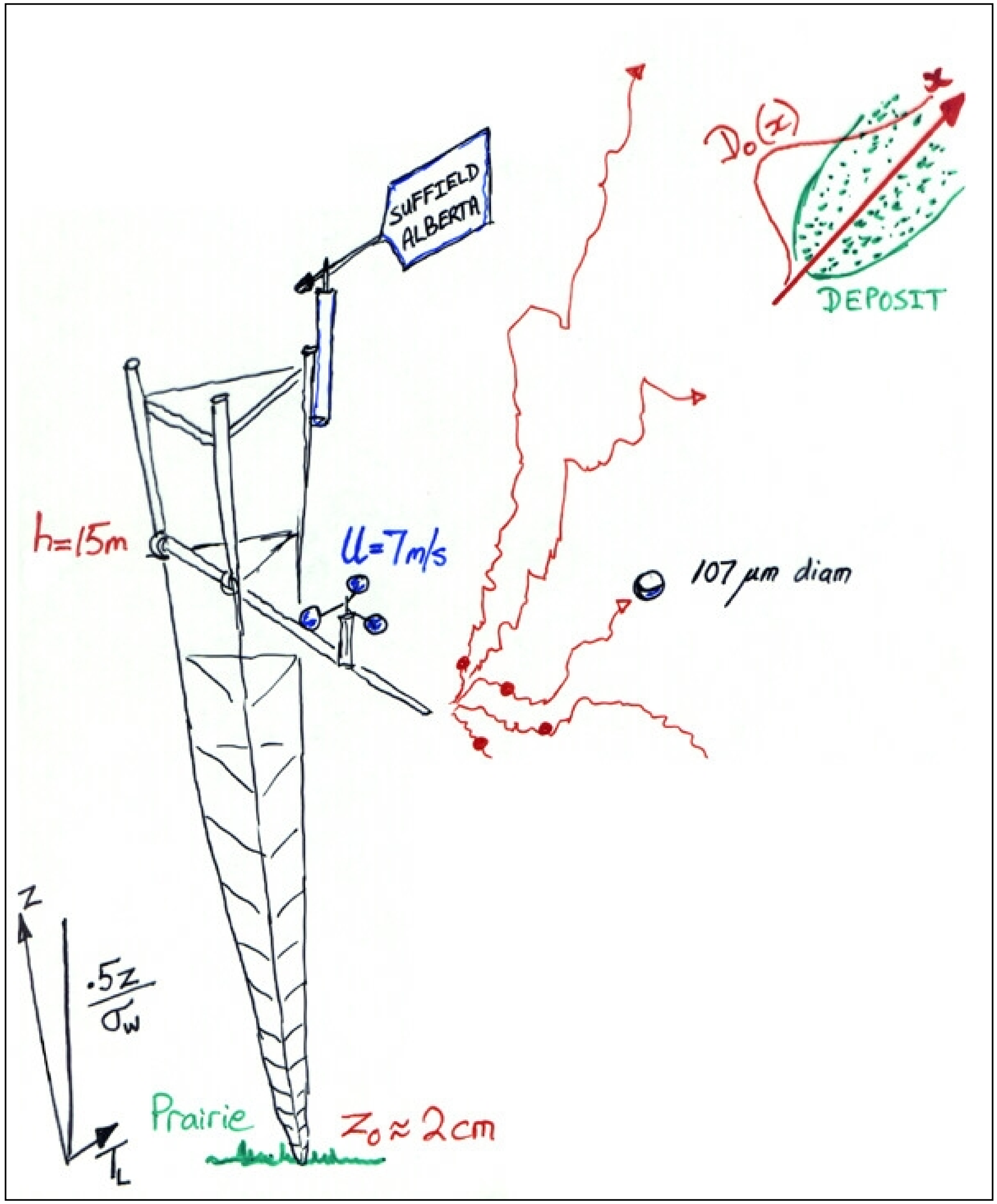
Application of Lagrangian stochastic model (in forward or backward mode) to various dispersion problems, covering both horizontally-homogeneous and fully 3-dimensional flows



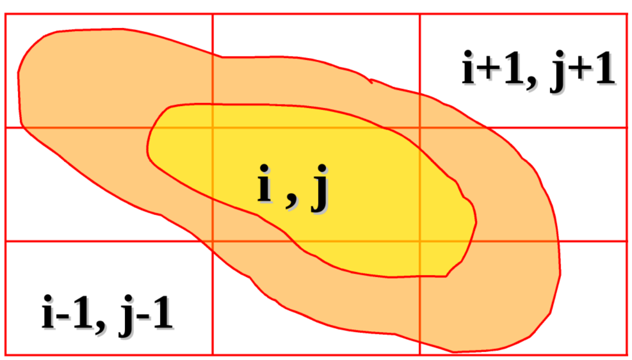
eas471_dispersionLS.odp
JD Wilson, EAS U. Alberta
Last modified 7 Apr. 2016

Eulerian approach:
"Mass is conserved…"

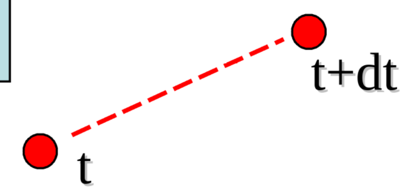
$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{w}\frac{\partial \bar{c}}{\partial z} = -\frac{\partial}{\partial x}\overline{u'c'} - \frac{\partial}{\partial z}\overline{w'c'}$$

+ closure $$\overline{w'c'} = -K\frac{\partial c}{\partial z}$$

"… during advection and 'diffusion' between control volumes… "



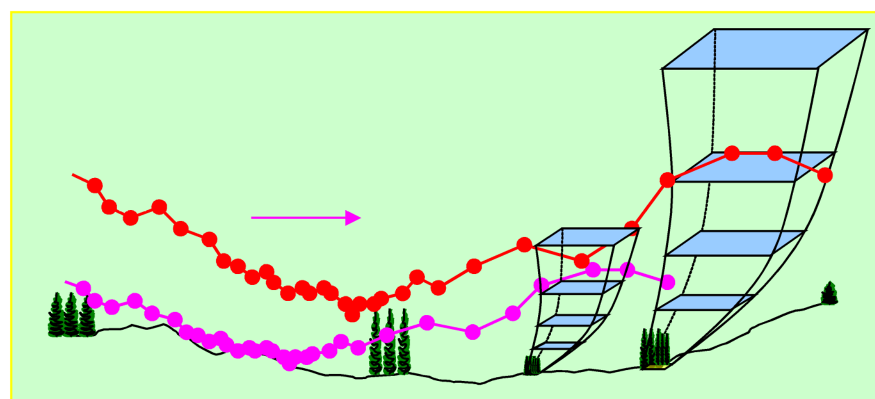
Lagrangian:
"Track motion…"



$$Z(t+dt) = Z(t) + W\ dt$$
$$W(t+dt) = W(t) + dW$$
$$dW = a(X,U)\ dt + b\ d\xi$$

memory

random forcing



Thomson's well-mixed LS model for 2-D Gaussian, horizontally-homogeneous turbulence

$$dU = -\frac{b^2}{2\sigma^2}\left[U\,{\sigma_w}^2 - W\,\overline{u'w'}\right]dt + \frac{\phi_u}{g_a}dt + b\,d\xi_u$$

$$dW = -\frac{b^2}{2\sigma^2}\left[W\,{\sigma_u}^2 - U\,\overline{u'w'}\right]dt + \frac{\phi_w}{g_a}dt + b\,d\xi_w$$

$$dX = [\,\overline{u}(Z) + U\,]\,dt$$

$$dZ = W\,dt$$

where $b^2 = C_0\epsilon$,

$$\sigma^2 = \sigma_u^2\,\sigma_w^2 - u_*^4 \qquad (\; u_*^2 \equiv \overline{u'w'}\;)$$

and $g_a = g_a(u',w';\,z)$ is the joint PDF of the Eulerian velocity fluctuations, specifically, the joint Gaussian:

$$g_a(u',w';z) = \frac{1}{2\pi\sigma}\;\exp\left[-\;\frac{\sigma_w^2\,(u')^2 + \sigma_u^2\,(w')^2 - 2u_*^2\,u'\,w'}{2\,\sigma^2}\right]$$

Thomson's well-mixed LS model for 2-D Gaussian, horizontally-homogeneous turbulence

$$\frac{\phi_u}{g_a} = \frac{1}{2}\frac{\partial\overline{u'w'}}{\partial z} + W\frac{\partial\overline{u}}{\partial z}$$
$$+ \frac{1}{2\sigma^2}\left[\frac{\partial{\sigma_u}^2}{\partial z}\left({\sigma_w}^2\,U\,W - \overline{u'w'}\,W^2\right) + \frac{\partial\overline{u'w'}}{\partial z}\left({\sigma_u}^2\,W^2 - \overline{u'w'}\,U\,W\right)\right]$$

$$\frac{\phi_w}{g_a} = \frac{1}{2}\frac{\partial{\sigma_w}^2}{\partial z}$$
$$+ \frac{1}{2\sigma^2}\left[\frac{\partial{\sigma_w}^2}{\partial z}\left({\sigma_u}^2\,W^2 - \overline{u'w'}\,U\,W\right) + \frac{\partial\overline{u'w'}}{\partial z}\left({\sigma_w}^2\,U\,W - \overline{u'w'}\,W^2\right)\right]$$

- necessary to include the *u*' fluctuation if, for instance, the turbulence intensity $\sigma_u/\bar{u}$ is large, as (for instance) within a plant (or urban) canopy

- however often there is little (if any) penalty to neglecting the correlation $\overline{u'w'}$ in which case the model above simplifies radically

- 3D generalization is straightforward

A TWO-DIMENSIONAL TRAJECTORY-SIMULATION MODEL FOR NON-GAUSSIAN, INHOMOGENEOUS TURBULENCE WITHIN PLANT CANOPIES

T. K. FLESCH and J. D. WILSON

Boundary-Layer Meteorology **61**: 349–374, 1992.

- tested the Thomson 2-D LS model (of previous page) and an alternative based on non-Gaussian velocity PDF (an added hypothesis of the alternative model is that a_i must be anti-parallel to the Lagrangian velocity fluctuation)

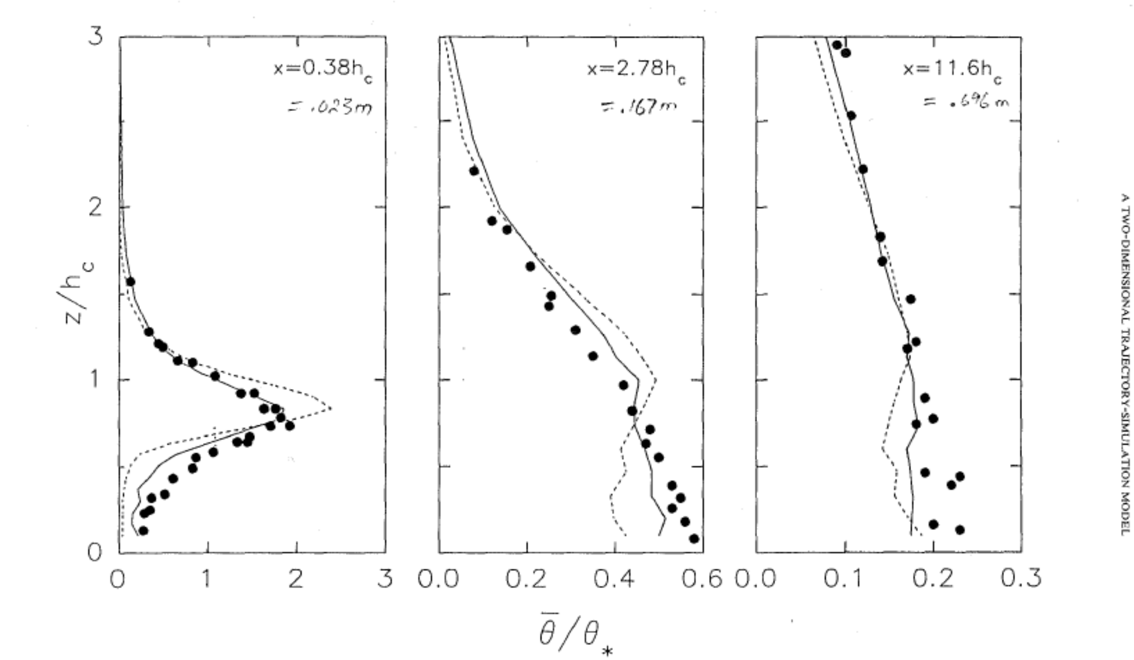
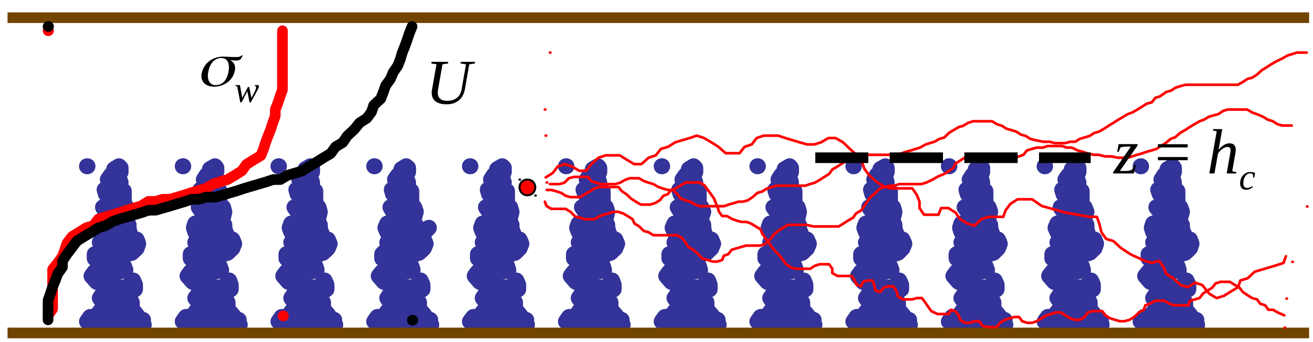


