Regulatory Models for Short-Range Air Quality Applications: Overview and Outlook

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In Air Quality Analysis and Prediction: The Interaction of Science and Policy

Background

- US Clean Air Act and Amendments
  - Need & emphasis on models
  - Models key for emission limits; NAAQS compliance
  - 1977 Amend. – EPA Guideline on Air Quality Modeling

- Regulatory models
  - Short-range: distance x < 50 km
  - Mesoscale, regional: x > few 10’s of kms
  - Hybrid: combination of above

- Early short-range models (1970 – 2005)
  - Gaussian plume model core
  - Old technology & deficiencies

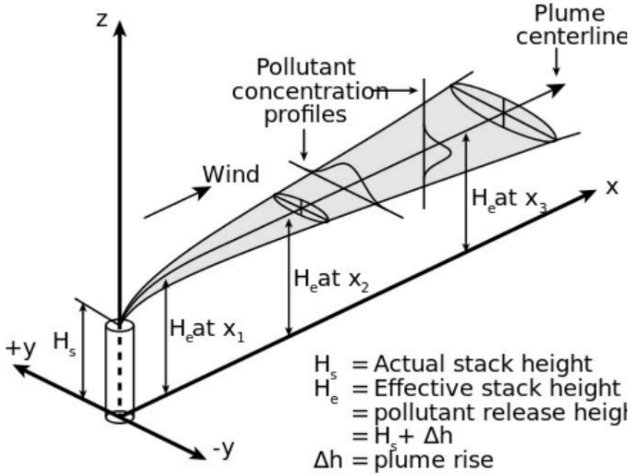
- Current key short-range models
  – AERMOD (since 2005): plume model, “workhorse”
  - CALPUFF: puff model

Figure 14. Keystone plume, May 25, 1968, 1047 EST.

Power plant plume in western Pennsylvania; 900 MW plant with 244 m stack

Background

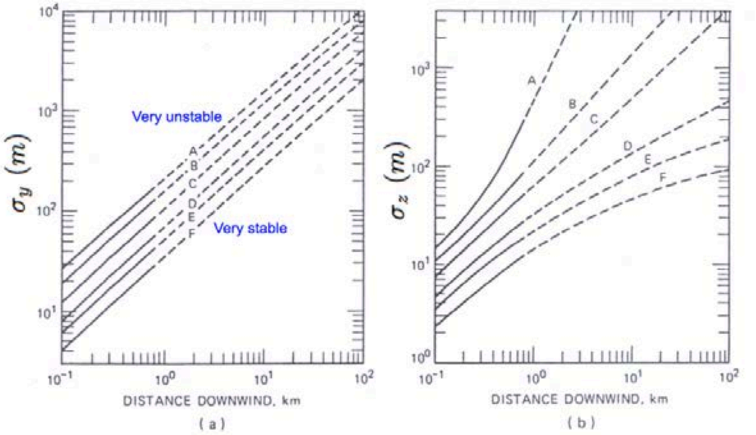
- Gaussian plume model
  - Simple, fast turnaround
  - Uniform wind, turbulence
- Meteorological data
  - Airport surface weather
  - Radiosondes – temperature profiles
- Earlier EPA models
  - Short & tall stacks – **Industrial Source Complex (ISC) Model**
  - Complex terrain – CTDM$^+$,
  - Roadway/line source – CALINE
- Implementation - NAAQS compliance; Models run for multiple years met
- Appendix W – use of alternative models



Mean Conc.

$$C = \frac{Q}{\pi U \sigma_y \sigma_z} \exp\left(\frac{-h_e^2}{2\sigma_z^2}\right) \exp\left(\frac{-y^2}{2\sigma_y^2}\right)$$

Dispersion curves, surface source



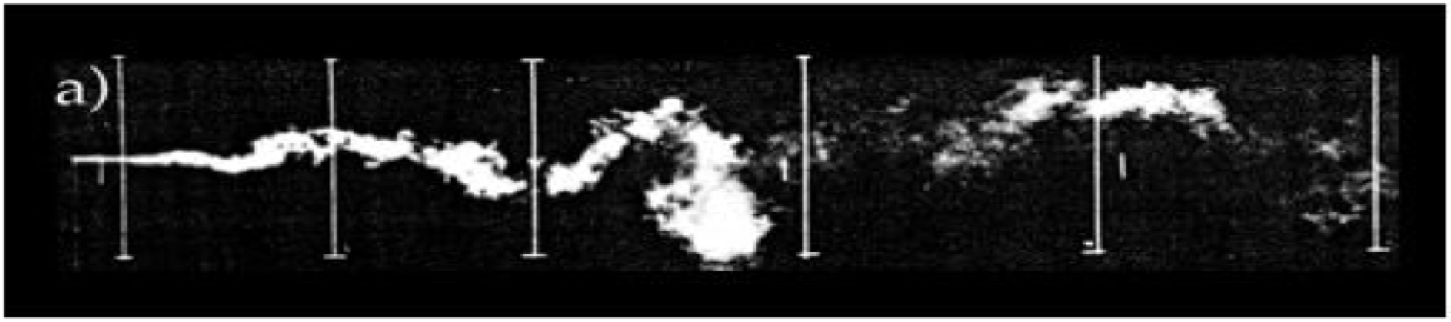
(Pasquill,1961; Gifford,1960)

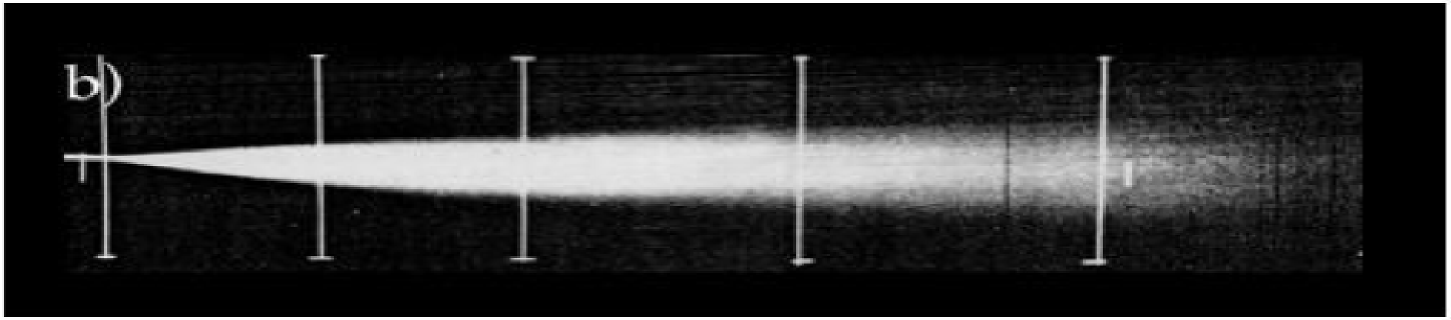
Effect of Averaging on Plumes & Dispersion

(From EPA Fluid Modeling Facility)

Smoke visualization downstream of a source in a turbulent, wind-tunnel flow

Instantaneous plume (short-time exposure)





Ensemble-average plume (long-time exposure)

ISC Model Deficiencies

- Meteorological model and inputs
  - Turbulence based on surface meteorology
  - Use of mixed layer (CBL) height (z_i)
- Dispersion parameters
  - Short-range dispersion; surface source
  - Surface meteorology, stability classes
- Plume rise & buoyancy effects
  - Briggs (1971) model; no convection
  - Plume penetration of inversions; all or none
- Complex/elevated terrain
  - No dividing streamline height
- Building downwash
  - Discontinuous in treatment of z_s ; no cavity concentrations

Figure 14. Keystone plume, May 25, 1968, 1047 EST.

Power plant plume in western Pennsylvania; 900 MW plant with 244 m stack

Understanding of Planetary Boundary Layer (PBL), Turbulence, & Dispersion (1970 – 1995)

- Large-eddy simulations (LES) of PBL structure, turbulence (Deardorff, 1972; etc)
- Minnesota, Aschurch & other PBL field campaigns (Kaimal,1972; Caughey, 1982)
- Convection tank measurements of turbulence (Willis & Deardorff, 1974)
- Convection tank dispersion experiments – convective scaling (Willis & Deardorff, 1976, 1978, 1981, 1984, etc)
- Lagrangian particle modeling of dispersion driven by LES fields (Lamb, 1978; 1982)
- CONDORS & other dispersion field experiments – 1975 to 1993 (e.g., Eberhard et al., 1988; Briggs, 1993; etc)
- Power plume studies, observations (EPRI, 1982; Maryland DNR, 1972 – 1986)

AERMOD: AMS – EPA Regulatory Model

- AMS – EPA Steering Committee AQ Modeling (1979 – 1993)
  - Advise EPA on scientific model aspects & evaluation
  - Conduct workshops, model reviews, etc
- AMS – EPA Regulatory Model Improvement Committee (AERMIC) (1991 – 2005)
  - Members: 3 AMS, 4 – 5 EPA (Weil, chair)
  - Proposed & developed AERMOD as an ISC replacement
  - Improve science & performance but keep simple
- AERMOD proposed November 2005; adopted 2006

