's surface and therefore for urban scale chemical transport models (Seinfeld and Pandis, 1998; p. 1212). Eq. (3.2) is in reality ensuring that the applied wind field is volume conserving. It should be noted that the concentration, c_i , for a fluid element is a conserved quantity as long as the wind field obeys (3.2), and therefore the mixing length representation of the turbulence terms in (3.1) is valid within this approximation.

3.2 The applied sigma coordinate transform

The vertical extent of the model is defined from the ground, $z = h(x,y)$, and up to a constant height, $z = H_0$, above sea level. This means that the model applies a stretched vertical coordinate, or a sigma-coordinate system, given by the following transformation:

$$x^* = x, \quad y^* = y, \quad \sigma = \sigma(x, y, z) = H_0 \frac{z - h(x, y)}{H_0 - h(x, y)} \quad \text{and} \quad t^* = t \quad (3.3)$$

Note that denominator of eq. (3.3) is identical to the total vertical depth of the model, i.e. $D(x,y)$ defined as:

$$D(x, y) \equiv H_0 - h(x, y) \quad \Leftrightarrow \quad h(x, y) = H_0 - D(x, y).$$

The physical extent of the model domain when applying the transform (3.3) is depicted in Figure 3.1.

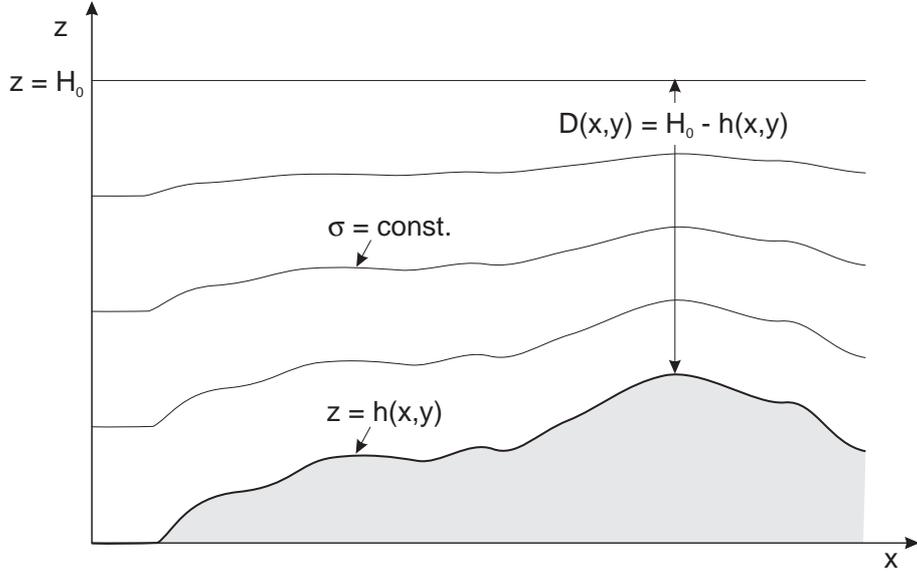


Figure 3.1: A schematic representation of the vertical extent of the model domain and the position of the model layers, when the transform of (3.3) is applied.

From (3.3) a grid volume element is given by: $\delta V = \delta x \cdot \delta y \cdot \delta z = \frac{D(x,y)}{H_0} \delta x^* \cdot \delta y^* \cdot \delta \sigma$, and $\sigma = 0$ for $z = h(x,y)$ and $\sigma = H_0$ for $z = H_0$, i.e. $\sigma \in [0, H_0]$. Note also that $\partial h / \partial \xi = -\partial D / \partial \xi$ where ξ is either x or y .

In this transformed coordinate system, with the additional assumptions that the wind field is incompressible and that a simplified parameterisation of the horizontal turbulent diffusion terms can be applied (Slørdal, 2002c), the advection/diffusion equations which are to be solved in EPISODE can be written as

$$\frac{\partial c_i}{\partial t} + \frac{1}{D} \left(\frac{\partial (u c_i D)}{\partial x^*} + \frac{\partial (v c_i D)}{\partial y^*} + \frac{\partial (\omega c_i D)}{\partial \sigma} \right) = \frac{\partial}{\partial x^*} \left(K^{(H)} \frac{\partial c_i}{\partial x^*} \right) + \frac{\partial}{\partial y^*} \left(K^{(H)} \frac{\partial c_i}{\partial y^*} \right) + \left(\frac{H_0}{D} \right)^2 \frac{\partial}{\partial \sigma} \left(K^{(Z)} \frac{\partial c_i}{\partial \sigma} \right) + R_i - S_i \quad (3.4)$$

The vertical velocity in the transformed system, $\omega \equiv \bar{V} \cdot \nabla \sigma$, is expressed as

$$\omega \equiv \frac{H_0}{D} w + (H_0 - \sigma) \frac{u}{D} \frac{\partial D}{\partial x} + (H_0 - \sigma) \frac{v}{D} \frac{\partial D}{\partial y}, \quad (3.5)$$

and the incompressible wind field satisfies the equation

$$\frac{\partial (uD)}{\partial x^*} + \frac{\partial (vD)}{\partial y^*} + \frac{\partial (\omega D)}{\partial \sigma} = 0. \quad (3.6)$$

The stretch factor $H_0/D(x,y)$, which enters the advection/diffusion equation through the vertical turbulent diffusion terms, will normally vary between 1.0 and ∞ . However, with large values of the stretch factor, the computation time increases severely. This is related to the stability requirements of the explicit numerical method applied for the vertical diffusion, see Section 3.6.5. Since the computation time increases as the square of the stretch factor, this problem can be reduced by choosing H_0 large enough compared to the variations in the topography, thereby keeping $H_0/D(x,y)$ close to one.

3.3 Parameterisations of the eddy diffusivities

In EPISODE the transport processes caused by turbulence are treated with a first order mixing length parameterisation, (first order closure or K-theory). Since the values of the applied horizontal and vertical diffusivities depend both on the spatial structure of the flow field and on the grid resolution, their values need to be parameterised so as to account for both effects.

3.3.1 The horizontal eddy diffusivity, $K^{(H)}$

For the horizontal eddy diffusion EPISODE applies horizontal diffusivities that are calculated according to the expression

$$K^{(H)}(k) = 0.1 \cdot \min(\Delta x, \Delta y) \cdot \max_{i,j} \sigma_v(i, j, k) \quad (3.7)$$

where k is the vertical layer index, Δx , Δy is the horizontal grid resolution, and $\sigma_v(i,j,k)$ is the horizontal turbulence intensity in gridcell i,j,k . σ_v is parameterized as recommended by Gryning et al. (1987). The inclusion of the grid resolution in (3.7) means that the horizontal turbulent length scale is proportional to the grid size.

3.3.2 The vertical eddy diffusivity, $K^{(z)}$

The applied vertical eddy diffusivity, $K^{(z)}$, in Episode, is defined as a sum of two terms

$$K^{(z)} = K^* + K_0(u_*, \Delta z_1), \quad (3.8)$$

where K^* is a standard parameterization depending on the stability conditions, and K_0 is an additional grid-size specific term which has been found necessary in stable, low wind situations.

Under unstable and neutral conditions the eddy diffusivity of Shir (1973) is applied

$$K^* = \kappa u_* z \exp\left(-\frac{8fz}{u_*}\right), \quad (3.9)$$

while the expression of Businger and Arya (1974) is applied under stable conditions

$$K^* = \frac{\kappa u_* z}{0.74 + 4.7(z/L)} \exp\left(-\frac{8fz}{u_*}\right). \quad (3.10)$$

The values of u_* , and L are calculated by the AirQUIS meteorological pre-processor MEPDIM (Böhler, 1996). $\kappa = 0.41$ is the von Karman constant, and f is the Coriolis parameter. For applications at low latitudes the use of eqs. (3.9) and (3.10) should be reconsidered since their region of validity is at mid-latitudes. At present a minimum value of $1 \cdot 10^{-5} \text{ s}^{-1}$ is applied for the Coriolis parameter (the value at a latitude of about 20°).

As alluded to above, eqs. (3.9) and (3.10) have been found to give unrealistic low values for K^* during stable low-wind conditions in Norwegian cities. In order to reduce this problem the empirical term $K_0(u_*, \Delta z_1)$ has been added to the equation of $K^{(z)}$. This term is defined as

$$K_0(u_*, \Delta z_1) = (2 \cdot \Delta z_1)^2 / 3600 \quad \text{for } u_* > 0.2 \text{ m/s.} \quad (3.11)$$

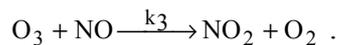
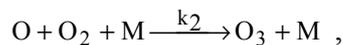
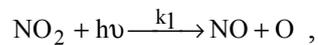
$$K_0(u_*, \Delta z_1) = \Delta z_1^2 / 3600 \quad \text{for } u_* < 0.1 \text{ m/s.}$$

with a linear variation of K_0 for values of u_* in between 0.1 m/s and 0.2 m/s. In the expression above Δz_1 is the thickness of the most shallow layer (i.e. the lowermost layer) of the dispersion model. This particular choice of K_0 is based on a scale analysis where it is assumed that the minimum values of $K^{(z)}$ should be large enough, during a one hour period, to mix an air-column of thickness Δz_1 and $2 \cdot \Delta z_1$, when u_* is less than 0.1 m/s and larger than 0.2 m/s, respectively. For u_* less than 0.1 m/s and a value of Δz_1 equal to 20 m, K_0 becomes equal to $0.11 \text{ m}^2/\text{s}$, which is a very low value. For u_* greater than 0.2 m/s and with Δz_1 equal to 20 m, K_0 becomes equal to $0.44 \text{ m}^2/\text{s}$.

3.4 Chemistry in the grid model

3.4.1 The photo-stationary state assumption

Presently EPISODE uses the photostationary state assumption that is based on an instantaneous equilibrium between the following three reactions:



The steady-state assumption implies that NO_x (the sum of nitrogen oxides) and O_x (oxidants) are conserved, where NO_x and O_x are defined as:

$$[\text{NO}_x] = [\text{NO}] + [\text{NO}_2] \quad , \quad \text{and} \quad [\text{O}_x] = [\text{O}_3] + [\text{NO}_2] \quad .$$

By these assumptions the three components NO , NO_2 and O_3 can be found by the solution of a second-degree equation in O_3 .

This is a valid assumption in urban areas from a short distance away from the emissions until a net ozone formation is starting. In polluted areas in the north in winter this will be a good assumption. However, when the solar UV-radiation is stronger, either because of a more southern location or in summer, a net ozone formation could take place even in urban areas a certain distance away from the main emission sources. Thus, the assumption of conservation of O_x and NO_x is then not valid and a more detailed chemical description is needed.