Fig. 6. Comparison of normalized temperature measurements from the LRC experiment (·) with predicted values using Gaussian (———) and non-Gaussian (-------) PDFs at three fetches (x).

- proved acceptable to aproximate the canopy velocity PDF as Gaussian

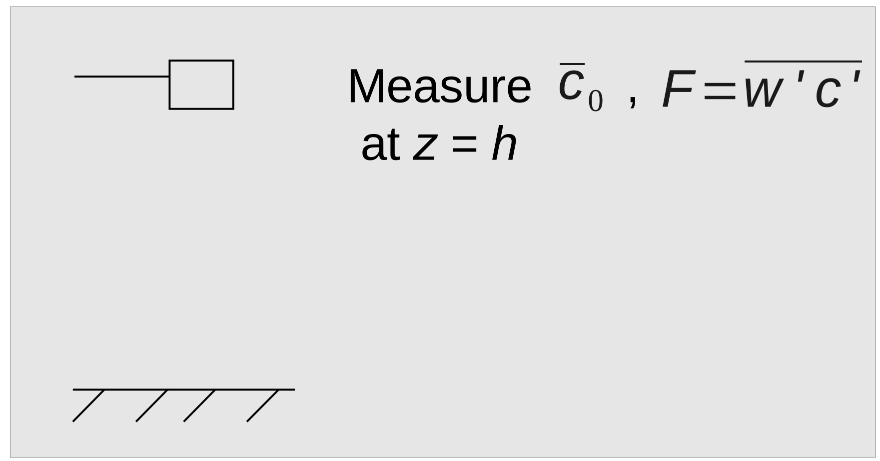
- inhomogeneity has greater influence than non-Gaussianity

Wind tunnel canopy – experiment by Legg, Raupach & Coppin
– crosswind line source of tracer heat



Deposition to ground or canopy

Uptake at ground is often parameterized in terms of a "deposition velocity," defined as the ratio $w_d = F/\bar{c}_0$ of the magnitude of the flux density to the surface to a mean concentration $\bar{c}_0$ measured at an arbitrary reference location above the surface (this only makes sense if the flux and concentration are measured within the constant flux layer)

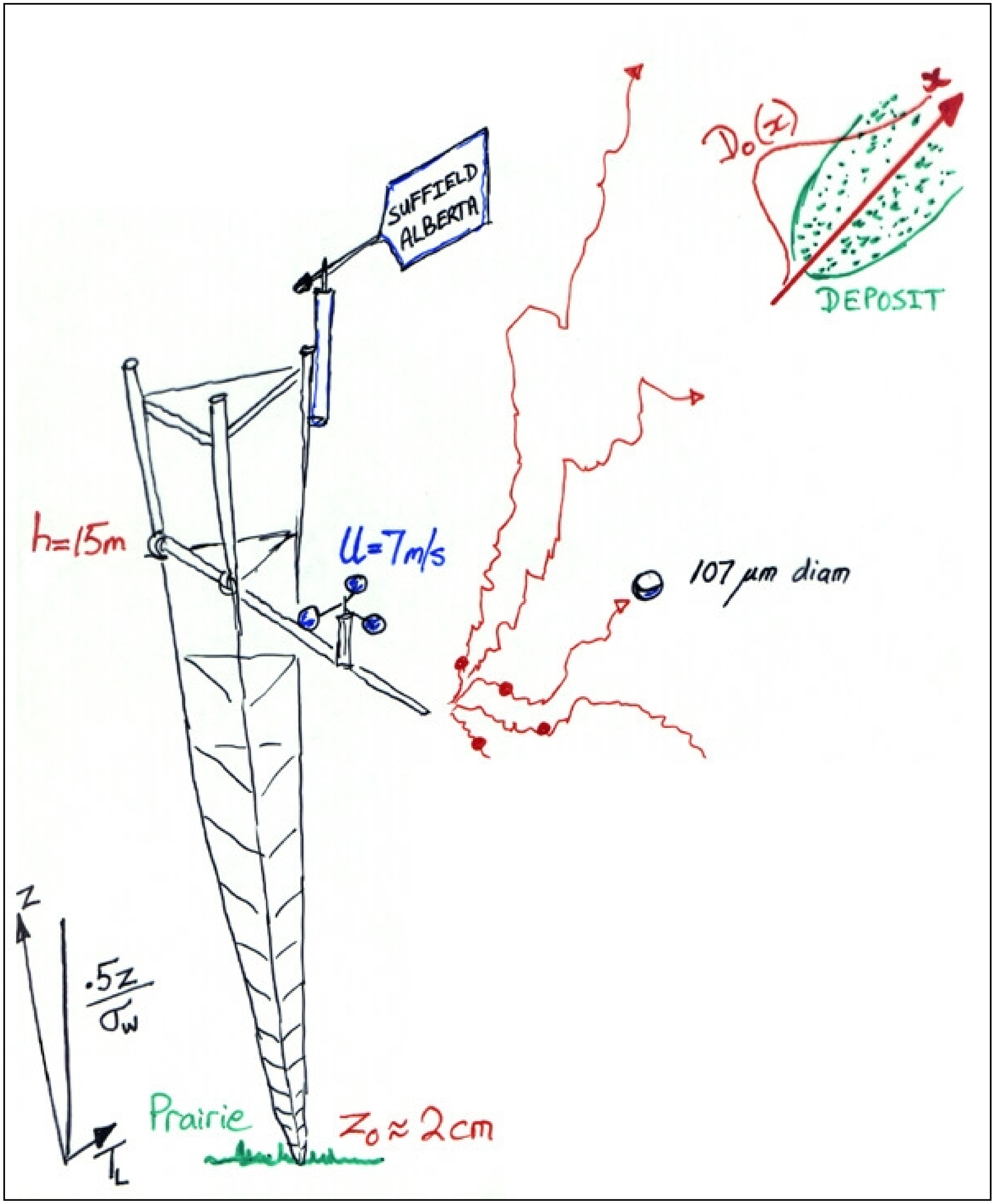


If deposition velocity known, can incorporate in LS model by performing *partial* reflection: a fraction *A* of particles contacting the surface is absorbed, and the complementary fraction *R=1-A* is reflected in the usual way. Wilson et al. (1989, Agric. Forest Meteo. Vol. 47) show *R* relates to w_d as:

$$\frac{1-R}{1+R} = \sqrt{\frac{\pi}{2}} \frac{w_d}{\sigma_w}$$

Heavy particle dispersion

- inertia
- gravitational settling
- deposition on ground
- what is the “well-mixed state”?
- lack rigorous criteria for LS models
- path of a heavy particle is not a fluid trajectory



Heavy particle dispersion

For spherical particles (diam. d) at low slip Reynolds number

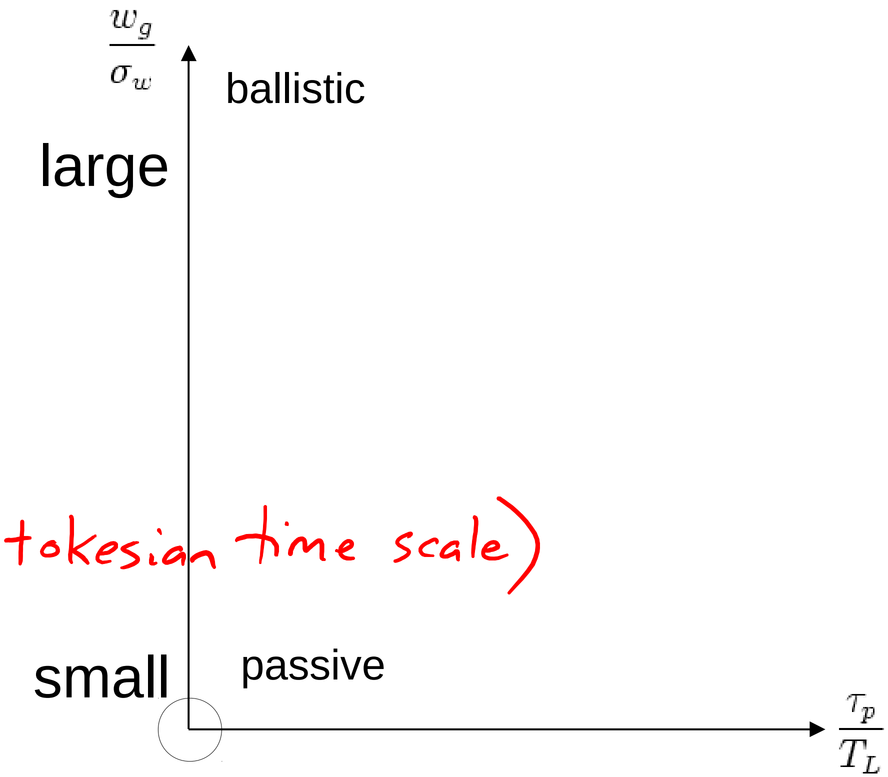
$$R = \frac{|\vec{U}_p - \vec{u}|\ d}{\nu}$$

the eqn of motion is

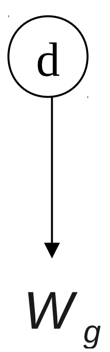
$$\frac{dW_p}{dt} = \frac{w(t) - W_p}{\tau_p} - g$$

inertial time scale (Stokesian time scale)

(drag depends linearly on relative velocity)



At steady state with Eulerian velocity w = const., the terminal velocity is $|W_g| = \tau_p\ g$



