Large-Eddy Simulation and Lagrangian Two-Particle Modeling of Mean and Fluctuating Concentrations in the Atmospheric Boundary Layer

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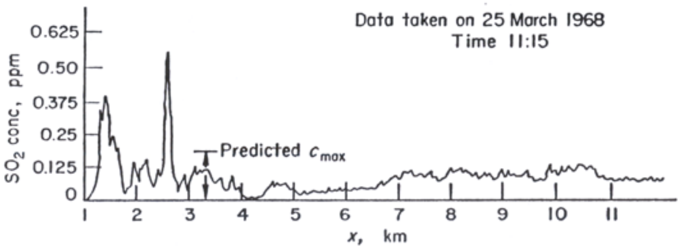
Davis, CA, 11 – 13 September, 2019

Background

- Importance of statistical variability
  - Estimate peak concentrations—toxics, air quality, odors, chemistry, etc.
  - Need: mean, variance, probability distrib.



- Statistics for variable averaging time, T_{av}
  - Requires "relative dispersion" of plume

- Approach
  - Lagrangian two-particle dispersion model (L2PDM) driven by large-eddy simulations (LES) of the convective boundary layer (CBL)

- Goal
  - Generate dispersion realizations & statistics for T_{av}'s: 40 s – 30 min
  - Demonstrate applicability of L2PDM to mean & fluctuating concentrations with convection tank data
  - Provide numerical data for testing simpler models

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- Importance of statistical variability
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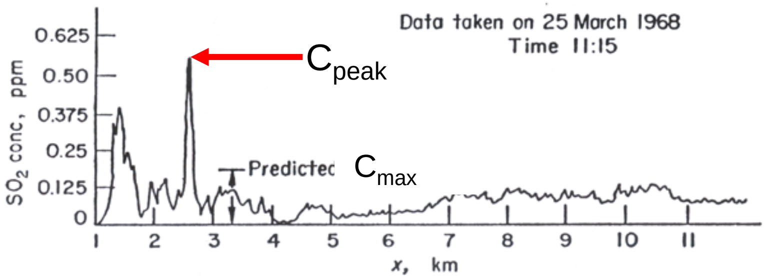
Figure 14. Keystone plume, May 25, 1968, 1047 EST.

- Statistics for variable averaging time, T_{av}
  - Requires "relative dispersion" of plume



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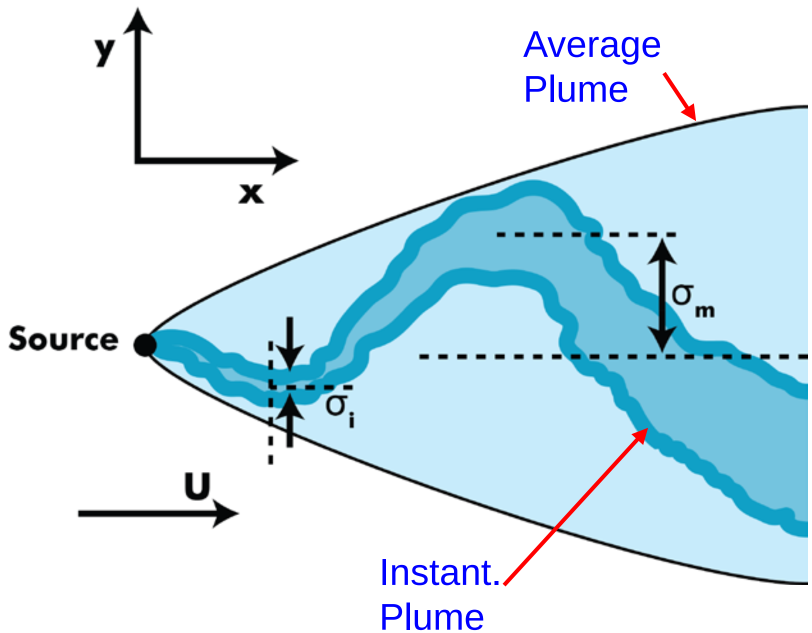
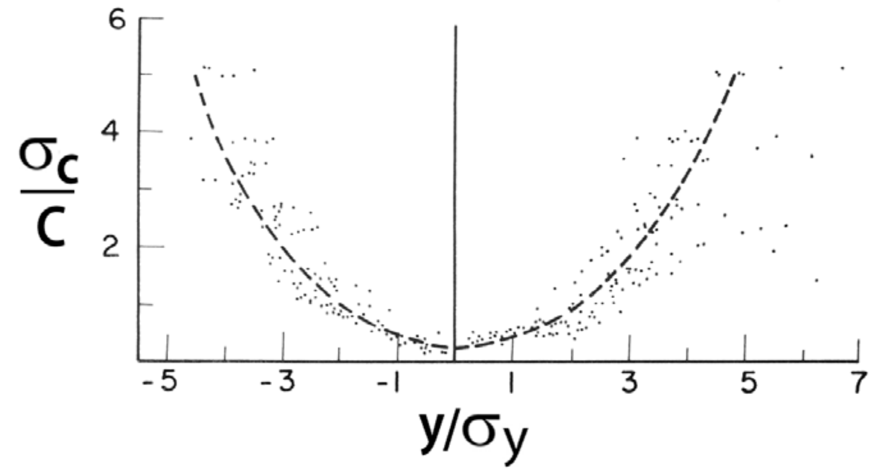
Generation of Concentration Fluctuations

Meandering Plume Model
(Gifford 1959)



Concentration Fluctuation Intensity
(Csanady 1973)



$$\sigma_y = (\sigma_i^2 + \sigma_m^2)^{1/2}$$

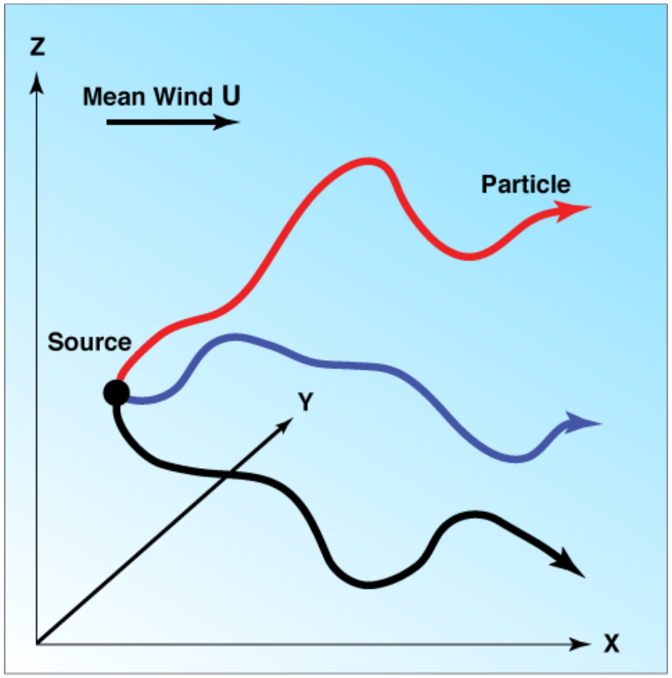
Short times

$$\sigma_i^2 = \sigma_r^2 \propto \epsilon t^3 \quad t \ll T_L$$ (Batchelor,1950)

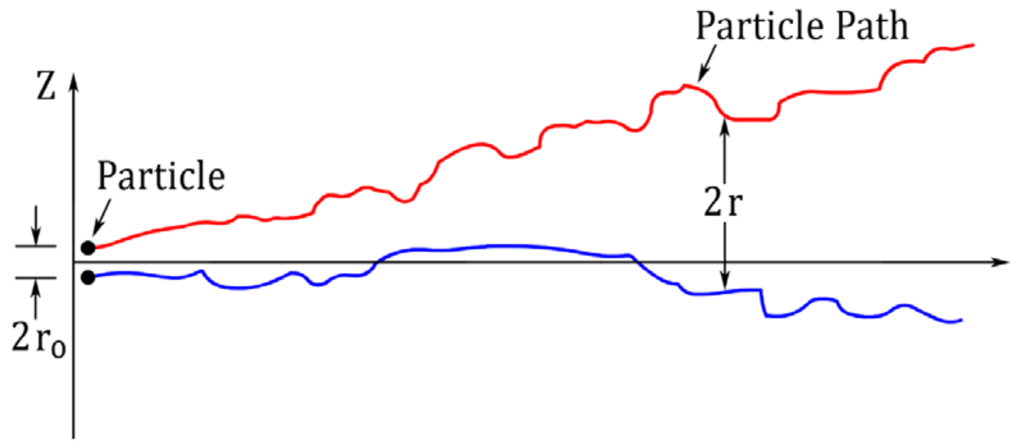
$$\sigma_m = \sigma_{vm} t$$ (Csanady,1973)

Lagrangian 1- & 2-Particle Dispersion Models

Applies to 1- & 2-particle models



2-particle model



$$v_1(x_{01},x_{02},t) = u_{R1}(x_{p1},t) + u_{S1}(x_{p1},x_{p2},t)$$
$$v_2(x_{02},x_{01},t) = u_{R2}(x_{p2},t) + u_{S2}(x_{p1},x_{p2},t)$$

u_{Ri} = resolved LES velocity, particle *i*
u_{Si} = stochastic subgrid-scale (SGS) velocity
Adopt Thomson's (1990) stochastic model for u_{Si}

Concentration

$$c(\mathbf{x},t) = Q\int p_1(\mathbf{x},t;\mathbf{x}_{S1},t'_1)\,dt'_1$$

$$t = nT_{av}$$

LPDMs Driven by LES

Large-Eddy Simulations (LES)

(Moeng & Sullivan, 1994, NCAR LES;
Prusa et al, 2008, EULAG)

- CBL Setup:
  5 km X 5 km X 2 km domain
  96^3 grid points
  z_i = 1000 m, w_* = 2 m/s,
  z_i/w_* = 500 s, U = 3 m/s, U/w_* = 1.5
  Highly convective: $-z_i/L$ = 106 (NCAR)
  = 78 (EULAG)

- 500 stored LES data files (NCAR)
  at 10 s intervals
  210 files (EULAG)