AMS = American Meteorological Society

AERMOD: AMS – EPA Regulatory Model

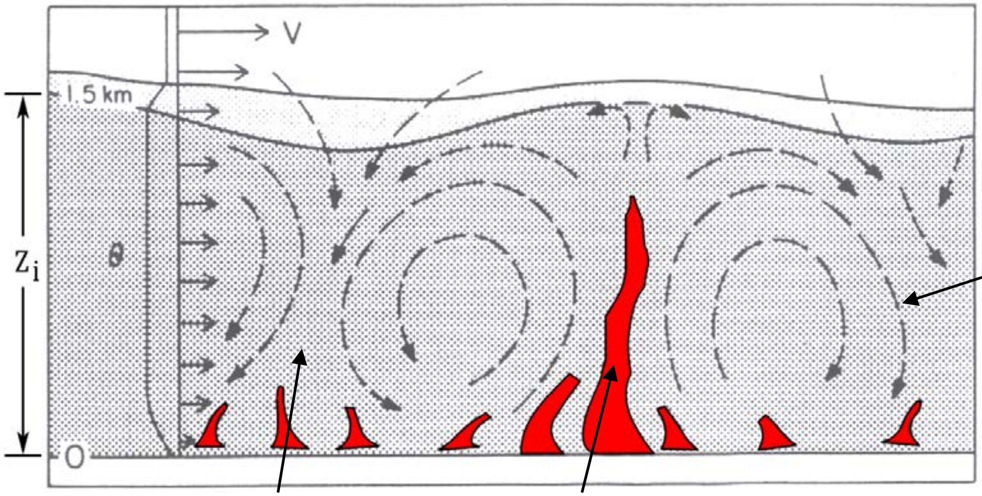
- AERMOD features
  - Parameterize wind, turbulence using PBL scaling concepts
  - Dispersion based on statistical theory with PBL inputs
  - “PDF” model for dispersion in convective boundary layer (CBL)
  - Gaussian plume model for stable boundary layer (SBL)
  - New techniques for building downwash, complex/elevated terrain, & urban dispersion
  - Evaluation with observations
- AERMOD proposed November 2005; adopted 2006

Key references:

Cimorelli et al., 2005: J. Appl. Meteor. Climatology, 44, 682—693.
Perry et al., 2005: J. Appl. Meteor. Climatology, 44, 694—708.

Planetary Boundary Layer

Convective boundary layer (CBL; day) Wyngaard (1985)



Downdrafts

Updrafts

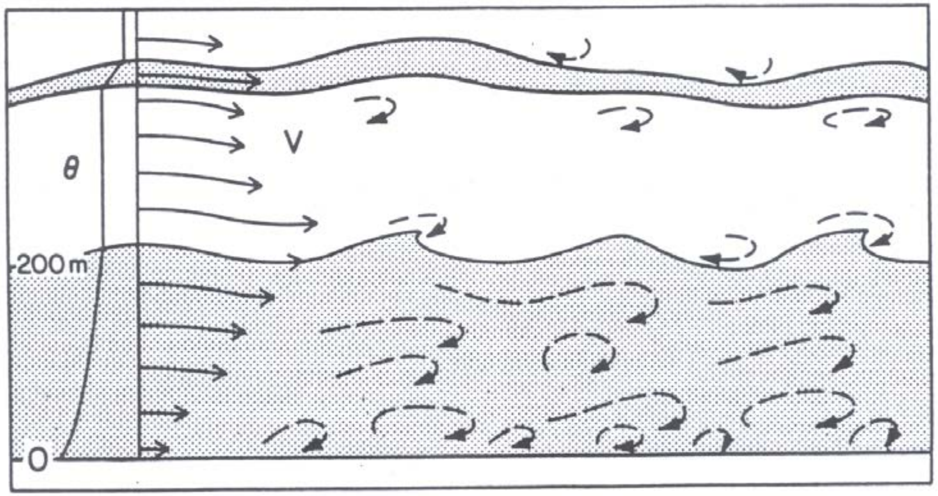
Long-lived circulations

Turbulence time scale

$$T_L \propto z_i / w_*$$

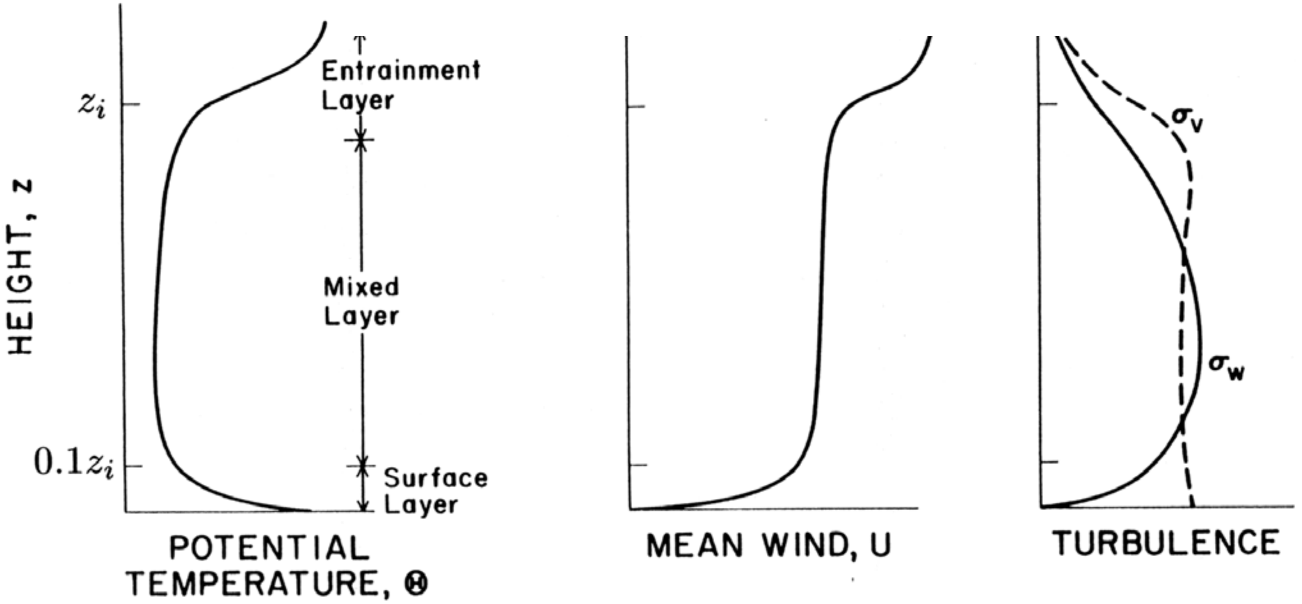
$$T_L \sim 5 - 10 \text{ min}$$

Stable boundary layer (SBL; night)



Key turbulence velocity, u_*

Convective Boundary Layer



Turbulence scales

Friction velocity u_*

Convective velocity scale $w_* \propto (\overline{w\theta_0} z_i)^{1/3}$

Lengths $z_i,\ L \propto -u_*^3/\overline{w\theta_0}$

Stability parameter:

$$-z_i/L,\ u_*/w_*,\ w_*/U$$

(Deardorff,1972; Willis & Deardorff, 1986)

Key variables

Near-surface wind speed U_{10}

Surface heat flux, net or solar rad

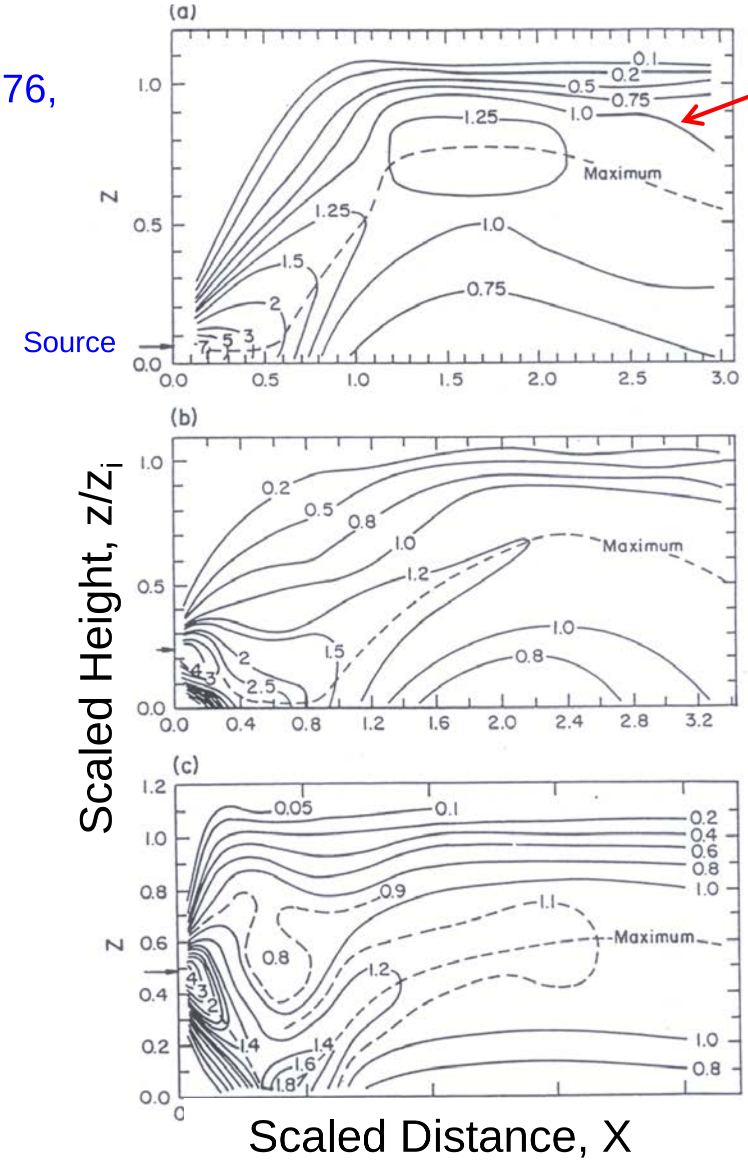
CBL depth (meas or modeled)