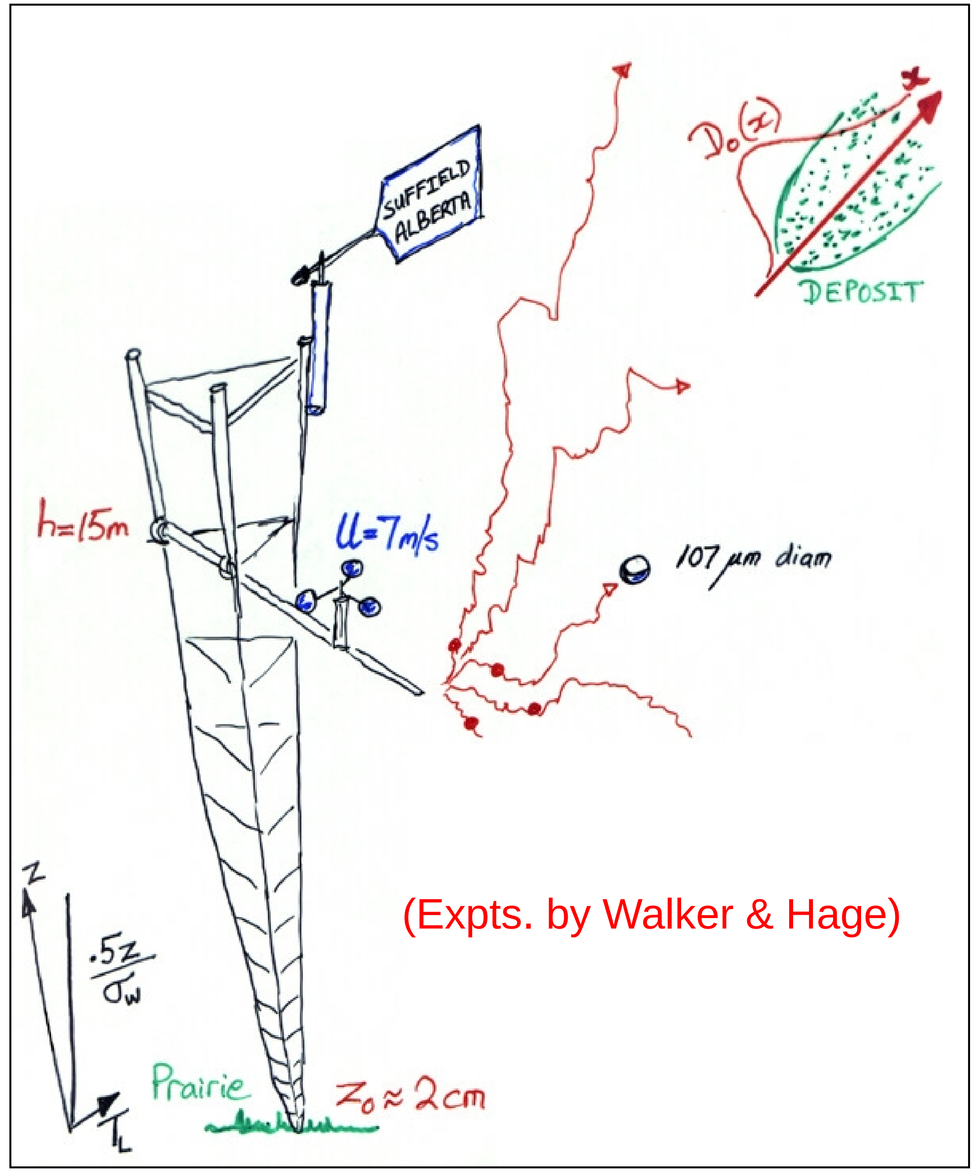
$\mu,\ \rho,\ \rho_p$

What does a dimensional analysis suggest for W_g ?

Stokes' analysis (linearized treatment) $$\frac{\tau_p}{d^2/\nu} = \frac{1}{18}\ \frac{\rho_p}{\rho}$$

Heavy particle dispersion – experiment measured deposition of glass beads

$$d = 107\ \mu\text{m}$$
$$\tau_p = 0.06\ \text{s}$$
$$w_g = 0.6\ \text{m s}^{-1}$$



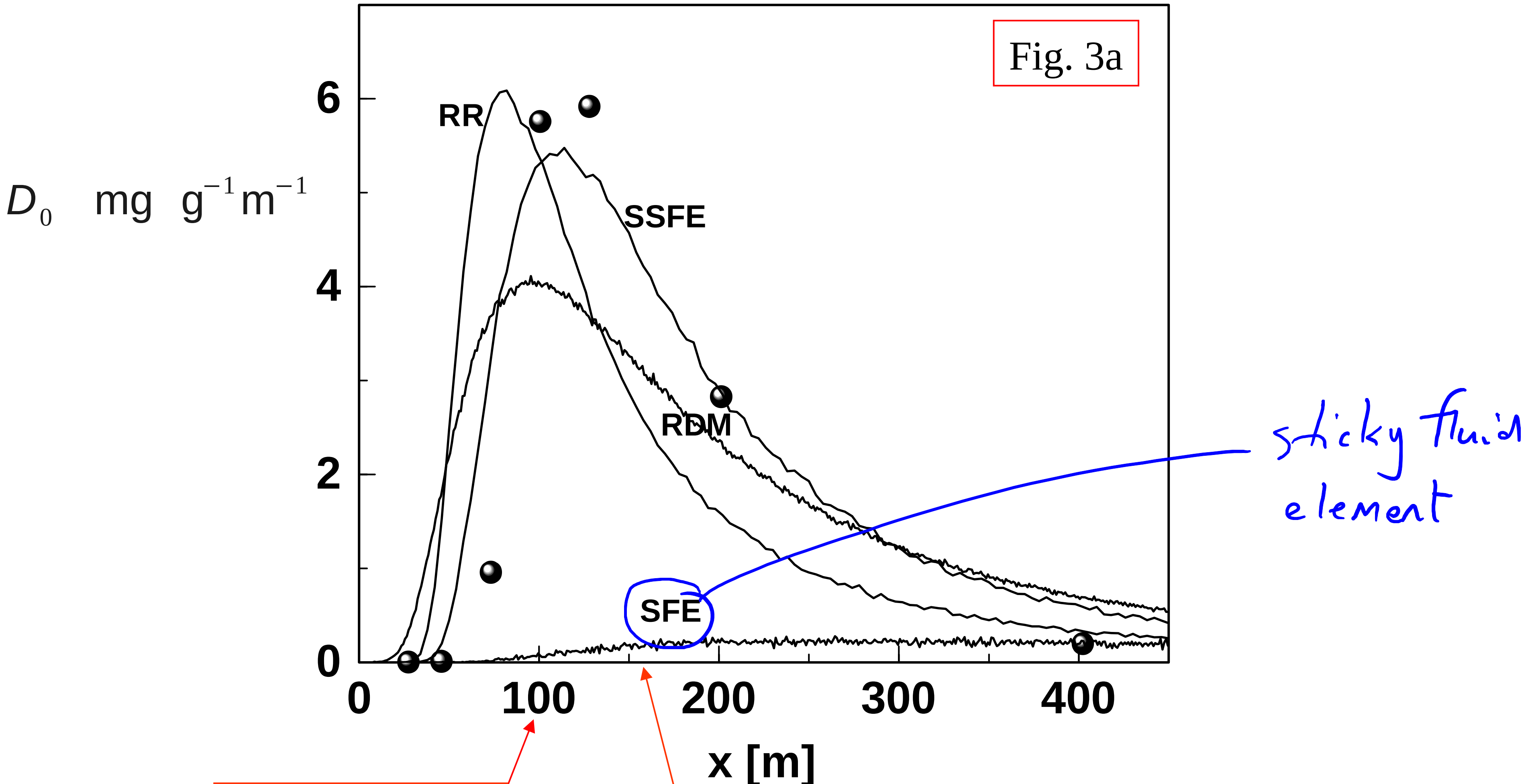
(Expts. by Walker & Hage)

Trajectory Models for Heavy Particles in Atmospheric Turbulence: Comparison with Observations

JOHN D. WILSON

JOURNAL OF APPLIED METEOROLOGY (2000) VOLUME 39

Run C: neutral stratification, L = 341 m. Comparison of obsv. with various models



$$\frac{x}{\overline{u}(h)\, T_L(h)} \approx 1$$

Ballistic impact point x=159 m

$$\mathrm{RR}:\;\; W = \mathrm{const.} = \sigma_w(h)\; r \;-\; w_g,\;\;\; r \in \mathrm{N}(0,1)$$

& $\bar{u}(z)$

$$\mathrm{RDM}:\;\; dZ = \frac{\partial(\sigma_w^2\, T_L)}{\partial z}\, dt + \sqrt{\frac{2\,\sigma_w^2\, dt}{T_L}}\; r \;-\; w_g\, dt,\;\;\; r \in \mathrm{N}(0,1)$$

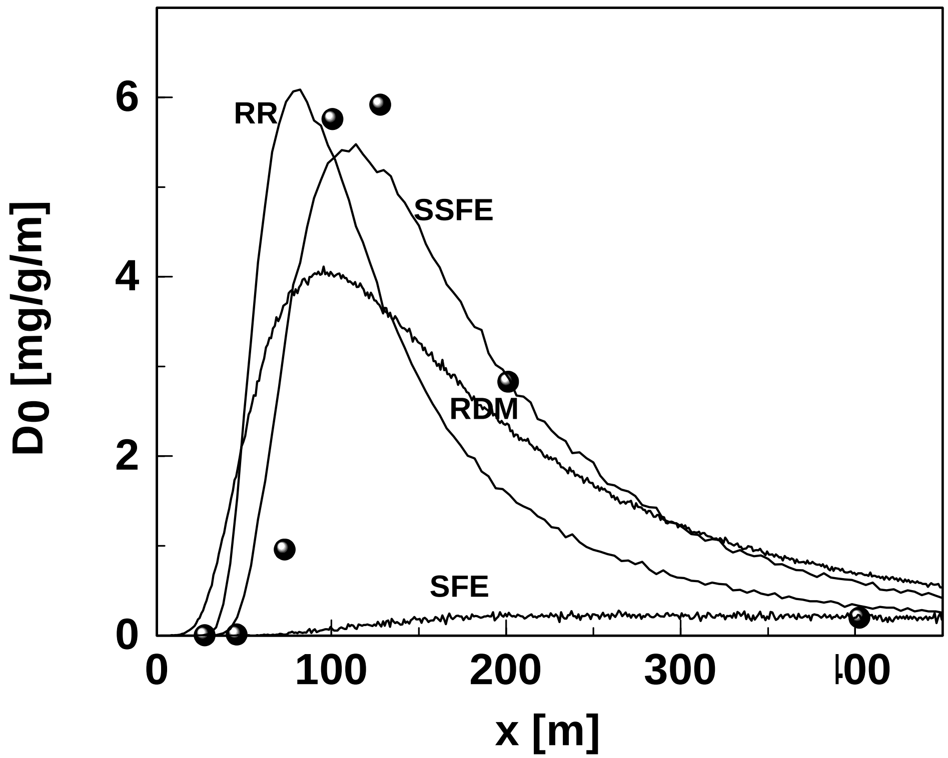
Run C: neutral stratification, L = 341 m. Comparison of obsv. with various models

SSFE ("Settling sticky fluid element" model):

$$
\begin{aligned}
dW &= a\ dt + \sqrt{C_0\ \epsilon}\ d\xi \\
W &= W + dW \\
W_p &= W - w_g \\
dZ_p &= W_p\ dt
\end{aligned}
$$

where $a(W) = -\dfrac{W}{T_L} + \dfrac{1}{2}\dfrac{\partial {\sigma_w}^2}{\partial z}\left(\dfrac{W^2}{{\sigma_w}^2} + 1\right)$

