ESSE 5203: Diffusion notes

March 16, 2020 - PAT

Text: J.R.Garratt, The Atmospheric Boundary Layer, 1994. Cambridge , Also some material from

J.C. Kaimal and J.J. Finnigan, 1994, Atmospheric Boundary-Layer Flows - Oxford.

Blackadar, A.K., 1997, Turbulence and Diffusion in the Atmosphere, Springer: Blackadar Chapter 10 is good, Morphology, Could use Blackadar Smoke model – but it is on a CD!.

Pasquill, F. and Smith, F.B., 1983, Atmospheric Diffusion, 3rd Edition, Ellis Horwood

Terminology – dependence on atmospheric stability. Not so many smoke plumes around these days! Also plumes may be buoyant, hot or releasing latent heat – effective source height with Gaussian plumes.

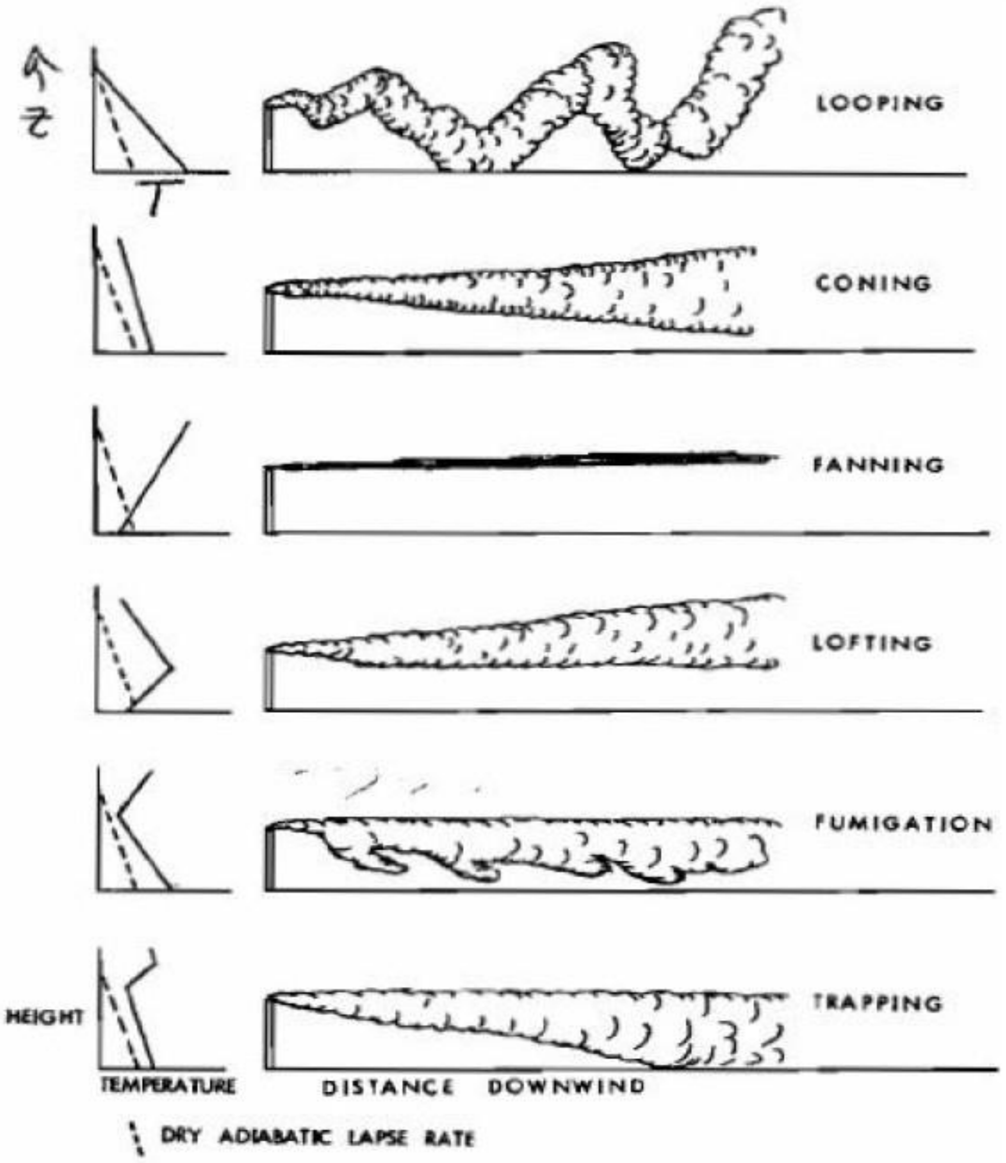
Continuity - passive contaminant, inert, no settling, no chemistry

Instantaneous and continuous point sources

IPS $Q = \int C(x, y, z, t)\, dxdydz$ is constant,
Q - kg, C - kg m^{-3}

CPS $Q = \int U\, C(x, y, z)\, dydz$ steady state, where Q is now a source rate kg s^{-1} and we assume U > 0 and unidirectional. Integral at fixed x.

Can also have a continuous line source model - a busy road.



Fickian Diffusion - analogue with molecular diffusion. Constant, isotropic, eddy diffusivity
Fickian diffusion equation, diffusion coefficient D (m^2s^{-1})

For IPS and uniform wind, move coordinate system with mean flow.

