## Use of Turbulence Measurements in Dispersion Model Applications

Jeff Weil CIRES, University of Colorado, and NCAR

## **Dispersion Models for Applications**

- Applications
  - Air quality: surface concentrations, AQ stds
  - National security: hazard zones, evacuation plans
- Model attributes
  - Numerically simple for fast turnaround
  - Capture essential physics of PBL & dispersion
  - Ensemble-average approaches (mostly)
- Development and testing
  - Lab & numerical (LES) simulations, field observations
- Use of turbulence measurements
  - Turbulence statistics input for dispersion (not much & why)
  - Develop turbulence parameterizations
  - Forcing in high resolution models (e.g., LES)

# Model Types

- Simple analytical, statistical
  - Probability density function (PDF) models, Gaussian plume AERMOD, SCIPUFF
- Lagrangian particle models
  - Stochastic displacement (NARAC)
  - Stochastic velocity (QUIC)
- Large-eddy simulations
  - Lagrangian particle
  - Diffusion equation
- CFD RANS approaches
- Eulerian grid models

# Outline

- Background
  - Plume behavior, statistical theory, PBL parameterization
- Convective boundary layer
  - PDF model
  - NARAC/LLNL (eddy diffusion)
  - Lagrangian particle model with LES
- Urban boundary layer
  - LES with real-time winds/turbulence (FEM3MP)
- Stable boundary layer
  - Lagrangian particle model with LES

# Dispersion in the Planetary Boundary Layer (PBL)

#### Convective boundary layer (CBL)



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

#### Stable boundary layer (SBL)



#### Surface concentrations from above case



## Effect of Averaging on Dispersion (From EPA Fluid Modeling Facility)

Smoke visualization downstream of a point source in a wind tunnel with turbulent flow

Instantaneous plume (short-time exposure)





Ensemble-average plume (long-time exposure)

# Statistical Dispersion Theory (Taylor, 1921)

Ensemble-average spread with time *t* Homogeneous, stationary turbulence



 $\sigma_v$  = Lateral rms velocity  $\sigma_y$  = Lateral spread  $T_L$  = Lagrangian time scale or "memory time"

$$\begin{split} t \ll T_L & \sigma_y = \sigma_v t & \text{Effective diffusivity} \\ t \gg T_L & \sigma_y = (2\sigma_v^2 T_L t)^{1/2} & K_y = \sigma_v^2 T_L \\ \text{All } t & \sigma_y = \sigma_v t f_y (t/T_L) \\ & f_y = (1 + 0.5t/T_L)^{-1/2} \end{split}$$

### Demonstration of Statistical Theory Using Turbulence Measurements & Dispersion Obs



## **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:

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

#### Key variables

Near-surface wind speed  $U_{10}$ Surface heat flux, net or solar rad CBL depth (meas or modeled) Surface roughness length  $\mathcal{Z}_0$ 

### Field Measurements for Parameterizing Turbulence



$$\sigma_v^2 = u_*^2 f_{SV} + w_*^2 f_{BV}$$
  
 $\sigma_w^2 = u_*^2 f_{SW} + w_*^2 f_{BW}$   
 $\overline{w^3} = w_*^3 f_3$   
 $f_{SV}, f_{BV}, f_{SW}, f_{BW}, f_3 \text{ are } f(z/z_i)$ 

## **Convection Tank Data**

Crosswind-Integrated Concentration (CWIC)



## Field vs. Convection Tank Data

Crosswind-Integrated Concentration (CWIC) (Moninger et al, 1983)



### PDF Model (Misra, 1982; Venkatram, 1983; Weil, 1986)

#### Key assumptions:

Uniform wind and turbulence with z Very large time scale  $\rm T_L$  Skewed w PDF

$$C^{y} = \frac{Qp_{z}}{U} \qquad p_{z} = p_{w}[w(z_{p})]|dw/dz_{p}|$$
$$p_{w} = \lambda_{1}G_{1}(w) + \lambda_{2}G_{2}(w)$$