and $T_L = \dfrac{2{\sigma_w}^2(z)}{C_0\ \epsilon(z)}$



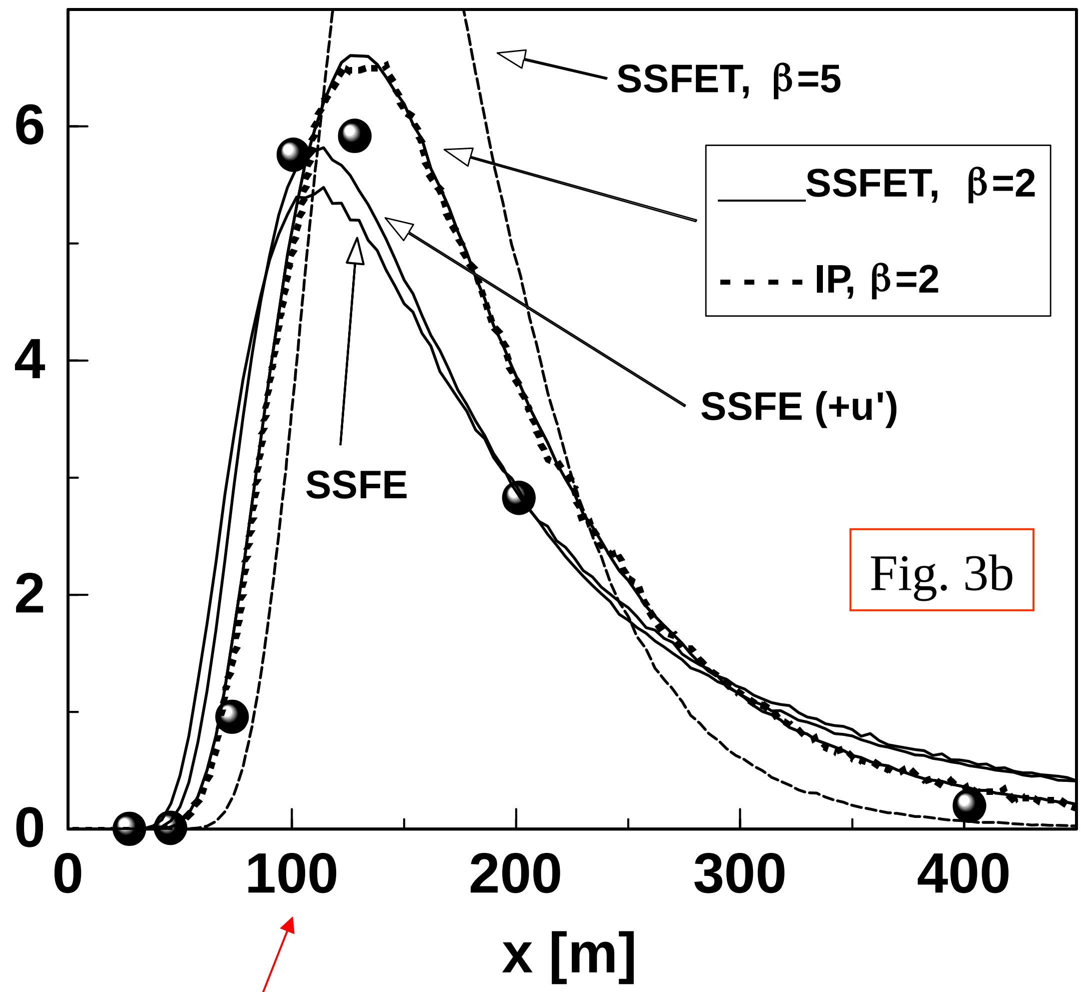
(a as for unique 1-D model for Gaussian inhomogeneous turbulence).

SSFET ("Settling sticky fluid element, reduced T" model):

Replace T_L in the above by T_p, a reduced timescale for the fluid velocity along the particle's path – this accounts empirically for the "crossing trajectories effect"

$$T_p = \frac{T_L}{\sqrt{1 + (\beta\ w_g / \sigma_w)^2}}$$

Run C: neutral stratification, L = 341 m



$$\frac{x}{\overline{u}(h)\, T_L(h)} \approx 1$$

Neither an Eulerian nor a Lagrangian sequence. Computed using Thomson's well-mixed 1st – order model, with timescale reduced relative to T_L

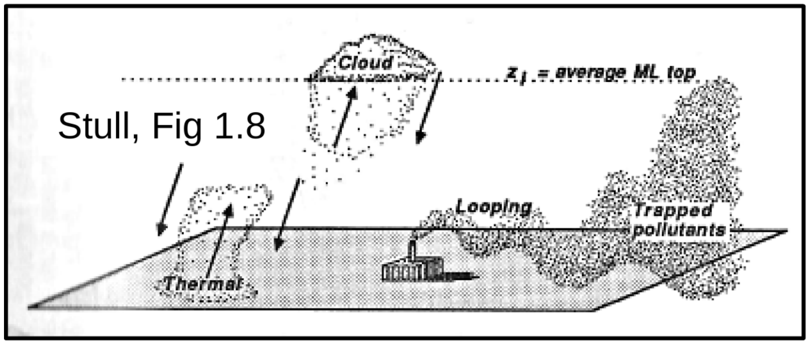
contrast with "IP" model

IP:

$$\frac{dW_p}{dt} = \frac{w(\mathbf{X}(t)) - W_p}{\tau_p} - g$$

$$dZ = W_p\, dt$$

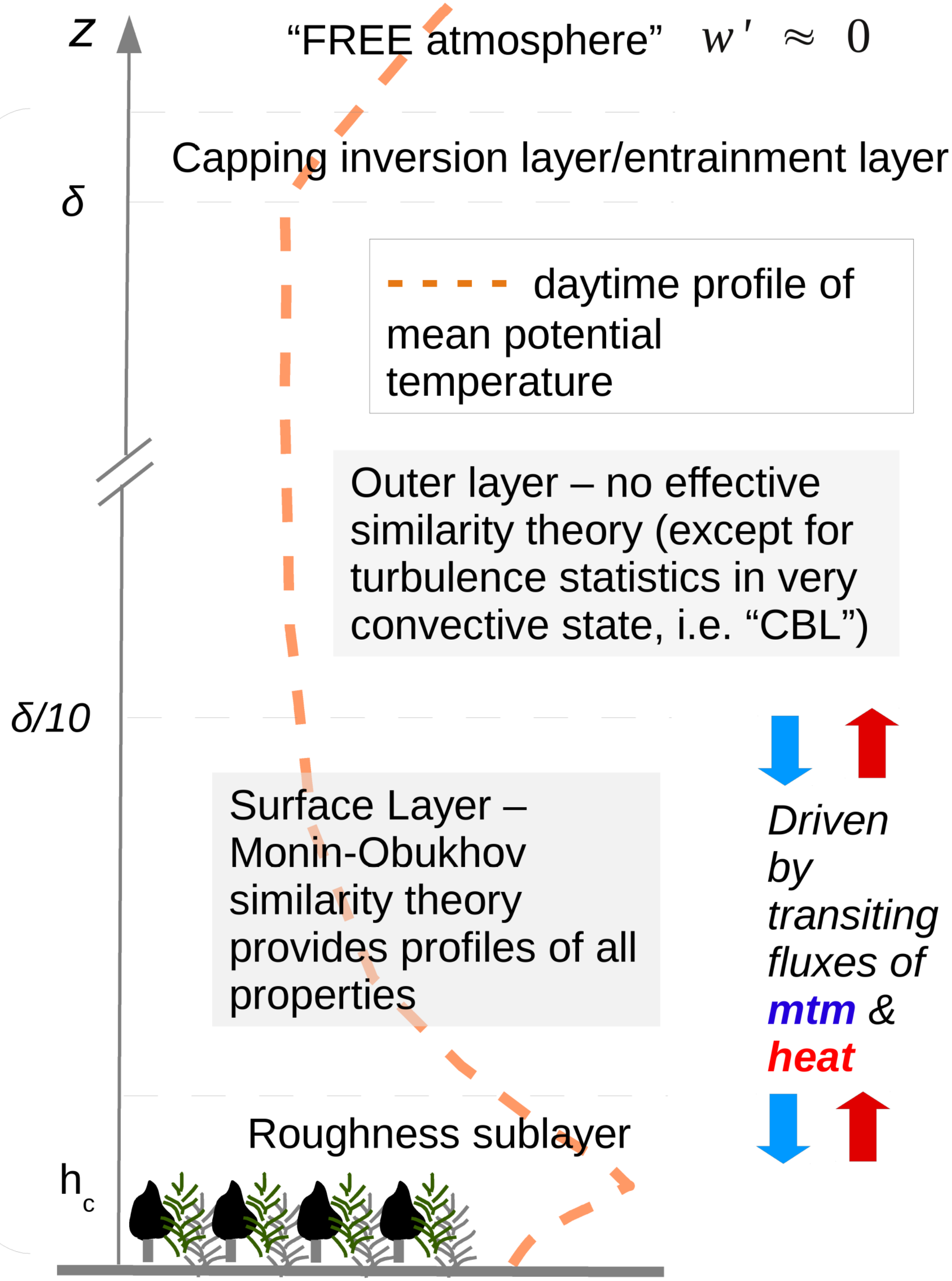
Modelling dispersion in the Convective Boundary Layer – non-Gaussian turbulence



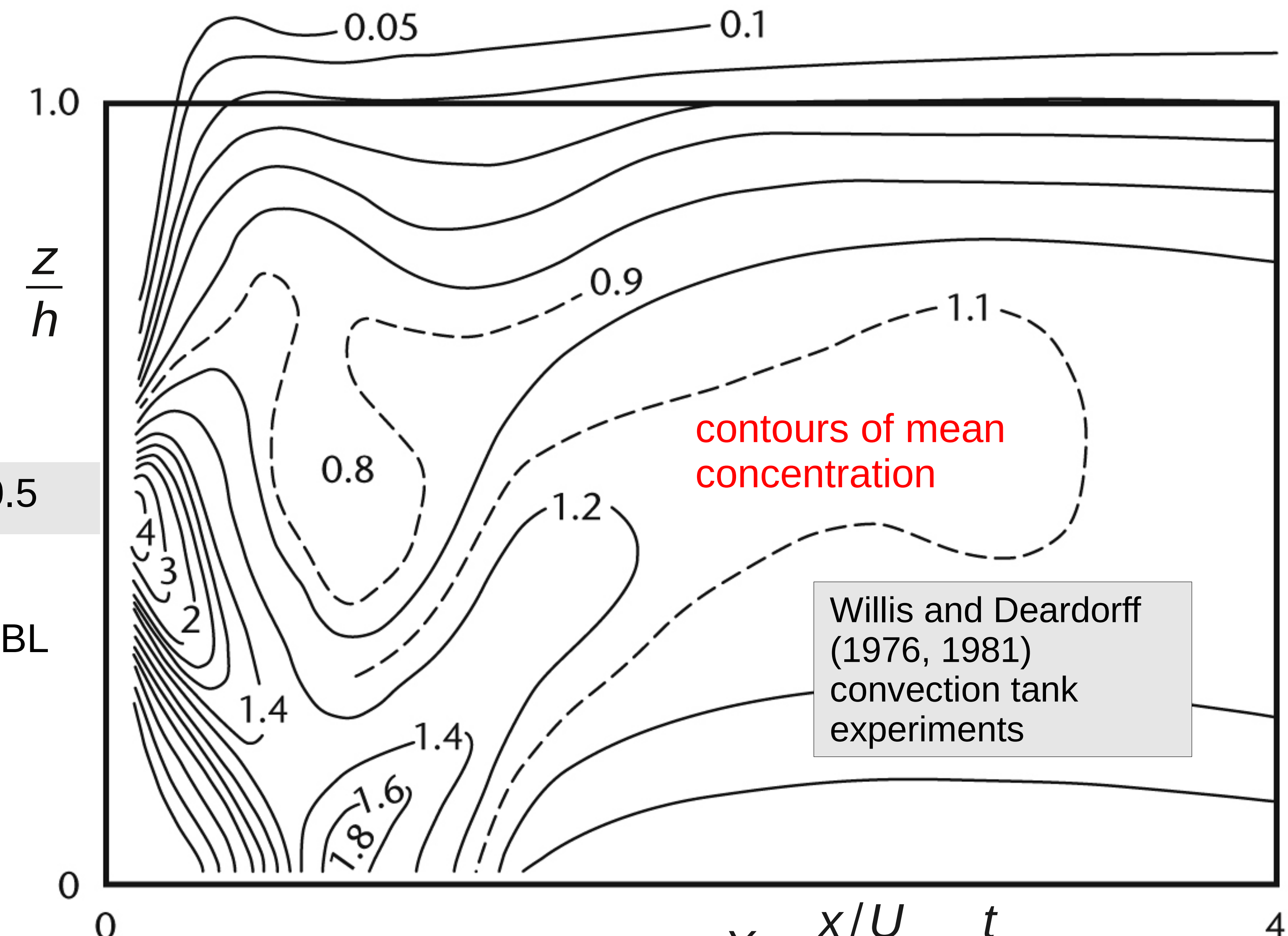
Atmospheric boundary layer
(Friction layer)

Unresolved (“turbulent”) velocity fluctuations

$$u' \approx v' \approx w' = \mathrm{O}[\mathrm{m\ s^{-1}}]$$



• a peculiarity of observed dispersion in the CBL, that Gaussian plume models cannot easily represent, is that the (time-average) plume centreline from an elevated continuous point source initially descends towards ground (with increasing downwind distance), then ascends