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right)$$

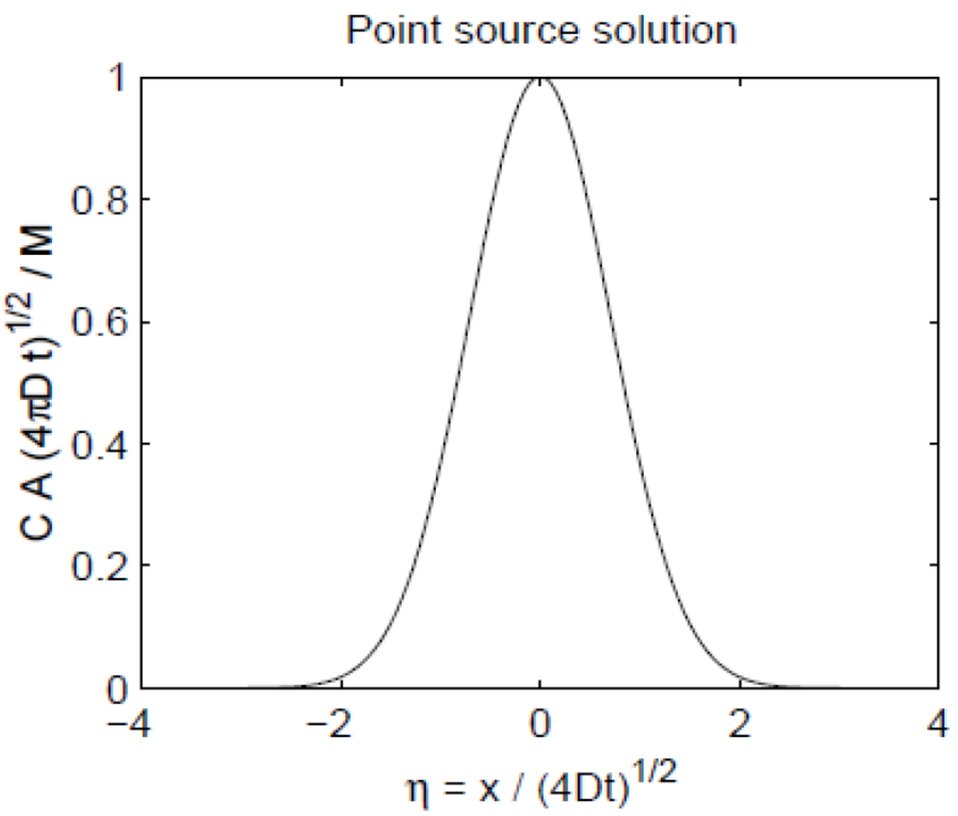
1-D case

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

Solution (1D), M is total mass in cross sectional area A

$$C(x,t) = \frac{M}{A\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)$$

Gaussian plumes – widely used



Solution of the 1-D equation $\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$ With M is total mass in cross sectional area A

Let $\eta = x/\sqrt{Dt}$

and $C = \frac{M}{A\sqrt{Dt}} f\left(\frac{x}{\sqrt{Dt}}\right)$

$$\frac{d^2 f}{d\eta^2} + \frac{1}{2}\left(f + \eta\frac{df}{d\eta}\right) = 0.$$

$$\int_{-\infty}^{\infty} f(\eta)d\eta = 1.$$

$$\frac{d}{d\eta}\left[\frac{df}{d\eta} + \frac{1}{2}f\eta\right] = 0.$$

$$f(\eta) = \frac{1}{2\sqrt{\pi}}\exp\left(\frac{-\eta^2}{4}\right)$$

$$C(x,t) = \frac{M}{A\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)$$

The Gaussian plume, or normal distribution.

$$\sigma^2 = 2Dt$$

In 3D, allowing for anisotropic diffusion coefficients,

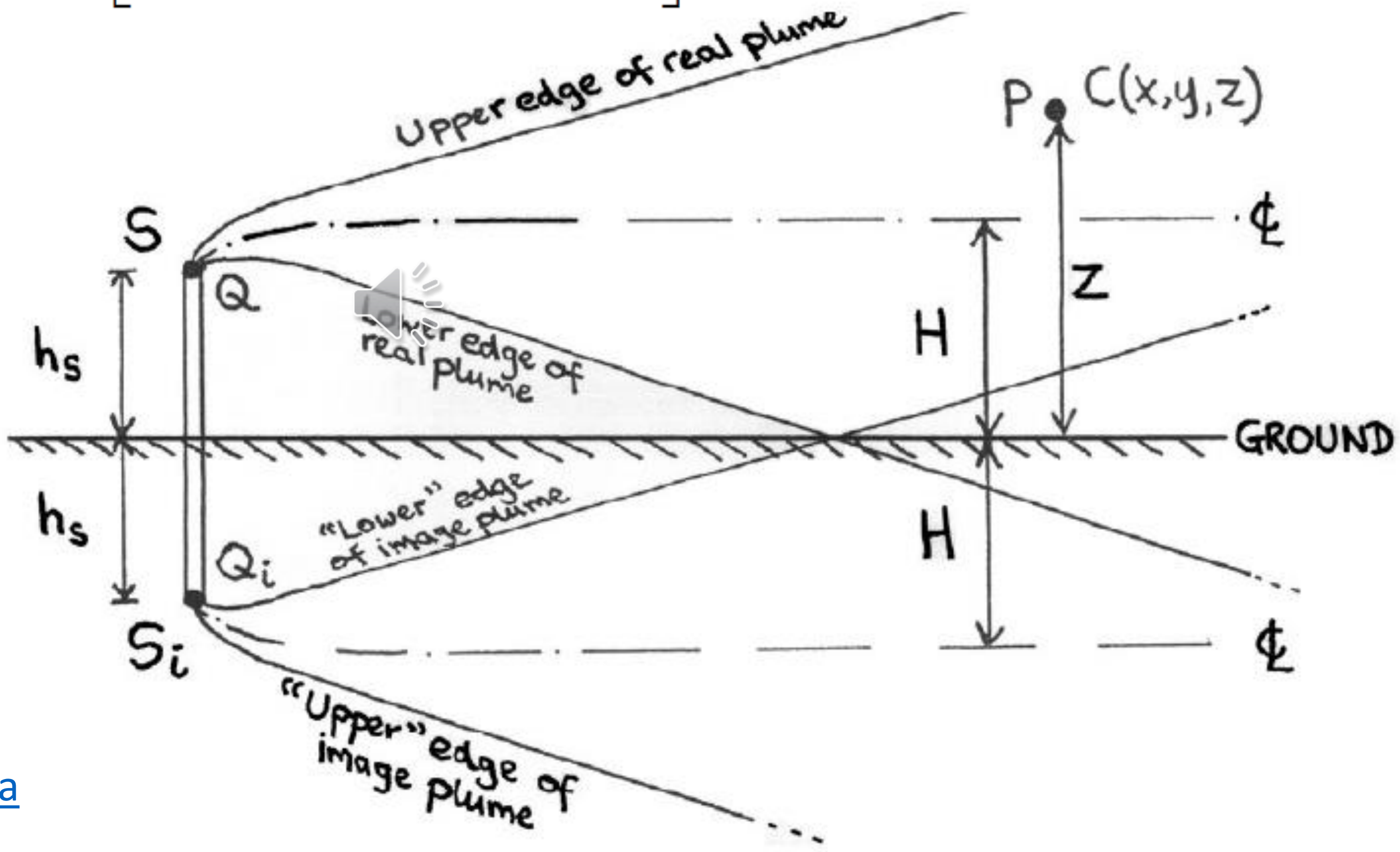
$$C(x,y,z,t) = \frac{M}{4\pi t\sqrt{4\pi D_x D_y D_z t}} \exp\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t} - \frac{z^2}{4D_z t}\right)$$