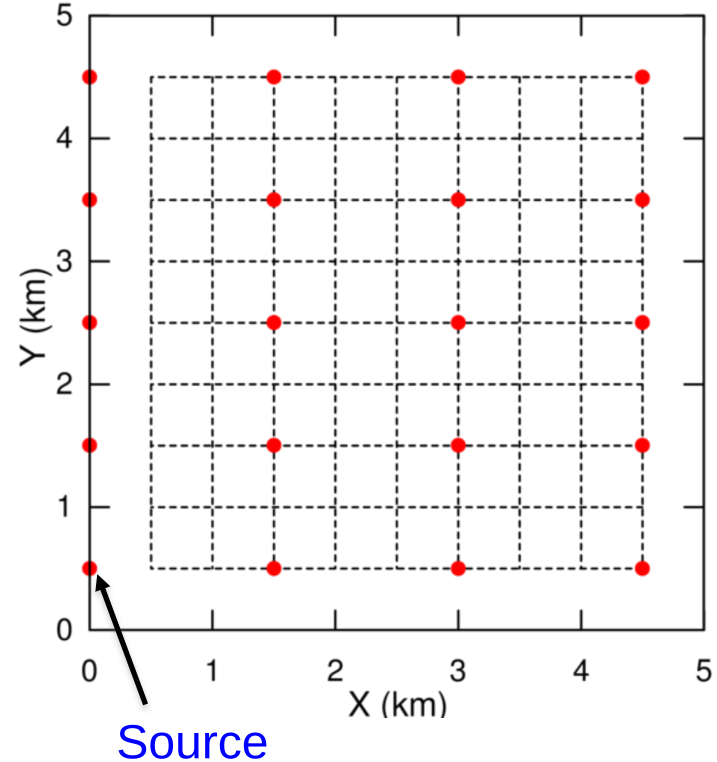
Subgrid TKE

$$e_s$$

Dissipation rate

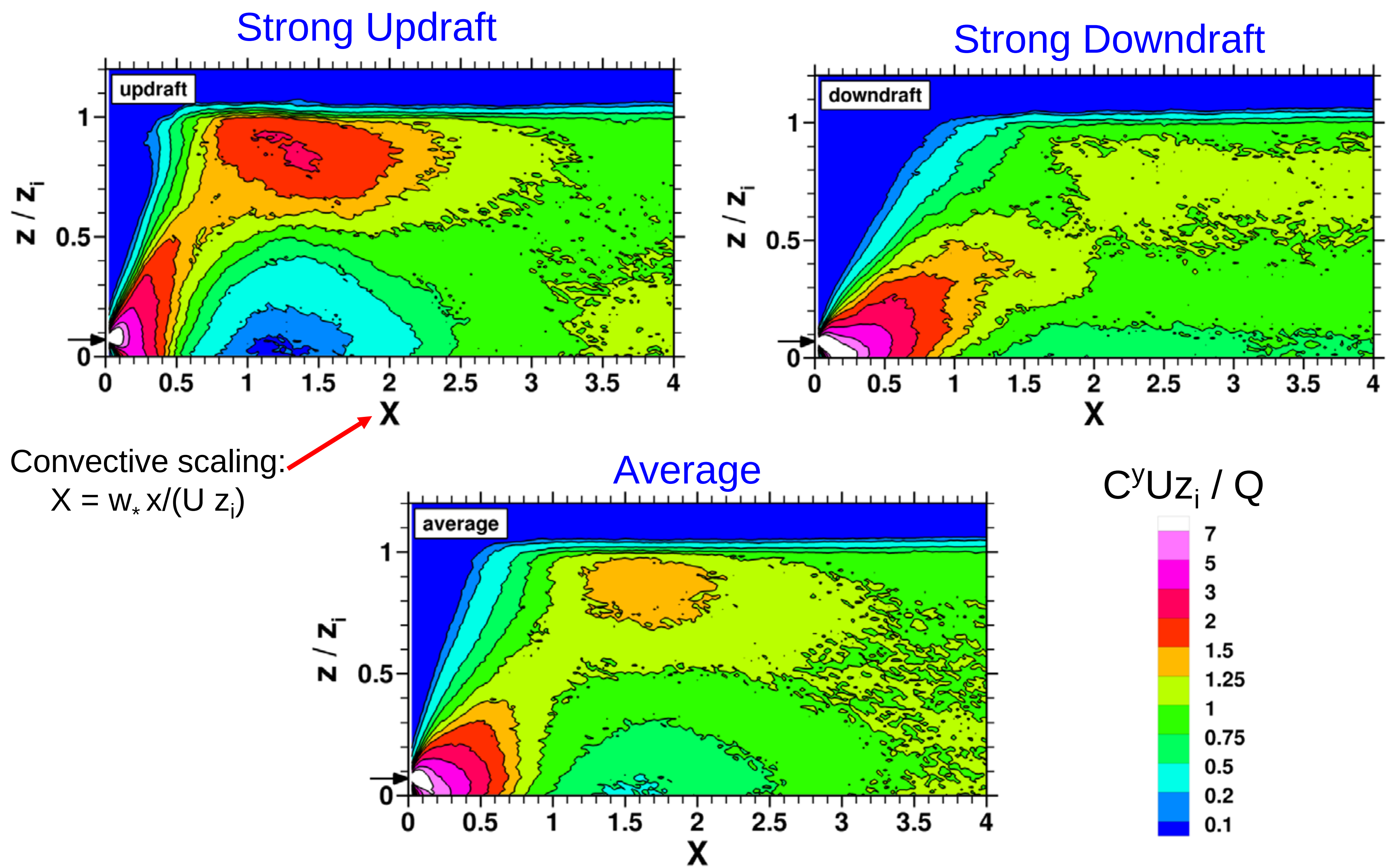
$$\epsilon = c_e e_s^{3/2}/\ell$$

Source Grid



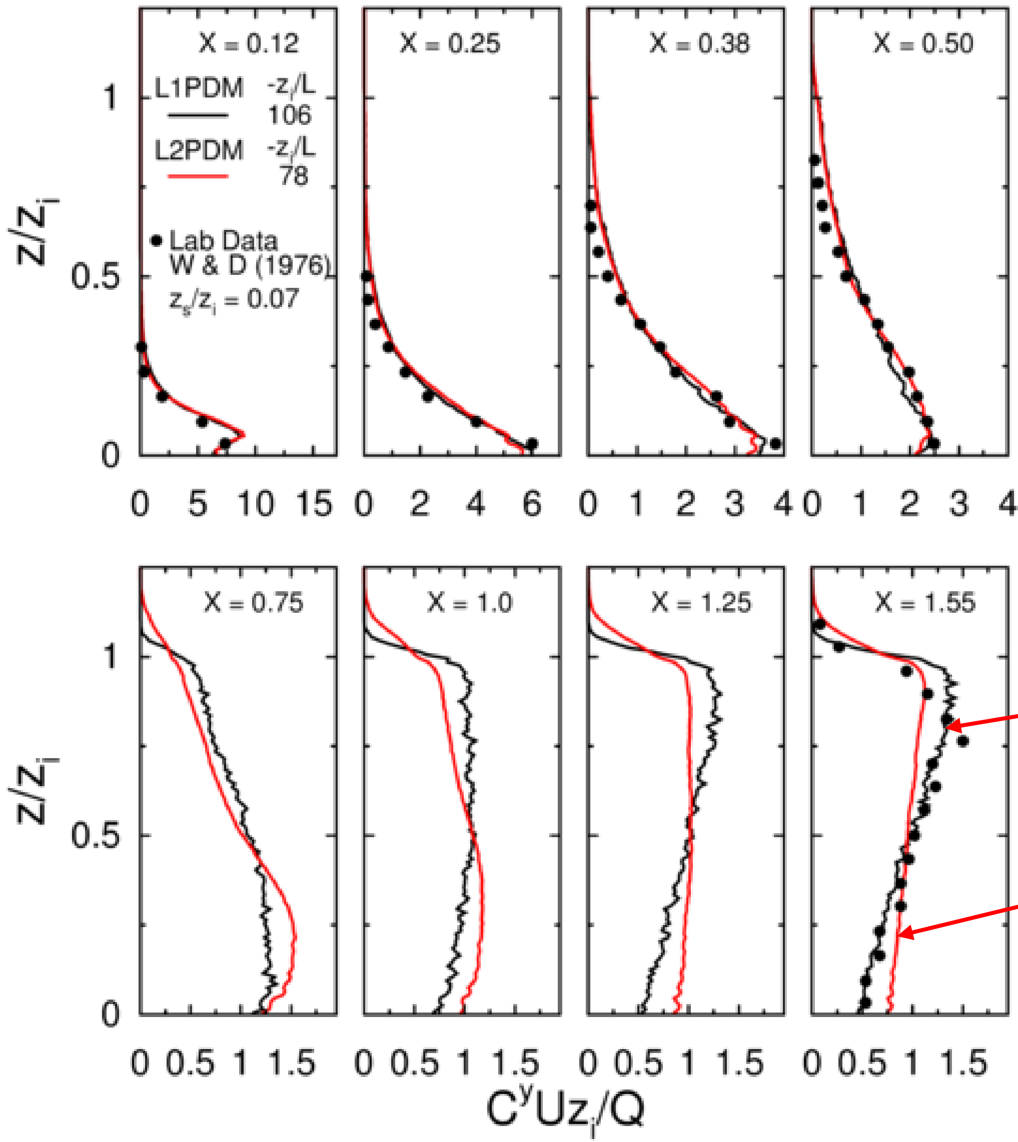
Crosswind-Integrated Concentrations (CWIC, C^y)

$z_s = 0.07\ z_i$, T_{av} = 30 min, L1PDM (Weil et al., 2012, BLM)



Vertical Profiles of Mean CWIC

$z_s = 0.07\ z_i$, T_{av} = 30 min, L1PDM & L2PDM

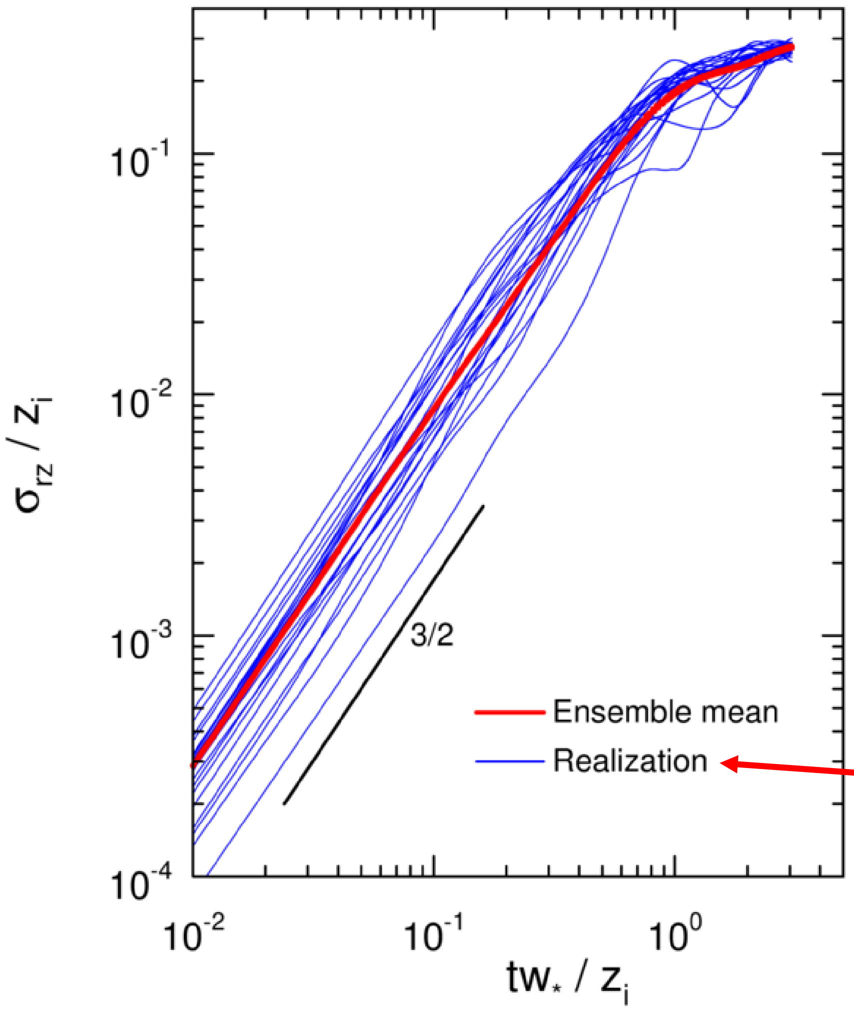


$$X = w_* x/(U z_i)$$

1-particle; Weil et al. (2004) $-z_i / L = 106$

2-particle; Current work $-z_i / L = 78$

2-Particle LPDM: Relative Dispersion



Batchelor (1950)