Surface roughness length z_0

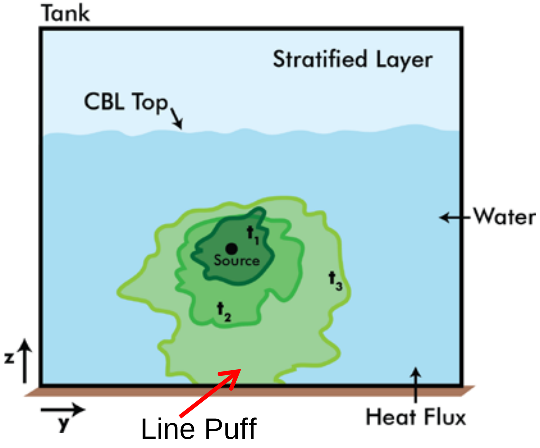
Convection Tank Experiments on Dispersion

Crosswind-Integrated Concentration (CWIC)

Willis & Deardorff (1976, 1978,1981)



$C^y U z_i / Q$



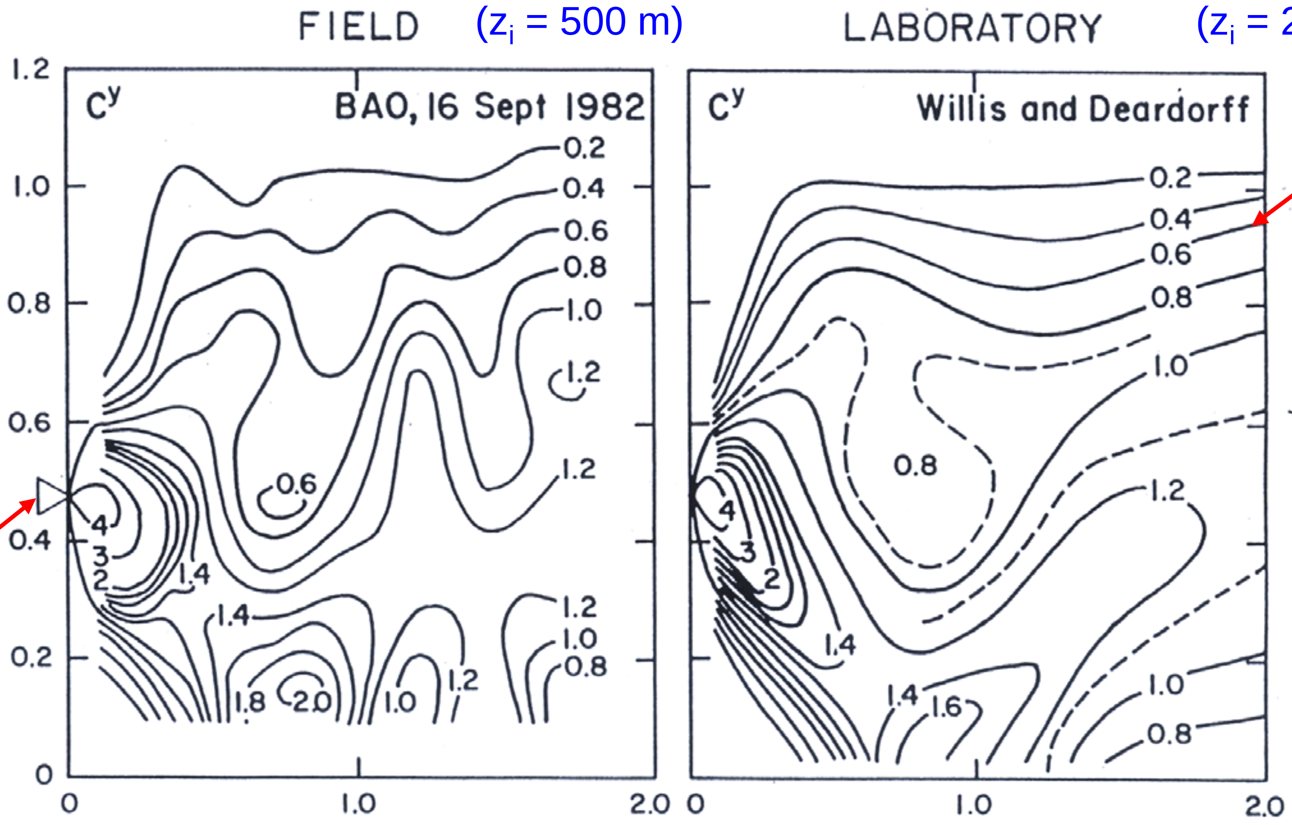
Applicable to Continuous Source, t = x/U

$$X = \frac{w_* x}{U z_i}$$

Field vs. Convection Tank Data

Crosswind-Integrated Concentration (CWIC)

(Moninger et al, 1983)



(z_i = 500 m)

(z_i = 25 cm)

z/z_i

Source

$$\frac{C^y U z_i}{Q}$$

$X = w_* x/(U z_i)$

PDF Model

(Misra, 1982; Venkatram, 1983; Weil & Furth, 1981)

Key assumptions:

Uniform wind and turbulence with z

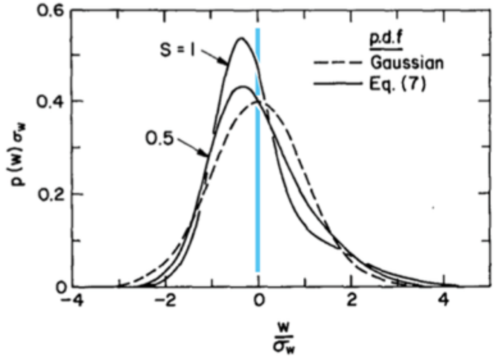
Skewed w PDF

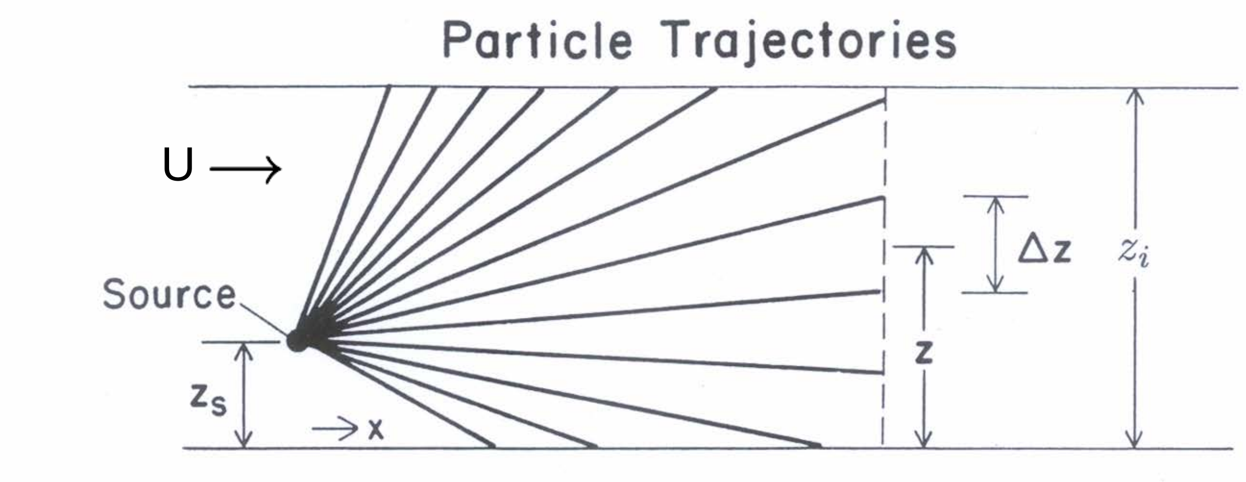
PDF = Probability density function

$$C^y = \frac{Q p_z}{U} \qquad p_z = p_w[w(z_p)]|dw/dz_p|$$

$$p_w = \lambda_1 G_1(w) + \lambda_2 G_2(w)$$

w PDF





PDF Model

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Uniform wind and turbulence with z