With stable stratification $D_z < D_x$ and D_y and the plume will spread more horizontally.

$$C(x,y,z) = \frac{Q}{U}\,\frac{1}{2\pi\sigma_y\sigma_z}\,e^{\left(\frac{-y^2}{2\sigma_y^2}\right)}\left[e^{\left(\frac{-(z-H)^2}{2\sigma_z^2}\right)} + e^{\left(\frac{-(z+H)^2}{2\sigma_z^2}\right)}\right]$$

Idealized reflection at the ground.

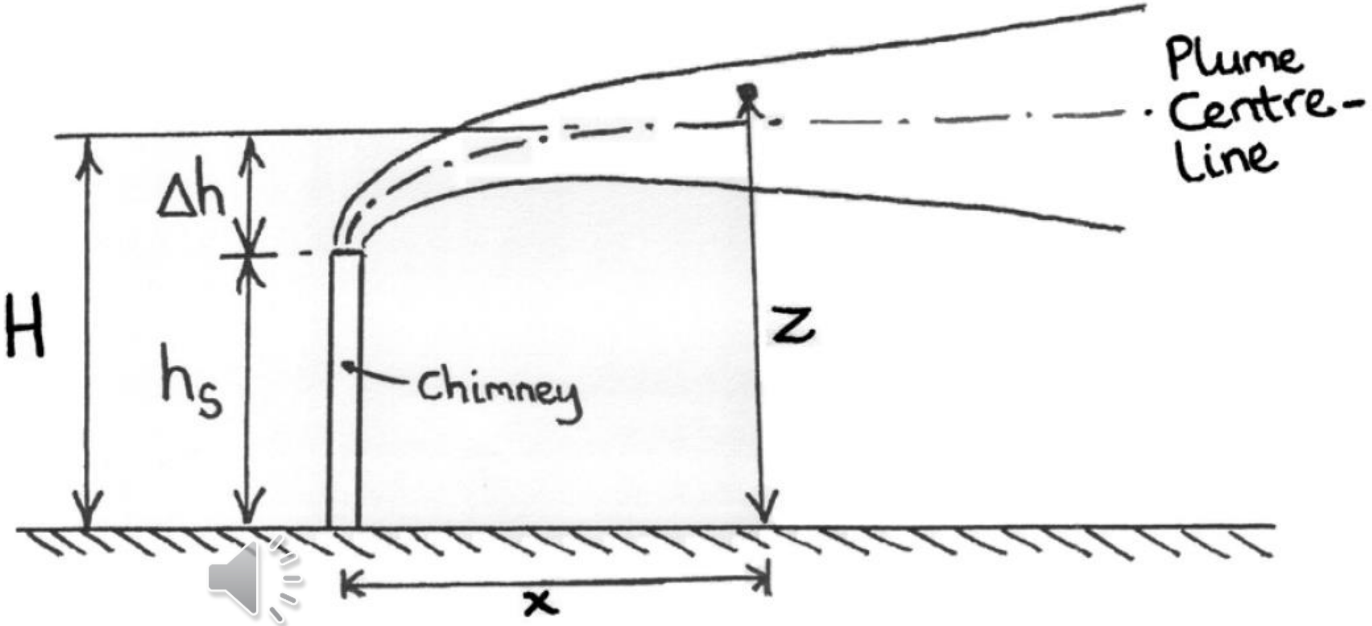
Ignores u(z) and any absorption at the ground



Notes from Eric Savory – Western U.

https://www.eng.uwo.ca/people/esavory/Gaussian%20plumes.pdf

Plume rise modifications



H = effective height of plume centre-line (m)
h_s = height of source above ground (m)
Δh = initial plume rise (m)
z = coordinate measured vertically from the ground to a point in the plume (m)

Typical turbulence intensities, σ_v/U, σ_w/U. But what we need are σ_y, σ_z

Thermal stratification	Lateral intensity (I_y)	Vertical intensity (I_z)
Extremely unstable	0.40 - 0.55	0.15 - 0.55
Moderately unstable	0.25 - 0.40	0.10 - 0.15
Near neutral	0.10 - 0.25	0.05 - 0.08
Moderately stable	0.08 - 0.25	0.03 - 0.07
Extremely stable	0.03 - 0.25	0 - 0.03