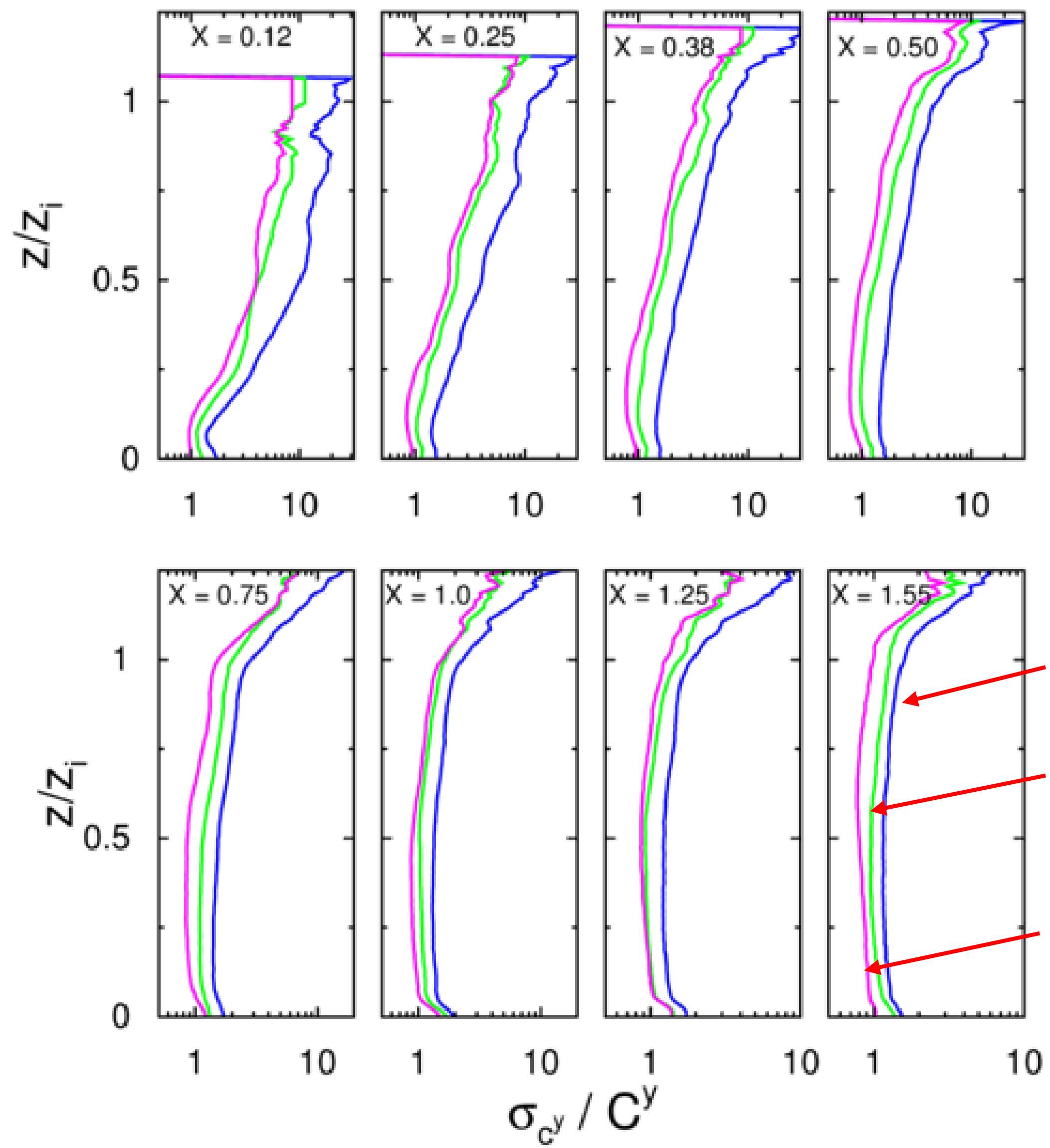
$$\sigma_r \propto \epsilon^{1/2} t^{3/2} \qquad t \ll T_L$$

$$\sigma_r \propto \sigma_v (T_L t)^{1/2} \qquad t \gg T_L$$

From 20 CBL sources

Vertical Profiles of CWIC Fluctuation Intensity, σ_{c^y}/C^y

$z_s = 0.07z_i$, L2PDM



Eddy turnover time

$t_* = z_i / w_*$

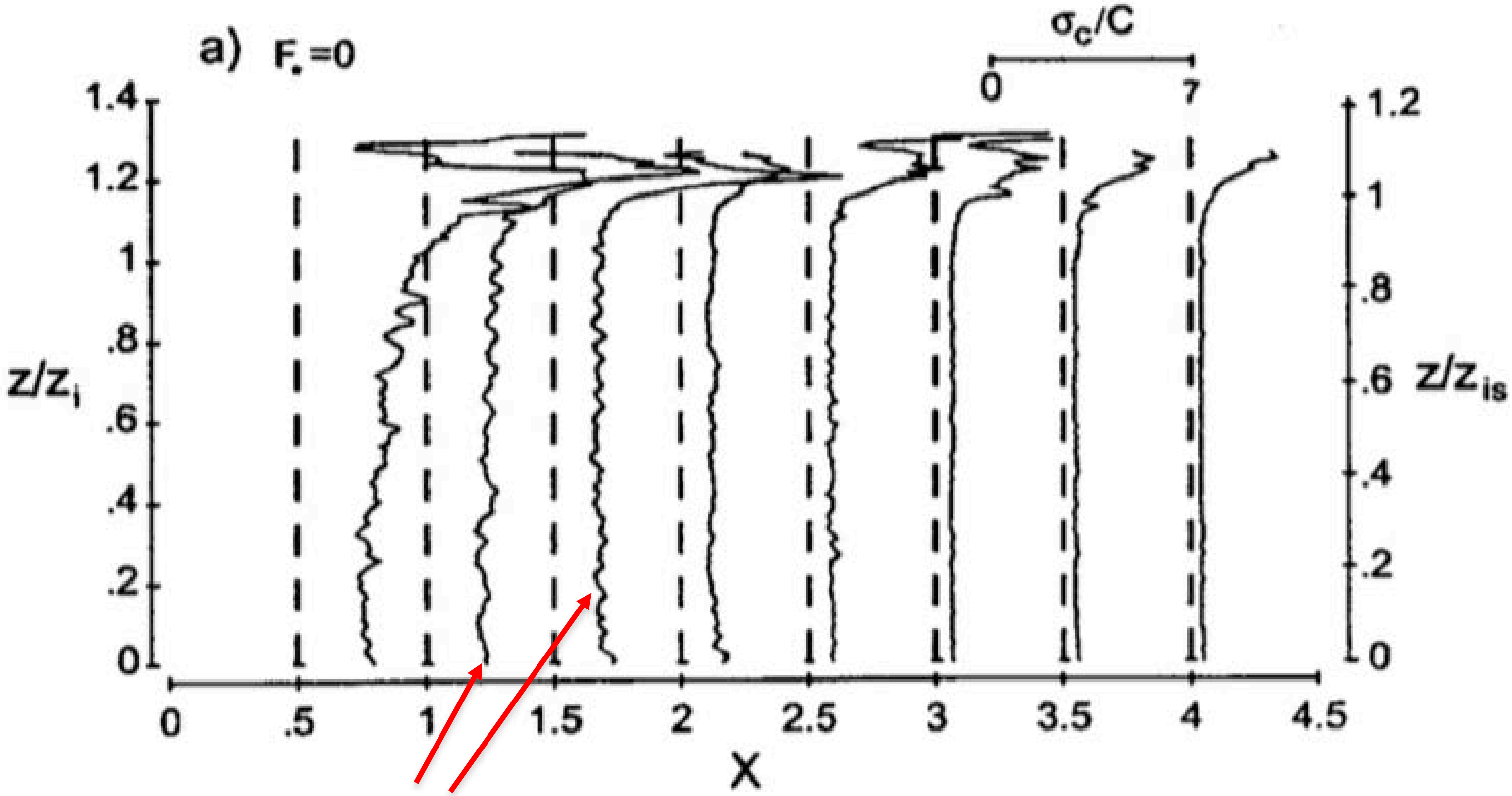
T_{av} = 60 s (= 0.12 t_*)

420 s (= 0.84 t_*)

700 s (= 1.36 t_*)

Vertical Profiles of Concentration Fluctuation Intensity, σ_c/C

Convection Tank Data, $z_s = 0.15z_i$ (Weil et al., 2002)