3.5 Deposition in the Eulerian grid model

3.5.1 Dry deposition

There is no treatment of dry deposition in the Eulerian grid model presently applied in AirQUIS₂₀₀₃.

3.5.2 Wet deposition

There is no treatment of wet deposition in the Eulerian grid model presently applied in AirQUIS₂₀₀₃.

3.6 Description of the applied numerical methods

3.6.1 Use of timesplitting

In order to solve (Eq. 3.1) numerically, timesplitting is used. Timesplitting means that the different parts of the equation are solved using a separate numerical method or algorithm that only deals with that isolated term.

In the EPISODE Eulerian model, timesplitting is used in order to separately solve the following processes

- Advection
- Diffusion
- Photochemical reactions

3.6.2 The horizontal advection

Horizontal advection in EPISODE is calculated by using Bott's 4th order scheme using 4th order polynomials positive definite scheme in combination with the timesplitting approach. The Bott scheme is known for having very good numerical properties with very low artificial numerical diffusion. The user is referred to the articles by Bott (1989, 1992, 1993) for a thorough description of this method. The method is also mass consistent. It is based on calculating fluxes between the gridcells based on a local area preserving 4th degree polynomial describing the concentration fluctuations locally.

Advection is first solved by applying a numerical advection operator in the x-direction followed by applying the same advection operator but now in the y-direction based on the result of the first operator thus:

$$c^{*n} = c^n + \Delta t \cdot ADV_x(c^n)$$

Here c^n denotes the 3D concentration field at timestep n , Δt is the timestep and ADV_x is the spatial advection operator in the x-direction based on the

concentration at level n . Since the operator only deals with advection along the x -direction the operator is applied to each row of gridcells along the x -axis for all cells in y - and z -direction.

Advection in the y -direction is then performed by applying the same advection operator in the y -direction based on the results of the x -advection:

$$c^{**n} = c^{*n} + \Delta t \cdot \text{ADV}_y(c^{*n})$$

The advection operator is applied in the y -direction for each gridcell in the x - z plane within the model 3D domain.

These operators are swapped in order every second timestep.

3.6.3 *The vertical advection*

For the vertical advection the simple upstream method is applied. This method is conditionally stable with the well known CFL-stability condition; $\Delta t \leq \Delta z/|w|$. The upstream method is known to be strongly diffusive, but is generally insignificant compared to the turbulent diffusion term.

3.6.4 *The horizontal diffusion*

Horizontal diffusion is calculated numerically by using a simple 2D fully explicit numerical scheme (Smith, 1985). Timesplitting is not used in the horizontal plane here, rather the x - and y -direction part of the diffusion is solved simultaneously using one single 2D numerical operator:

$$c^{***n} = c^{**n} + \Delta t \cdot \text{DIFF}_{xy}(c^{**n})$$

where c^{**n} here denotes the concentration grid values after the advection operator has been applied to the 3D grid field. DIFF_{xy} denotes the numerical diffusion operator. This operator is mass consistent.

3.6.5 *The vertical diffusion*

The numerical method applied for the vertical diffusion process is based on a simple forward in time, centred in space discretization. This method is conditional stable, with the stability condition given by: $\Delta t \leq \Delta z^2/2K^{(z)}$.

3.6.6 *Calculation of a numerical timestep*

The numerical timestep used in the EPISODE model is calculated internally from the critical timesteps associated with the horizontal advection and vertical advection and diffusion processes within the model. Let T_{ax} and T_{ay} be the critical timesteps associated with the horizontal advection operator in the x - and y -directions respectively and let T_{dh} be the critical timestep associated with the horizontal diffusion. Let T_{adv} be the critical timestep associated with the vertical advection and diffusion operator.

Then the timestep calculated and used by the model is given by

$$dt = \min(T_{ax}, T_{ay}, T_{dh}, T_v)$$

Thus it is the most critical of the operators that determines the actual time step to be used. The timestep is also adjusted slightly downward so that

$$nsteps = 3600./dt$$

is always an even integer. This makes it possible to perform all operations an even number of times so that every other operator sequence may be a mirror in the opposite direction of the first sequence to reduce time splitting errors.

4 The Subgrid Line Source Model applied in EPISODE

The main purpose of the line source model in EPISODE is to calculate hourly average ground level concentrations in different receptor points from line source emissions in the area. This also includes calculations for main grid cells as averages over the cell or in the midpoint of the cells.

The line source model is described in Section 4.1. while a detailed description of the coupling between the subgrid line source model and the Eulerian grid model is given in Section 4.2. The reader is referred to the AirQUIS2003 User documentation for a detailed description of the necessary input parameters for the line source model.

4.1 Model description

The subgrid line source model implemented in EPISODE is currently based on a steady-state integrated Gaussian plume model from US EPA, the HIWAY-2 model, (Petersen, 1980).

In order to describe the model, consider a single line source L and a given receptor point R as shown in Figure 4.1. The line source is assumed to have length D , and to be divided into two separate lanes, L_1 and L_2 , for traffic in each direction. The widths of the two lanes is denoted by w_1 and w_2 respectively. The emission intensity on each of the lanes is assumed to be constant (uniform) along the line source. The concentration value at the receptor point R may be found by adding the contribution from each of the two lanes. We therefore only need to describe the contribution from one of the two lanes, say from lane L_1 .

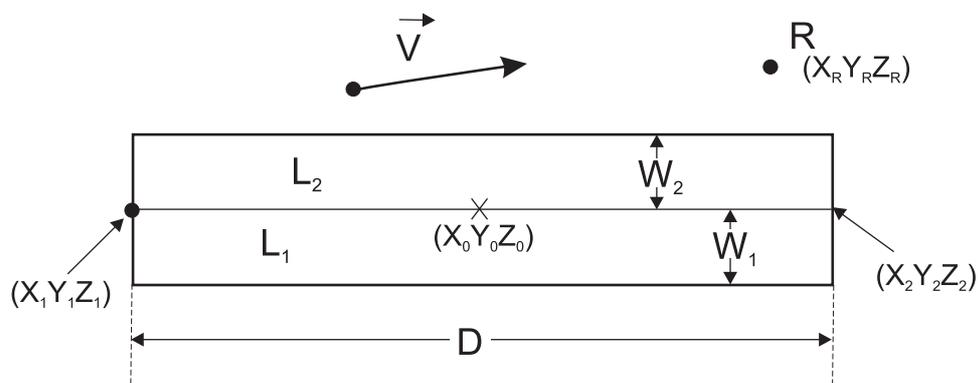


Figure 4.1: Example of a line source, L , consisting of two lanes, L_1 and L_2 . L_1 and L_2 have widths of w_1 and w_2 , respectively. The line source length (D) and direction is defined from its centreline start position (x_1, y_1, z_1) to its end position (x_2, y_2, z_2) . Each lane has identical length as the line source, and the distance between the centre line of lane i and the line source centreline is $w_i / 2$. By applying the wind velocity of the grid square containing the line source midpoint position, (x_0, y_0, z_0) , the concentration contribution from the line source at a receptor point, R , is calculated.

4.1.1 Line Source Model Equations

Consider now the line source L_i (lane i) being partitioned into an infinite number of infinitesimal "point" sources, where each such "point" source has an emission intensity $q_i \cdot dL$, where dL is an infinitesimal line segment. Each of the point sources is placed in the middle of the lane m_i with distance $w_i/2$ from the middle of the road L .

The concentration value at the receptor point R from emissions in lane i is now found by integrating (adding) the concentration contributions from each of the infinitesimal "point" sources along the line source L_i :

$$C = \frac{q_i}{u} \int_0^D f dl, \quad (4.1)$$

where

- q_i = emission intensity from the line source [$\mu\text{g}/\text{ms}$]
- u = wind speed [m/s]
- D = line source length [m]
- f = point source dispersion function [m^{-2}]

The value of the integral of eq. (4.1) is approximated by use of the Richardson extrapolation of the trapezoidal rule. Estimates are made dividing the line source into a number of intervals equal to 3, 6, ..., $3 \cdot 2^9$. Calculations are successively repeated for each partition class until the concentration estimates converge to within 2 percent of the previous estimate (Petersen, 1980).

The model uses local meteorology for dispersion, i.e., meteorology taken from the lowermost main gridcell where the midpoint of the line source is situated. Since expression (4.1) is invalid for wind speeds approaching zero, a lower bound is specified for the applied wind speeds. In the present version of EPISODE this minimum value is set to 1 m/s, and this limit value is applied when the calculated (or observed) wind speed is less than 1 m/s.

For *stable* conditions, or *if the mixing height is larger than 5000 meters*, the following ordinary point source Gaussian dispersion function is used in eq. (4.1):

$$f = \frac{1}{2\pi\sigma_y\sigma_z} \cdot e^{-\frac{y^2}{2\sigma_y^2}} \cdot \left\{ e^{-\frac{(z-H)^2}{2\sigma_z^2}} + e^{-\frac{(z+H)^2}{2\sigma_z^2}} \right\}, \quad (4.2)$$

where

- H = effective emission height [m]
- z = receptor height above the ground [m]
- σ_y = standard deviation of the concentration distribution in the crosswind direction [m]
- σ_z = standard deviation of the concentration distribution in the vertical direction [m]

For *unstable* or *neutral* conditions, if σ_z is larger than 1.6 times the height of the mixing height, h , the concentration distribution below the mixing layer is considered to be uniform with height, regardless of either source or receptor height, provided that both are less than the mixing height, h :

$$f = \frac{1}{\sqrt{2\pi} \cdot \sigma_y h} \cdot e^{-\frac{y^2}{2\sigma_y^2}} \quad (4.3)$$

For *all other unstable or neutral conditions*, the following Gaussian dispersion function is used, which includes multiple reflections from the ground:

$$f = \frac{1}{2\pi\sigma_y\sigma_z} \cdot e^{-\frac{y^2}{2\sigma_y^2}} \cdot \left\{ e^{-\frac{(z-H)^2}{2\sigma_z^2}} + e^{-\frac{(z+H)^2}{2\sigma_z^2}} + \sum_{n=1}^{\infty} \left(e^{-\frac{1}{2}\left(\frac{z-H-2nh}{\sigma_z}\right)^2} + e^{-\frac{1}{2}\left(\frac{z+H-2nh}{\sigma_z}\right)^2} + e^{-\frac{1}{2}\left(\frac{z-H+2nh}{\sigma_z}\right)^2} + e^{-\frac{1}{2}\left(\frac{z+H+2nh}{\sigma_z}\right)^2} \right) \right\} \quad (4.4)$$

The infinite sum series in eq. 4.4 converges rapidly, and more than four or five terms ($n = 1-5$) are seldom required.