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## PDF Model vs Tank Data



### PDF Model vs Field Data: Buoyant Releases





Centerline concentrations; 1 hr avgs.  $h_s$ : 107 m -- 305 m x : 0.5 km -- 50 km (Weil et al., 1997)

## AERMOD -- New EPA Regulatory Model

- Adopted December 2006
- Key EPA model for industrial source applications
- Parameterizes turbulence using PBL scaling; accepts wind & turbulence measurements
- Includes PDF model for CBL
- Gaussian model for SBL
- Addresses building downwash, elevated terrain, urban dispersion, etc
- Committee (AERMIC) 14 years

### National Atmospheric Release Advisory Center (NARAC) Model; Lawrence Livermore Natl. Lab. (LLNL) (Nasstrom et al., 2000)

- Uses: emergency response; national security
- Meteorological assimilation model (ADAPT)
  - Surface, tower, radiosonde data
  - Diagnostic wind field
- Lagrangian stochastic displacement model (LODI); ideally for t >> T<sub>L</sub>

$$dz_p = \frac{\partial K_z}{\partial z} dt + (2K_z)^{1/2} d\xi$$
$$K_z = \frac{ku_*}{\phi(z/L)} \exp\left(\frac{-c_k z}{z_i}\right)$$



## LODI Evaluation with Copenhagen Data

Copenhagen Field Experiment (Gryning & Lyck, 1984) SF<sub>6</sub> release;  $z_s = 115$  m; 23 1-h periods; 9 days; CBL Tower winds & temp.; radiosondes; turbulence info;  $1.4 \le -z_i/L \le 14$ Sampling arcs: x = 2, 4, 6 km; 1-h avg. SF<sub>6</sub> concs.



Figure 4. Experiment on September 26, 1978. The bars indicate the mean measured tracer concentrations for the period 11:40-12:40 (run 1-3, Table 11-12), for the individual measuring positions.

### **Observed Surface Concentrations vs LODI Predictions** (Weil & Dillon, 2005)

Arc-maxima only



### Observed Surface Concentrations vs LODI Predictions (Weil & Dillon, 2005)



## **Generation of Concentration Fluctuations**

#### Meandering Plume Model Gifford (1959)

#### Concentration Fluctuation Intensity Csanady (1973)



Figure 7.3. Schematic representation of Gifford's meandering-plume model.



Fig. 7.11. Rms to mean concentration ratio at fixed *nondimensional* distances from center of gravity (distance scale: standard deviation of concentration distribution). Dots represent data at four different sections (Murthy and Csanady, 1971).

### Variability of Predicted/Observed Concentration



"Bowtie" or "Butterfly" Pattern

### Variability of Predicted/Observed Concentration in Vertical



Lagrangian Particle Model Driven by LES Fields (Weil, et al., 2004, J. Atmos. Sci.)



 $\mathbf{v}(\mathbf{x}_{0},t) = \mathbf{u}_{RES}(\mathbf{x}_{p},t) + \mathbf{u}_{SGS}(\mathbf{x}_{p},t)$  $\mathbf{u}_{RES}$  = resolved LES velocity  $\mathbf{u}_{SGS}$  = stochastic subgrid-scale (SGS) velocity Adopt Thomson's (1987) stochastic model for  $\mathbf{u}_{SGS}$ 

Concentrations (CWIC)

$$C^{y} = Q \int p_{1}(x - x_{s}, z - z_{s}, t_{d}) dt_{d}$$
$$t_{d} = t - t_{em}$$

### Mean and Realizations of Vertical CWIC Profiles

(Weil, Sullivan, Moeng, Patton, 2006)

#### LES conditions:

96<sup>3</sup> grid points; 5 km X 5 km X 2 km domain; 1/2 h release  $z_i = 1000$  m,  $w_* = 2$  m/s,  $z_i/w_* = 500$  s, U = 3 m/s,  $-z_i/L = 106$ 