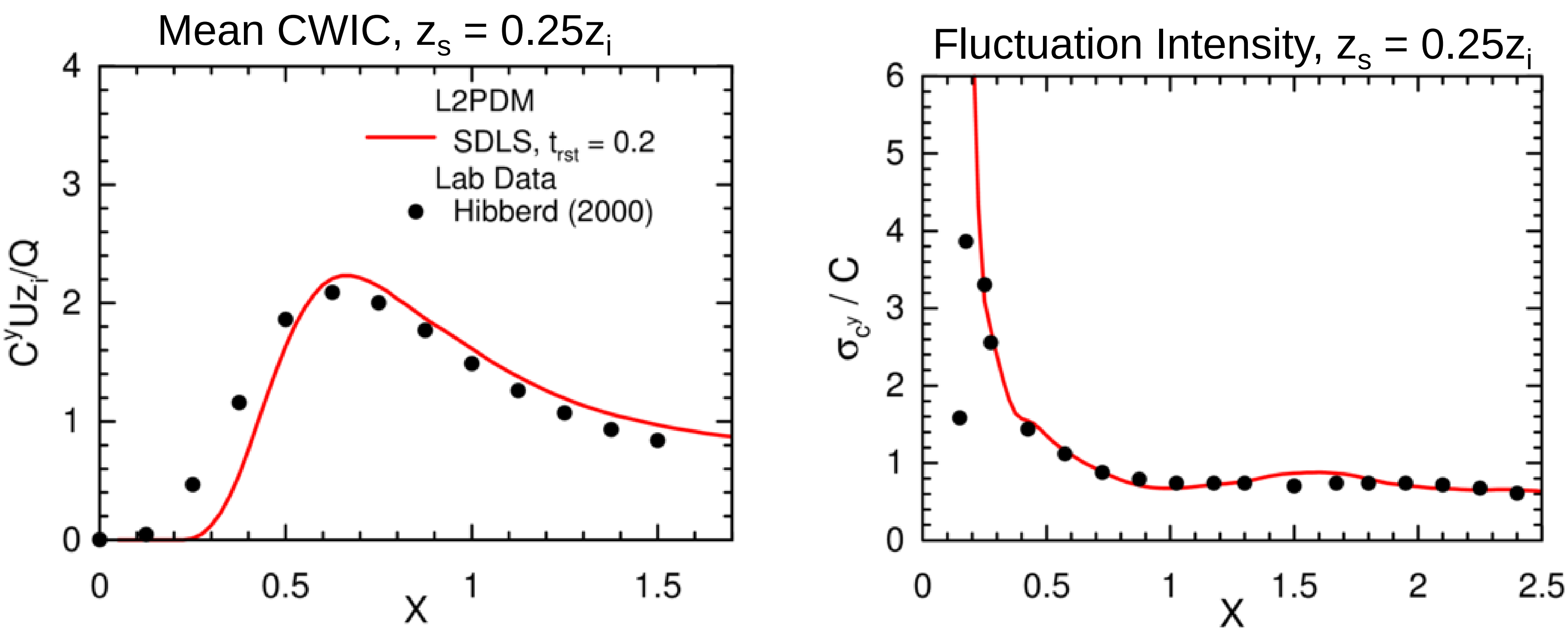


Well-mixed intensity

Surface Mean CWIC & Fluctuation Intensity

Short Duration Line Source (SDLS), $0 \leq t_r \leq 0.2t_*$

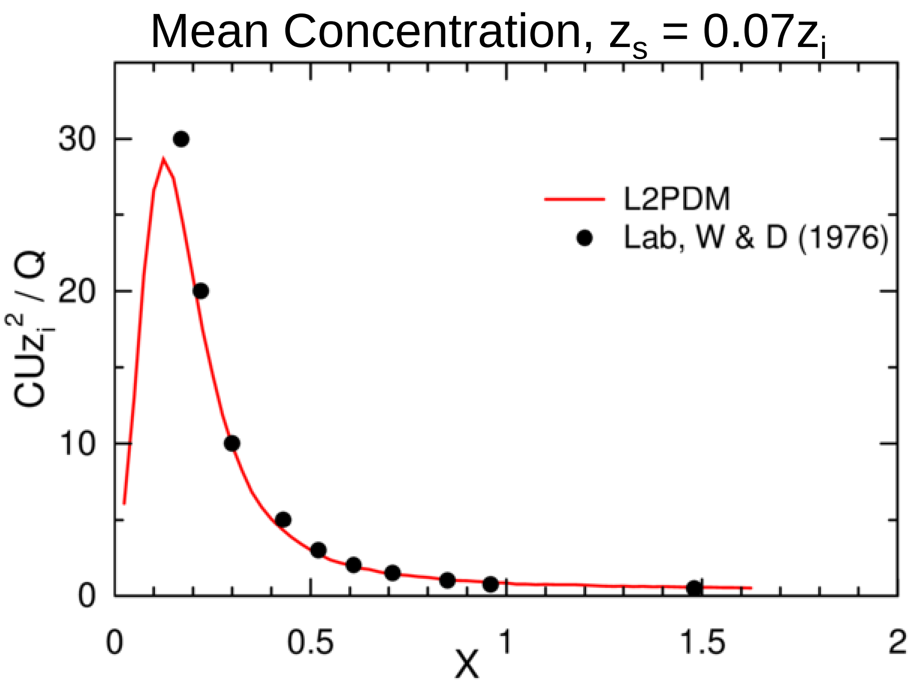
L2PDM vs Convection Tank Experiments (Hibberd, 2000)

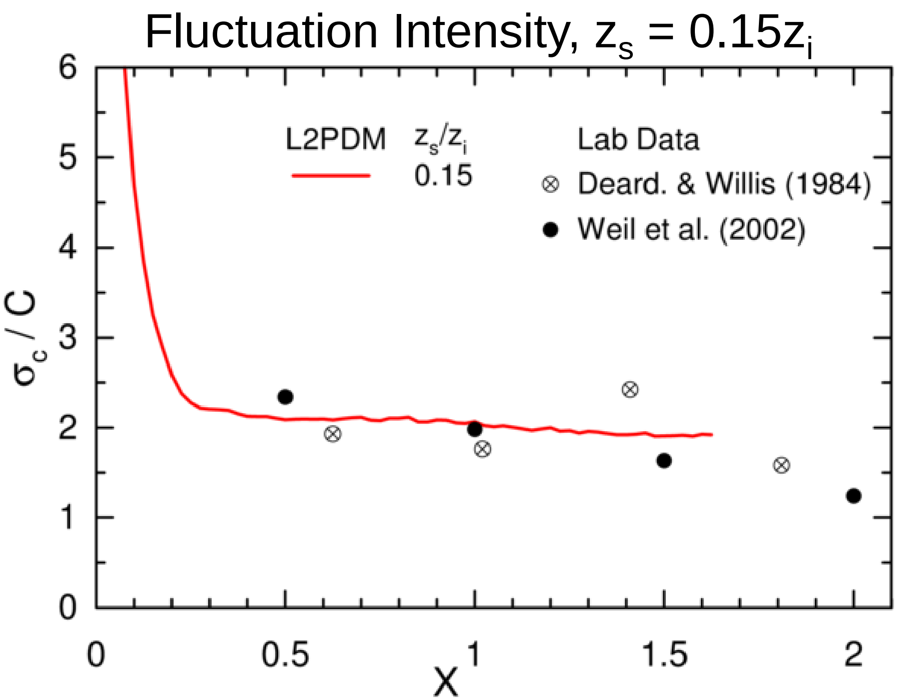


T_{av} = 1 min

Surface Mean Concentration & Fluctuation Intensity

Along plume centerline (y = 0)

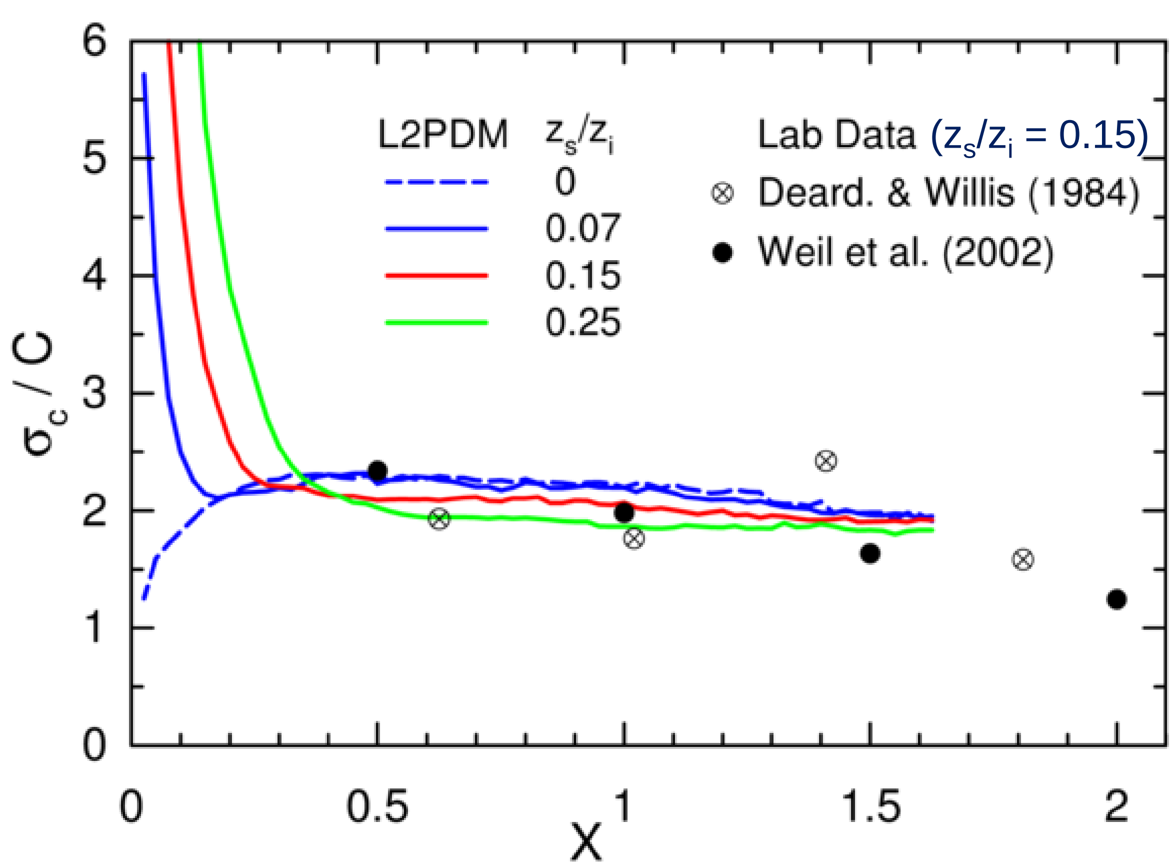




T_{av} = 1 min

$T_{av} = 0.12\ t_*$

Concentration Fluctuation Intensity at Surface: L2PDM vs Lab Data, Multiple Source Heights



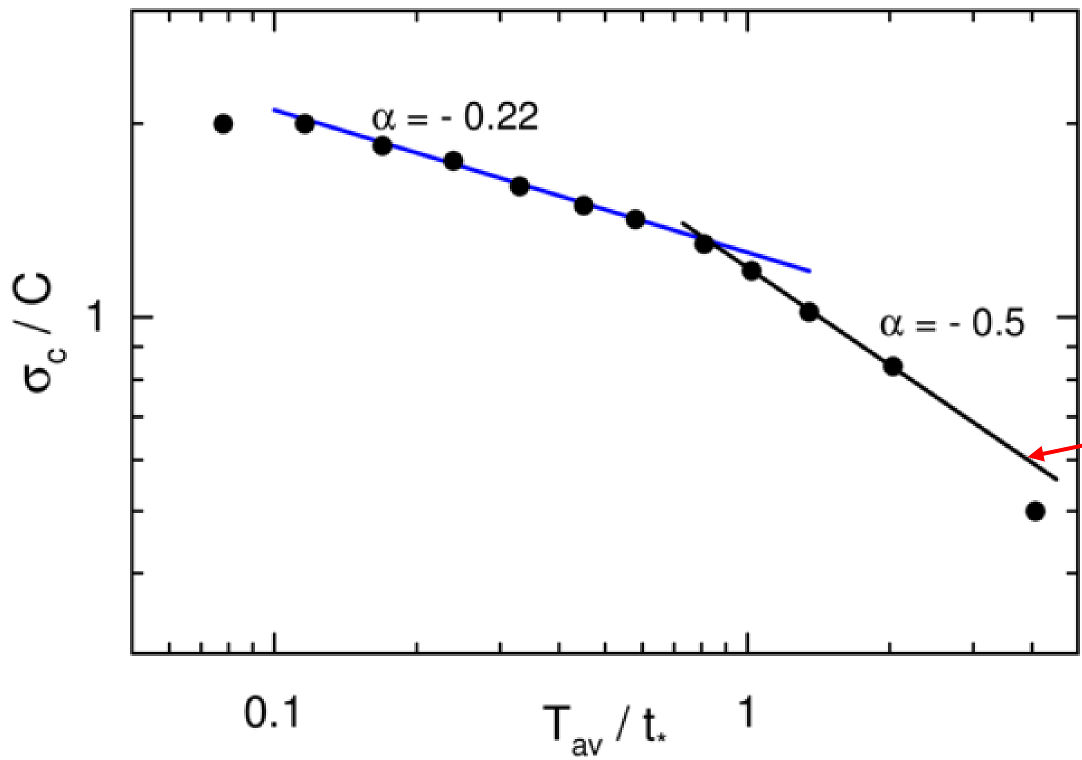
T_{av} = 1 min
L2PDM

Concentration Fluctuation Intensity at Surface: Averaging Time Effect

$$\left(\frac{\sigma_c}{C}\right)^2 = \frac{2(\sigma_{ci}/C)^2}{T_{av}} \cdot \int_0^{T_{av}} (1 - t/T_{av})\rho_c(t)dt$$ (Tennekes & Lumley, 1972)

$$\sigma_c = \sqrt{2}\sigma_{ci}\ (\tau_c/T_{av})^{1/2} \qquad T_{av}/\tau_c \gg 1$$