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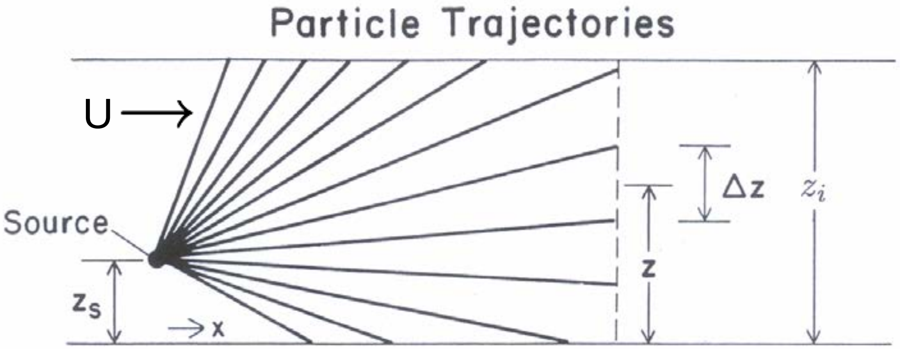
$$C^y = \frac{Q p_z}{U} \qquad p_z = p_w[w(z_p)]\left|dw/dz_p\right|$$

$$p_w = \lambda_1 G_1(w) + \lambda_2 G_2(w)$$

$$\frac{C^y U z_i}{Q} = \frac{\lambda_1}{\sqrt{2\pi}X}\exp\left(-\frac{\Psi^2}{2b_1^2X^2}\right) + \frac{\lambda_2}{\sqrt{2\pi}X}\exp\left(-\frac{\Psi^2}{2b_2^2X^2}\right)$$

$$\Psi = \frac{z}{z_i} - \frac{z_s}{z_i} - a_j X \qquad j = 1, 2$$



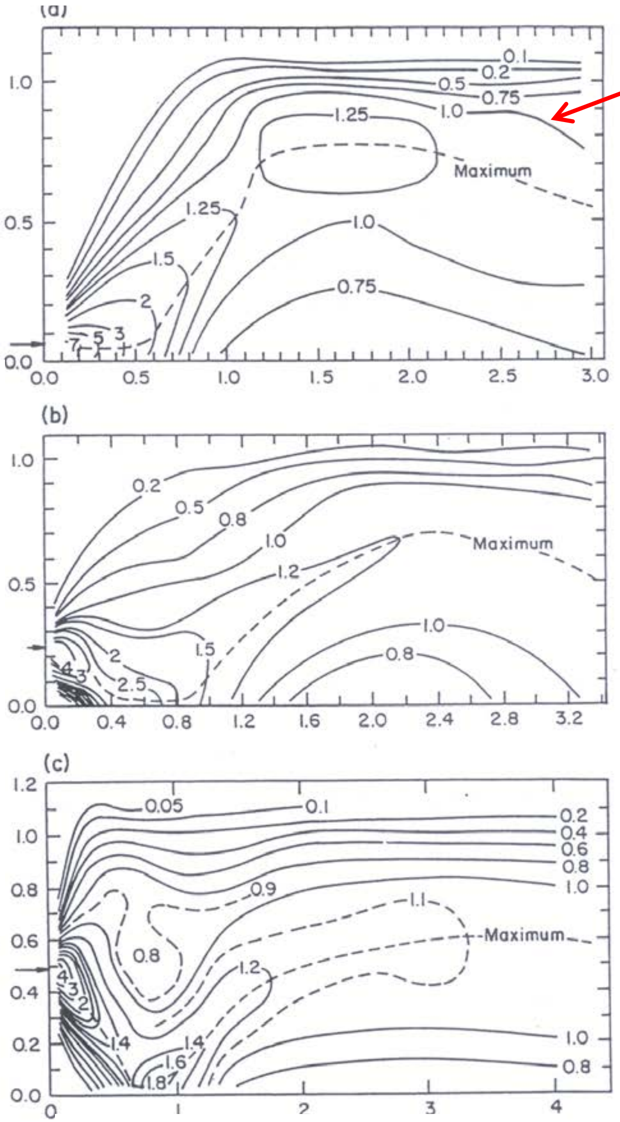
Crosswind-Integrated Concentration Fields

Convection Tank Data

$C^y U z_i / Q$

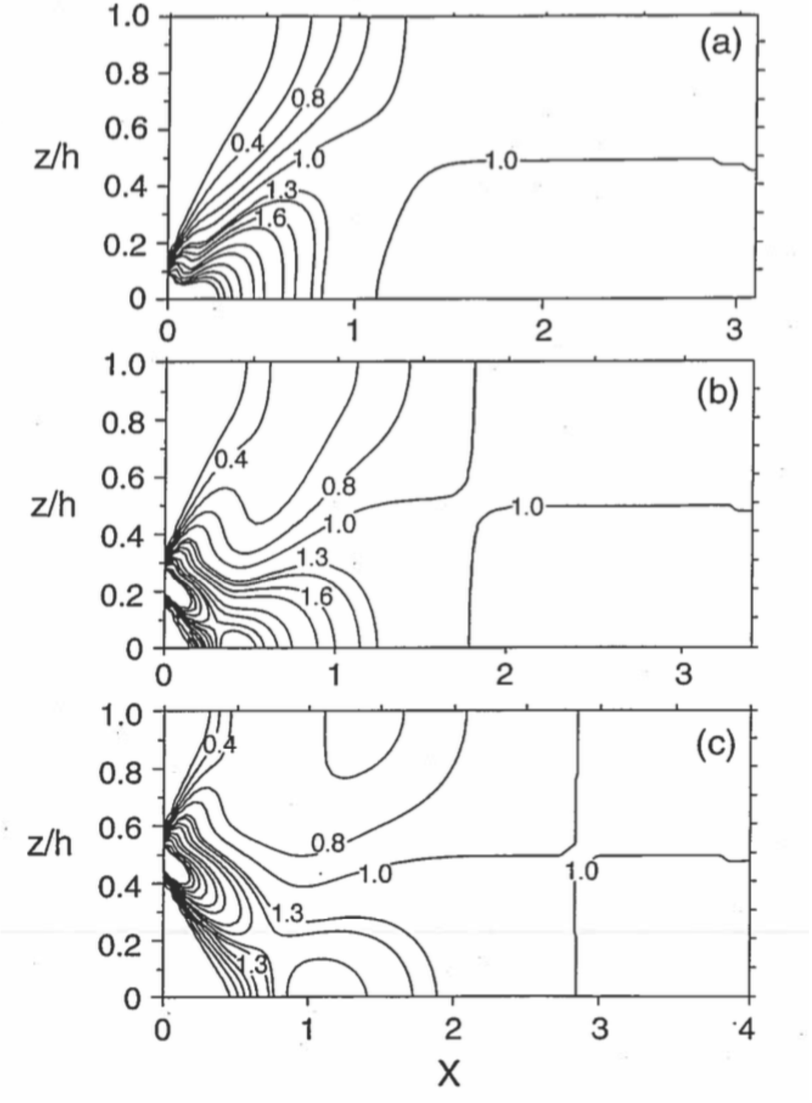
Source

Scaled Height, z/z_i



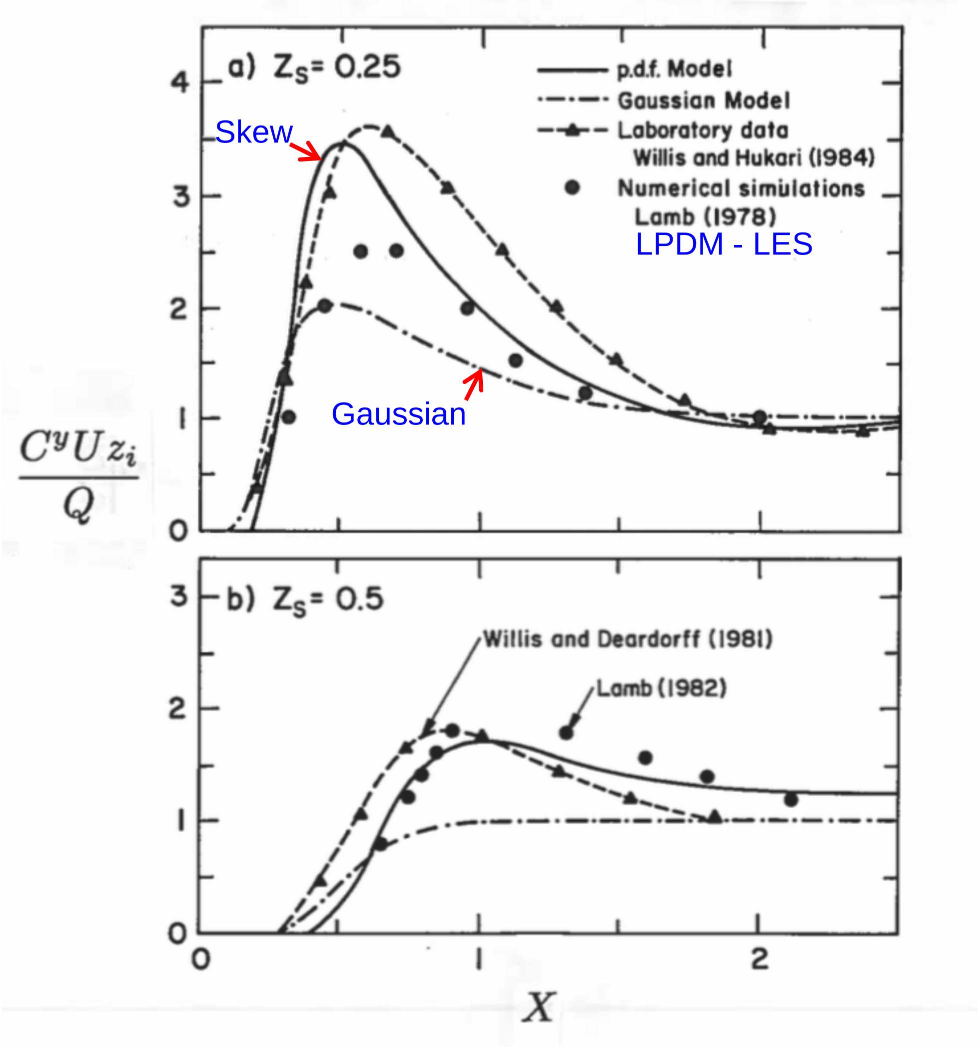
Scaled Distance, X

PDF Model (Weil, 1988)