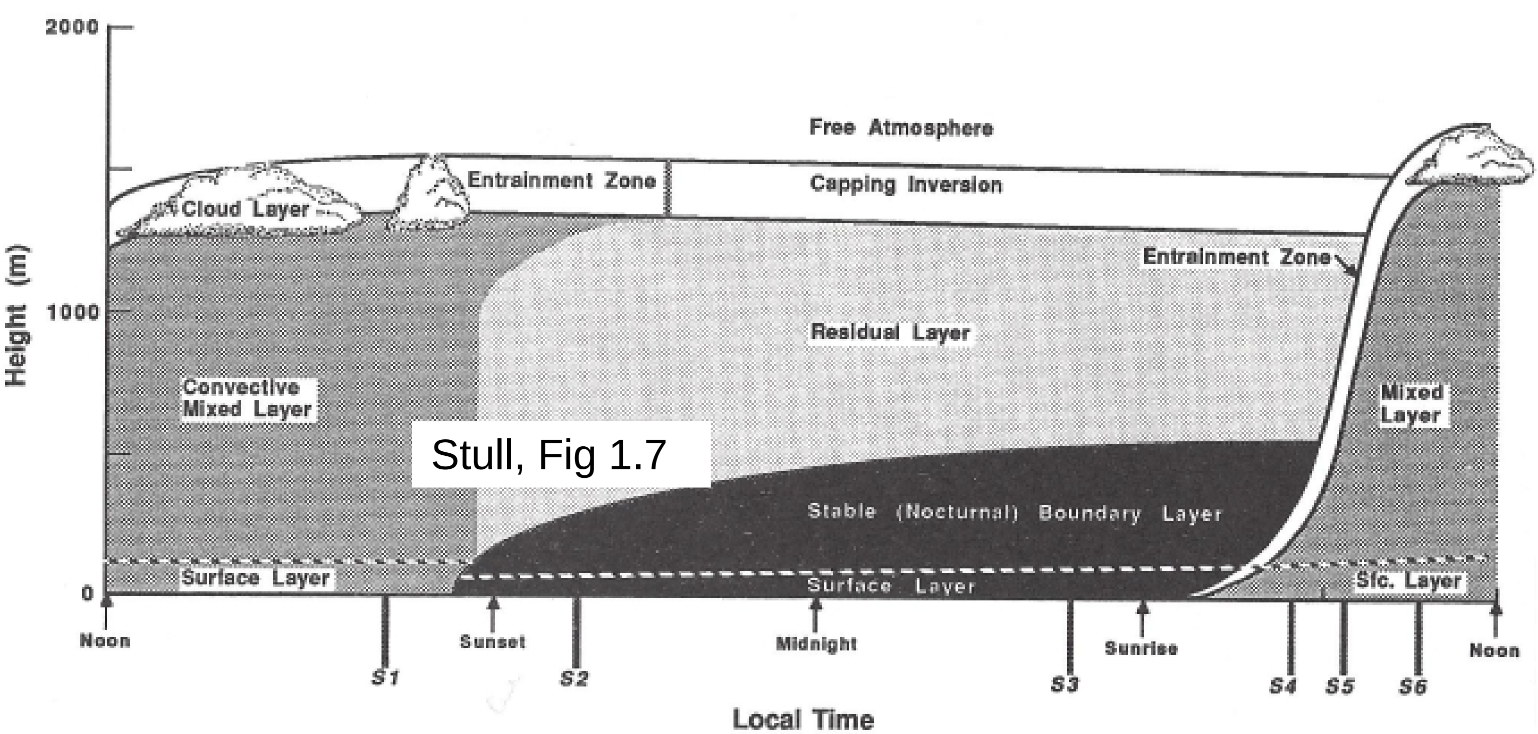
$z_s/h = 0.5$

Willis and Deardorff (1976, 1981) convection tank experiments

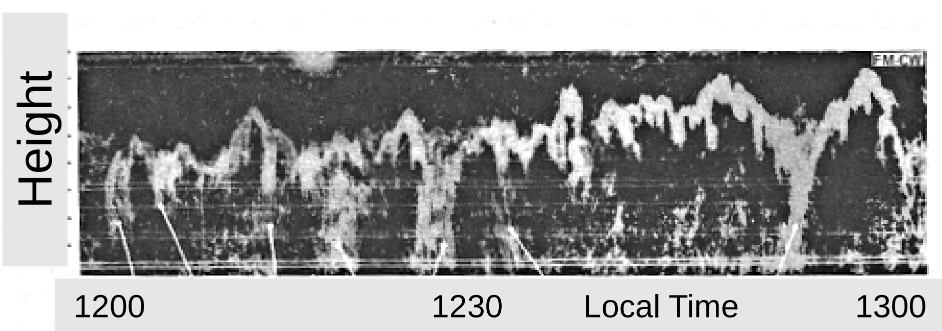
$$X = \frac{x/U}{h/w_*} = \frac{t}{T_L}$$

- *h* (or z_i or *δ*), ABL depth
- *U*, horiz. wind speed
- *w**, convective velocity scale