$z_s/z_i = 0.07$, $y = 0$, $X = 1.55$



$\sigma_c/C \propto (T_{av}/t_*)^{\alpha}$

Concentration Fluctuation Intensity at Surface: Averaging Time (T_{av}) Effect

$$\left(\frac{\sigma_c}{C}\right)^2 = \frac{2(\sigma_{ci}/C)^2}{T_{av}} \cdot \int_0^{T_{av}} (1 - t/T_{av})\rho_c(t)dt$$

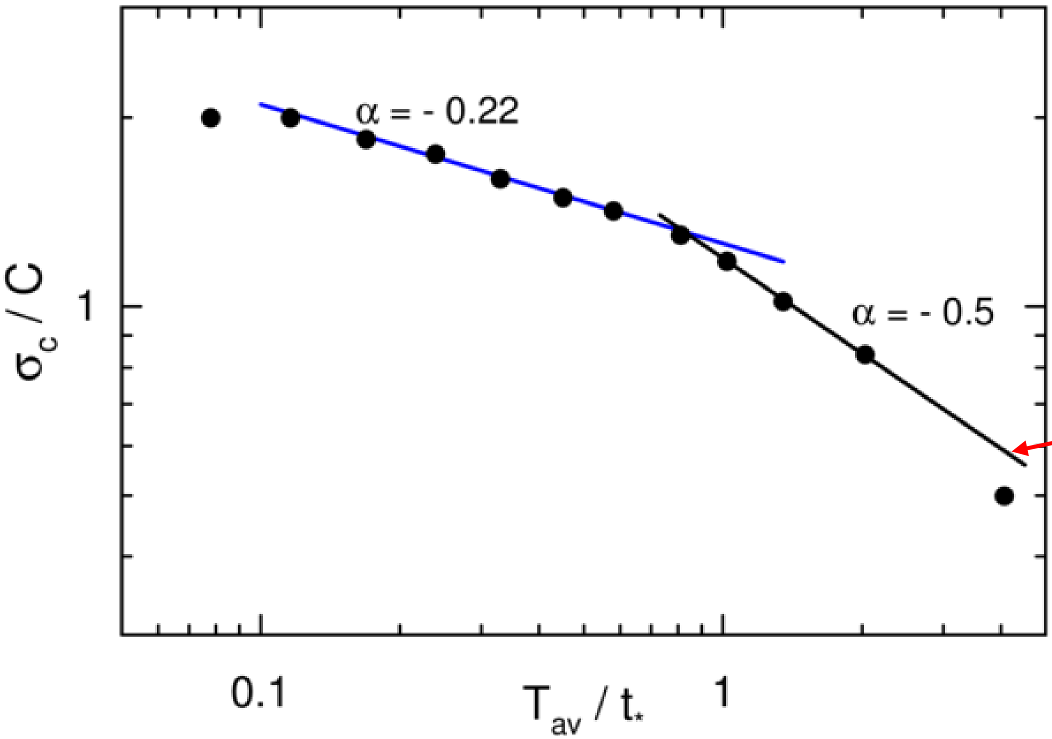
(Tennekes & Lumley, 1972)

Ensemble Variance (T_{av} = 0)

Concentration autocorrelation

$$\sigma_c = \sqrt{2}\sigma_{ci}\ (\tau_c/T_{av})^{1/2} \qquad T_{av}/\tau_c \gg 1$$

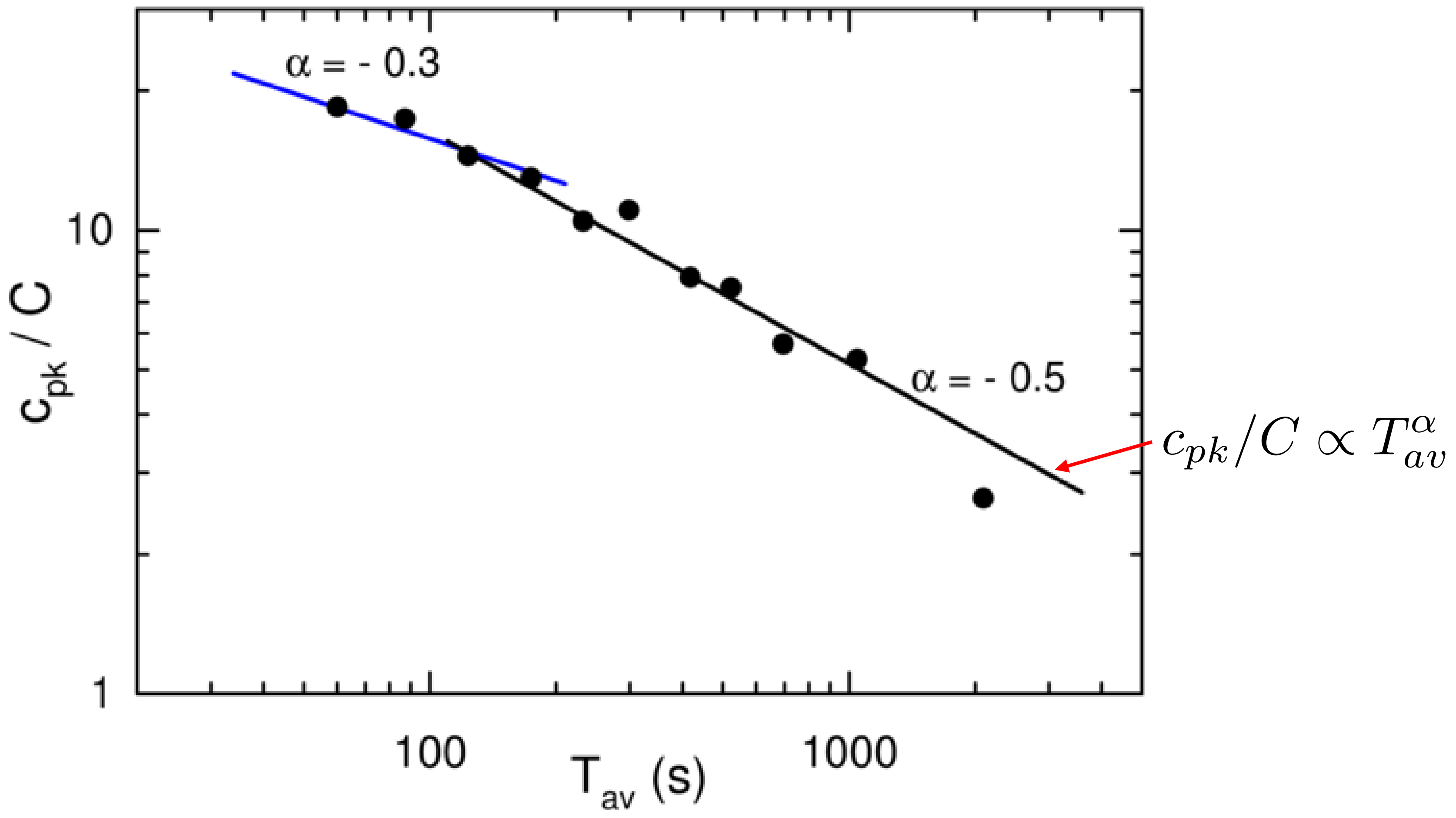
z_s/z_i = 0.07, y = 0, X = 1.55



$$\sigma_c/C \propto (T_{av}/t_*)^\alpha$$

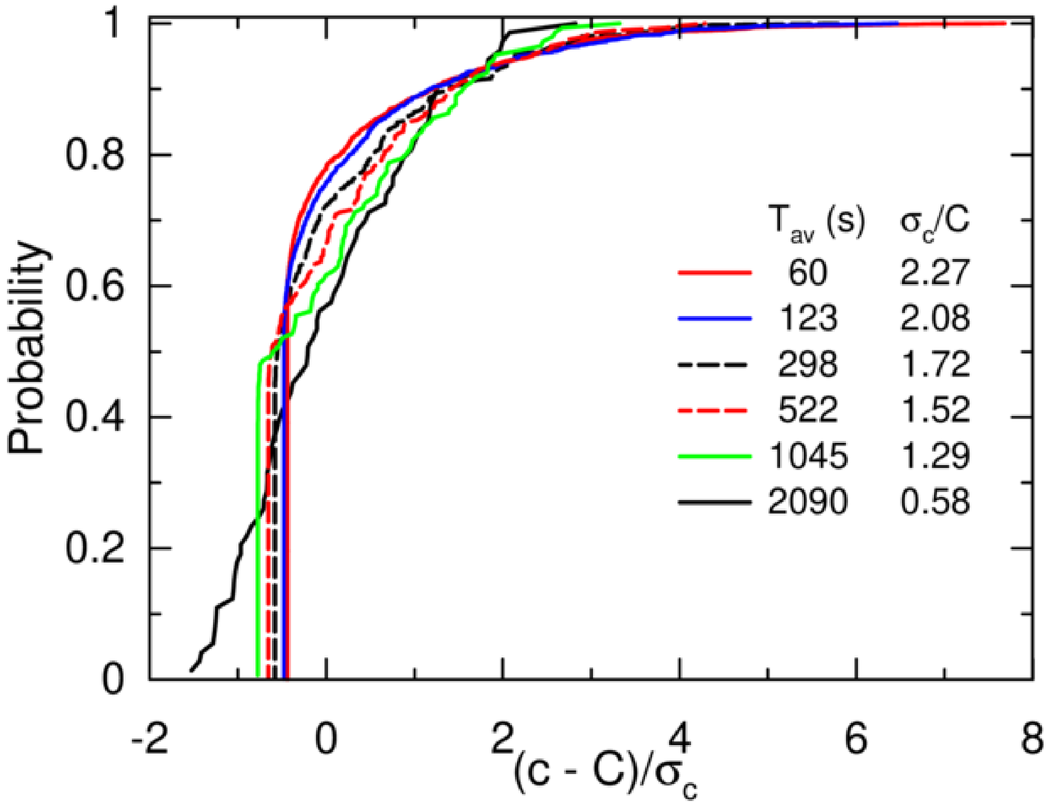
Peak Surface Concentration as Function of T_{av}