Can we estimate σ_y, σ_z ? Pasquill and Gifford schemes, One option,.

$$\sigma_y = I_y \, . \, x \qquad \text{and} \qquad \sigma_z = I_z \, . \, x$$

Stability description	Stability Class
Extremely unstable	A
Moderately unstable	B
Slightly unstable	C
Neutral conditions	D
Slightly stable	E
Moderately stable	F

Need to find plots such as those below, from about 1960. Or equations of the curves https://www.osti.gov/servlets/purl/5591108/ p29 - Steve Hanna

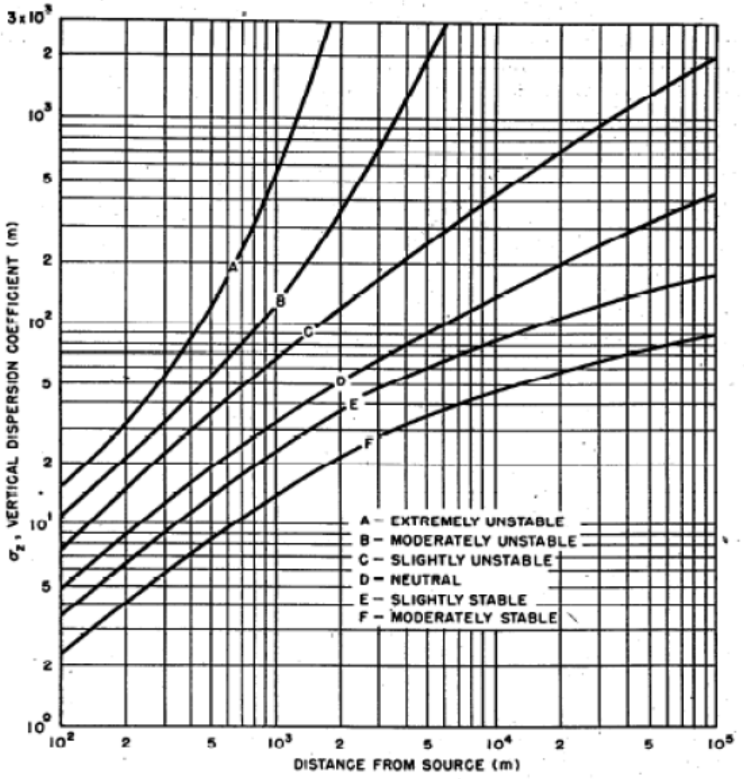


Fig. 3.11—Vertical diffusion, σ_z, vs. downwind distance from source for Pasquill's turbulence types.

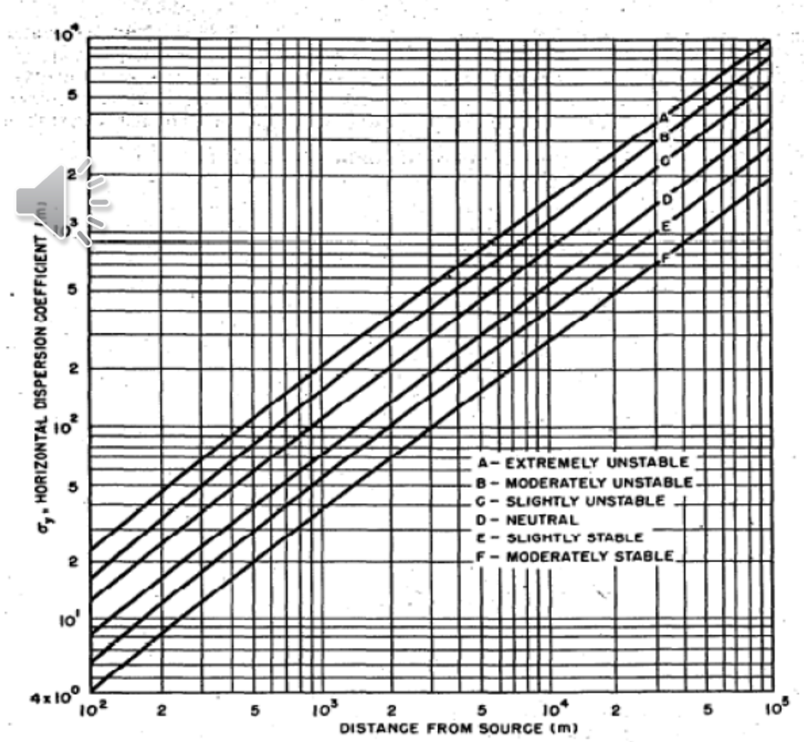
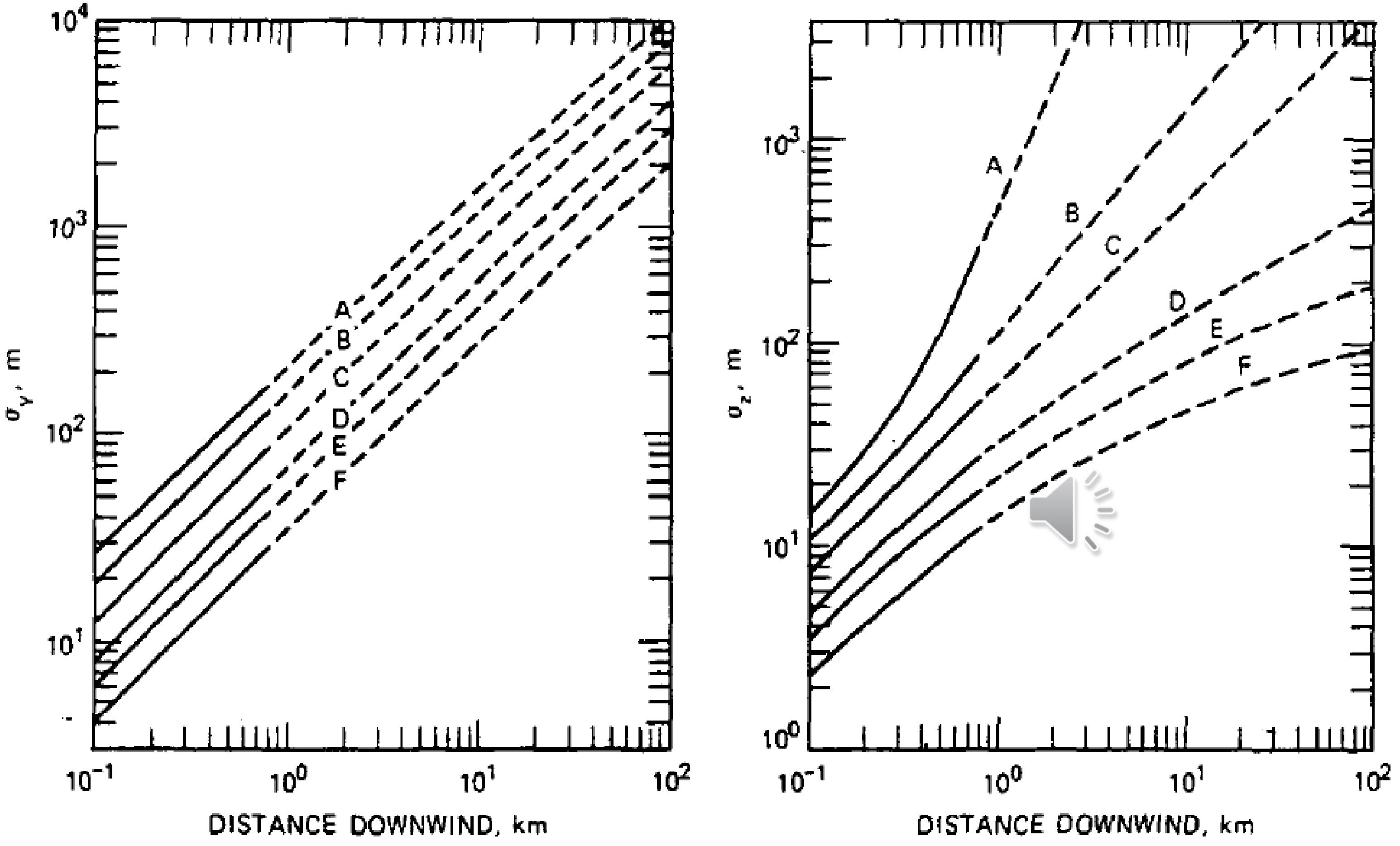