### Ensemble Mean and Realizations: Average Plume Height & CWIC Profiles



# LES of an Urban 2000 Experiment: Salt Lake City (Chan & Leach, 2004)

- LES with FEM3MP (LLNL model)
- Massively parallel CFD model
- Finite element method
- Smagorinsky SGS
- Forcing by COAMPS mesoscale model and field measurements

## LES of an Urban 2000 Experiment

## IOP7 Release 1 of Urban 2000

Wind velocity:very low and varying (mean speed: 0.4-0.65 m/s)Friction velocity:~0.05 m/sSource rate:1 g/s (line source of SF<sub>6</sub> released near ground for 1 hr)Neutral stability

### **Model Simulations**

Domain size(m): 943 x 945 x 210 (graded mesh)

Grid points: 229 x 227 x 35 (~1.82M)

Boundary conditions:

No slip on ground surface & no penetration on top boundary Time-dependent boundary conditions on inlet and side planes

### Sonic Data in Salt Lake City; Roof of City Center Building; z = 44 m

Measured data used to construct time-dependent boundary conditions with logarithmic variation in the vertical

Conditions applied on South, North, and East boundary of domain



### Average Concentration Patterns for Sequential 10-min Periods: Time-dependent BCs



### Predicted vs. Observed Concentrations Using Various Time-dependent Wind Forcings



Imposing proper time-dependent forcing by large scale flows has led to accurate prediction of tracer concentrations for complex and usually more hazardous dispersion scenarios under light and highly variable winds Lagrangian Particle Model (Weil, et al., 2004, J. Atmos. Sci.)



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# Large-Eddy Simulations (LES)

(Moeng & Sullivan, 1994; Sullivan et al., 1994; GABLS, Beare et al., 2005)

- Filtered Navier-Stokes equations with parameterized SGS fluxes to produce 3D volume of wind fields
- Stable boundary layer (SBL)
- Horizontally homogeneous
- Conditions:

400 m X 400 m X 400 m domain 200 X 200 X 192 grid points,  $\Delta \approx 2$  m  $z_i = 200$  m,  $u_* = 0.28$  m/s,  $z_i/u_* = 714$  s, U = 7 m/s, L = 125 m,  $z_i/L = 1.6$ 

• 640 stored LES data files at 5 s intervals





## **Extra Slides**

### NARAC Model Urban Modifications (Delle Monache and Weil, 2008)

- Capture average effects of urban surface on wind & turbulence
- Triple-layer UBL structure canopy, roughness sublayer, inertial sublayer
- Mean wind, turbulence, K<sub>z</sub> parameterization fractional frontal area, average building height h<sub>b</sub>
- Tests with Joint Urban 2003 data (OKC)

## NARAC Comparisons with JU03 Data



### Surface CWIC: LODI, LPDM-LES, & Observations



# **Vertical Dispersion**



# Dispersion in the CBL



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



Figure 13. Keystone plume, October 31, 1968, 0920 EST.

# Dispersion in a Stable Environment





#### Surface Concentrations: Observations vs LODI Predictions (Weil & Dillon, 2005)

Copenhagen Field Experiment (Gryning & Lyck, 1984) SF<sub>6</sub> release;  $z_s = 115$  m; 23 1-h periods; 9 days; Tower winds & temp.; radiosondes; turbulence info;  $1.4 \le -z_i/L \le 14$ Sampling arcs: x = 2, 4, 6 km; 1-h avg. SF<sub>6</sub> concs.



### PDF Model vs Convection Tank Data



### **Observed Surface Concentrations vs LODI**



## **Urban Boundary Layer**



# Fractional Bias: $2(C_p - C_o)/(C_p + C_o)$



# Convection Tank Experiments Willis & Deardorff (1976, 1978, 1981)



#### Basis for experiments: "Mixed layer" & uniform wind