$z_s/z_i = 0.07$; $y = z = 0$; $X = X_{mx} = 0.125$



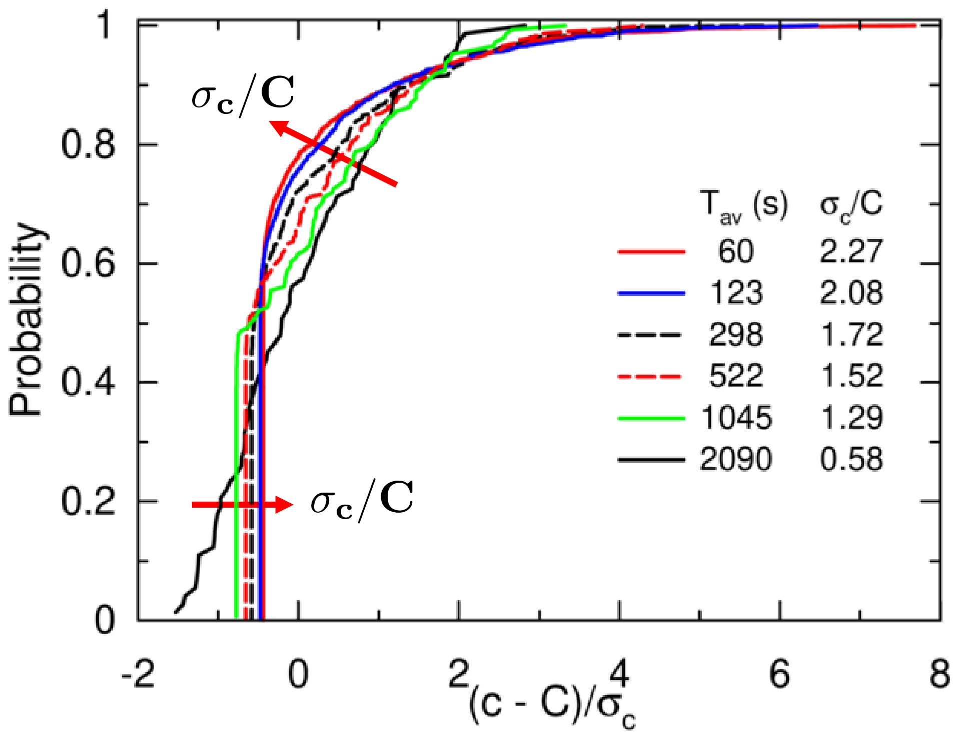
Cumulative Distribution Function (CDF) of Concentration Fluctuation, $(c - C)/\sigma_c$

$z_s/z_i = 0.07$; $y = z = 0$; $X = X_{mx} = 0.125$

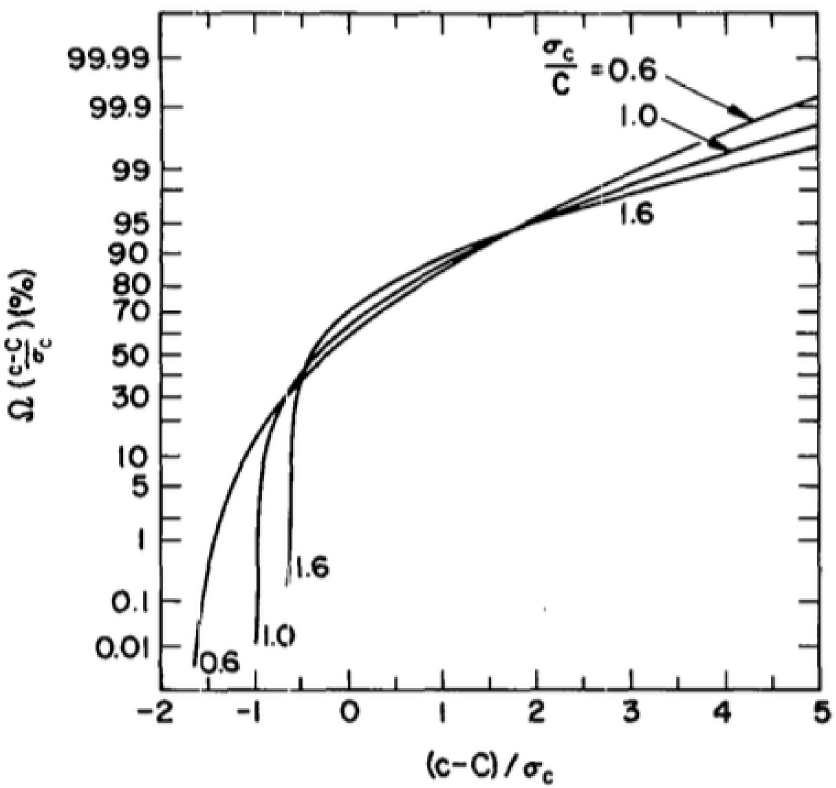


Cumulative Distribution Function of Concentration Fluctuations

L2PDM - LES; X = 0.125



Gamma CDF



Weil et al. (1992)

Applications: Estimate c_{peak}

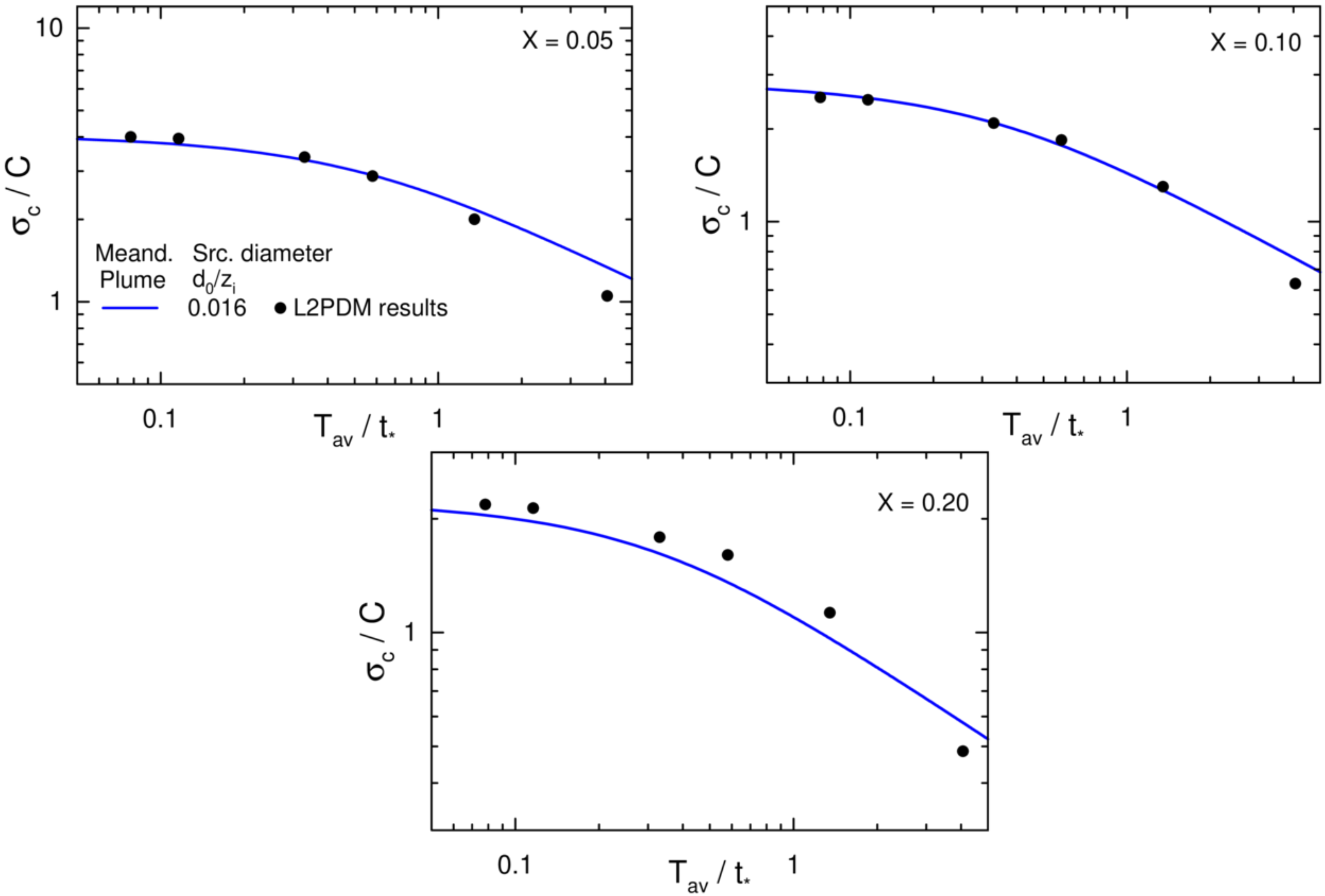
- Parameterized CDF
  - Mean (C), Rms ($\sigma_{\mathbf{c}}$), CDF shape
  - Compare L2PDM and Gamma CDFs

- Estimate $\sigma_{\mathbf{c}}$ with simpler model
  - Lagrangian “1-particle” model (e.g., Manor, 2014; Ferrero et al, 2017, 2019)
  - Extended meandering plume for T_{av} effects
  - Compare with L2PDM results

Extended Meandering Plume for T_{av} (Sykes, 1984)

Short times/distances: $\sigma_i^2 = \sigma_0^2 + \alpha\epsilon t^3, \;\; \sigma_m = \sigma_{vm} t$

$z_s/z_i = 0.07$; $y = z = 0$



Summary

- L2PDM matches mean CWIC and surface concentration fields of earlier 1-particle model and laboratory data in a CBL
- Modeled concentration fluctuation intensity agrees with convection tank fluctuation intensity profiles
- L2PDM gives fluctuation intensity, probability distributions of c, and c_{peak} as function of T_{av} over 60 s – 2090 s (35 min)
- L2PDM provides data for testing simpler models and applications

Further Work:

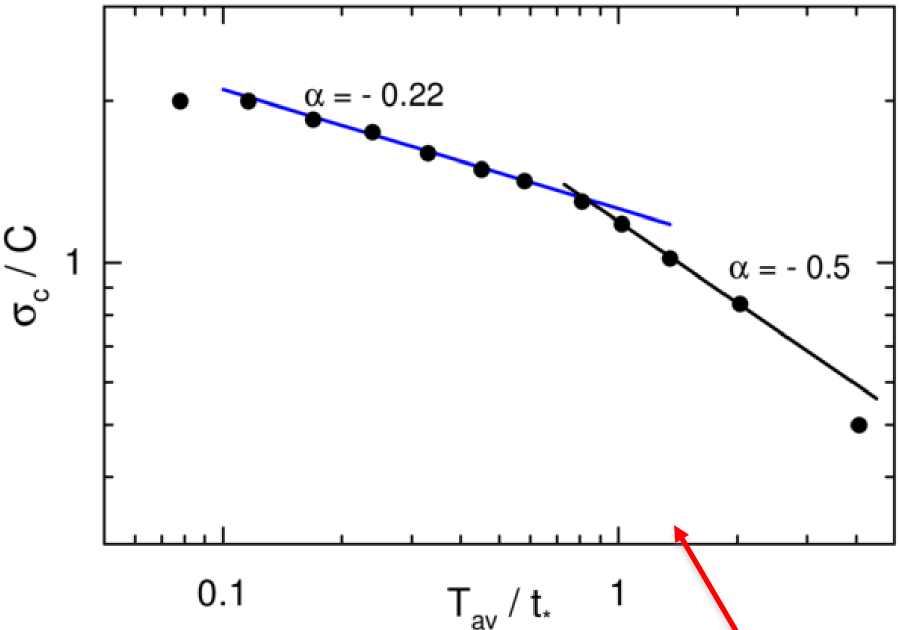
Finer resolution LES (CBL) and greater simulation time

Finer resolution LES and higher wind speeds ($U/w_* > 1.5$)