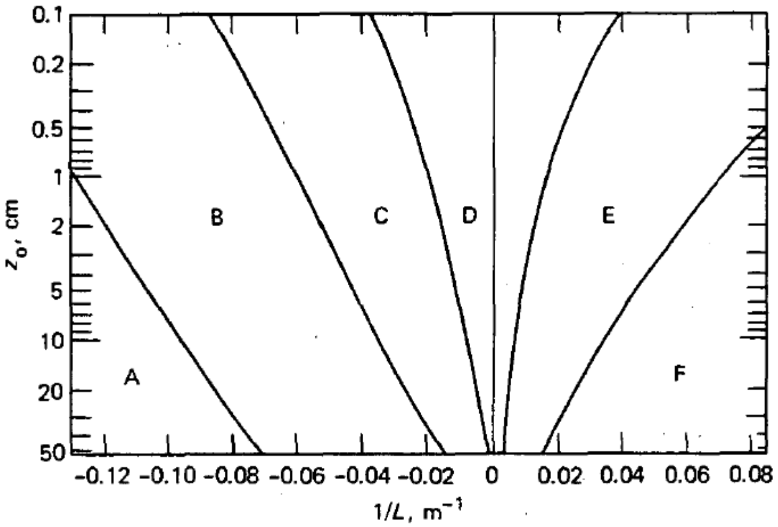
Fig. 3.10—Lateral diffusion, σ_y, vs. downwind distance from source for Pasquill's turbulence types.



(a) (b)

Table 4.5 Formulas Recommended by Briggs (1973) for $\sigma_y(x)$ and $\sigma_z(x)$ ($10^2 < x < 10^4$ m)

Pasquill type	σ_y, m	σ_z, m
	Open-Country Conditions	
A	$0.22x(1 + 0.0001x)^{-1/2}$	$0.20x$
B	$0.16x(1 + 0.0001x)^{-1/2}$	$0.12x$
C	$0.11x(1 + 0.0001x)^{-1/2}$	$0.08x(1 + 0.0002x)^{-1/2}$
D	$0.08x(1 + 0.0001x)^{-1/2}$	$0.06x(1 + 0.0015x)^{-1/2}$
E	$0.06x(1 + 0.0001x)^{-1/2}$	$0.03x(1 + 0.0003x)^{-1}$
F	$0.04x(1 + 0.0001x)^{-1/2}$	$0.016x(1 + 0.0003x)^{-1}$
	Urban Conditions	
A–B	$0.32x(1 + 0.0004x)^{-1/2}$	$0.24x(1 + 0.001x)^{1/2}$
C	$0.22x(1 + 0.0004x)^{-1/2}$	$0.20x$
D	$0.16x(1 + 0.0004x)^{-1/2}$	$0.14x(1 + 0.0003x)^{-1/2}$
E–F	$0.11x(1 + 0.0004x)^{-1/2}$	$0.08x(1 + 0.00015x)^{-1/2}$



A cleaner version, P-G curves from Hanna (1982)

How to determine stability class. See https://ready.arl.noaa.gov/READYpgclass.php
Air Resources Lab., NOAA – Hysplit model, trajectory and dispersion versions →

Pasquill Stability Classes

A: Extremely unstable conditions	D: Neutral conditions
B: Moderately unstable conditions	E: Slightly stable conditions
C: Slightly unstable conditions	F: Moderately stable conditions
G: Extremely Stable	

Meteorological conditions defining Pasquill stability classes.