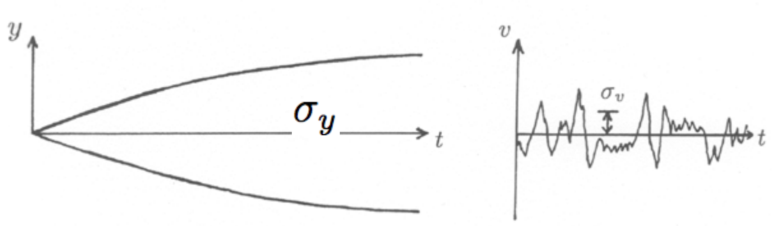
PDF Model vs Tank Data

Surface CWIC



Statistical Dispersion Theory (Taylor, 1921)

σ_v = Lateral rms velocity
σ_y = Lateral rms spread
T_L = Lagrangian time scale

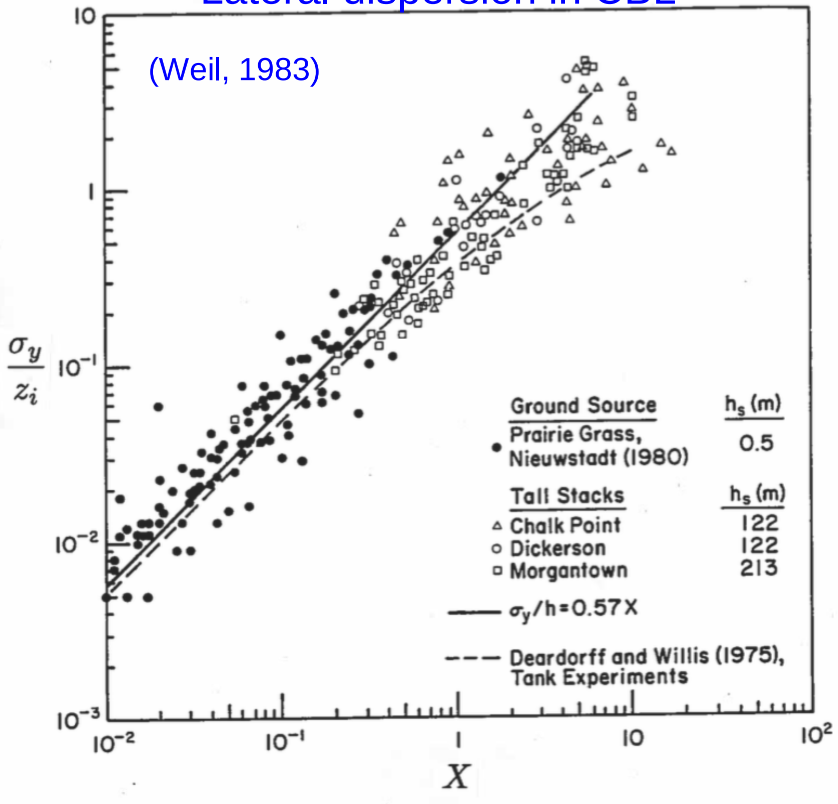


$$t \ll T_L \quad \sigma_y = \sigma_v t$$

$$t \gg T_L \quad \sigma_y = (2\sigma_v^2 T_L t)^{1/2}$$

All *t* : $$\sigma_y = \frac{\sigma_v t}{(1 + 0.5t/T_L)^{1/2}}$$

Lateral dispersion in CBL

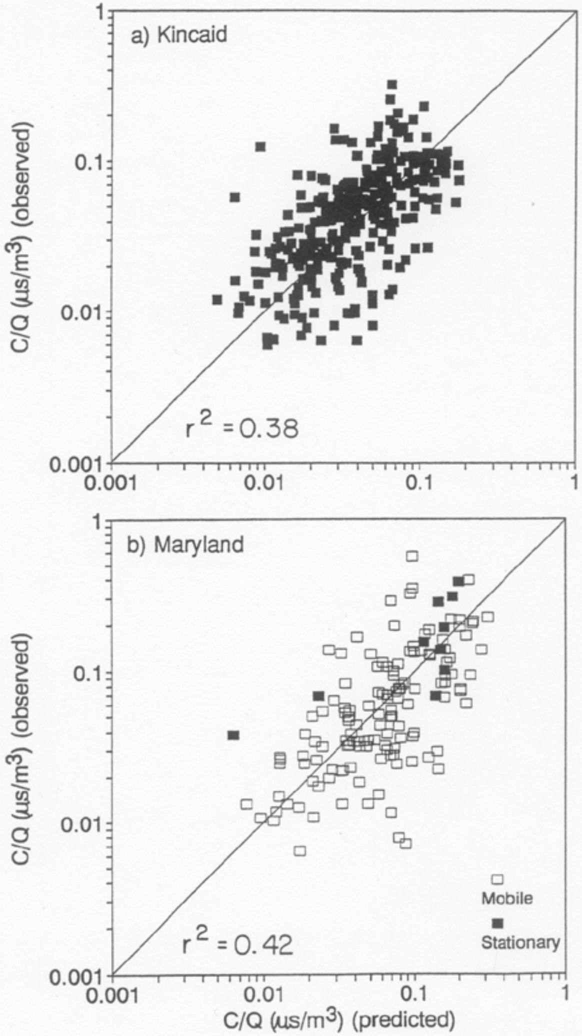


(Weil, 1983)

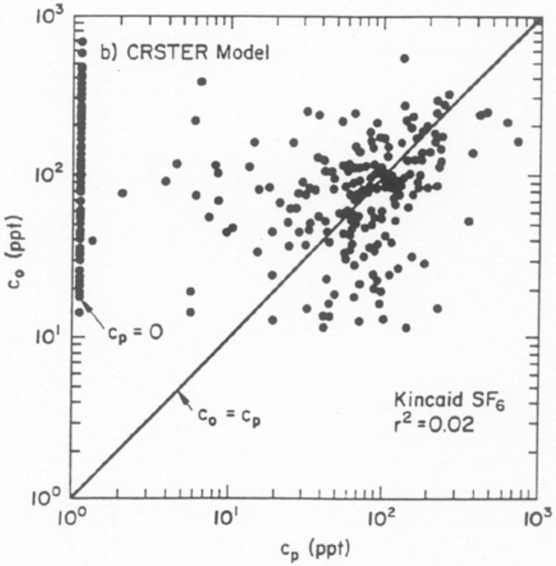
PDF Model vs Field Observations: Buoyant Releases from Tall Stacks

Ground-level concentrations

PDF Model



EPA Gaussian Model



Centerline concentrations; 1 hr avgs.