For all line sources, the emission height H is always set equal to 1 m above the ground. The receptor height is also defined as 1 m above the ground for all main grid cells. For individual receptor points, the receptor height is defined by the user (input data).

The Gaussian formulas above do not take into account any topographical effects (height differences between emission points and receptor points). The model should therefore only be applied in areas where there are relatively uncomplicated (smooth) terrain.

4.1.2 Determination of the dispersion parameters σ_y and σ_z

In each of the three equations above (eqs. 4.2 – 4.4), σ_y and σ_z are calculated based on functions depending on the Pasquill-Gifford (PG) stability class and downwind distance.

The meteorological pre-processor applied in EPISODE, see Section 2.4, distinguish between 4 stability classes:

- Stability class 1: Unstable
- Stability class 2: Neutral
- Stability class 3: Moderately stable
- Stability class 4: Stable

In the EPISODE the following one-to-one mapping relation is used between the 4 stability classes of EPISODE and the P-G stability categories:

EPISODE Stability class 1 = P-G Stability class B
 EPISODE Stability class 2 = P-G Stability class D-day
 EPISODE Stability class 3 = P-G Stability class E
 EPISODE Stability class 4 = P-G Stability class F

The horizontal and vertical dispersion parameters, σ_y and σ_z , are composed of dispersion due to ambient turbulence, σ_{ya} and σ_{za} , plus the initial dispersion due to the turbulence induced by the vehicles, σ_{y0} and σ_{z0} , and are thus calculated as

$$\sigma_y = \sqrt{\sigma_{ya}^2 + \sigma_{y0}^2} \quad (4.5)$$

and

$$\sigma_z = \sqrt{\sigma_{za}^2 + \sigma_{z0}^2} \quad (4.6)$$

Based on data by Zimmermann and Thompson (1975) the vehicle induced turbulence are given by the constant values:

$$\sigma_{y0} = 3.0 \text{ m}, \quad (4.7)$$

and

$$\sigma_{z0} = 1.5 \text{ m}. \quad (4.8)$$

Note that Petersen (1980) indicates that the values given in eqs. (4.7) and (4.8) might be too low especially in low wind conditions.

σ_{ya} is given by

$$\sigma_{ya} = 1000 \cdot x / (2.15 \cdot \tan \theta_p) \quad (4.9)$$

where again x is the downwind distance (in km) and θ_p is the half angle of horizontal plume spreading (in degrees). θ_p is given by

$$\theta_p = c - d \cdot \ln(x/x_0), \quad (4.10)$$

where c and d are constants depending on stability, and the normalizing distance, x_0 , is 1 km. For neutral conditions $c = 14.333$ and $d = 1.7706$, while for stable conditions $c = 12.5$ and $d = 1.0857$.

σ_{za} is specified by the formula

$$\sigma_{za} = a \cdot x^b, \quad (4.11)$$

where x is downwind distance (in km) and the constants a and b depends on the stability. For neutral conditions $a = 86.49$ and $b = 0.92332$, while for stable conditions $a = 61.14$ and $b = 0.91465$.

Sufficiently far downwind the atmospheric dispersion process dominates. At 300 m downwind the above described dispersion curves are merged into the

P-G dispersion curves. For a more detailed description of these functions the reader is referred to Petersen (1980).

Monitoring results from roadside stations and tracer gas experiments show that the parameterisation of dispersion for stable atmospheric conditions coupled with the fixed initial dispersion from traffic induced turbulence provide too little dispersion of the roadside emissions during such conditions. Since the application of the model is in urban areas, and the subscale model is used in close vicinity to the roads, the present EPISODE version assume always neutral conditions. Thus stability class D is used, the mixing height is equal to 1000 meters, and dispersion eq. (4.4) is applied.

4.1.3 Definition of line source influence zones

The line source model is typically used to calculate ground level hourly average concentrations at individual receptor points (including grid points) over relatively small distances from the individual line sources, e.g., up to 500 m, ($\Delta X/2$) in most of the applications. In the model an *influence distance* is defined for each line source. In Figure 4.2 the resulting rectangular influence zone is depicted when the influence distance is R_{inf} . The line source model will only calculate concentrations for receptor points that lay within this influence zone. In addition, for receptor points that are closer than a minimum distance of R_{min} from the line source, the receptor point is moved away to a distance R_{min} from the line source (along the minimum distance vector). The inclusion of R_{min} has proved necessary in order to avoid that building point concentrations are estimated on the road due to the idealization of the line sources as straight line segments. Typically R_{min} is specified as $5 \text{ m} + w/2$, i.e. 5 m from the roadside.

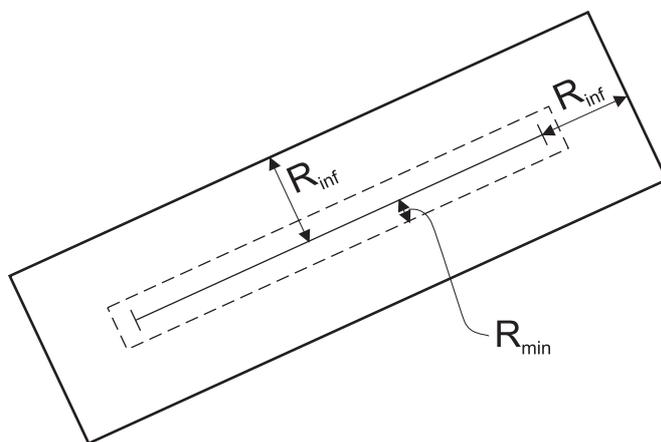


Figure 4.2: The resulting rectangular influence zone around a line source when the maximum and minimum influence distance is R_{inf} and R_{min} , respectively.

For any given receptor point, contributions from all line sources with influence zones containing the receptor point will be added. This is done at the end of each hour of calculation. In order to estimate the total “ground level” concentration at the receptor point the lower layer Eulerian grid concentrations is then added. The

hourly ($t = n \cdot h$) “ground level” concentration in an arbitrary receptor point ($x_r, y_r, z_r = 1 \text{ m}$) is thus estimated as

$$C(x_r, y_r, z_r = 1 \text{ m}, t = nh) = C_{i,j,1}^{nh} + \sum_{m=1}^M C_m^{nh}; \quad (4.12)$$

where $C_{i,j,1}^{nh}$ is the hourly Eulerian grid concentration in the lowermost layer at the end of hour n , and C_m^{nh} is the line source contribution from line source m , assuming that M line sources are contributing, and that the receptor point is within the grid cell with indices $(i,j,1)$. The Eulerian grid concentration applied in eq. (4.12), $C_{i,j,1}^{nh}$, is modified (see Section 4.3) so that the emissions from the contributing line sources are not counted twice.

An estimate of the hourly ground level grid square concentration, $\overline{C_{i,j}^{nh}}_{z=1 \text{ m}}^{xy}$, is similarly computed as the sum of $C_{i,j,1}^{nh}$ and an average of P·P evenly distributed receptor point values within each main grid cell, thus

$$\overline{C_{i,j}^{nh}}_{z=1 \text{ m}}^{xy} = C_{i,j,1}^{nh} + \frac{1}{P^2} \sum_{p=1}^{P^2} \left(\sum_{m=1}^M C_m^{nh} \right) \quad (4.13)$$

where the only change from eq. (4.12) is that the line source contribution is computed as a spatial average.

The expressions in (4.12) and (4.13) are used to store hourly “ground level” output concentrations in EPISODE, i.e. (4.12) for individual receptor points and (4.13) for gridded values. However, as the model steps forward in time, an accurate account of the total pollutant mass from area- and line-sources is kept within the Eulerian grid model. A detailed description of this (mass consistent) book-keeping procedure is given in Section 4.3 below.

The CPU time used by the subgrid scale line source model is approximately proportional to the number of line sources. The CPU time spent for a given line source depends on the number of receptor points within the influence distance from the line source, in addition to actual local meteorological data. By adjusting the influence distance for individual line sources, the CPU time used by the line source model may be controlled by the user. If the influence distance for a given line source is reduced, fewer receptor points will fall within the influence zone and less CPU time will be spent.

One way to adjust the influence distances, so that CPU time is spent where it is most useful, is to define larger influence zones for larger line sources with high emissions, and smaller influence zones for smaller line sources with lower emissions. In this way, CPU time will be spent where it is most useful, in calculating subgrid scale concentration distributions from the larger (more significant) line sources.

4.2 Coupling of the subgrid line source model and the Eulerian grid model – mass consistency of the coupled system

Generally the hourly concentration in an arbitrary receptor point (x_r, y_r, z_r) is calculated as described in eq. (4.12) in Section 4.1 above, i.e.

$$C(x_r, y_r, z_r, t = nh) = C_{i,j,k}^{nh} + \sum_{m=1}^M C_m^{nh} \quad (4.14)$$

where $C_{i,j,k}^{nh}$ is the hourly Eulerian grid concentration after n hours, and C_m^{nh} is the line source contribution from line source m , assuming that M line sources are contributing, and that the receptor point is within the grid cell with indices (i,j,k) .

If the influence distance for all of the line sources are defined as zero, then all of the C_m^{nh} -terms are zero, and the emissions from the road traffic will be redistributed as grid emissions in the Eulerian model for each timestep of the hour. If this redistribution is performed by EPISODE (and not in the emission module in AirQUIS) this redistribution procedure is as described in Appendix A.1.

If, on the other hand, the influence distance is taken as infinite, the line sources do not contribute to the Eulerian grid model emissions during each hour of calculation. At the end of the hour eq. (4.14) is applied to calculate the hourly receptor point concentrations, and the line source contributions during the last hour is given by the sum of the C_m^{nh} terms in eq. (4.14). After application of eq. (4.14), and before the start of the model calculation for the next hour, the emitted mass from all of the line sources during the last hour are introduced to the Eulerian grid model cell as an instantaneous contribution to the grid cell concentrations, $C_{i,j,k}^{nh}$. A description of this mass adjustment process is given in Appendix A.2.

Normally, the prescribed influence distance of a line source is less than (or equal to) $\Delta X/2$ (i.e. 500 m). This means that we are in a situation in between the two limiting cases described in Appendix A.1 and Appendix A.2. In this situation the line source will contribute to the gridded Eulerian emissions during each model timestep of the first part of the hour, (defined as: 1 hour - T_{inf}). During the remaining part of the hour (i.e. during T_{inf}) the line source emissions are not contributing to the Eulerian model, but are distributed among the grid cells at the beginning of the next hour. The applied methodology is described further in Appendix A.3.