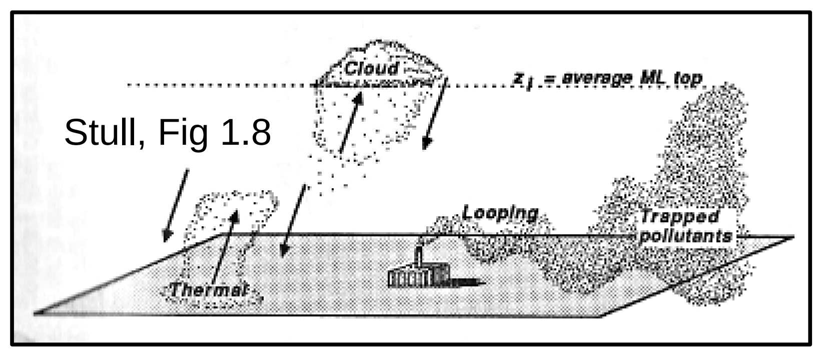
Time evolution of the ABL



Stull, Fig 1.7

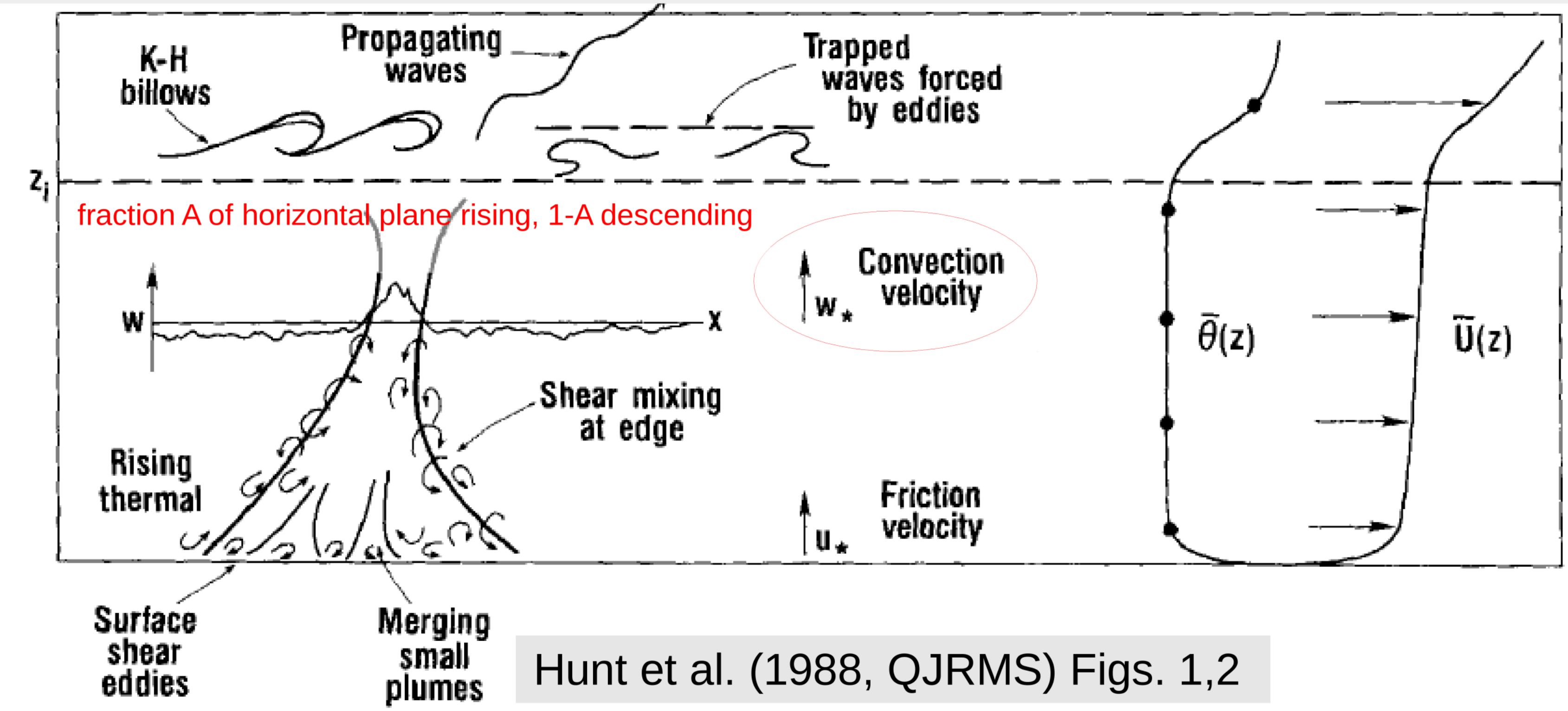


Garratt, Fig 6.4



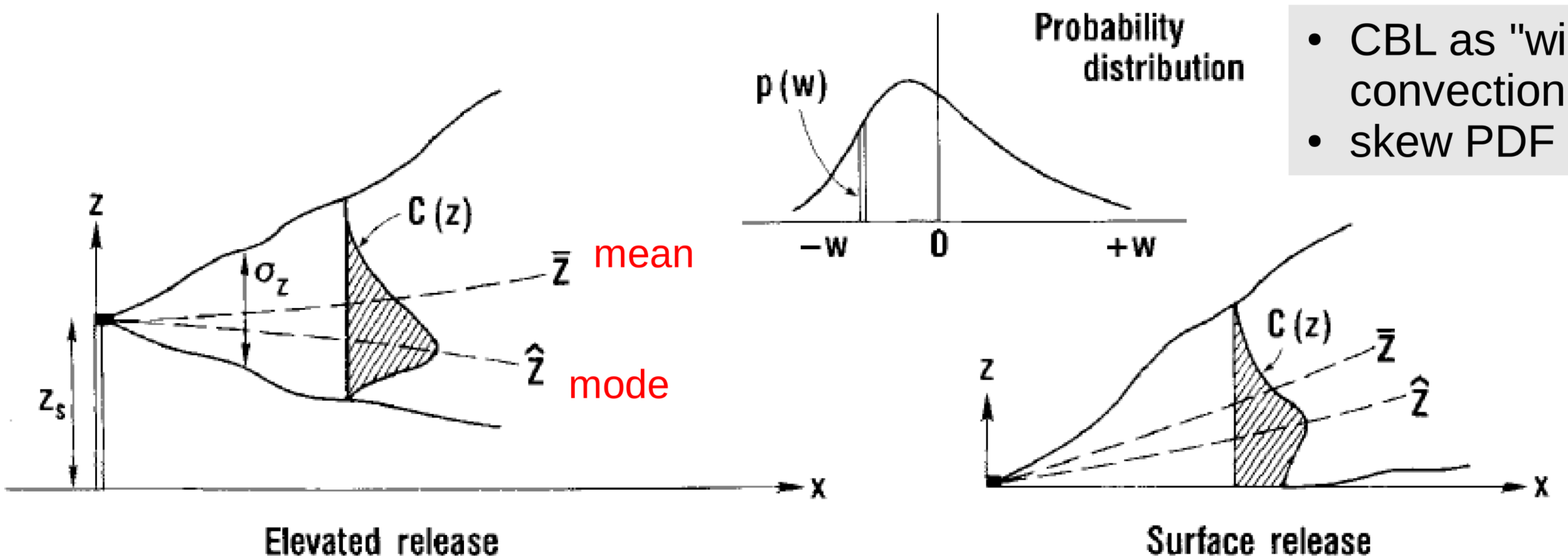
Stull, Fig 1.8

Qualitative properties of the CBL



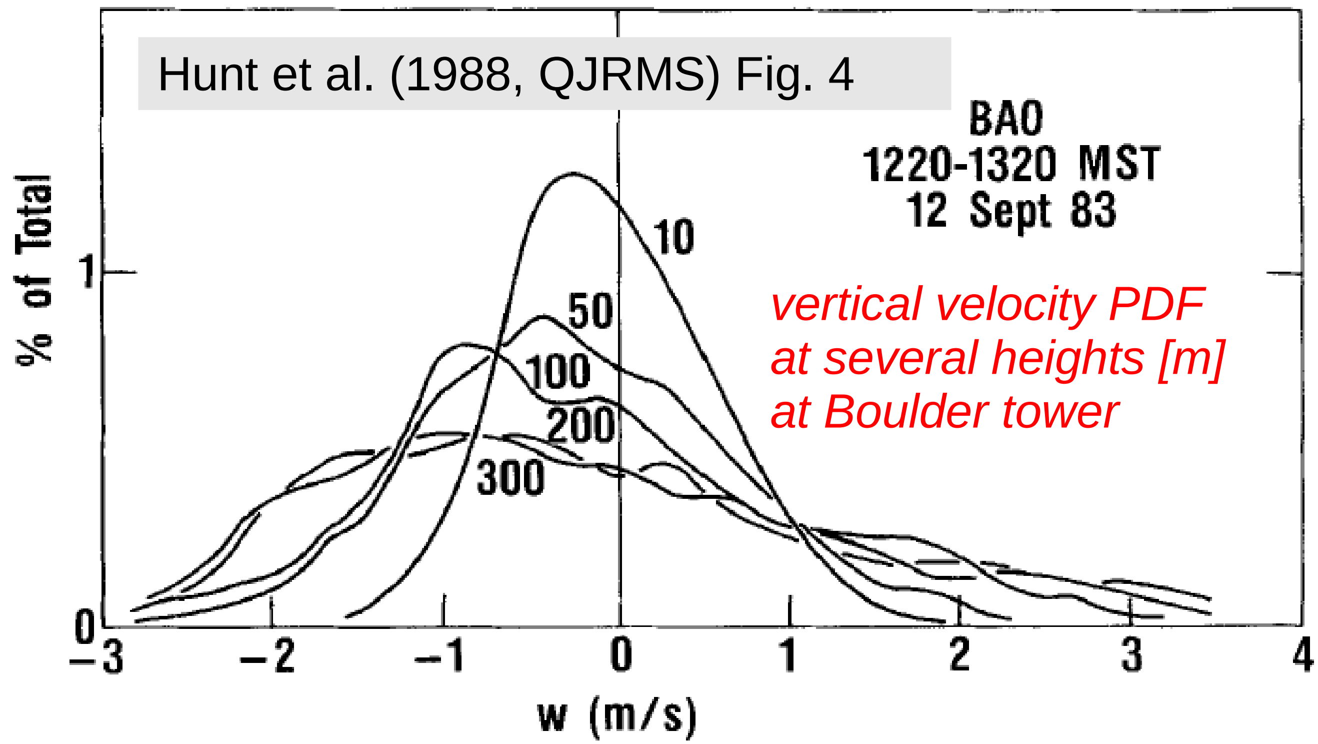
Hunt et al. (1988, QJRMS) Figs. 1,2

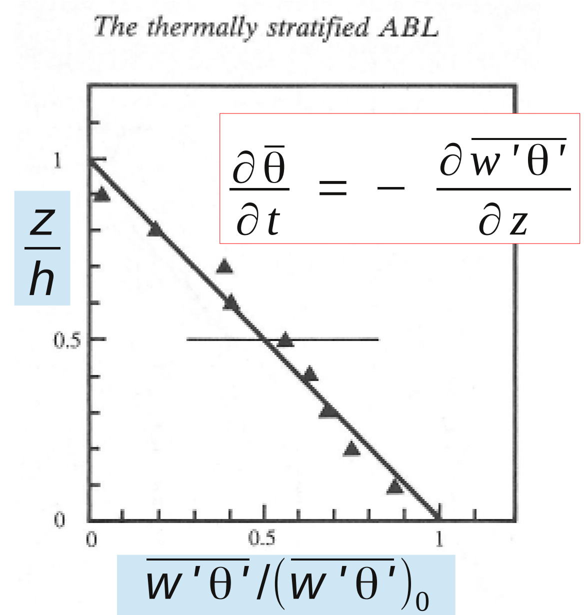
Figure 1. Schematic diagram of the flow, temperature and eddy structure of the convective boundary layer.



- CBL as "windless convection layer"
- skew PDF of *w*

CBL velocity statistics & mixed layer similarity theory



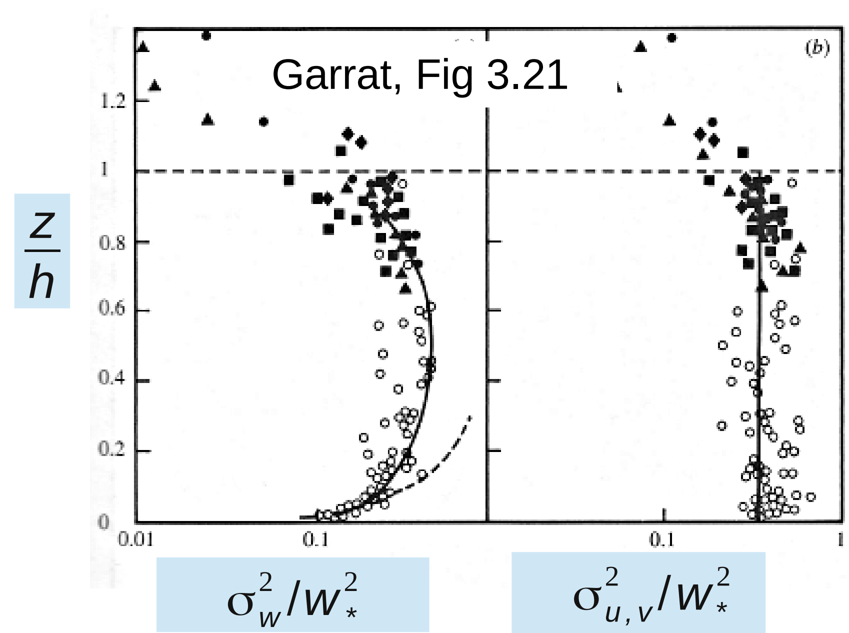


Garratt, Fig 6.13

Mixed-layer turbulence scales: *δ, w*, θ**

$$w_* = \left[\frac{g}{\theta_0} \, \delta \, \left(\overline{w'\theta'}\right)_0 \right]^{1/3}$$

$$\theta_* = -\left(\overline{w'\theta'}\right)_0 / w_*$$



Dispersion in the CBL – well-mixed Lagrangian stochastic model

• ignore specifics of thermals; consider ABL horiz. homog; then, the vertical velocity PDF is skewed (as shown earlier). Ignore the shear in horiz. velocity (constant advection veloc. *U*)

• fractional area (*A*) of "updrafts" (wherein mean velocity is upward, but instantaneous velocity need not be) and complementary fractional area (*B=1-A*), considered the (predominantly) subsiding environmental region. Obsv. give *A* ~ 0.2 – 0.4

• choose a suitable representation of the vertical velocity PDF, e.g.

$$g_a(w;z) = A(z)\, P_A(w;z) + [1 - A(z)]\, P_B(w;z)$$

(Luhar & Britter, 1989, Atmos. Env. Vol. 23) where P_A, P_B are Gaussians (whose moments vary with *z*)... may or may not require *A*=*A*(*z*)

• setting aside the details of "fitting" the parameters of the PDF's, the form of the model is (again)

$$dW = a(Z, W)\, dt + \sqrt{C_0\, \epsilon(z)}\;\; d\xi$$

• applying the well-mixed condition gives $$a = -\frac{\sigma_w^2(Z)}{\tau(Z)}\;\frac{Q(W)}{g_a(W;Z)} + \frac{\phi(W)}{g_a(Z;W)}$$

First “well-mixed” Lagrangian stochastic model for the CBL

Atmospheric Environment Vol. 23, No. 9, pp. 1911–1924, 1989.
Printed in Great Britain.
0004-698
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A RANDOM WALK MODEL FOR DISPERSION IN INHOMOGENEOUS TURBULENCE IN A CONVECTIVE BOUNDARY LAYER

ASHOK K. LUHAR and REX E. BRITTER

δ = CBL depth
*W** = CBL veloc., scale

$$w_* = \left[\frac{g}{T_0} \left(\overline{w'T'} \right)_0 \delta \right]^{1/3}$$

$$Q(W) = \frac{A}{\sigma_{wA}^2} (W - \overline{w}_A)\, P_A(W) + \frac{1-A}{\sigma_{wB}^2} (W + \overline{w}_B)\, P_B(W)$$

$$\begin{aligned}
\phi(W) = & -\frac{1}{2} \left(A \frac{\partial \overline{w}_A}{\partial z} + \overline{w}_A \frac{\partial A}{\partial z} \right) erf\left(\frac{W - \overline{w}_A}{\sqrt{2}\, \sigma_{wA}} \right) \\
& + \frac{1}{2} \left(B \frac{\partial \overline{w}_B}{\partial z} + \overline{w}_B \frac{\partial B}{\partial z} \right) erf\left(\frac{W + \overline{w}_B}{\sqrt{2}\, \sigma_{wB}} \right) \\
& + \left[\frac{A}{2} \frac{\partial \sigma_{wA}^2}{\partial z} \left(\frac{W^2}{\sigma_{wA}^2} + 1 \right) + \sigma_{wA}^2 \frac{\partial A}{\partial z} \right] P_A(W) \\
& + \left[\frac{B}{2} \frac{\partial \sigma_{wB}^2}{\partial z} \left(\frac{W^2}{\sigma_{wB}^2} + 1 \right) + \sigma_{wB}^2 \frac{\partial B}{\partial z} \right] P_B(W)
\end{aligned}$$

Mean horiz. wind in CBL sometimes treated as const. *U* – a "shearless convection layer"

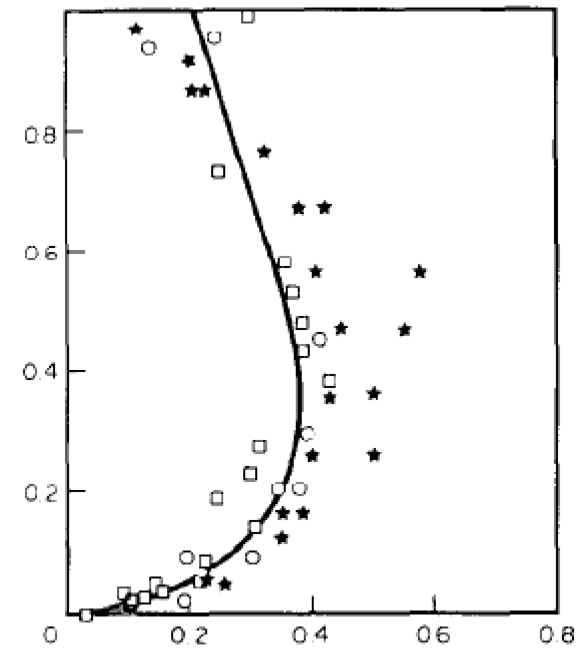
The moments $\overline{w}_A(z),\ \sigma_{wA}(z)\ldots$ of the component Gaussians vary with height and are related to suitable empirical profiles of $\overline{w'^2},\ \overline{w'^3},\ \overline{w'^4}$ for the CBL

First "well-mixed" Lagrangian stochastic model for the CBL

Atmospheric Environment Vol. 23, No. 9, pp. 1911–1924, 1989.
Printed in Great Britain.