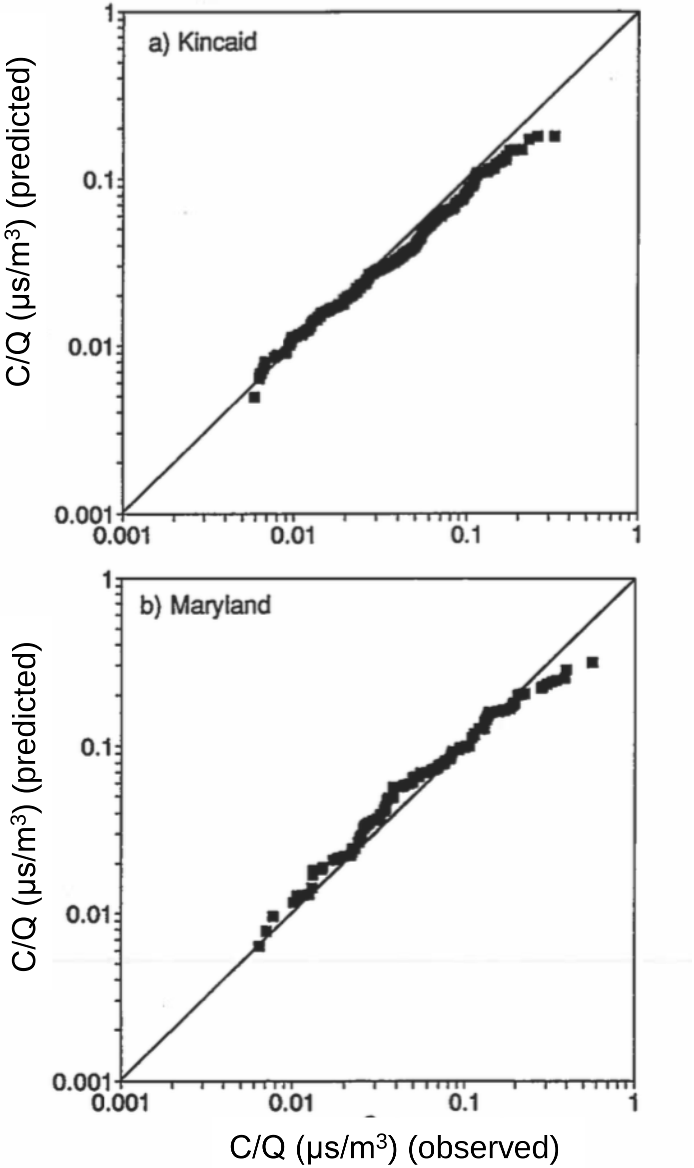
h_s: 107 m -- 305 m

x : 0.5 km -- 50 km

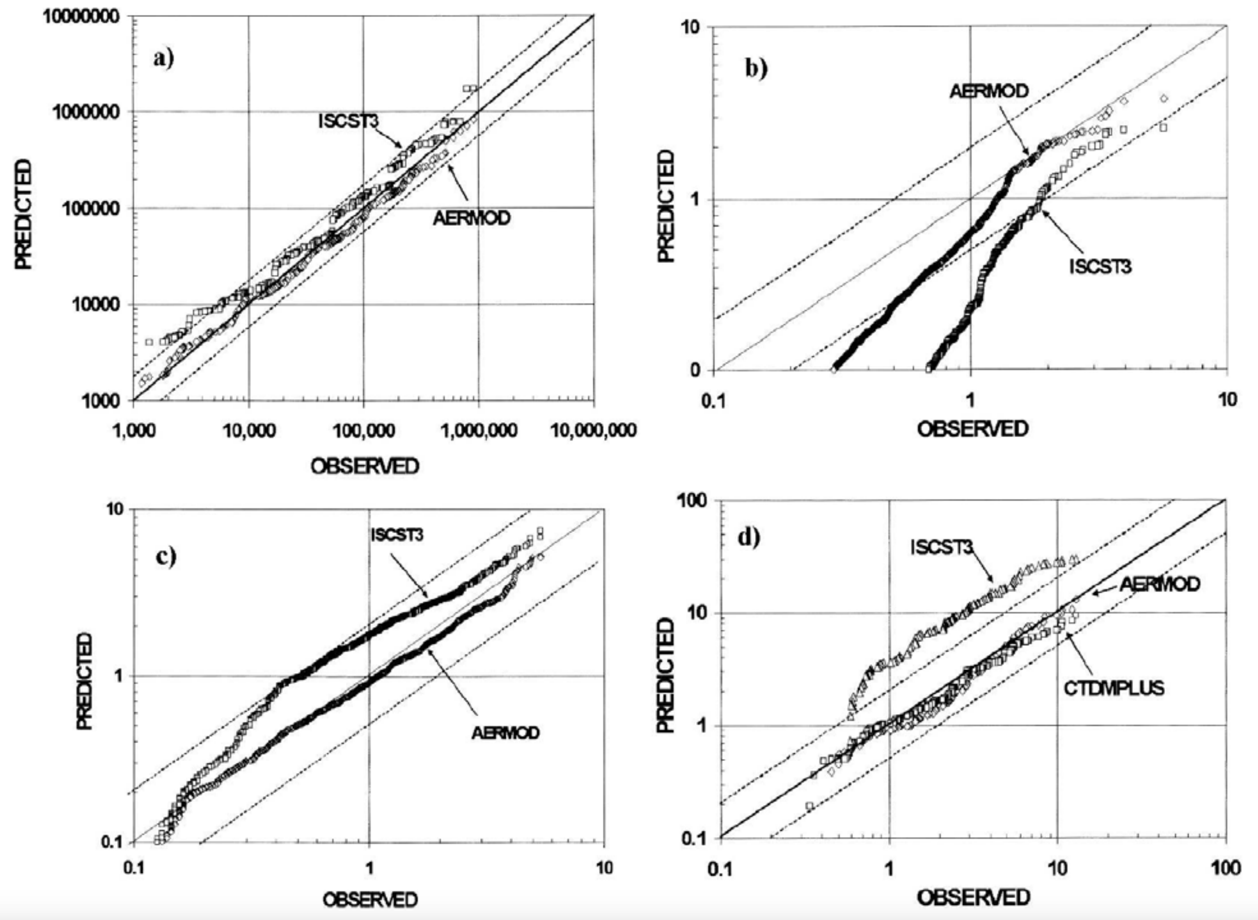
(Weil et al., 1997)

PDF Model: Quantile – Quantile Plot

(Weil et al., 1997)



AERMOD: Predicted vs Observed Concentrations Quantile – Quantile (Perry et al., 2005)



Prairie Grass, surface src.

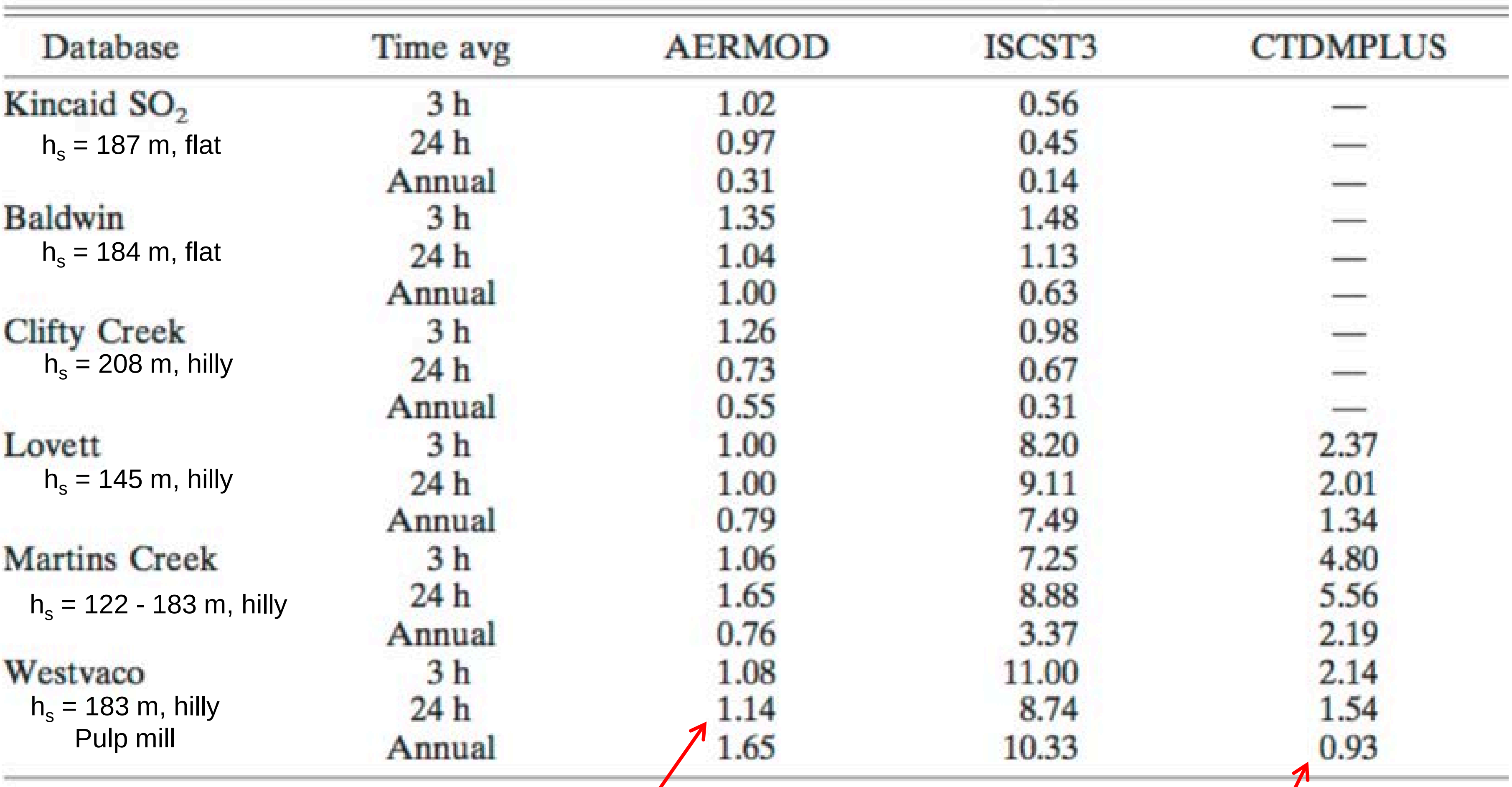
Kincaid Power Plnt., rural

Indianapolis Power Plnt., urban

Tracy Power Plnt., complex terrain

Centerline concentrations; 1 hr avgs.
h_s: 0.5 m -- 187 m
x : 0.5 km -- 50 km

AERMOD: Ratio of Predicted-to-Observed Robust Highest Concentration (Perry et al., 2005)