	Daytime insolation			Night-time conditions	
Surface wind speed (m/s)	Strong	Moderate	Slight	Thin overcast or > 4/8 low cloud	<= 4/8 cloudiness
< 2	A	A - B	B	E	F
2 - 3	A - B	B	C	E	F
3 - 5	B	B - C	C	D	E
5 - 6	C	C - D	D	D	D
> 6	C	D	D	D	D

Source: Pasquill, 1961.

NOTES:

1. Strong insolation corresponds to sunny midday in midsummer in England; slight insolation to similar conditions in midwinter.

2. Night refers to the period from 1 hour before sunset to 1 hour after sunrise.

3. The neutral category D should also be used, regardless of wind speed, for overcast conditions during day or night and for any sky conditions during the hour preceding or following night as defined above.

PG classes for fluctuations in wind direction and the vertical temperature gradient.

Pasquill Class	Sigma Theta (degrees)	Delta T/Delta Z (Deg C/100 m)
A	25	-1.9
B	20	-1.9 to -1.7
C	15	-1.7 to -1.5
D	10	-1.5 to -0.5
E	5	-0.5 to 1.5
F	2.5	1.5 to 4.0
G	1.7	>4.0

Modified: December 4, 2019
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US Dept. of Commerce | NOAA | NOAA Research | ARL
webmaster

https://ready.arl.noaa.gov/READYtransp.php

Get/Run the HYSPLIT Model - Download the PC or Mac version or run the model on the web. Registration may be required to access some portions of this page. Additional documentation on the HYSPLIT model and its meteorological data can also be found here.

- HYSPLIT Basic Tutorial - Want to learn more about HYSPLIT and how to run the PC/Mac version? Then this online tutorial is the place to start as it will provide you with a good starting point for running the model appropriately.
- HYSPLIT Forum - Have a question about HYSPLIT? Register for the HYSPLIT Forum and search for an answer to your question or ask the user community for ideas and answers to your specific application.
- HYSPLIT Workshops - NOAA Air Resources Laboratory presents a PC/Mac HYSPLIT Workshop in the spring or early summer each year and follows the material found in the HYSPLIT Tutorial.
- HYSPLIT Automated Forecasts - HYSPLIT has been configured to automatically produce atmospheric dispersion forecasts for several locations four times daily. These locations may change based on the needs of NOAA and its partners. The model assumes a unit of mass emission over 60 hours and produces graphics for two concentration grids: a fine grid (~ 1km horizontal resolution) and a coarse grid (~10 km horizontal resolution). Output on the fine grid extends from hour 1 to hour 12 each hour, while the coarse extends from hour 2 to hour 60 every 2 hours. world.
- Volcanic Ash - Volcanic ash from an erupting volcano can seriously impact the aviation community. This section presents links to current and hypothetical eruptions within the Washington and Anchorage Volcanic Ash Advisor Center (VAAC) areas of responsibilty. Users can also run the HYSPLIT model for many volcanoes around the world.
- Fukushima NPP Transfer Coefficient Matrix (TCM) - Previously computed HYSPLIT simulations of the Fukushima Daiichi nuclear power plant accident are used to calculate Cesium-137 and Iodine-131 air concentrations and depositions from user selected source term estimates. The TCM allows provides an easy method to view the impacts of source term estimates without having to rerun the model for each case.
- Short-Range Ensemble Forecast (SREF) Dispersion Forecasts - The NOAA National Centers for Environmental Prediction (NCEP) run a series of model forecasts called the Short-Range Ensemble Forecasting (SREF) system to provide an estimate of the variability of a single forecast. ARL is experimenting with using the SREF to provide an estimate of the variability one might expect in the dispersion forecast due to variations in the meteorology used by the model. The source location may vary.
- Gaussian Plume Model - A simple model that was once considered the standard dispersion model for routine calculations is called the Gaussian plume model because it assumes the air pollutant dispersion has a Gaussian distribution (normal probability distribution). It assumes a constant wind direction and speed and uniform terrain, which limits its applicability to many atmospheric dispersion problems especially cases where the meteorology is changing and for calculations distant from the source location. It is still used by some regulatory agencies due to its simplicity. A simple version of the Gaussian plume model is provided here only to demonstrate its functionality and should not be used for most transport and dispersion simulations. HYSPLIT is a better choice if looking to use a model to calculate transport and dispersion.
- Balloon Flight Forecasting Tools - A tool for manned balloon flight planning has been developed that allows the user to visualize the potential flow combinations from up to three different starting heights, multiple times along the flight track. This tool uses the HYSPLIT model trajectories to determine where a balloon might travel if the height of the balloon is changed along the flight path and can help "steer" a balloon to a particular location or avoid a location such as calm winds.

G.I. Taylor's Diffusion Equation (from 1921) (Blackadar 10.5). Extract:

In a recent communication to the Royal Society, Mr. L. F. Richardson has described some experiments on the diffusion of smoke emitted from a fixed point in a wind. Similar observations have been made on the smoke from factory chimneys by Mr. Gordon Dobson. Both these observers came to the conclusion that, at small distances from the origin of the smoke, the surface containing the standard deviations of the smoke from a horizontal straight line to leeward of the source, is a cone. If the mean velocity of the wind is assumed to be uniform, the standard deviation in a short interval of time is therefore proportional to the time. At greater distances their observations indicate that this surface becomes like a paraboloid, so that the deviation of the smoke is proportional to the square root of the time.

DIFFUSION BY CONTINUOUS MOVEMENTS

By G. I. Taylor.

[Received May 22nd, 1920.—Read June 10th, 1920.]