5 The Point Source Model(s) applied in EPISODE

Two different point-source sub-grid models are implemented in EPISODE. One is based on a segmented plume/trajectory model (Walker et al. 1992), while the other is a puff/trajectory model (Petersen and Lavdas, 1986; Knudsen and Hellevik, 1992). In both models the emissions from individual point sources are treated as a temporal sequence of instantaneous releases of a specified pollutant mass. The subsequent position and concentration distribution within each of the plume segments or puffs are then estimated by the models. The segmented plume/trajectory model is described in detail in Section 5.1, while a technical description of the puff/trajectory model is presented in Section 5.2.

5.1 The Segmented Plume Trajectory Model

5.1.1 Overview

In the segmented plume trajectory model the emissions from individual point sources are treated as discrete emissions of finite length plume segments, emitted at time intervals ΔT . The length of ΔT is given by $\Delta T = 3600/2 \cdot N$, where N is an integer. The value of N depends on the meteorological conditions and becomes larger as the wind speed increase. Since the meteorology is kept constant within one hour, so does N and thereby also ΔT . The finite plume segments are redirected at every grid point and every hour according to the changing wind field.

Each individual plume segment is defined by the following set of parameters:

- horizontal position: x, y [m]
- vertical position: H [m]
- length in wind direction: L [m]
- direction: θ [deg]
- time since release: T [s]
- horizontal standard deviation: σ_y [m]
- vertical standard deviation: σ_z [m]
- emission rate: q [g/s]
- total mass of segment: Q [g]

Initially, the above parameters are specified as follows:

- The horizontal position of the plume segment, (x, y) , is at the source.
- The vertical position, or the plume segment height H , is estimated from plume rise formulas that are based on input information on stack height, velocity of the emitted gas, and buoyancy of the effluent.
- The length of the plume segment is prescribed as

$$L = U \cdot \Delta t,$$

where U is the wind speed at the plume height, H .

- The direction of the plume, θ , is set equal to the wind direction at the source.

- The Gaussian dispersion parameters, σ_y and σ_z , are set equal to the stack-top diameter, D_s .
- The emission rate, q , is set equal to the source emission rate, and the corresponding plume segment mass, Q , is thus:

$$Q = q \cdot \Delta t.$$

The ground level concentration for a given plume segment is calculated as

$$C(x, y, z) = \frac{qe^{-\lambda_w T}}{2\pi \cdot U \sigma_y \sigma_z} \cdot \exp\left[-\frac{y^2}{2\sigma_y^2}\right] \cdot \left\{ \exp\left[-\frac{(z-H)^2}{2\sigma_z^2}\right] + \alpha \cdot \exp\left[-\frac{(z+H)^2}{2\sigma_z^2}\right] \right\}, \quad (5.1)$$

where

x, y, z = receptor point location (here with the x-axis parallel with the wind direction [m],

q = emission intensity for the point source [g/s],

H = effective emission height [m],

U = wind speed [m/s],

σ_y = standard deviation of the concentration distribution in the cross wind direction [m],

σ_z = standard deviation of the concentration distribution in the vertical direction [m],

α = partial reflection coefficient due to dry deposition [non-dimensional].

NOTE: α is predefined as 1, i.e. the effect of dry deposition is not included in the AirQUIS₂₀₀₃ version.

λ_w = wet scavenging coefficient due to wet deposition [s^{-1}].

NOTE: λ_w is predefined as 0, i.e. the effect of wet scavenging is not included in the AirQUIS₂₀₀₃ version.

T = total time since rain started [s].

When the segmented plume reaches a predefined horizontal or vertical extent, it is inserted into the Eulerian grid cell containing its center of mass. This size is optimally set as $\sigma_y/\Delta y = 4$ or $\sigma_z/\Delta z = 4$, where σ_y and σ_z are the horizontal and vertical length scales of the plume segment, and Δy and Δz are the grid spacing in the horizontal and vertical direction, respectively. This is also done if the segmented plume experiences a large change in wind direction.

5.1.2 Input Requirements

The following point source characteristics are required:

- geographical position of stack (x, y),
- stack height, h_s , and stack diameter, D_s ,
- temperature and vertical velocity of emitted gas,
- height and width of surrounding building(s),
- the emission rate [g/s],
- topography,
- deposition and gravitational settling velocities (Not included in AirQUIS₂₀₀₃).

5.1.3 Stack Downwash

An effluent emitted vertically from a stack can rise due to its momentum, or be brought downward by the low pressure in the wake of the stack. What happens in a given situation depends on the ratio of the exit gas velocity to the wind velocity.

The physical stack height, h_s , is modified according to Briggs (1974)

$$h'_s = \begin{cases} h_s + 2(W_s / U - 1.5) \cdot D_s & \text{for } W_s < 1.5U \\ h_s & \text{for } W_s \geq 1.5U \end{cases} \quad (5.2)$$

where W_s is the exit gas velocity, U is the wind speed, and D_s is the inside stack-top diameter. The modified stack height h'_s is further used to calculate the effective plume height.

5.1.4 Plume Rise Equations

The plume rise due to momentum or buoyancy is estimated using Briggs algorithm (Briggs, 1969, 1971 and 1975). The calculated values of ΔH_m and ΔH_b in this Section, and h'_s in Section 5.1.3 are further used to evaluate the effects of buildings, penetration and topography in the following chapters to end up with the final plume height, H .

5.1.4.1 Neutral-Unstable Conditions

Regardless of the atmospheric stability, *neutral-unstable momentum rise*, ΔH_m , is calculated. This rise is calculated as

$$\Delta H_m = 3D_s W_s / U. \quad (5.3)$$

Equation (5.3) is most applicable when W_s / U is greater than 4. Since momentum rise occurs quite close to the point of release, the distance to final rise is set equal to zero.

The value of the boundary flux parameter, F , is needed for computing the distance to final rise, x_f , and the *buoyant plume rise*, ΔH_b .

$$F = (g W_s D_s^2 \Delta T) / (4 T_s), \quad (5.4)$$

where $\Delta T = T_s - T_a$, T_s is the stack gas temperature (K), and T_a is the ambient air temperature (K). The dimension of F is thus m^4/s^3 .

The distance to final rise, x_f (km), is the distance at which atmospheric turbulence begins to dominate entrainment. The expression of x_f depends on the boundary flux parameter, F , and is given as

$$x_f = 0.049 \cdot F^{5/8} \quad \text{for } F < 55, \quad (5.5)$$

and

$$x_f = 0.119 \cdot F^{2/5} \quad \text{for } F \geq 55. \quad (5.6)$$

The buoyant plume rise, ΔH_b (m), is finally determined from the equations

$$\Delta H_b = 21.425 \cdot F^{3/4} / U \quad \text{for } F < 55, \quad (5.7)$$

and

$$\Delta H_b = 38.71 \cdot F^{3/5} / U \quad \text{for } F \geq 55. \quad (5.8)$$

If the neutral-unstable momentum rise, calculated from eq. (5.3), is larger than the neutral-unstable buoyancy rise calculated here, momentum rise applies and the distance to final rise is set equal to zero.

5.1.4.2 *Stable Conditions*

For stable situations, the stability parameter s is calculated from the equation

$$s = g(\partial\theta/\partial z) / T_a. \quad (5.9)$$

As an approximation the vertical gradient of the potential temperature, $\partial\theta/\partial z$, is taken as 0.02 K/m for the light stable class, and as 0.035 K/m for the stable class.

When the stack gas temperature is less than the ambient air temperature, it is assumed that the plume rise is dominated by momentum. The plume *momentum rise*, ΔH_m , is then calculated by the equation

$$\Delta H_m = 1.5 \cdot \left[(W_s^2 D_s^2 T_a) / (4 T_s U) \right]^{1/3} \cdot s^{-1/6}. \quad (5.10)$$

This value of ΔH_m is compared with the value for neutral-unstable momentum rise (eq. 5.3) and the *lower* of the two values is used as the resulting plume height.

For situations where $T_s \geq T_a$, *buoyancy* is assumed to dominate. The distance to final rise (in kilometres) is determined by the equation

$$x_f = 0.0020715 \cdot U \cdot s^{-1/2}, \quad (5.11)$$

and the *buoyant plume rise* is determined by

$$\Delta H_b = 2.6 \cdot [F / (U \cdot s)]^{1/3}. \quad (5.12)$$

In addition to the general expression in (5.12), the stable buoyancy rise for *calm conditions* is also evaluated

$$\Delta H_b = 4 \cdot F^{1/4} s^{-3/8}, \quad (5.13)$$

and then the *lower* of the two values obtained from eqs. (5.12) and (5.13) is taken as the final estimate of the buoyant plume rise.

If the stable momentum rise is higher than the stable buoyancy rise calculated here, momentum rise applies and the distance to final rise is set to equal to zero.

5.1.5 Building Effects

Briggs (1974) has outlined a useful procedure for estimating the effective height of emission incorporated building-induced disturbances to the flow. The procedure is as follows:

Calculate the height, h' , according to the formula

$$h' = h_s + \Delta H_m \quad (5.14)$$

where ΔH_m is the momentum plume rise, eqs. (5.3) or (5.10).

If stack downwash occurs, $h' = h'_s$ from eq. (5.2) in Section 5.1.3.

Let L_B be the smaller of the frontal building dimensions H_B or W_B .

a) If h' is greater than $H_B + 1.5L_B$, the plume is above the region of building influence. Continue to Section 5.1.6 to check for penetration by using $h_e = h' + \Delta H$ as the effective plume height. ΔH is the plume rise from Section 5.1.4.

b) If h' is less than H_B , set

$$h'' = h' - 1.5L_B \quad (5.15)$$

c) If h' is between H_B and $H_B + 1.5L_B$, set

$$h'' = 2h' - (H + 1.5L_B) \quad (5.16)$$

For the cases b) and c) the plume may remain aloft or may be entrained into the wake cavity and become essentially a ground level source.

If h'' is greater than $0.5L_B$, the plume remains elevated and concentrations can be calculated by using standard formulas with modified stack height equal h'' , and effective plume height $h_e = h'' + \Delta H$. Continue to Section 5.1.6 to check for penetration by using h_e as the effective plume height.

If h'' is less than $0.5L_B$, the plume is influenced by the buildings, an additional dispersion factor is combined with the standard dilution factor as follows (Briggs, 1971).

$$\sigma_y = (\sigma_z^2 + cA/\pi)^{1/2} \quad (5.17)$$

$$\sigma_z = (\sigma_z^2 + cA/\pi)^{1/2} \quad (5.18)$$

where $c = 1.0$ and $A = H_B W_B$.

5.1.6 Plume Penetration

A buoyant plume rising into a well-mixed layer capped by stable air may partially or completely penetrate the elevated stable layer. To compute ground level concentrations for this situation, the fraction of the plume that penetrates the stable layer is first estimated and then the emission rate, q_s , and effective plume height, h_e , for the material remaining within the mixed layer are modified.