Database	Time avg	AERMOD	ISCST3	CTDMPLUS
Kincaid SO_2 h_s = 187 m, flat	3 h	1.02	0.56	—
	24 h	0.97	0.45	—
	Annual	0.31	0.14	—
Baldwin h_s = 184 m, flat	3 h	1.35	1.48	—
	24 h	1.04	1.13	—
	Annual	1.00	0.63	—
Clifty Creek h_s = 208 m, hilly	3 h	1.26	0.98	—
	24 h	0.73	0.67	—
	Annual	0.55	0.31	—
Lovett h_s = 145 m, hilly	3 h	1.00	8.20	2.37
	24 h	1.00	9.11	2.01
	Annual	0.79	7.49	1.34
Martins Creek h_s = 122 - 183 m, hilly	3 h	1.06	7.25	4.80
	24 h	1.65	8.88	5.56
	Annual	0.76	3.37	2.19
Westvaco h_s = 183 m, hilly Pulp mill	3 h	1.08	11.00	2.14
	24 h	1.14	8.74	1.54
	Annual	1.65	10.33	0.93

Ideal value = 1.0

CTDM$^+$ = earlier EPA complex terrain model

AERMOD Technical Issues – Short Term: Review of EPA 11th AQ Modeling Conference

Issues raised by AERMOD users

- Light wind transport, low turbulence (u_*) & potential overestimation of surface concentrations
- Elevated buoyant plumes & low CBL heights (z_i): plume penetration of elevated inversion & rapid dispersion/re-entry.

  - Possible overestimation of concentrations.
- Building downwash model fidelity: several conditions, e.g., low winds in SBL and building fugitive heating with plume lift-off
- Validity of AERMOD (steady flow) & CALPUFF (unsteady) for near-source distances, complex terrain, and long-range transport
- Modeling of single-source contributions to O_3 and $PM_{2.5}$: Is it possible instead of using CMAQ or photochemical grid model?
- Representative surface conditions, especially roughness (z_0)

Short-Range Dispersion Modeling – Long Term:

Use of Lagrangian Particle Dispersion Model (LPDM) Driven by LES Fields

- LPDM – LES for special cases: particular scientific issues requiring hi-fidelity modeling. Can simulate both convective & stable PBLs.
  - “1-particle” LPDM for typical mean concentration issues; can do neutral/passive and positively- or negatively-buoyant releases
  - “2-particle” LPDM for concentration fluctuation/variance fields probability distribution of concentration.
- LPDM – LES for providing hi-fidelity “numerical data” for development and evaluation of simple models, AERMOD or other.
- Routine applications using a GPU – LES code to drive a parallelized LPDM. Key advantage – speed.

Background

- Gaussian plume model
  - Mass conservation
  - Uniform wind, turbulence
- Meteorological data
  - Airport surface weather
  - Radiosondes – temperature profiles
- Earlier EPA models
  - Short & tall stacks – Industrial Source Complex (ISC) Model
  - Complex terrain – CTDM^{+},
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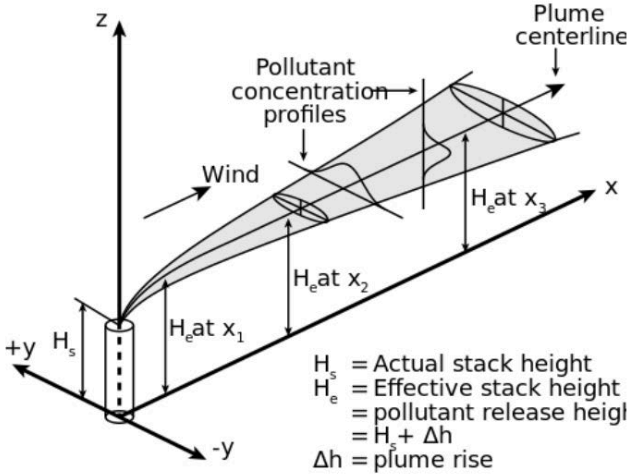
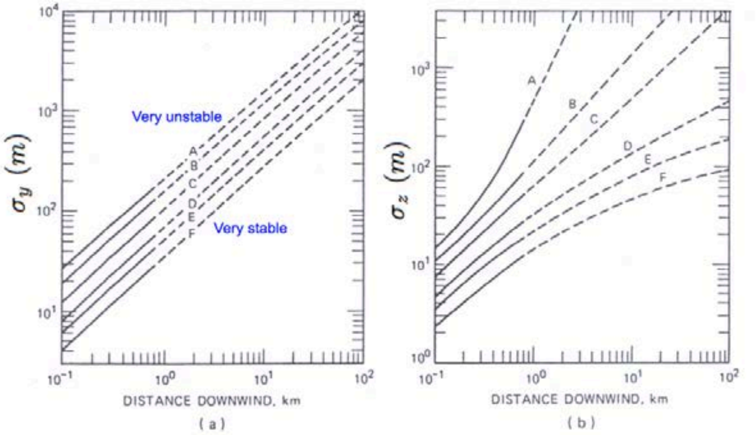
- Implementation - NAAQS compliance; Models run for multiple years met
- Appendix W – use of alternative models



Mean Conc.

$$C = \frac{Q}{\pi U \sigma_y \sigma_z} \exp\left(\frac{-h_e^2}{2\sigma_z^2}\right) \exp\left(\frac{-y^2}{2\sigma_y^2}\right)$$

Dispersion curves, surface source

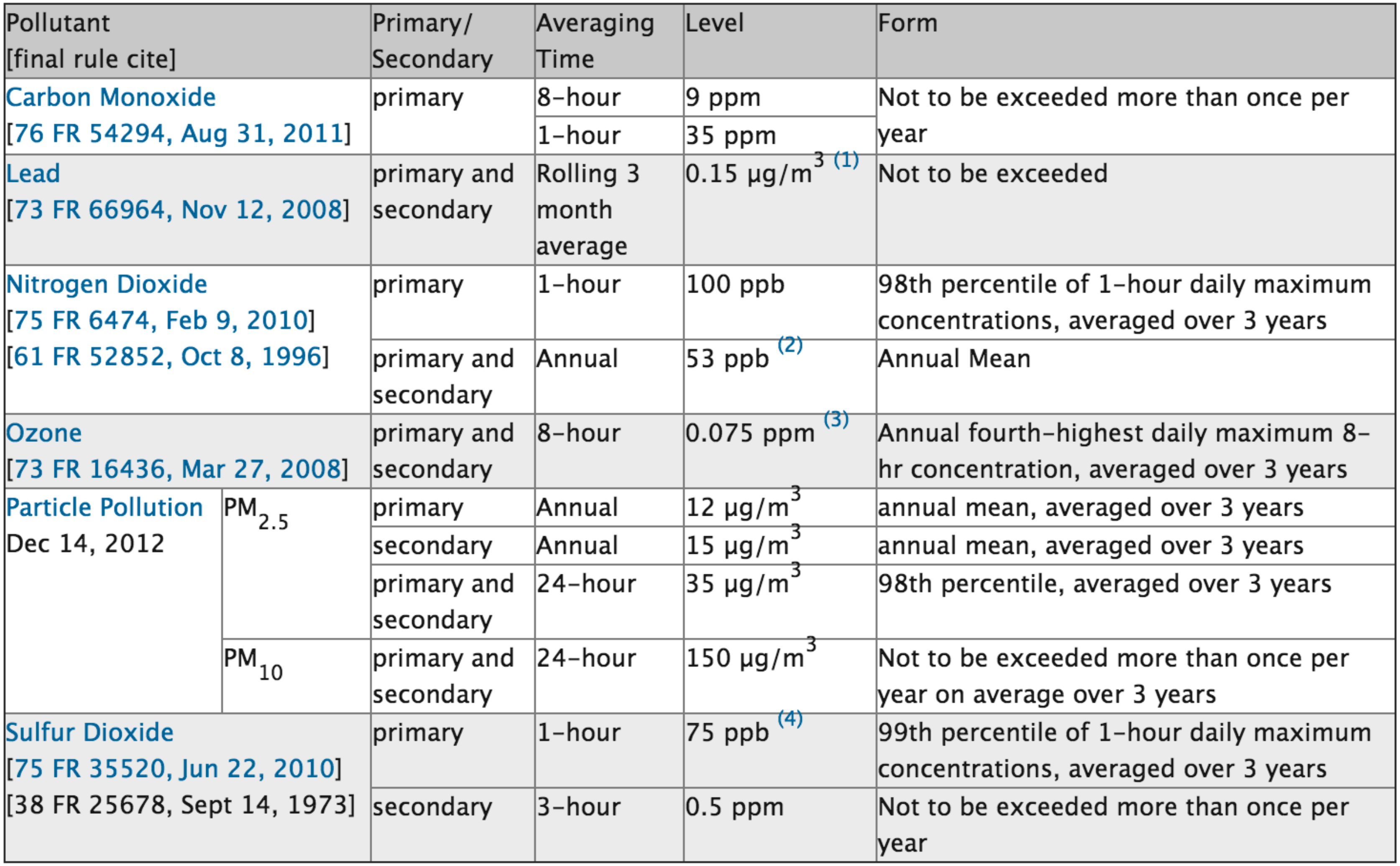


(Pasquill,1961; Gifford,1976)