Introduction.

It has been shown by the author,* and others, that turbulent motion is capable of diffusing heat and other diffusible properties through the interior of a fluid in much the same way that molecular agitation gives rise to molecular diffusion. In the case of molecular diffusion the relationship between the rate of diffusion and the molecular constants is known; a large part of the Kinetic Theory of Gases is devoted to this question. On the other hand, nothing appears to be known regarding the relationship between the constants which might be used to determine any particular type of turbulent motion and its "diffusing power."

The propositions set down in the following pages are the result of efforts to solve this problem.

Also G.I.Taylor 1935, Proc Roy Soc A.

Is the conical pattern compatible with Fickian diffusion? Would always grow as $x^{1/2}$. Eulerian and Lagrangian autocorrelations $R(\xi) = \langle v(t)v(t+\xi)\rangle/\sigma_v^2$: Blackadar p131,132

10.5 Taylor's Diffusion Equation

An important contribution to our understanding of turbulent diffusion was made by Taylor (1935). The theory recognized diffusion as a continuous process, in contrast to exchange theory, which is based on a model of discrete mixing events interspersed with undisturbed displacements over paths of undetermined lengths. While Taylor's equation falls short of providing a complete theory of diffusion, it focuses attention on those processes that are most important and on the statistics that must be known for further progress.

We shall discuss only dispersion in the y-direction, but the outcome can also be applied to the z-direction. The turbulence is presumed to be stationary. Particles are released from a source one by one, and each particle's motion is independent of that of its predecessor. The aim is to predict the variance of the y values of all the particles at a time interval T after leaving the source.

We define the Lagrangian autocorrelation $R(\xi)$ by the equation

$$R(\xi) \equiv \frac{\overline{v(t)\,v(t+\xi)}}{\overline{v^2}} \tag{10.17}$$

where $v(t)$ is $dy dt$ for a single particle at some time t, and $v(t+\xi)$ is the value for the same particle ξ seconds later. The average is extended over all the particles released at the same point. Under *stationary* conditions, the Lagrangian autocorrelation is a function of ξ only. Its value for $\xi = 0$ is unity.

We can integrate $R(\xi)$ from the moment of release ($t = 0$) to a time t seconds later:

$$\overline{v^2} \int_0^t R(\xi)\,\mathrm{d}\xi = \overline{v(t)\,y(t)} = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,\overline{y^2}(t)\ . \tag{10.18}$$

A second integration, treating t as a dummy variable over the range 0 to T, gives, in principle, the mean squared value of y.

Key points are: Lagrangian autocorrelation,

$$R(\xi) \equiv \frac{\overline{v(t)\,v(t+\xi)}}{\overline{v^2}}$$

$$\overline{v^2} \int_0^t R(\xi)\,\mathrm{d}\xi = \overline{v(t)\,y(t)} = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,\overline{y^2}(t)$$

Notes from Blackadar, Next step is to integrate wrt time (or distance if x = Ut)

$$\overline{y^2}(T) = \int_0^T \frac{\mathrm{d}}{\mathrm{d}t}\,\overline{y^2}\mathrm{d}t = 2\sigma_v^2 \int_0^T \mathrm{d}t \int_0^t R(\xi)\,\mathrm{d}\xi\ . \tag{10.19}$$

In this equation we have replaced, $\overline{v^2}$ by our previously used symbol σ_v^2. T now represents the time interval after leaving the point source. The statistic $\overline{y^2}$ is not exactly what we have previously defined as σ_y^2: the latter refers to the standard deviation of the values of y of all the particles that lie a distance $X = \overline{u}T$ downwind of the source, while $\overline{y^2}$ refers to all the particles that have travelled a time T since leaving the source. Some of these will be situated closer and some further from the source than distance X. The difference is seldom very great, and for most purposes we can identify the two statistics as the same. Thus we may interpret Taylor's equation as

$$\sigma_y^2(X) \cong 2\sigma_v^2 \int_0^T \mathrm{d}t \int_0^\xi R(\xi)\,\mathrm{d}\xi \tag{10.20}$$

where X is the mean distance from the point of release of all the particles that have traveled an interval of time T since leaving the source.

The problem of diffusion is thus reduced to finding R as a function of ξ. There are two special cases of interest. The first concerns the dispersion rate immediately following the time of release from the source. We may define the word *immediately* as T small enough that we can put $R(\xi) \approx 1$. In this case, (10.20) gives

$$\overline{y^2} = \sigma_v^2 T^2 \quad \text{or} \quad \sigma_y \approx \sigma_v T = \frac{\sigma_v X}{\overline{u}}\ . \tag{10.21}$$

Thus initially σ_y is a linear function of time T or X. Initially the plume spreads linearly with a constant angular width, which is proportional to σ_α, the standard deviation of wind directions measured by a wind vane situated at the point of release. If the angles are small, this standard deviation is given quite well by

$$\sigma_\alpha \cong \frac{\sigma_v}{\overline{u}} \quad \text{and} \quad \sigma_y \cong \sigma_\alpha X\ . \tag{10.22}$$

The second special case concerns the behavior a very large distance away from the source. We shall assume that an integral time scale, in this case the Lagrangian time scale defined by

$$T_{\mathrm{L}} \equiv \lim_{t\to\infty} \int_0^t R(\xi)\,\mathrm{d}\xi \tag{10.23}$$

exists. At a sufficiently long time after release, the Taylor equation becomes

$$\sigma_y^2 = 2\sigma_v^2 T_{\mathrm{L}} T \tag{10.24}$$

or

$$\sigma_y \propto \sqrt{T}\ . \tag{10.25}$$

This limiting behavior is identical to the result obtained from the Fick equation. The reasons for this behavior will be explored in the next section.