A RANDOM WALK MODEL FOR DISPERSION IN INHOMOGENEOUS TURBULENCE IN A CONVECTIVE BOUNDARY LAYER

Ashok K. Luhar and Rex E. Britter



- L&B fitted empirical curves to observations:

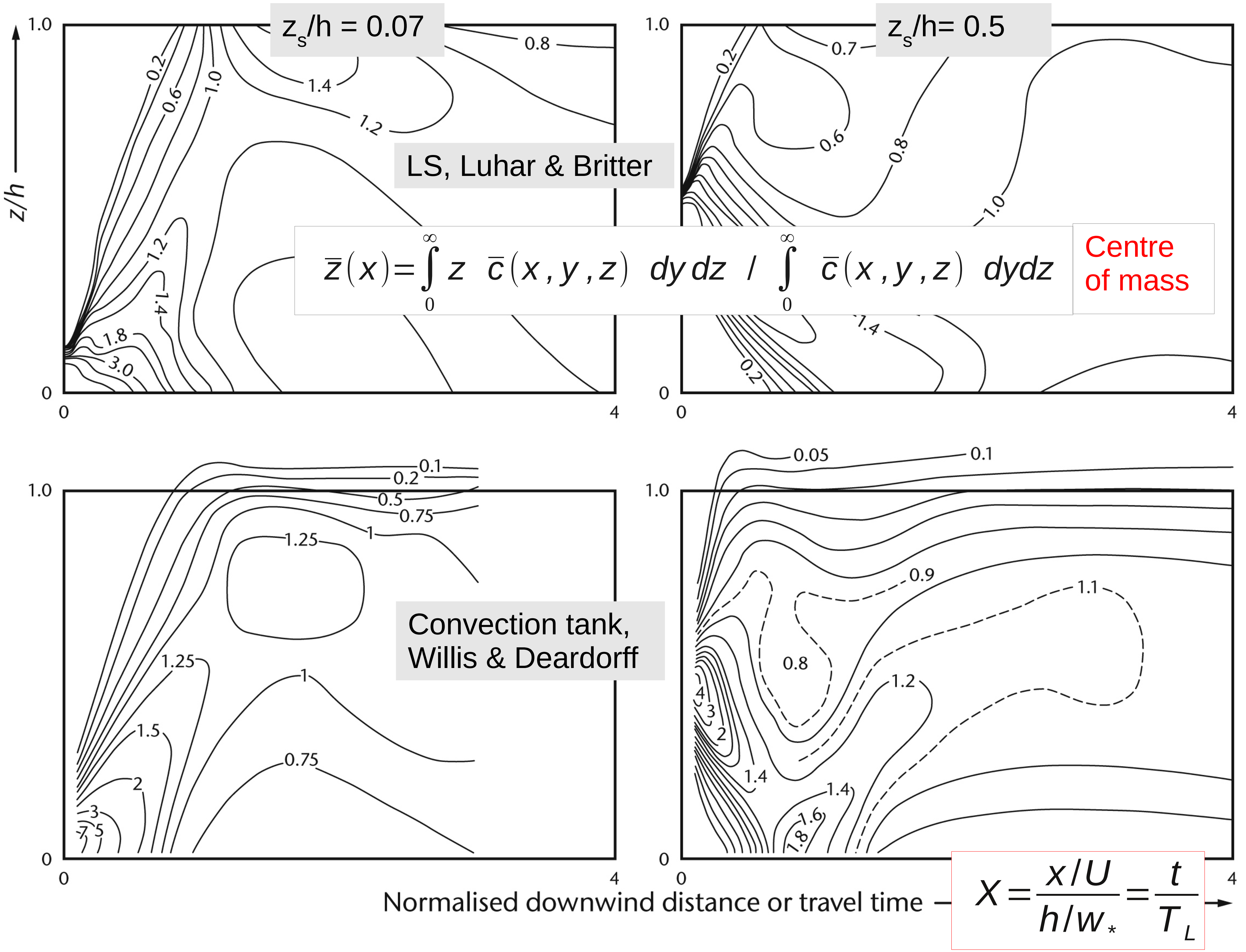
$$\frac{\sigma_w^2(Z)}{w_*^2} = 1.1 \left(\frac{Z}{\delta}\right)^{2/3} \left(1-\frac{Z}{\delta}\right)^{2/3} \left[1-4\frac{(Z/\delta-0.3)}{(2+|Z/\delta-0.3|)^2}\right]$$

$$\frac{\overline{w'^3}}{w_*^3} = 0.8 \left(\frac{\sigma_w^2}{w_*^2}\right)^{3/2}$$

$$\frac{w_*\tau(Z)}{\delta} = \left[1.5-1.2\left(\frac{Z}{\delta}\right)^{1/3}\right]^{-1} \frac{\sigma_w^2(Z)}{w_*^2}$$

$$\frac{\delta\,\epsilon(Z)}{w_*^3} = \left[1.5-1.2\left(\frac{Z}{\delta}\right)^{1/3}\right]$$

Note: these profiles do not resolve an ASL



$$\bar{z}(x) = \int_0^\infty z \; \bar{c}(x,y,z) \; dy\,dz \;\; / \int_0^\infty \bar{c}(x,y,z) \; dy\,dz$$

Centre of mass

$$X = \frac{x/U}{h/w_*} = \frac{t}{T_L}$$

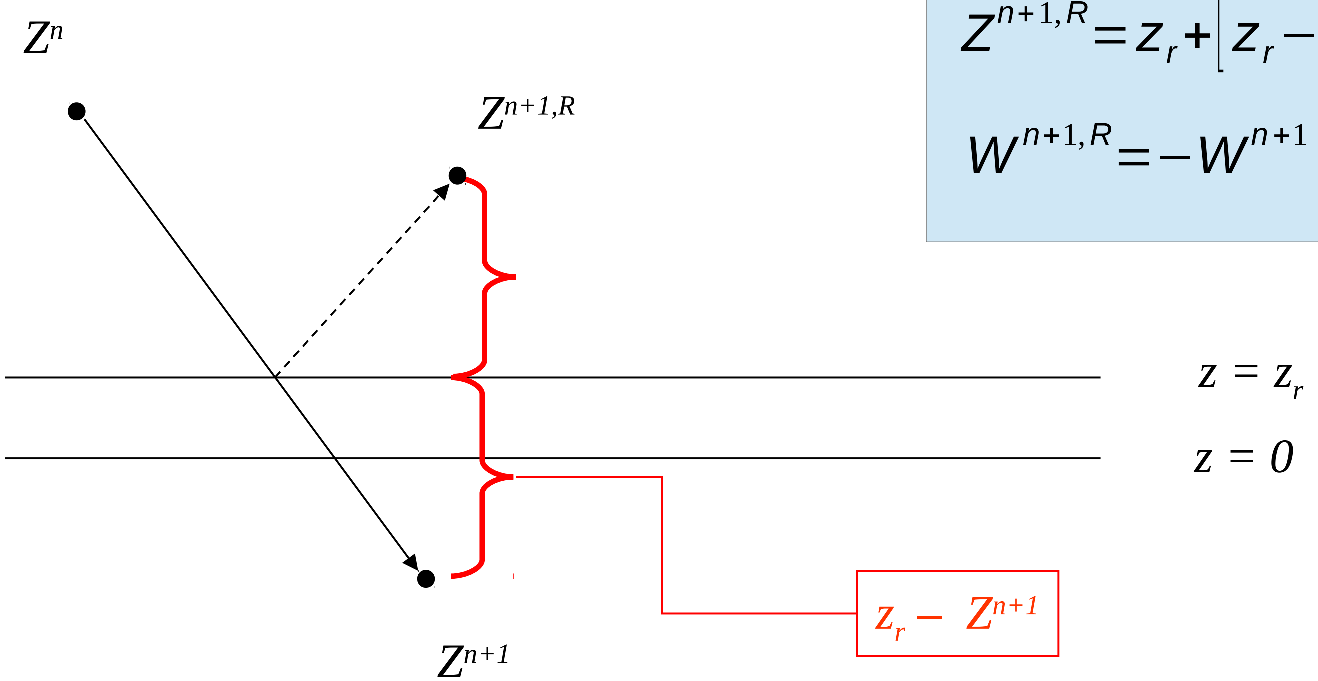
Reflection of trajectories in LS models

- a reflection algorithm tacked to a well-mixed LS model can cause violation of the w.m.c. (e.g. Wilson & Flesch, 1993, “Flow boundaries in random flight dispersion models: enforcing the well-mixed condition," J. Appl. Meteorol. 32, 1695-1707)

- however “perfect reflection” (“smooth wall reflection”) at an artificial boundary (reflection height z_r) is acceptable in Gaussian turbulence provided $\partial \sigma_w / \partial z \rightarrow 0$ as $z \rightarrow z_r$

$$Z^{n+1,R} = z_r + \left[z_r - Z^{n+1} \right]$$

$$W^{n+1,R} = -W^{n+1}$$



- in practice acceptable to set z_r much larger than z_0 to reduce computation time
- if simulating whole ABL may need reflection at $z = \delta$ as well

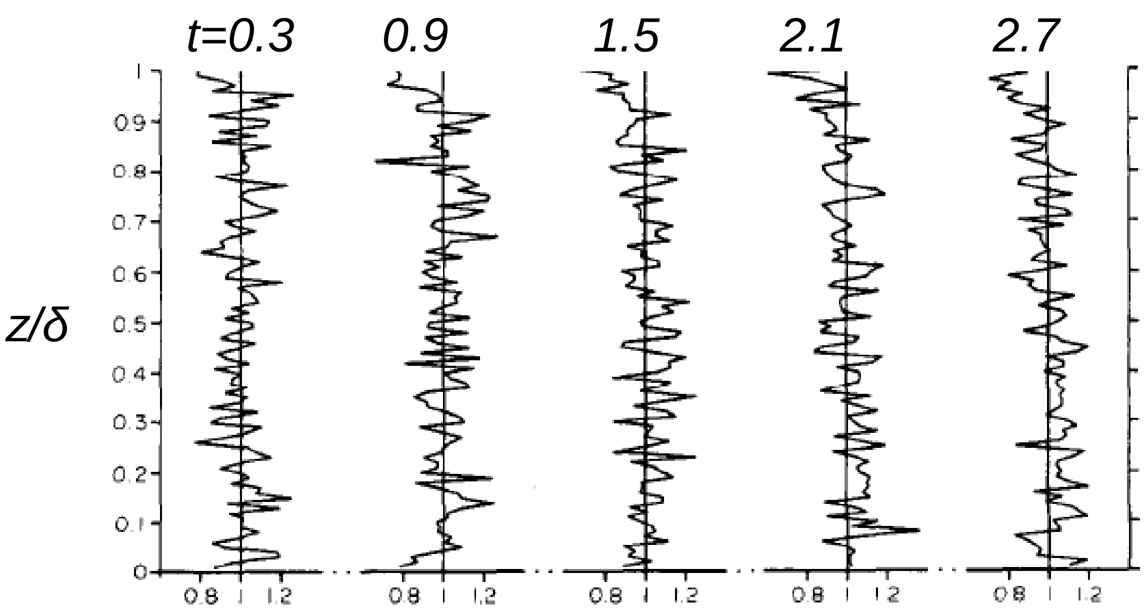
How to judge if reflection is problematic?

Compute the evolution of an initially well mixed particle distribution… e.g. release N_P particles, with the initial height chosen $Z^0 \in U\left[z_r,\, \delta\right]$ which implies $p(z,0) = \dfrac{1}{\delta - z_r}$

MONTE CARLO SIMULATION OF PLUME DISPERSION IN THE CONVECTIVE BOUNDARY LAYER

J. HØGNI BÆRENTSEN* and RUWIM BERKOWICZ

Atmospheric Environment Vol. 18, No. 4, pp. 701–712, 1984
Printed in Great Britain.



This work done prior to Thomson's (1987) well-mixed condition

Fig. 4. Distribution of particles after different travel times as simulated by the Monte Carlo model. The source is distributed uniformly through the whole boundary layer. 10,000 particles were used in the simulation.