The fraction P of the plume that penetrates the elevated stable layer is estimated as follows (Weil and Brower, 1984)

$$P = 0 \quad \text{if} \quad \frac{z_i'}{\Delta H} \geq 1.5 \quad (\text{i.e. no penetration}) \quad (5.19)$$

$$P = 1 \quad \text{if} \quad \frac{z_i'}{\Delta H} \leq 0.5 \quad (\text{i.e. total penetration}) \quad (5.20)$$

$$P = 1.5 - \frac{z_i'}{\Delta H} \quad \text{if} \quad 0.5 < \frac{z_i'}{\Delta H} < 1.5 \quad (\text{i.e. partial penetration}) \quad (5.21)$$

where ΔH is the predicted plume rise and $z_i' = z_i - h_s$, where z_i is the height of the stable layer aloft, and h_s is the stack height.

The plume material remaining within the mixed layer is assumed to contribute to ground level concentrations. The modified source strength, q , is then

$$q = q_s \cdot (1 - P) \quad (5.22)$$

where q_s is the emission rate on top of the stack.

To modify the effective plume height for plumes trapped within the mixed layer, it is assumed that the plume rise due to penetration, ΔH_p , is linearly varying between $0.62 z_i'$ for no penetration and z_i' for total penetration.

Thus for partial penetration ($0 < P < 1$)

$$\Delta H_p = (0.62 + 0.38 \cdot P) \cdot z_i' \quad (5.23)$$

The modified plume height to be used further, h_m , is the lowest value of the height in the unlimited atmosphere, h_e , from Section 5.1.5, and the height due to penetration, such as:

$$h_m = \min(h_e, h_p) ; \quad h_p = h_s' + \Delta H_p \quad (5.24)$$

Continue to Section 5.1.7 to check for terrain effects by using h_m for the effective plume height.

5.1.7 Topography

The effect of elevated terrain on the ground level concentrations is included by reducing the effective plume height, h_m , assuming

$$H = h_m - \Delta H_t ; \quad \Delta H_t = k \cdot h_t \quad (5.25)$$

where h_t is the height of terrain above stack base level and k is a terrain factor ($0 < k < 1$) dependent upon steepness, distance from source, stability etc. The method used to evaluate the effect of a hill on a source as a function of distance from the source is given in Table 5.1 below. The effect of elevated terrain on the ground level concentrations decreases as the distance from the source increases.

Table 5.1: Terrain factor, k , to evaluate the effect of a hill on a source with stack height h_s .

Distance (x)	k
$0 < x \leq 5 h_s$	0.7
$5 h_s < x \leq 10 h_s$	0.5
$10 h_s < x \leq 20 h_s$	0.3
$20 h_s < x \leq 30 h_s$	0.1
$30 h_s < x$	0.0

5.1.8 Advection

Horizontal advection of each plume segment is performed by calculating a new horizontal plume position

$$X(t + \Delta t) = X(t) + U \cdot \Delta t \quad \text{and} \quad Y(t + \Delta t) = Y(t) + V \cdot \Delta t \quad (5.26)$$

where U and V are the X- and Y-components of the wind and Δt is the current timestep.

Vertical advection of plume segments is not taken into account in the present model.

5.1.9 Dispersion

Horizontal dispersion of each plume segment is calculated according to the following formula (Irwin, 1983)

$$\sigma_y(t) = \sigma_v \cdot t \cdot \frac{1}{1 + 0.9\sqrt{t/1000}} \quad (5.27)$$

where t is the travel time (time since release) and σ_v is the standard deviation in the horizontal turbulent wind fluctuations. If onsite measurements of σ_v are available, these values are used in (5.27). However, most often such measurements are not available and then estimated values of σ_v are applied. These values are calculated by use of the meteorological pre-processor as described in Section 2.3 above.

Vertical dispersion is calculated according to the following formula (Venkatram et al., 1984)

$$\sigma_z(t) = \sigma_w \cdot t \cdot \left(1 + \frac{t}{2T_L}\right)^{-1/2} \quad (5.28)$$

and where T_L denotes the Lagrangian timescale (see also Section 2.5) defined as

$$T_L = \frac{\lambda}{\sigma_w}, \quad (5.29)$$

where the dispersion length scale λ is specified as

$$\frac{1}{\lambda} = \frac{1}{\lambda_s} + \frac{1}{\lambda_n} \quad (5.30)$$

and where λ_s and λ_n are defined respectively as:

$$\lambda_s = \frac{\gamma^2 \sigma_w}{N} \quad (5.30 \text{ a})$$

and

$$\lambda_n = \alpha z. \quad (5.30 \text{ b})$$

In (5.30 a) and (5.30b) $N = \sqrt{\frac{g}{T} \frac{d\theta}{dz}}$ is the Brunt-Vaisala frequency, $\gamma = 0.52$, and $\alpha = 0.36$.

In EPISODE the vertical Gaussian plume dispersion parameter σ_z is calculated according to eq. (5.28), with T_L defined as in eq. (5.29) and with the length scale given by eq. (5.30). For stable conditions EPISODE applies the total interpolation formula (5.30) for the calculation of the length scale λ , while for neutral and unstable conditions only (5.30 b) is applied, i.e.

$$\lambda = \lambda_n = \alpha z. \quad (5.31)$$

Note that expressions like eqs. (5.27) and (5.28) automatically make the σ -values proportional to t and \sqrt{t} for small and large values of t , respectively.

5.1.10 Dry Deposition

Dry deposition is not included in the Segmented Plume Trajectory Model in AirQUIS2003. The parameter α in Eq. (5.1) is predefined as 1.

5.1.11 Wet Deposition

Wet deposition is not included in the Segmented Plume Trajectory Model in AirQUIS2003. The parameter λ_w in Eq. (5.1) is predefined as 0.

5.2 The puff trajectory model (INPUFF)

5.2.1 Overview

INPUFF (Petersen and Lavdas, 1986; Knudsen and Hellevik, 1992) is a Gaussian integrated puff model with a wide range of applications. The Gaussian puff diffusion equation is used to compute the contribution from multiple point sources to the concentration at each user defined receptor point for every time step. The implied modelling scale is from tens of meters to tens of kilometres. The model is capable of addressing the accidental release of a substance over several minutes, or of modelling the more typical continuous plume from a stack.

INPUFF is primarily designed to model a single event during which a meteorological transition period occurs, such as, going from afternoon to evening conditions. A spatially varying wind field can be specified at time intervals defined by the user. These intervals may range from minutes to an hour. In Episode these intervals are typically one hour.

Three dispersion algorithms are available within INPUFF for simulating dispersion downwind of the source. The user may choose between the Pasquill-Gifford (P-G) scheme (Turner, 1970) or the on-site scheme (Irwin, 1983) for short travel time dispersion. The on-site scheme, so named because it requires specification of the variances of the vertical and the lateral wind direction, is a synthesis of work performed by Draxler (1976) and Cramer (1976). The third dispersion scheme is for long travel times in which the growth of the puff becomes proportional to the square root of time. Optionally the user can incorporate his own subroutine for estimating atmospheric dispersion.

INPUFF utilizes the deposition algorithms given by Rao (1982). In the limit when pollutant settling and dry deposition velocities become zero, these expressions reduce to the Gaussian diffusion algorithms.

INPUFF is in addition equipped with the following features:

- Optional stack downwash
- Wind speed extrapolated to release height
- Temporally variable source characteristics
- Optional user-supplied temporally and spatially variable wind field
- Consideration of terrain effects through the applied wind field
- Optional buoyancy induced dispersion
- Optional user-supplied plume rise algorithm
- Optional user-supplied dispersion algorithm
- Optional deposition and settling (*Not included in AirQUIS₂₀₀₃*)
- Optional source update
- Optional intermediate concentration output
- Optional puff information output

Although INPUFF, as applied in EPISODE, has several advantages over its continuous plume counterpart, it still retains several limitations, including:

- Wind direction constant with height
- No consideration of chemical reactions
- No explicit treatment of complex terrain.

The dimension of the modelling grid must be specified. In the case when a user-supplied wind field option is implemented, which is the normal case when applied in EPISODE, then the dimension of the meteorological grid must also be indicated. (It is recommended that both grids be given a common origin.) If a puff travels outside the modelling region, it is deleted from further consideration. If it travels outside the meteorological grid, but is still within the modelling region, the last wind experienced by the puff is used to advect it further.

The puff-formula applied in INPUFF calculates the concentration, C , of a pollutant at the position x , y , and z and at time t , from an instantaneous puff release, Q , with an effective emission height, H , according to

$$C(\bar{r}, t) = \frac{Q}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \cdot \exp\left(-\frac{(x-ut)^2}{2\sigma_x^2}\right) \cdot \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \cdot \left\{ \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) \right\} \quad (5.32)$$

By assuming isotropic diffusion in the horizontal, $\sigma_x = \sigma_y = \sigma_r$, and introducing the radial distance from the advecting centre of mass of the puff, $r^2 = (x-ut)^2 + y^2$, the above equation can be rewritten:

$$C(r, z, t) = \frac{Q}{(2\pi)^{3/2} \sigma_r^2 \sigma_z} \cdot \exp\left(-\frac{r^2}{2\sigma_r^2}\right) \cdot \left\{ \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) \right\} \quad (5.33)$$

When σ_z becomes larger than 0.8 times the mixing height, h_{mix} , the puff is assumed to be well mixed and the concentration is simplified to

$$C(r, h_{\text{mix}}, t) = \frac{Q}{2\pi\sigma_r^2 h_{\text{mix}}} \cdot \exp\left(-\frac{r^2}{2\sigma_r^2}\right) \quad \text{for} \quad \sigma_z > 0.8 \cdot h_{\text{mix}} \quad (5.34)$$

Each individual puff is defined by the following set of parameters:

- horizontal position of centre of mass: x, y [m]
- vertical position of centre of mass: H [m]
- horizontal distance to centre of mass: r [m]
- vertical distance to ground: z [m]
- time since release: t [s]
- lateral standard deviation: $\sigma_r(t)$ [m]
- vertical standard deviation: $\sigma_z(t)$ [m]
- emission rate: q [g/s]
- total mass of puff: $Q = q \cdot \Delta t$ [g]

Initially, the above parameters are specified as follows:

- The horizontal position of the centre of mass of the puff, (x, y) , is at the source.

- The vertical position, or the puff height H , is estimated from plume rise formulas that are based on input information on stack height, velocity of the emitted gas, and buoyancy of the effluent.
- The lateral and vertical extent of the puff is prescribed as σ_{r0} and σ_{z0} .
- The horizontal position of the centre of mass of each puff is subsequently advected along with the applied wind field according to

$$X(t + \Delta t) = X(t_0) + U \cdot \Delta t, \quad \text{and} \quad Y(t + \Delta t) = Y(t_0) + V \cdot \Delta t$$

where U , V are the horizontal components of the wind and Δt is the timestep between each puff release.