US Air Quality Standards

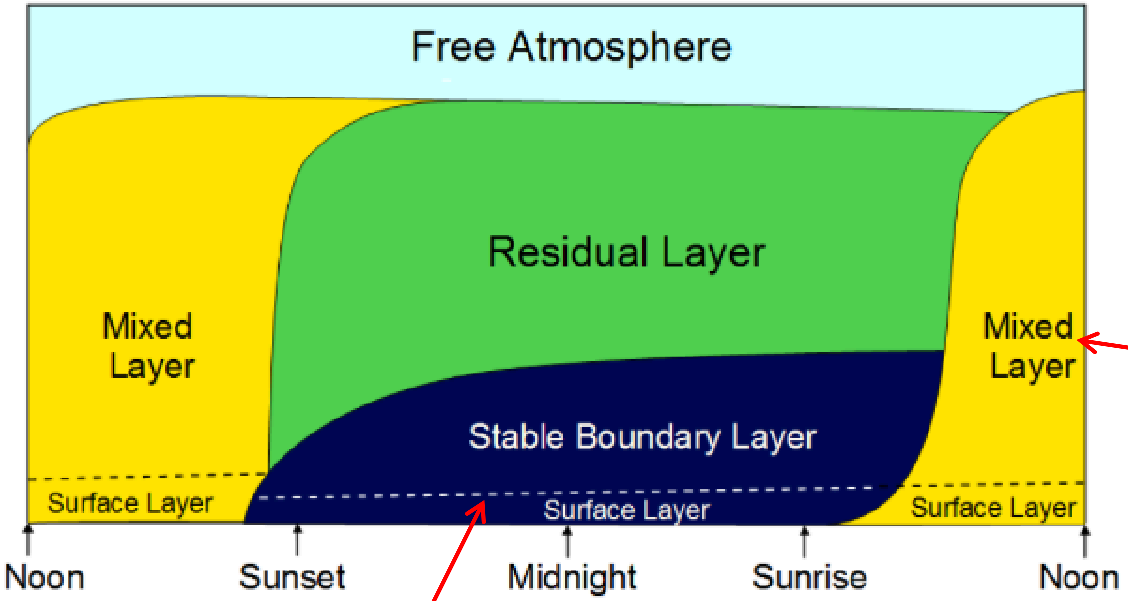
Jack Rabbit II

- Accidental releases of dense gas (DG)



Pollutant [final rule cite]		Primary/ Secondary	Averaging Time	Level	Form
Carbon Monoxide [76 FR 54294, Aug 31, 2011]		primary	8-hour	9 ppm	Not to be exceeded more than once per year
			1-hour	35 ppm	
Lead [73 FR 66964, Nov 12, 2008]		primary and secondary	Rolling 3 month average	0.15 $\mu g/m^3$ (1)	Not to be exceeded
Nitrogen Dioxide [75 FR 6474, Feb 9, 2010] [61 FR 52852, Oct 8, 1996]		primary	1-hour	100 ppb	98th percentile of 1-hour daily maximum concentrations, averaged over 3 years
		primary and secondary	Annual	53 ppb (2)	Annual Mean
Ozone [73 FR 16436, Mar 27, 2008]		primary and secondary	8-hour	0.075 ppm (3)	Annual fourth-highest daily maximum 8-hr concentration, averaged over 3 years
Particle Pollution Dec 14, 2012	$PM_{2.5}$	primary	Annual	12 $\mu g/m^3$	annual mean, averaged over 3 years
		secondary	Annual	15 $\mu g/m^3$	annual mean, averaged over 3 years
		primary and secondary	24-hour	35 $\mu g/m^3$	98th percentile, averaged over 3 years
	PM_{10}	primary and secondary	24-hour	150 $\mu g/m^3$	Not to be exceeded more than once per year on average over 3 years
Sulfur Dioxide [75 FR 35520, Jun 22, 2010] [38 FR 25678, Sept 14, 1973]		primary	1-hour	75 ppb (4)	99th percentile of 1-hour daily maximum concentrations, averaged over 3 years
		secondary	3-hour	0.5 ppm	Not to be exceeded more than once per year

Diurnal Cycle of Planetary Boundary Layer (PBL)



Convective boundary layer (day); strong turbulence

Stable boundary layer (night); weak turbulence

From Stull (1988)

Statistical Dispersion Theory (Taylor, 1921)

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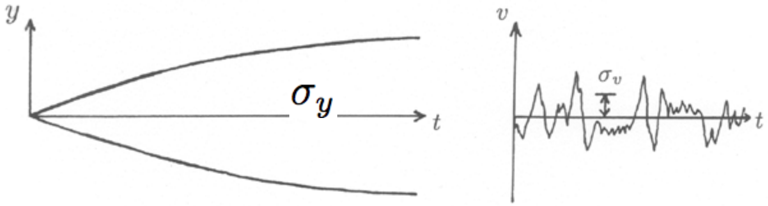
σ_y = Lateral rms spread
T_L = Lagrangian time scale

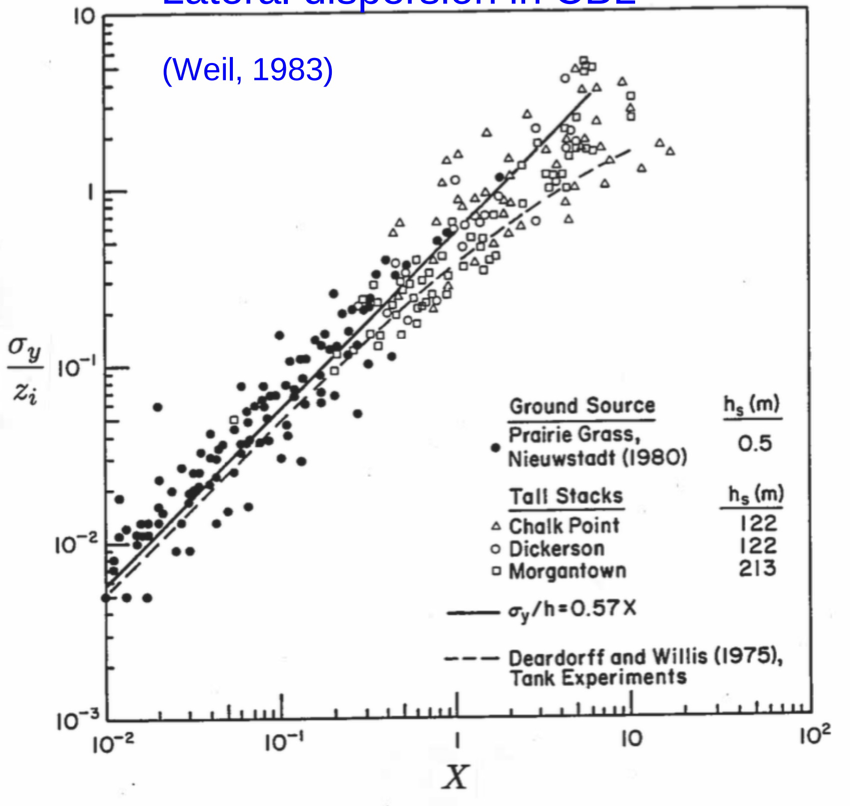
$$t \ll T_L \quad \sigma_y = \sigma_v t$$

$$t \gg T_L \quad \sigma_y = (2\sigma_v^2 T_L t)^{1/2}$$



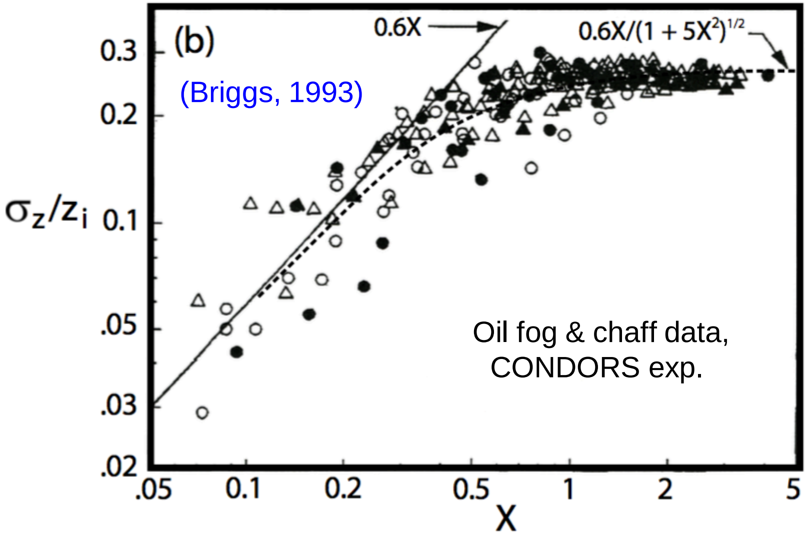
All *t* : $\sigma_y = \dfrac{\sigma_v t}{(1 + 0.5t/T_L)^{1/2}}$

Lateral dispersion in CBL



(Weil, 1983)

Vertical dispersion in CBL



(Briggs, 1993)

Oil fog & chaff data,
CONDORS exp.