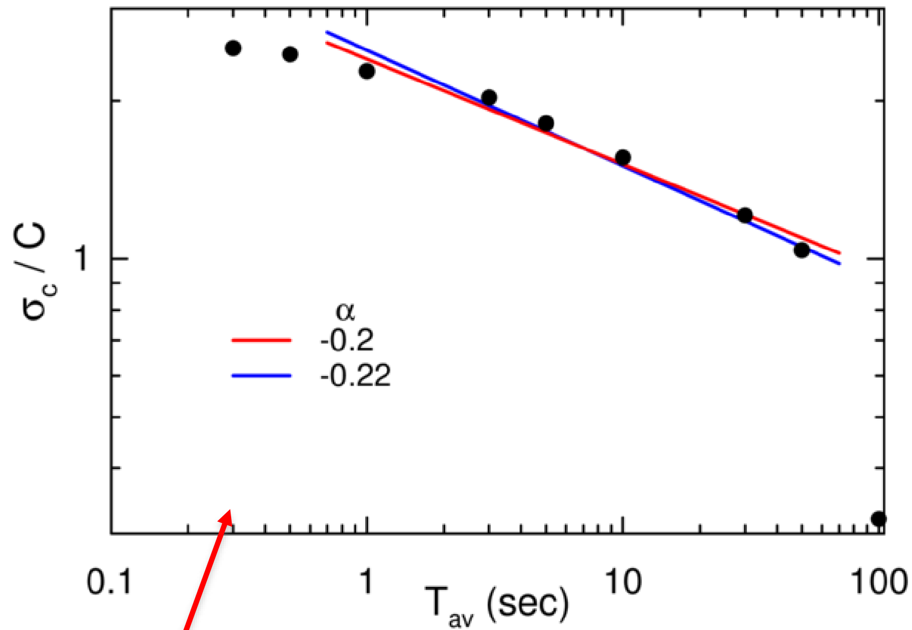
Weakly stable boundary layer

Concentration Fluctuation Intensity vs T_{av}: Comparison with Field Data

$z_s/z_i = 0.07$, $y = 0$



Field data: surface source in neutral conds.; Mylne & Mason (1991)



Similar slope/dependence on T_{av} at small T_{av}

Background

- Importance of statistical variability
  - Estimate peak concentrations—toxics, air quality, odors, chemistry, etc.
  - Need: mean, variance, probability dist.

Borex (Denmark,1992)

"Passive" or non-buoyant source.

- Statistics for variable averaging time, T_{av}
  - Requires "relative dispersion" of plume

- Approach
  - Lagrangian two-particle dispersion model (L2PDM) driven by large-eddy simulations (LES) of the convective boundary layer (CBL)

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  - Provide numerical data for testing simple models

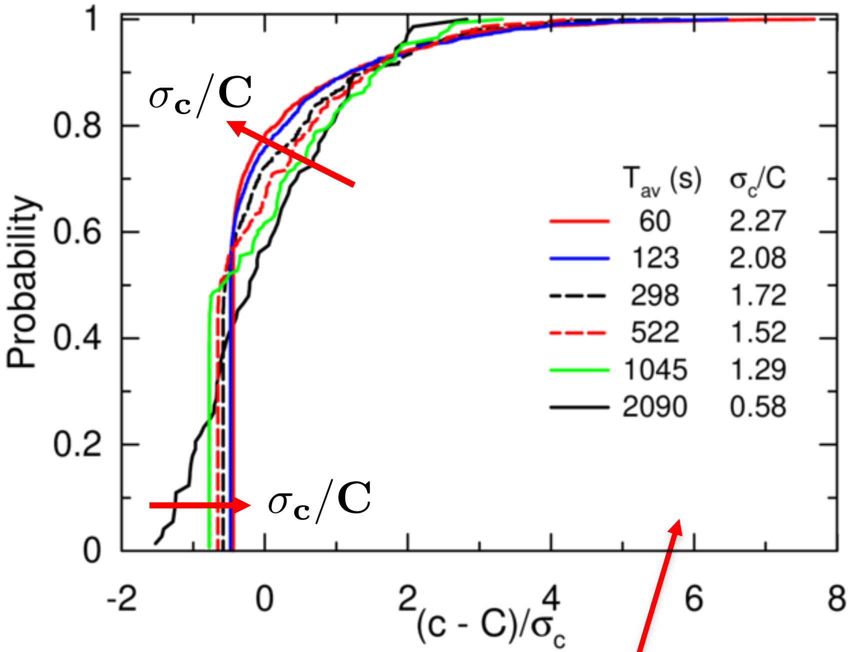
Applications: Estimate $C, \sigma_c, \underline{c_{peak}}$

- Parameterized CDF
  - Mean (C), Rms ($\sigma_{\mathbf{c}}$), CDF shape
  - Compare L2PDM with Gamma CDF

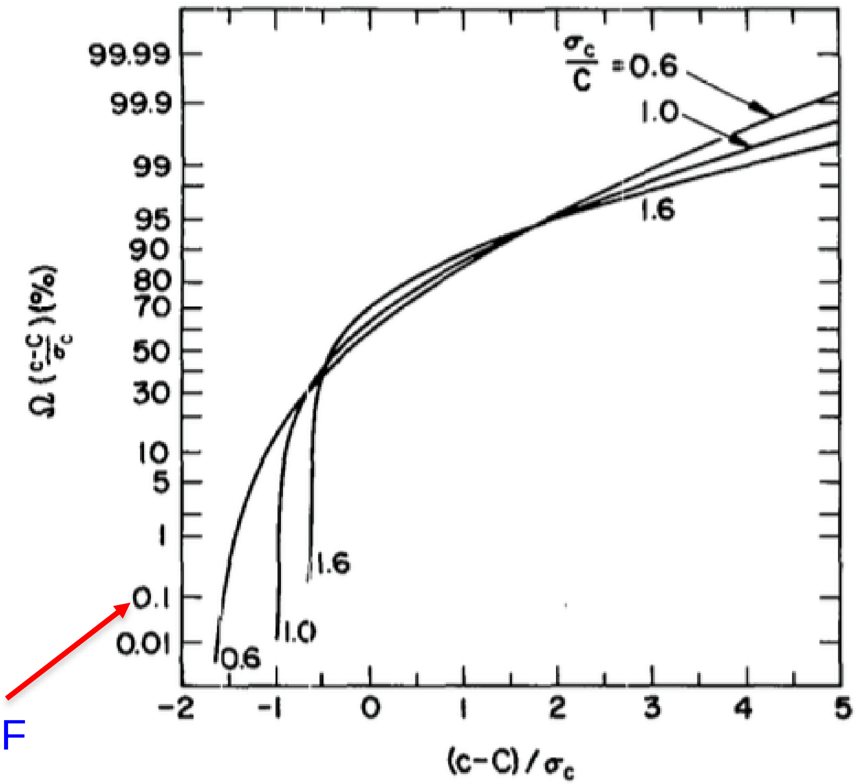
- Estimate $\sigma_{\mathbf{c}}$ with simpler model
  - Lagrangian “1-particle” model (e.g., Manor, 2014; Ferrero et al, 2017, 2019)
  - Extended meandering plume for T_{av} effects

Cumulative Distribution Function of Concentration Fluctuations

L2PDM - LES; X = 0.125



Gamma CDF



Weil et al. (1992)

Rescaled L2PDM CDF similar to Gamma CDF

Get similar c_{pk}/C to Gamma CDF with $\sigma_c/C = 3.5$

Summary

- Lagrangian particle & LES approach extended to concentration fluctuations with a 2-particle model (L2PDM)
- L2PDM matches mean CWIC and surface concentration fields of earlier 1-particle model and laboratory data in a CBL
- Modeled concentration fluctuation intensity agrees with convection tank data of vertical and surface fluctuation intensity profiles
- L2PDM provides fluctuation intensity, probability distributions of c, and c_{peak} as function of T_{av} over 60 s – 2090 s (35 min)
- L2PDM provides data for testing simpler models and applications

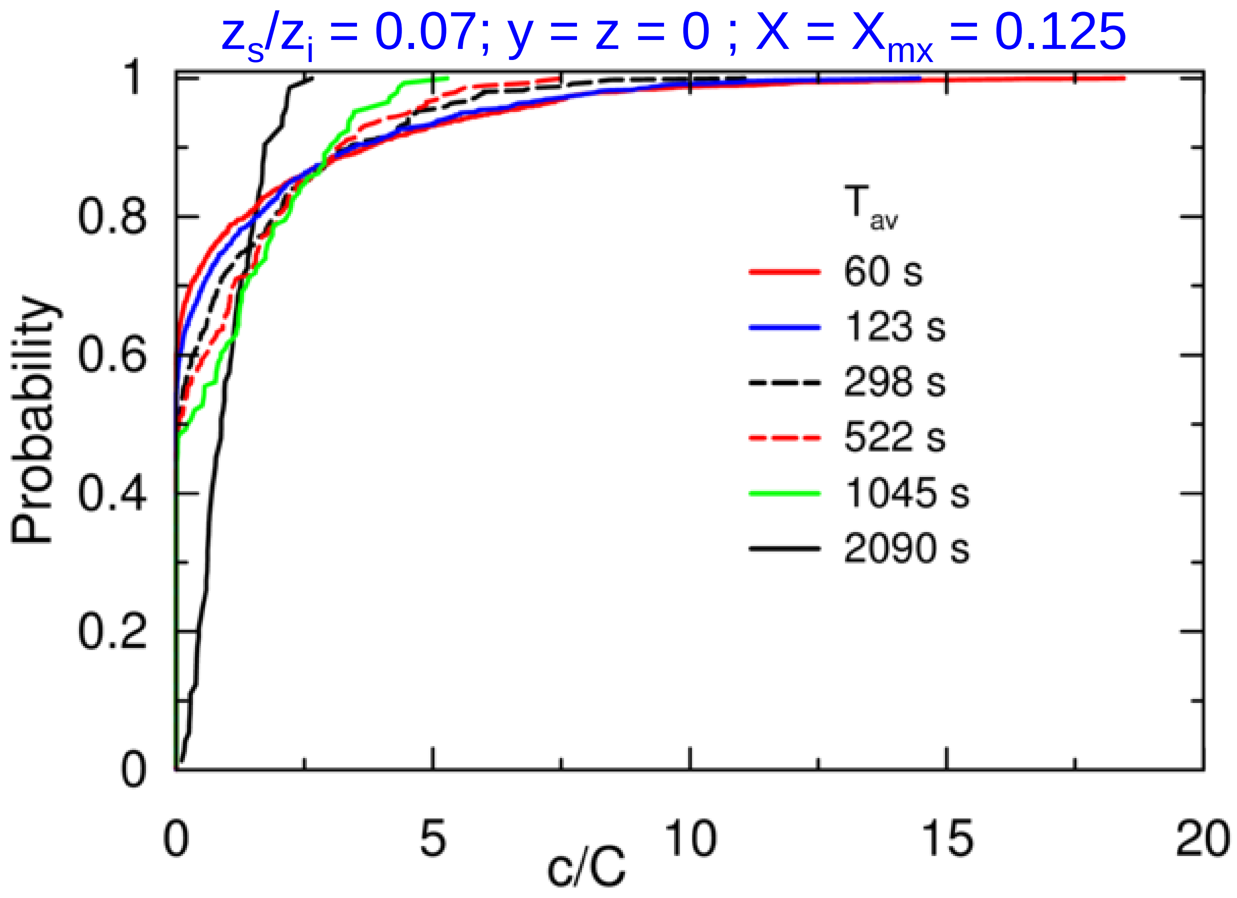
Further Work:

Finer resolution LES (CBL) and greater simulation time

Finer resolution LES and higher wind speeds ($U/w_* > 1.5$)