A schematic representation of the treatment of the puffs in the INPUFF model is given in Figure 5.1. In order to simplify the description, a spatially homogeneous wind field is applied in this example. The first puff (puff A) was initially advected with an east-southeast directed wind, followed by a slightly stronger wind from the south, and finally by an even stronger wind from south-southeast. The second puff (puff B) was released at the time when the wind shifted from east-southeast to south, and the third puff (puff C) was released at the next wind shift. Note that the stability conditions, and thus the growth rate of the individual puffs, will normally vary from one meteorological condition to the next. INPUFF assumes that $\sigma_x = \sigma_y$, and therefore the horizontal spread of each puff remains circular throughout their lifetime.

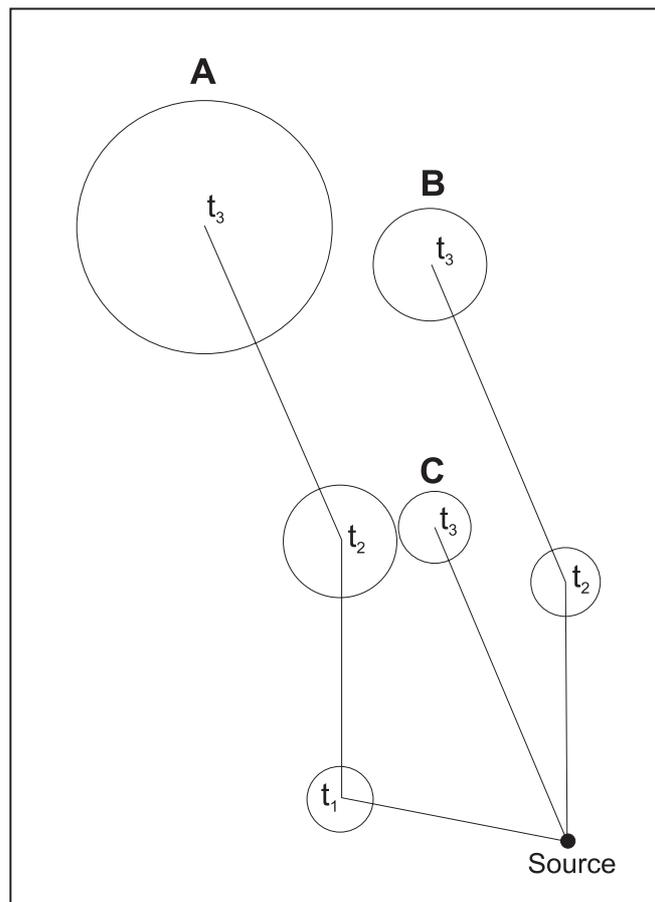


Figure 5.1: Schematic picture of the time-evolution of three individual puffs.

5.2.2 *Input Requirements*

The following point source characteristics are required:

- geographical position of stack (x,y),
- stack height and stack diameter, [m]
- temperature and vertical velocity of emitted gas, [K] and [m/s]
- stack gas volume flow, [m³/s]
- height and width of surrounding building(s) [m]
- the emission rate, [g/s]

The meteorological data needed for the computation are as follows:

- wind speed [m/s]
- wind direction [degrees]
- mixing height [m]
- stability class [dim. less]
- standard deviation of elevation angle; $\arctan(\sigma_z/U)$, [rad],
- standard deviation of azimuth angle; $\arctan(\sigma_r/U)$, [rad],
- ambient air temperature, [K],
- Height of wind speed and direction, [m].

5.2.3 *Stack Downwash*

Optionally, stack downwash can be considered using the method (Briggs, 1974) described in Section 5.1.3 above. Use of this option primarily affects computations from stacks having small ratios of exit velocity to wind speed.

5.2.4 *(Plume) Rise Equations*

Plume rise is optionally calculated using the methods of Briggs; i.e. the methods described above in Section 5.1.4 (Briggs, 1969, 1971 and 1975).

5.2.5 *Building Effects*

Building downwash, and gradual plume rise are not treated by INPUFF.

5.2.6 *Penetration*

Puff penetration across the top of the mixed layer is not treated in INPUFF. However, see Section 5.2.10 for a description on the influence of the mixing height, h_{mix} .

5.2.7 *Topography*

INPUFF does not explicitly handle the effect of sloping terrain. The topography only influences the results by its modifying effect on the direction of the applied wind field.

5.2.8 *Advection*

Horizontal advection of each puff is performed by tracking the horizontal position of its centre of mass according to the following formula

$$X(t + \Delta t) = X(t) + U \cdot \Delta t \quad \text{and} \quad Y(t + \Delta t) = Y(t) + V \cdot \Delta t \quad (5.35)$$

where U and V are the X- and Y-components of the wind and Δt is the model timestep.

After the final rise of the puff, H , has been calculated, no further effect of *vertical advection* is taken into account in the present model.

5.2.9 Dispersion

Several dispersion algorithms are incorporated in the INPUFF model to account for initial dispersion, short travel time dispersion, and long travel time dispersion.

5.2.9.1 Initial dispersion

The initial dispersion of the puff at the source is modelled by specifying the initial horizontal and vertical dispersion parameters, σ_{r0} and σ_{z0} . For tall stacks these parameters generally, have little influence on downwind concentrations. However, if the source is large enough or close enough to the ground, then initial size is important in determining ground level concentrations near the source.

In the INPUFF version presently implemented in EPISODE, the values of σ_{r0} and σ_{z0} are defined equal to the inside stack-top diameter, D_s , i.e.

$$\sigma_{r0} = \sigma_{z0} = D_s \quad (5.36a)$$

(However, these values can easily be modified and values similar to the ones recommended in the INPUFF model description (Petersen and Lavdas, 1986),

$$\sigma_{r0} = D_s / 4.3, \quad \text{and} \quad \sigma_{z0} = h_s / 2.15, \quad (5.36b)$$

can be applied instead. Here h_s is the physical height of the source. According to Petersen and Lavdas (1986), these values of σ_{r0} and σ_{z0} for the initial size of near ground releases gives reasonable concentration estimates at downwind distances greater than about five times the initial horizontal dimension of the source.)

5.2.9.2 Buoyancy induced dispersion

The buoyancy-induced dispersion feature is offered because emitted plumes undergo a certain amount of growth during the plume rise phase, due to the turbulent motions associated with the conditions of plume release and the turbulent entrainment of ambient air. Pasquill (1976) suggested that this buoyancy-induced dispersion could be approximated by $\Delta H/3.5$, and that the effective dispersion, σ_{ze} , could be determined by adding variances, i.e.

$$\sigma_{ze} = \sqrt{\sigma_{z0}^2 + (\Delta H/3.5)^2}, \quad (5.37a)$$

where ΔH is the plume rise (calculated as described in Section 5.1.4), and σ_{z0} is the initial value specified in eq. (5.36a) or (5.36b). At the distance of final rise and beyond, the buoyancy-induced dispersion is constant using ΔH of final rise. At distances closer to the source, the ΔH is itself determined using gradual rise.

Since in the initial growth phases of release the plume is nearly symmetrical about its centreline, buoyancy-induced dispersion in the horizontal direction equal to that in the vertical is used, i.e.

$$\sigma_{ye} = \sqrt{\sigma_{y0}^2 + (\Delta H/3.5)^2} , \quad (5.37b)$$

In general, buoyancy-induced dispersion will have little effect upon maximum concentrations unless the stack height is small compared to the plume rise.

It should be clarified here that the buoyancy-induced dispersion close to the source is calculated using gradual rise in INPUFF, even if the gradual plume rise option is not being used to determine the effective plume height.

5.2.9.3 *Short travel time dispersion*

The subsequent dispersion downwind of the source can be estimated by either the Pasquill-Gifford (P-G) scheme, which is a function of stability class and downwind distance, or by the on-site scheme (Irwin, 1983), which is a function of travel time.

5.2.9.3.1 *Pasquill-Gifford scheme*

The P-G values that appear as graphs in Turner (1970) are used in the model. However, for neutral atmospheric conditions two dispersion curves as suggested by Pasquill (1961) are incorporated into the model. Dispersion curves D1 and D2 are appropriate for adiabatic and sub-adiabatic conditions, respectively. The D2 curve is used in Turner (1970) for neutral conditions. From a practical point of view, since temperature soundings may not be available we refer to the D1 and D2 curves as D-day and D-night. P-G stability classes are numerical inputs to the puff model. Stability classes A through D-day are specified by 1-4, and classes D-night through F are specified by 5-7, respectively.

The meteorological pre-processor applied in EPISODE, see Section 2.4, distinguish between 4 stability classes:

- Stability class 1: Unstable
- Stability class 2: Neutral
- Stability class 3: Moderately stable
- Stability class 4: Stable

In the present implementation of INPUFF the following one-to-one mapping relation is used between the 4 stability classes of EPISODE and the P-G stability categories:

EPISODE Stab. class 1 = INPUFF Stab. class 2 (= P-G Stab. class B)
 EPISODE Stab. class 2 = INPUFF Stab. class 4 (= P-G Stab. class D-day)
 EPISODE Stab. class 3 = INPUFF Stab. class 6 (= P-G Stab. class E)
 EPISODE Stab. class 4 = INPUFF Stab. class 7 (= P-G Stab. class F)

(In the present application of INPUFF in EPISODE the on-site dispersion scheme (Irwin, 1983; see below) is preferred instead of the P-G scheme.

5.2.9.3.2 On-site dispersion scheme (Irwin, 1983)

The *horizontal* and *vertical diffusion* are specified for each puff according to the following formulas (Irwin, 1983)

$$\sigma_y(t) = \sigma_v \cdot t \cdot \frac{1}{1 + 0.9\sqrt{t/1000}}, \quad (5.38)$$

$$\sigma_z(t) = \sigma_w \cdot t \cdot f_z, \quad (5.39a)$$

where

$$f_z = 1 \quad \text{for unstable conditions, and} \quad (5.39b)$$

$$f_z = \frac{1}{1 + 0.9\sqrt{t/50}} \quad \text{for stable conditions.} \quad (5.39c)$$

In these expressions t is the puff's travel time from the source. Stable conditions are considered if the stability class (KS) is greater than 4, i.e. when the EPISODE stability class is 3 (moderately stable) or 4 (stable), i.e. eq. (5.39b) is applied for stability class 1 (unstable) and stability class 2 (neutral).