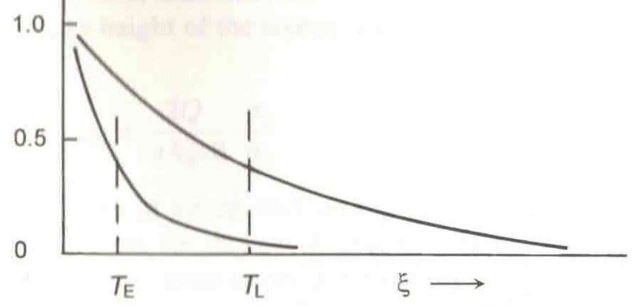

Fig. 10.7 Idealized Lagrangian and Eulerian autocorrelation functions

AQ models, See https://www.epa.gov/scram/air-quality-dispersion-modeling

Air Quality Dispersion Modeling

Dispersion modeling uses mathematical formulations to characterize the atmospheric processes that disperse a pollutant emitted by a source. Based on emissions and meteorological inputs, a dispersion model can be used to predict concentrations at selected downwind receptor locations. These air quality models are used to determine compliance with National Ambient Air Quality Standards (NAAQS), and other regulatory requirements such as New Source Review (NSR) and Prevention of Significant Deterioration (PSD) regulations. These models are addressed in Appendix A of EPA's Guideline on Air Quality Models (also published as Appendix W (PDF) of 40 CFR Part 51), which was originally published in April 1978 to provide consistency and equity in the use of modeling within the U.S. air quality management system. These guidelines are perodically revised to ensure that new model developments or expanded regulatory requirements are incorporated.
This site provides links for dispersion models and other related tools and information as follows ………

https://www.ontario.ca/document/guideline-11-air-dispersion-modelling-guideline-ontario-0

Regulation 346
Ontario's approved dispersion models include SCREEN3 for screening analyses and AERMOD for more sophisticated modelling analyses. In addition, the ASHRAE model must be used as necessary to assess potential for contamination of building air intakes that are located on the same structure as the source of the contaminant (see section 9 of the Regulation). SCREEN3 or AERMOD are used for assessment of POI concentrations at receptors that are not located on the same structure as the source of contaminant. A brief overview of each of these models can be found in the following subsections. For appropriate model selection, please review Chapter 2.3.1 – 2.3.3, as appropriate that outline the details of the following air dispersion models:
AERMOD SCREEN3 ASHRAE (same structure contamination).
NOTE: Older regulatory air dispersion models (known as Regulation 346 models) used under O. Reg. 419/05 will be phased out on February 1, 2020, as specified in the regulation. [PK Misra and I had worked on these 20-30 years ago!]

https://www.epa.gov/scram/air-quality-dispersion-modeling-preferred-and-recommended-models

AERMOD Modeling System - A steady-state plume model that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, and both simple and complex terrain.
CAL3QHC/CAL3QHCR - CALINE3 based CO model with queuing and hot spot calculations and with a traffic model to calculate delays and queues that occur at signalized intersections.
CTDMPLUS - A refined point source gaussian air quality model for use in all stability conditions for complex terrain.
OCD - A straight line Gaussian model developed to determine the impact of offshore emissions from point, area or line sources on the air quality of coastal regions.

Air quality management – multiple sources.

AERMOD Modeling System

The American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee (AERMIC) was formed to introduce state-of-the-art modeling concepts into the EPA's air quality models. Through AERMIC, a modeling system, AERMOD, was introduced that incorporated air dispersion based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, and both simple and complex terrain.
There are two input data processors that are regulatory components of the AERMOD modeling system: AERMET, a meteorological data preprocessor that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, and AERMAP, a terrain data preprocessor that incorporates complex terrain using USGS Digital Elevation Data. Other non-regulatory components of this system include: AERSCREEN, a screening version of AERMOD; AERSURFACE, a surface characteristics preprocessor, and BPIPPRIM, a multi-building dimensions program incorporating the GEP technical procedures for PRIME applications.

AERMOD

From : https://files.ontario.ca/admgo-id50_aoda_v2b.pdf

AIR DISPERSION MODELLING GUIDELINE FOR ONTARIO [GUIDELINE A-11] Version 3.0

1.1 Application of the Dispersion Models in the Regulation

The Regulation requires the use of specified approved dispersion models to assess compliance with ministry POI Limits when using the air standards compliance approach. Earlier versions of the regulation (previously known as Regulation 346 – General Air Pollution Regulation) included a set of suggested air dispersion models in the Appendix to Regulation 346. The models in the Appendix to Regulation 346 are being phased out and replaced with new air dispersion models developed by the United States Environmental Protection Agency (US EPA)

The models work in conjunction with the standards as follows:

 To demonstrate compliance with the half-hour average air standards listed in Schedule 2 of the Regulation, any of the approved dispersion models may be used (after appropriate conversion of time averaging periods is made as per section 17 of the Regulation, if necessary).

 To demonstrate compliance with the air standards listed in Schedule 3 of the Regulation, any of the approved dispersion models, except for the models in the Appendix to Regulation 346, may be used (after appropriate conversion of time averaging periods is made as per section 17 of the Regulation, if necessary).

https://weather.gc.ca/aqfm/index_e.html

Regional Air Quality Deterministic Prediction System (RAQDPS)

The current operational air quality forecast model is GEM-MACH (Global Environmental Multi-scale - Modelling Air quality and CHemistry). This model is a comprehensive air quality model containing a full description of atmospheric chemistry and meteorological processes. GEM-MACH is an in-line model, meaning that the meteorology is integrated in-step with the chemistry. The model uses the emissions inventory to assess the source of tropospheric ozone precursors. GEM-MACH is run twice a day over North America and is used to provide guidance for the production of air quality forecasts for Canadians.

Regulatory models run over a year or more of historic met data, usually small domain. Forecast models run over larger domains’