Weakly stable boundary layer

Cumulative Distribution Function / Probability of c/C as Function of T_{av}



Generation of Concentration Fluctuations

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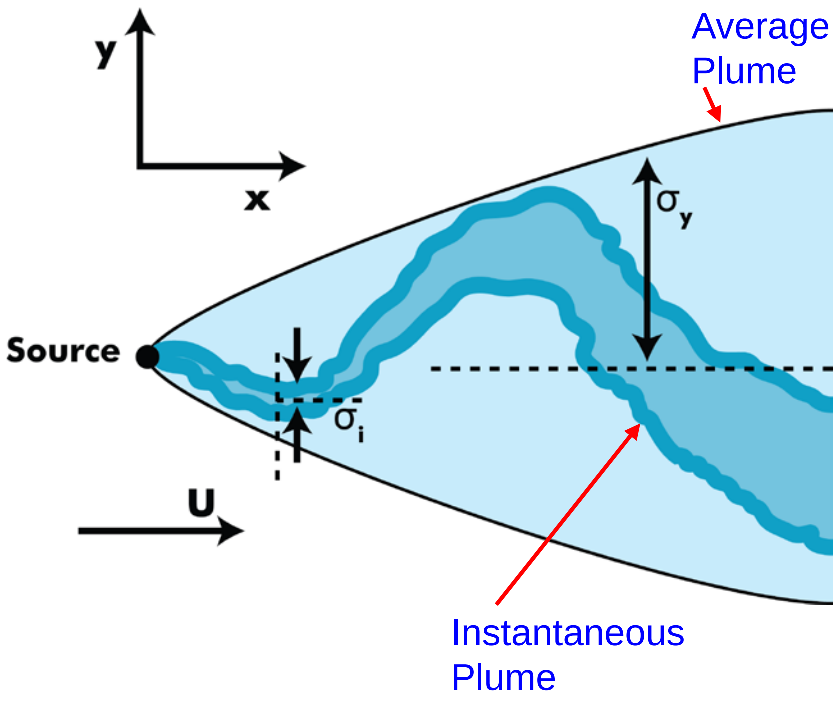
(Gifford 1959)



Concentration Fluctuation Intensity
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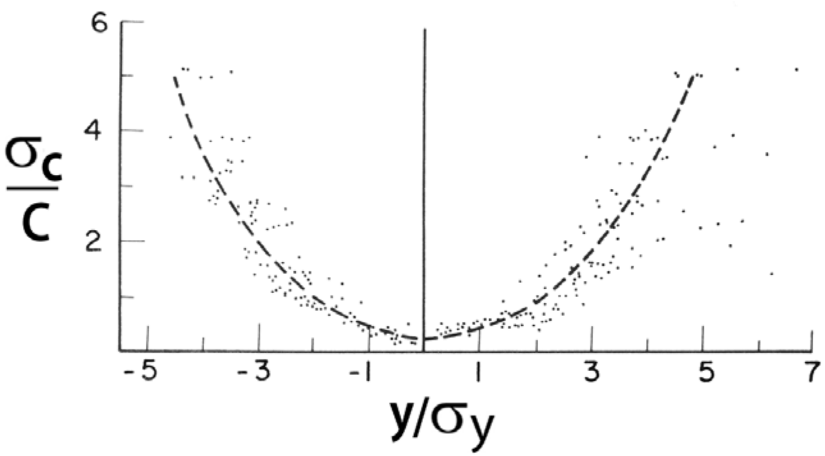
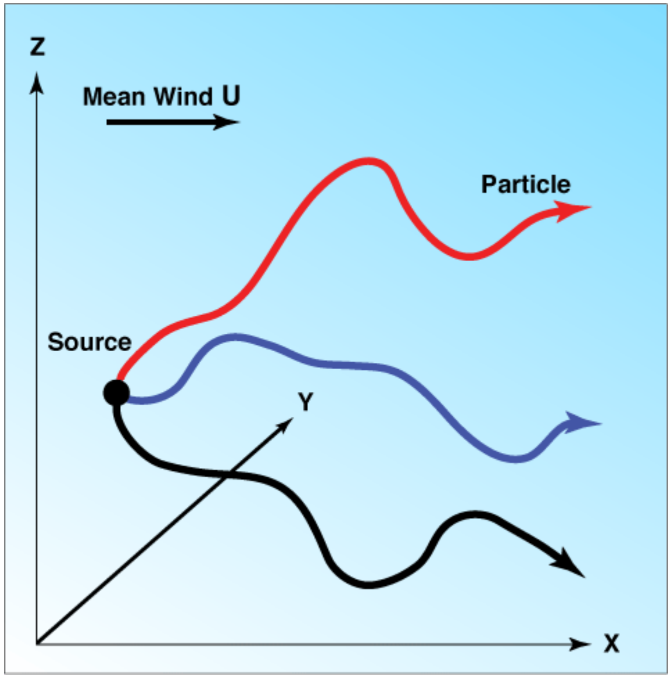


Lagrangian 1- & 2-Particle Dispersion Models

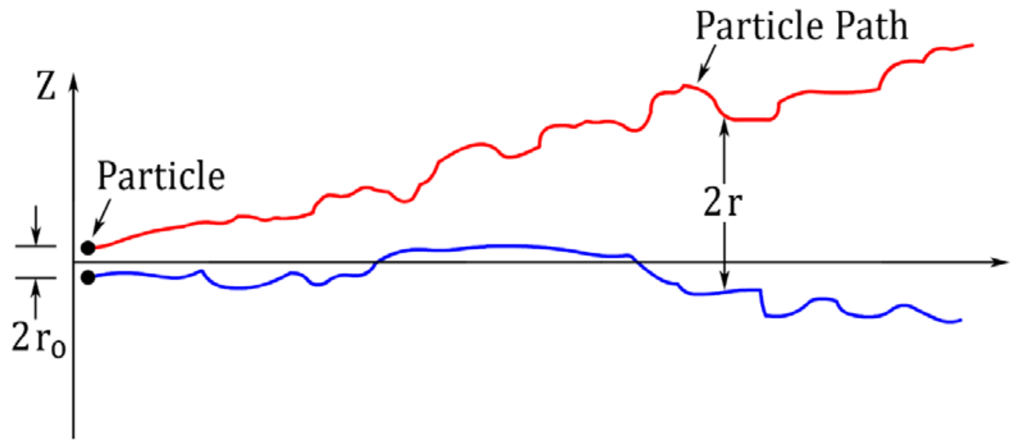
Applies to 1- & 2-particle models



Concentration

$$c(\mathbf{x},t) = Q\int p_1(\mathbf{x},t;\mathbf{x}_{S1},t_1')dt_1'$$

2-particle model



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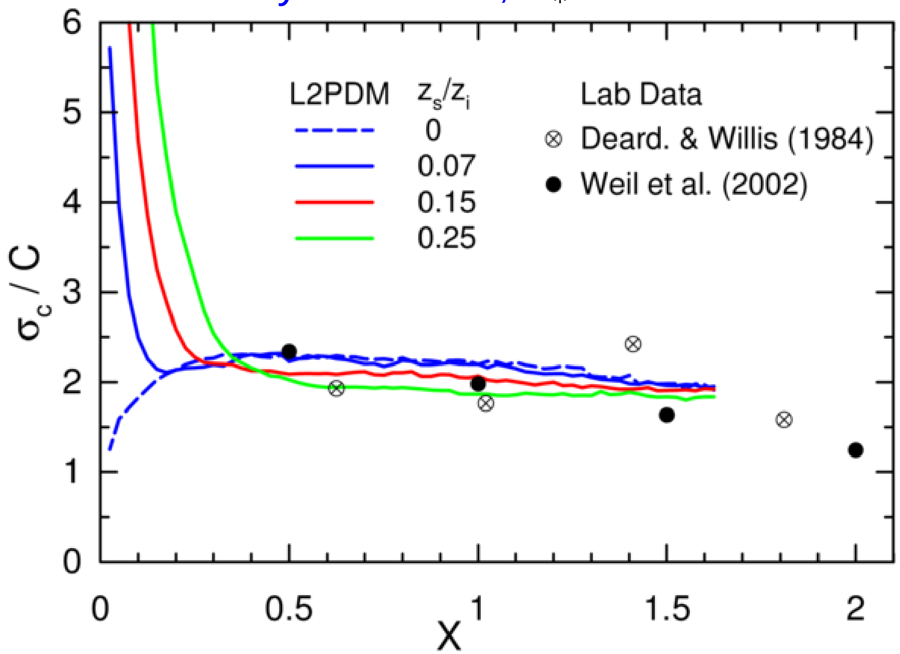
u_{Ri} = resolved LES velocity, particle *i*
u_{Si} = stochastic subgrid-scale (SGS) velocity

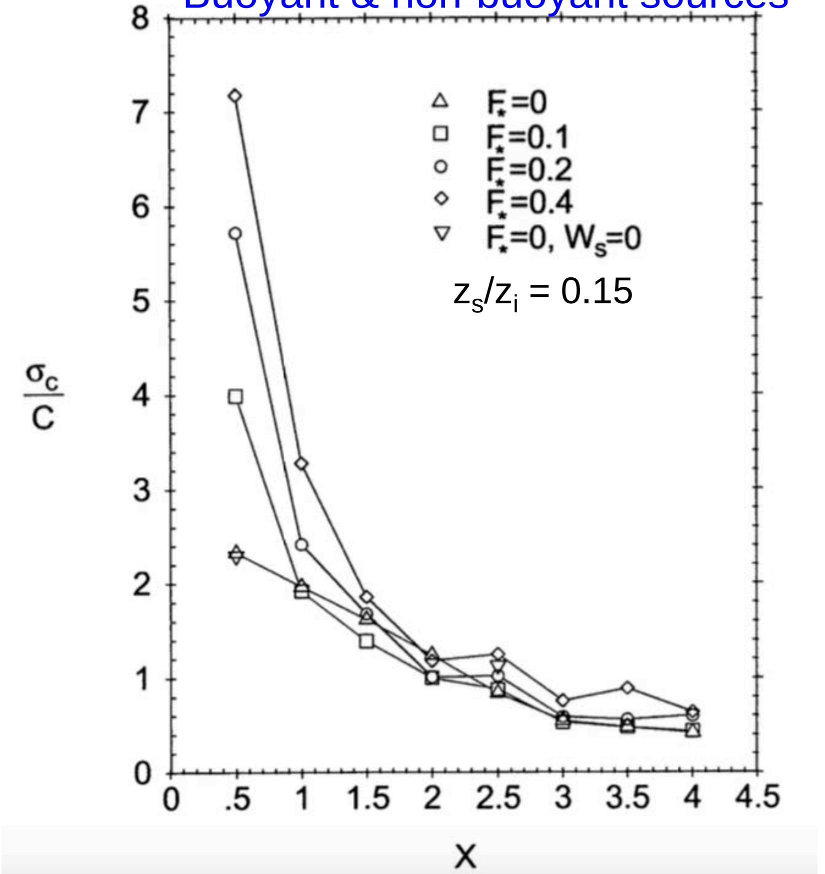
Adopt Thomson's (1990) stochastic model for u_{Si}

Concentration Fluctuation Intensity at Surface: L2PDM vs Lab Data, Multiple Source Heights

Non-buoyant source, $F_* = 0$



Conv. Tank Data (Weil et al., 2002)
Buoyant & non-buoyant sources



Peak Surface Concentration as Function of T_{av}