In addition to the stability class, needed for determining the functional form of σ_z , the on-site scheme requires values of the turbulence parameters, σ_v and σ_w , which are assumed to be representative for the conditions at final plume height, H . (For small angles, $\sigma_v = \sigma_a \cdot U$ and $\sigma_w = \sigma_e \cdot U$, where U is the wind speed at measurement height and σ_a and σ_e are the standard deviations of the horizontal and vertical wind angle, respectively.) Since the INPUFF model requires σ_a and σ_e as input data, these quantities are computed from σ_v and σ_w by the following relations

$$\sigma_a = \arctan(\sigma_v/U) \quad \text{and} \quad \sigma_e = \arctan(\sigma_w/U). \quad (5.40)$$

For small angles (5.40) can be approximated by:

$$\sigma_a \approx \sigma_v/U \quad \text{and} \quad \sigma_e \approx \sigma_w/U.$$

5.2.9.4 Long travel time dispersion scheme

That the dispersion parameters used in INPUFF satisfy the diffusion theory developed by Taylor (1921) is desirable. Taylor showed that while the growth of the puff is linear with time near the source, the growth becomes proportional with the square root of time at large distances. In the model, therefore, after the puff has attained a user specified horizontal dimension, $(\sigma_y)_{\max}$, the algorithm automatically goes to a long travel time growth rate proportional to the square root of time. In the present implementation in EPISODE this length scale is specified as

$$(\sigma_y)_{\max} = 1000 \text{ m.} \quad (5.41)$$

A very large value of $(\sigma_y)_{\max}$ results in the long travel time code not being executed. The incremental growth of σ_y in this long travel time regime is calculated as

$$\sigma_y^{n+1} = A \sqrt{\frac{\sigma_y^n}{A} + \Delta t} \quad (5.42)$$

where A is a constant of value 10.4446. Note, that the On-site scheme (Irwin 1983) already contains the square root of time growth at large travel times, and therefore the formula in eq. (5.42) need not be considered.

5.2.10 The effect of the mixing height, h_{mix}

Depending on the stack height and final plume rise, the puffs can be above or below the height of the mixed layer, $z = h_{mix}$.

a) Puff above h_{mix} .

If the puffs are above h_{mix} , there are two cases that govern their growth. Initially the puffs are allowed to grow according to the P-G, F curve (i.e. stable conditions), or if the On-site scheme is used, the puffs are restricted to a vertical growth rate characterized by:

$$\sigma_w = 0.01 \text{ m/s} , \quad \text{if } H > h_{mix} \quad (5.43)$$

After the puffs attain a given size of $(\sigma_r)_{lim}$, (not actual puff size) specified by the user, the horizontal growth rate is specified by the long travel time sigmas.

NOTE: If the stability conditions continue to be neutral (D-day) or unstable from one hour to the next, the value of h_{mix} is not allowed to decrease between these two hours. If a lower value of h_{mix} is estimated from the meteorological pre-processor, this value is reset to the previous value by INPUFF.

b) Puff below h_{mix} .

When the puffs are below h_{mix} , there are four cases that must be considered. Cases one and two are puffs that are not well mixed vertically and whose growth rates are characterized by the short travel time sigmas or by a growth proportional to \sqrt{t} . Cases three and four are puffs that are well mixed vertically and whose growth for σ_r is for short travel times or according to \sqrt{t} .

During the simulation, each puff is given a dispersion key to indicate whether it is above or below h_{mix} , whether its growth rate is characterized by the short travel time sigmas or by the long travel time expression, and whether the puff is well mixed or not. Thus, a puff can attain one of six possible dispersion keys. In the modelling design, puffs are allowed to change their dispersion keys. When the height of h_{mix} becomes greater than the puff height, the puffs are allowed to grow at the rate characterized by surface measurements. Normally this is a neutral or unstable situation. This transition period is likely to occur in the morning hours. In the afternoon, despite the decay of active mixing, a puff remains well mixed through the maximum mixing lid as shown in Figure 5.2. The maximum height of h_{mix} is stored for each puff and is never allowed to decrease. This method assures that concentration does not increase with downwind distance or travel time, so as to violate the second law of thermodynamics (avoiding anti-diffusion).

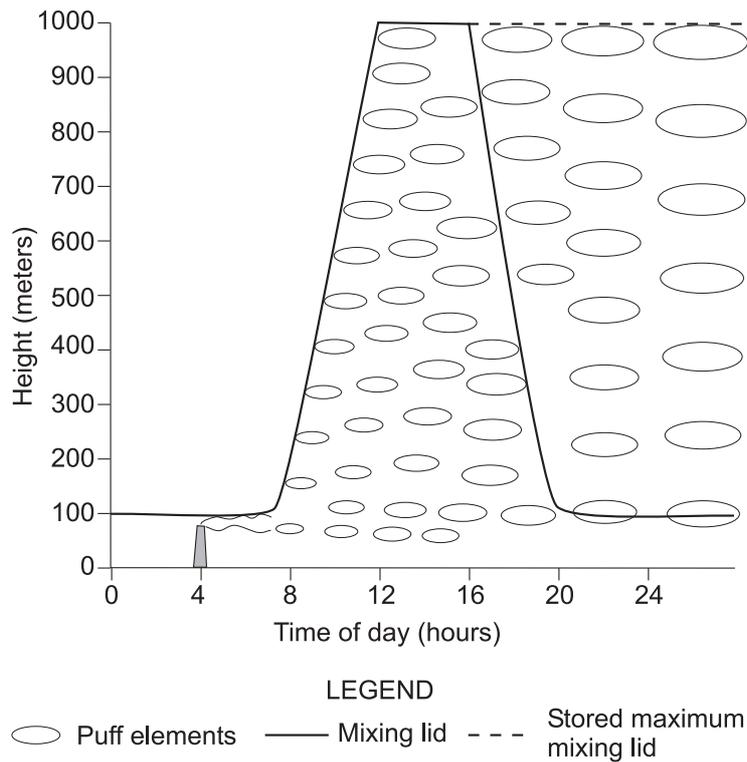


Figure 5.2: The effect of variable mixing height on puff dispersion.

5.2.11 Merging of puffs

To reduce computing time INPUFF contains functionality for combining neighbouring puffs, i.e. puff merging. Combination of puffs occur only for adjacent puffs in the release sequence which have identical values of the above defined dispersion keys. The merging depends on a user specified input parameter, SDCMBN, and two puffs are combined when their centres are within a horizontal distance of $SDCMBN \cdot \sigma_r$. A value of SDCMBN equal to 0 results in no puff combination. Normally, a value of 1.0 is assigned to SDCMBN. If the user specifies a negative value for SDCMBN, INPUFF will automatically assign a value for this parameter.

Upon combining puffs, the position, displacement, and travel time are combined based on the weighted (based on total mass within puff) average between the two puffs. The puff sigmas are calculated according to the weighted geometric means. The mass of the puffs are summed. For more details on user defined input parameters, see pp. 50 – 60 in Knudsen and Hellevik (1992).

5.2.12 Dry deposition and gravitational settling

Dry deposition and gravitational settling are not included in the version of INPUFF presently applied in AirQUIS₂₀₀₃.

5.2.13 Wet Deposition

Wet deposition is not included in the version of INPUFF presently applied in AirQUIS₂₀₀₃.

6 References

About AirQUIS: <http://www.nilu.no/aqm/>

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Appendix A

Coupling of the subgrid line source model and the Eulerian grid model

Appendix A.1 Redistribution of line source emissions in the Eulerian grid model when the line source influence distance is zero

If the influence distance for a given line source is zero, the subgrid line source model will not be applied. All of the pollutant mass emitted from the line source will then go directly into the Eulerian grid model as emissions in the gridcell(s) containing the line source. If the line source is distributed over several grid cells, the emissions will be split over the affected gridcells. This can be viewed as a mechanism to deactivate individual line sources and effectively turning them into (distributed) area sources.

In detail the procedure for this redistribution is as follows:

Consider a line source, m , with length L . If the length of the line source is greater than half the horizontal grid distance, the line source is split into a minimum number, N , of equally long segments, each being less than half of the horizontal grid distance, thus

$$N = \text{INT}\left(\frac{2 \cdot L}{\text{MIN}(\Delta X, \Delta Y)}\right) + 1. \quad (1)$$

Each of the segments have length L/N , and the distance from the start node of the line source to the midpoint of each segment is

$$X_m^i = (2i - 1) \cdot \frac{L}{2N} \quad i = 1, \dots, N. \quad (2)$$

where X_m^1 is the midpoint of the segment closest to the start node. Each segment then contribute with its emission to the grid cell (i, j, k) containing the segment midpoint. The emission intensity (in g/s) of each segment is $Q_m = q_m \cdot L/N$, where q_m is the line source emission intensity given in g/(m·s). [NOTE: All of the segment emission intensities are equal for a given line source. Furthermore, this emission intensity is found by summing over all lanes.] For every time step the line segment then contributes to the gridded Eulerian model source field, $S_{i,j,k}$, in the following way

$$S_{i,j,k} = S_{i,j,k} + \frac{Q_m}{V_{i,j,k}} \cdot \Delta t \quad (3)$$

where $V_{i,j,k}$ is the volume of the grid cell containing the midpoint of the segment considered.

Appendix A.2 Mass redistribution in the case of infinite influence distances

With an infinite influence distance no line source emissions are introduced as gridded emissions into the Eulerian model during the model computation from one hour to the next. In this case the mass emitted from all of the line sources during the last hour are introduced to the grid cell concentrations, $C_{i,j,k}$, as an instantaneous contribution at the beginning of the next hour. Each line source contributes to this process according to the following formula:

$$C_{i,j,k} = C_{i,j,k} + (w_m)_{i,j,k} \cdot \frac{\Omega_m}{V_{i,j,k}} \quad (4)$$

Here Ω_m is the mass emitted from line source m during the last hour, $V_{i,j,k}$ is the volume of grid cell (i,j,k) , and $(w_m)_{i,j,k}$ is a weight function that determines how much of the mass, emitted from line source m , is introduced into the grid cell (i,j,k) . The weight function is simply given as

$$(w_m)_{i,j,k} = \frac{(C_m)_{i,j,k}}{\sum_{\forall i,j,k} (C_m)_{i,j,k}} \quad (5)$$

here $(C_m)_{i,j,k}$ is the concentration contribution from line source m in the midpoint of grid cell (i,j,k) , and $\sum_{\forall i,j,k} (C_m)_{i,j,k}$ is the sum of the concentration contributions from this line source to all of the grid cell midpoints within the Eulerian model domain. Thus the weight function satisfy the familiar conditions

$$0 \leq (w_m)_{i,j,k} \leq 1 \quad \text{and} \quad \sum_{i,j,k} (w_m)_{i,j,k} \equiv 1 \quad (6)$$

A similar contribution is found from all of the line sources and they therefore add up to the following expression

$$C_{i,j,k} = C_{i,j,k} + \sum_m^M (w_m)_{i,j,k} \cdot \frac{\Omega_m}{V_{i,j,k}} \quad (7)$$

where M is the total number of line sources that contribute to the mid point of grid cell (i,j,k) . The change of the Eulerian grid model concentrations specified in eq. (7) should be considered as an adjustment of the initial concentration distribution before starting the model calculations for the next hour.

A special case occurs when the line source, say m^* , is close to the model boundary and the wind direction is such that the denominator in eq. (5) becomes zero. In this case the mass from this line source is distributed within the grid cell containing the line source midpoint, i.e. (i^*,j^*,k^*) :

$$C_{i^*,j^*,k^*} = C_{i^*,j^*,k^*} + \frac{\Omega_{m^*}}{V_{i^*,j^*,k^*}} \quad (8)$$

Appendix A.3 Mass redistribution in the case of influence distances with finite lengths

Normally, the prescribed influence distance of a line source is less than (or equal to) $\Delta X/2$ (i.e. 500 m). This means that we are in a situation in-between the two limiting cases described in Appendix A.1 and Appendix A.2. In this situation each of the line source segments (see Appendix A.1 for the definition of the segments) will contribute to the gridded Eulerian emissions during each model timestep of the first part of the hour, (defined as: 1 hour - T_{inf}) and then the segment emissions during the remaining part of the hour (i.e. during T_{inf}) will be redistributed among the grid cells at the beginning of the next hour. The method described in Appendix A.1 is applied during the first period, while the redistribution method of Appendix A.1 is applied for the line source emissions during the last period. The only aspect that needs to be described further is the determination of the influence time, i.e. T_{inf} for each line segment.

In Figure A.1 an example situation is depicted in which a line source, with total length L_m , is divided in two segments ($N = 2$) and where the local coordinate system is defined with the origin at the start node and the x-axis directed along the line source. Each of the segments have length $L_m/2$ and the midpoints of each segment are denoted X_m^1 and X_m^2 , respectively. A separate influence time is defined for each line segment, T_{inf}^i .

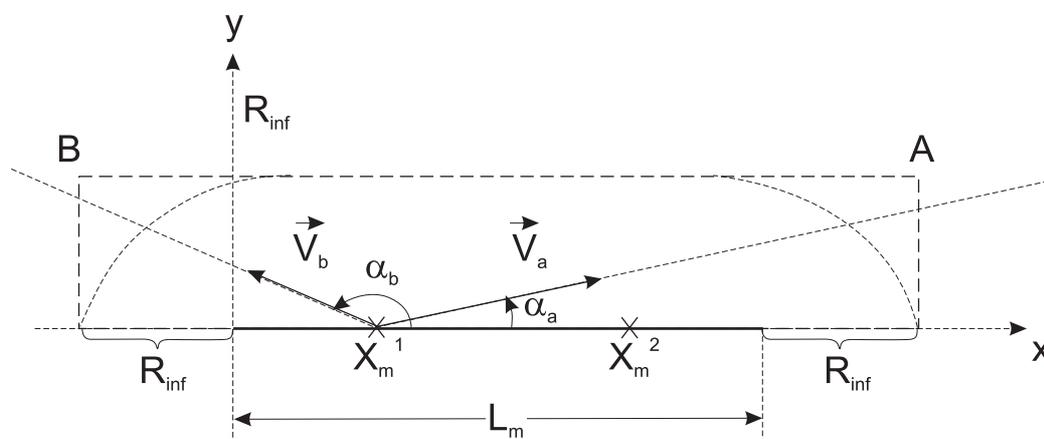


Figure A.1: Example of a line source with length L_m , and with a prescribed influence distance of R_{inf} . The line source which is aligned with the x-axis, is divided in two equally long segments, each with midpoint co-ordinates X_m^1 and X_m^2 . Two examples of the wind velocities are depicted, one with a component towards the end node of the line source (**Error! Objects cannot be created from editing field codes.**) and one with a component in the other direction (**Error! Objects cannot be created from editing field codes.**).

Assuming that the prescribed line source influence distance is given as R_{inf} , and the wind direction is normal to the line source, the estimated influence time for all of the segments is simply given by:

$$T_{inf}^i = \text{MIN} \left(\frac{R_{inf}}{|\vec{V}|}, 3600. \right) \quad (9)$$

where $|\vec{V}|$ is the wind speed. With R_{inf} equal to 500 m, the upper limit of 1 hour is only applied for wind speeds less than 0.14 m/s.

For other wind directions we need to distinguish between directions with components along the road towards the end node, and directions with components in the other direction.

a) With a wind component from the start node towards the end node (ref. \vec{V}_a and α_a in Figure 4):

In this case a new line segment influence distance, R_{new}^i , is computed for each line segment. With reference to Figure 4, this length is found in the interval:

$$R_{new}^i \in < R_{inf}, R_{inf} + L_m - X_m^i] \quad (10)$$

The lower boundary, $R_{new}^i = R_{inf}$, is applied for near normal winds ($\alpha_a \approx 90^\circ$ or 180°) and the upper boundary, $R_{new}^i = L_m + R_{inf} - X_m^i$, is applied for along road winds ($\alpha_a = 0^\circ$). For wind directions in between R_{new}^i is gradually varying between these bounds. Since there is no limit of the length of the line source, L_m , the new influence distance can become very large.

b) With wind in the opposite direction (ref. \vec{V}_b and α_b in Figure A.1):

The new line segment influence distance is in this case limited by the interval:

$$R_{new}^i \in < R_{inf}, R_{inf} + X_m^i] \quad (11)$$

Again the lower boundary is applied for near normal winds ($\alpha_b \approx 90^\circ$) and the upper boundary for along road winds ($\alpha_b = 180^\circ$).

Note that the additional terms in the upper boundary of both (10) and (11) is just the distance from the segment midpoint to the alongwind end-point of the line source.

By applying the above a) and b) expressions, the line segment influence time is given by:

$$T_{\text{inf}}^i = \text{MIN} \left(\frac{R_{\text{new}}^i}{|\bar{V}|}, 3600. \right) \quad (12)$$

The total mass emitted from a line source, named m , during the different influence times of each line segment is then found as

$$\Omega_m = \sum_{i=1}^N \frac{q_m L_m}{N} \cdot T_{\text{inf}}^i = q_m L_m \sum_{i=1}^N \frac{T_{\text{inf}}^i}{N} = q_m L_m \cdot (\overline{T_{\text{inf}}})_m \quad (13)$$

Here q_m is the line source emission intensity given in $\text{g}/(\text{m}\cdot\text{s})$, L_m is the line source length, and N is the number of line source segments. $(\overline{T_{\text{inf}}})_m$ is the average value of the various influence times. Following the same procedure as described in Appendix A.2, see eq. (7), the masses, Ω_m , from the different line sources are then introduced in the Eulerian grid model concentrations at the beginning of the next hour as:

$$C_{i,j,k} = C_{i,j,k} + \sum_m^M (w_m)_{i,j,k} \cdot \frac{\Omega_m}{V_{i,j,k}} \quad (14)$$

where M is the total number of line sources that contribute to the mid point of grid cell (i,j,k) and $(w_m)_{i,j,k}$ is a weight function determining how much of the mass emitted from line source m that is introduced into grid cell (i,j,k) . The only difference between the redistribution formulae of (7) and (14) is that while the weight in (7) (defined in (5)) is normalised by the sum of line source contributions in all of the grid cell midpoints within the model domain, (14) just consider the grid cell midpoints within the influence zone of each line source. This influence zone is simply defined as a rectangle centred around the line source with along-road length of $(L_m + 2R_{\text{inf}})$ and cross-road width of $(2R_{\text{inf}})$, where L_m is the line source length, and R_{inf} is the prescribed line source influence distance, see Figure A.2.

Thus $(w_m)_{i,j,k}$ in (4.28) is given by:

$$(w_m)_{i,j,k} = \frac{(C_m^{\text{nh}})_{i,j,k}}{\sum_{i,j,k} (C_m^{\text{nh}})_{i,j,k}} ; \quad i, j, k \text{ within the influence zone of line source } m. \quad (15)$$

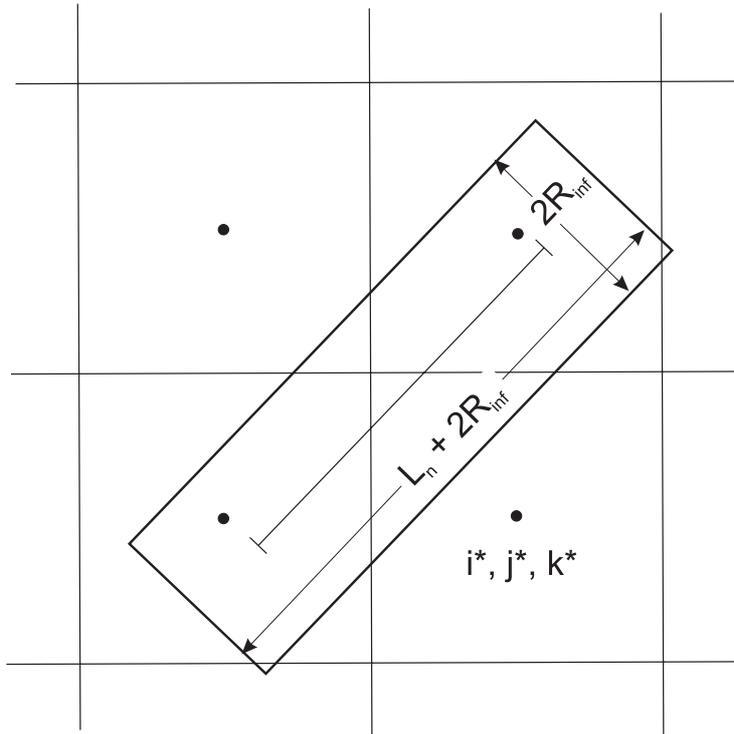


Figure A.2: An example of the selection of grid cell midpoints affected by the rectangular influence zone around a line source when the prescribed influence distance is R_{inf} .

In the special case when no grid cell midpoints are within the influence zone of line source m , the mass Ω_m is introduced to the grid cell containing the line source midpoint, i.e. (i^*, j^*, k^*) as:

$$C_{i^*, j^*, k^*} = C_{i^*, j^*, k^*} + \frac{\Omega_m}{V_{i^*, j^*, k^*}} \quad (16)$$

Note that the change of the Eulerian grid model concentrations specified in eq. (14) should be considered as an adjustment of the initial concentration distribution before starting the model calculations for the next hour.