Using an LS model to compute the concentration field due to a gas source in urban winds

QUARTERLY JOURNAL OF THE ROYAL METEOROLOGICAL SOCIETY
Q. J. R. Meteorol. Soc. 135: 1586–1602 (2009)
Published online 28 July 2009 in Wiley InterScience
(www.interscience.wiley.com) DOI: 10.1002/qj.452

RMetS
Royal Meteorological Society

Lagrangian simulation of wind transport in the urban environment

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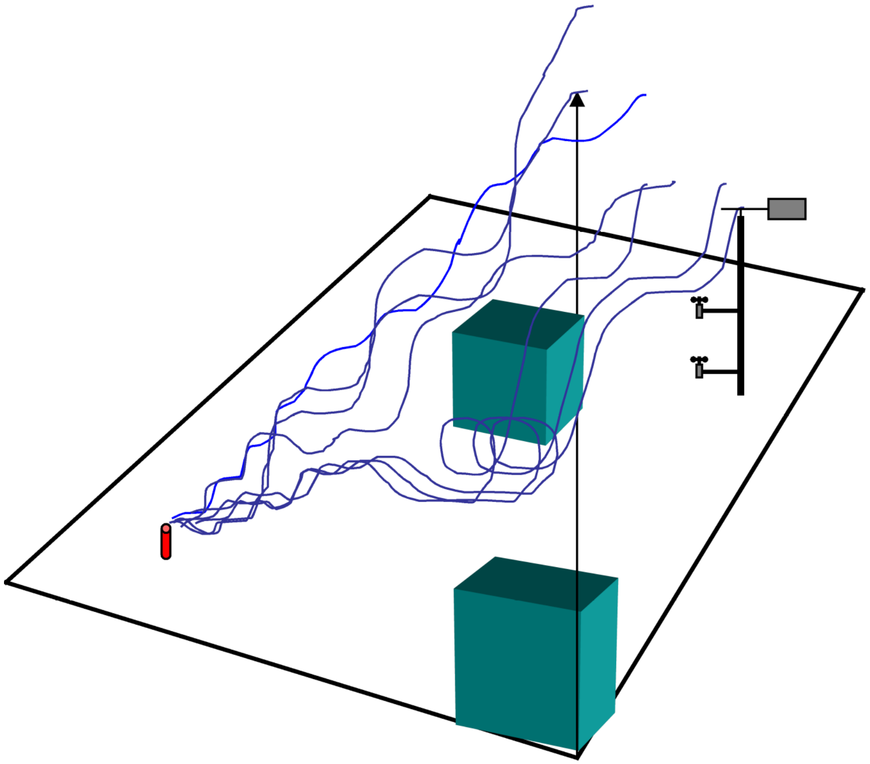
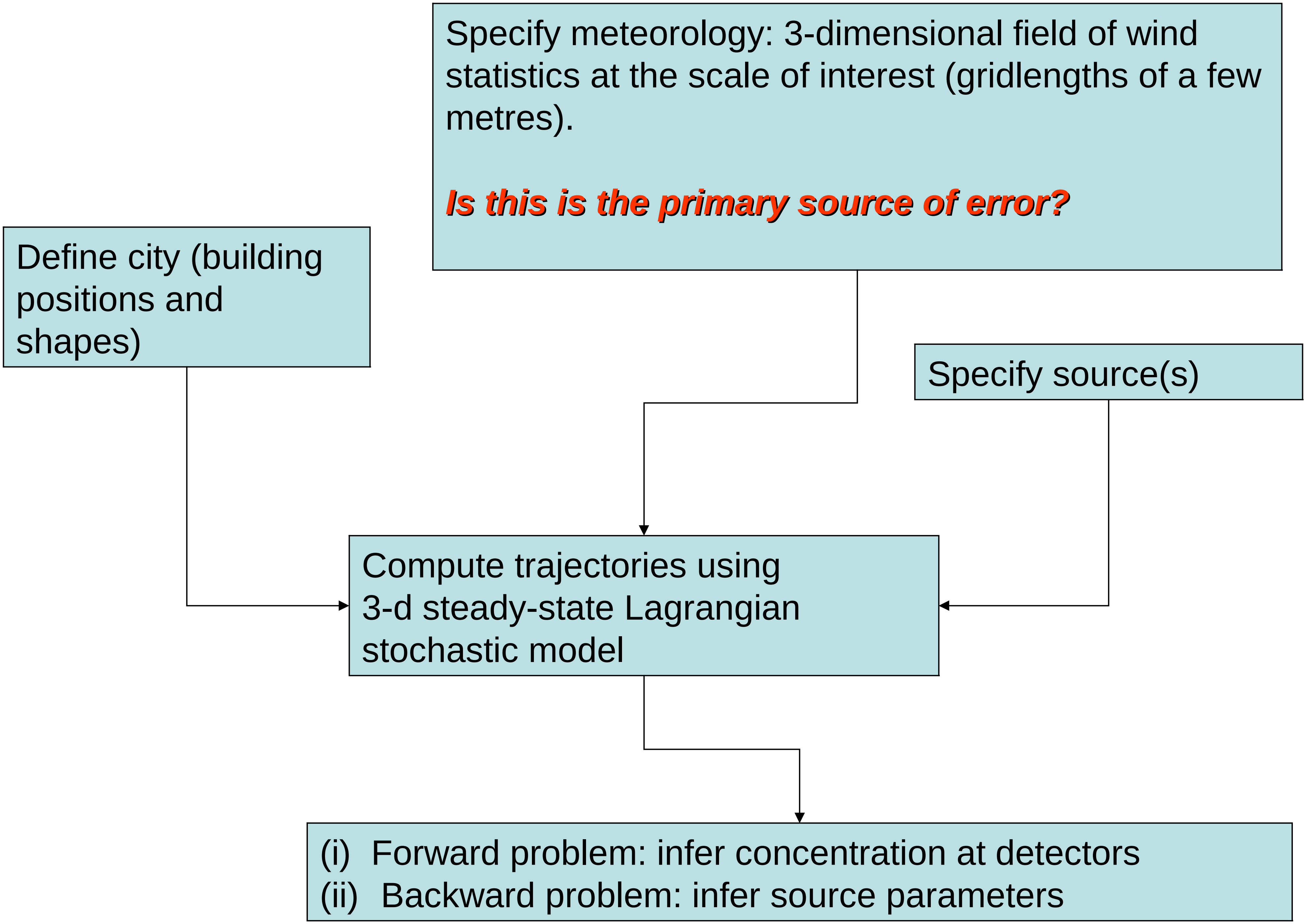
[a]*Department of Earth and Atmospheric Sciences, University of Alberta, Edmonton, Alberta, Canada*
[b]*Defence R&D Canada–Suffield, Medicine Hat, Alberta, Canada*
[c]*Canadian Meteorological Centre, Dorval, Quebec, Canada*



- a three-dimensional LS model for fully-inhomogeneous Gaussian turbulence, "driven" by another model providing the needed velocity statistics

Salient property of wind in a city: short term (order one hour) wind statistics in a city are ***extremely*** inhomogeneous on all three axes

Using an LS model to compute the concentration field due to a gas source in urban winds



Using an LS model to compute the concentration field due to a gas source in urban winds

High resolution weather analysis/prediction: “Urban GEM-LAM”

Provides upwind and upper boundary conditions

Building-resolving *k*-ε turbulence model: “**urbanSTREAM**” (steady state, no thermodynamic equation, control volumes congruent with walls)

Provides computational mesh over flow domain and gridded fields of needed Eulerian velocity statistics:

$$\overline{u_j}\ ,\ \overline{u_i'u_j'}\ ,\ \partial\overline{u_i'u_j'}/\partial x_k\ ,\ \varepsilon$$

Lagrangian stochastic model “**urbanLS**” to compute ensemble of paths from source(s)

Adopt D.J. Thomson's 3D well-mixed LS trajectory model for Gaussian turbulence

- assumes probability density function for velocity is Gaussian
- given the Eulerian velocity statistics $\bar{u}_i\ ,\ R_{ij} \equiv \overline{u_i' u_j'}\ ,\ \epsilon$ ⇒ coefficients (***T*** 's) determining paths

$$dU_i = a_i\ dt + \sqrt{C_0\ \epsilon}\ d\zeta$$

(*dζ* is a standardized Gaussian random variate: mean is zero, variance is *dt*)

$$a_i = \frac{1}{2}\frac{\partial R_{il}}{\partial x_l} - \frac{1}{2} C_0\ \epsilon\ R_{ij}^{-1}\ U_j + \frac{1}{2} R_{lj}^{-1}\ \frac{\partial R_{il}}{\partial x_k}\left(U_j\ \ \bar{u}_k + U_j\ U_k\right)$$

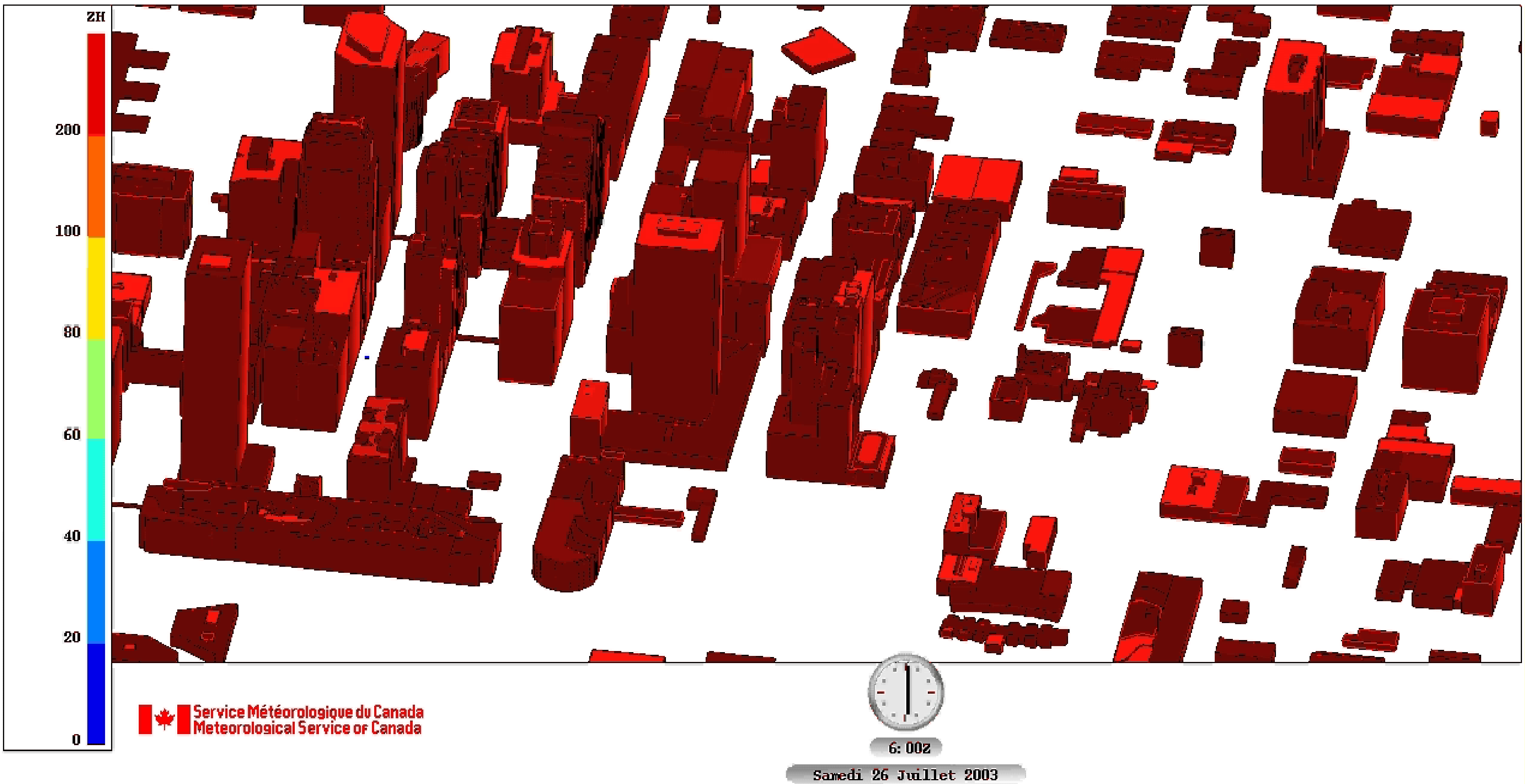
$$= T_i^0 + T_{ij}^1 U_j + T_{ijk}^2 U_j\ U_k$$

The ***T*** matrices are computed and stored on the grid prior to computing the ensemble of paths. At each timestep, use ***T*** 's from gridpoint closest to particle (ie. no interpolation to particle position). Note that the cond'tl mean accel'n in Thomson's model comprises a constant term, a term linear in the velocity fluctuation, and a term quadratic in the velocity fluctuation

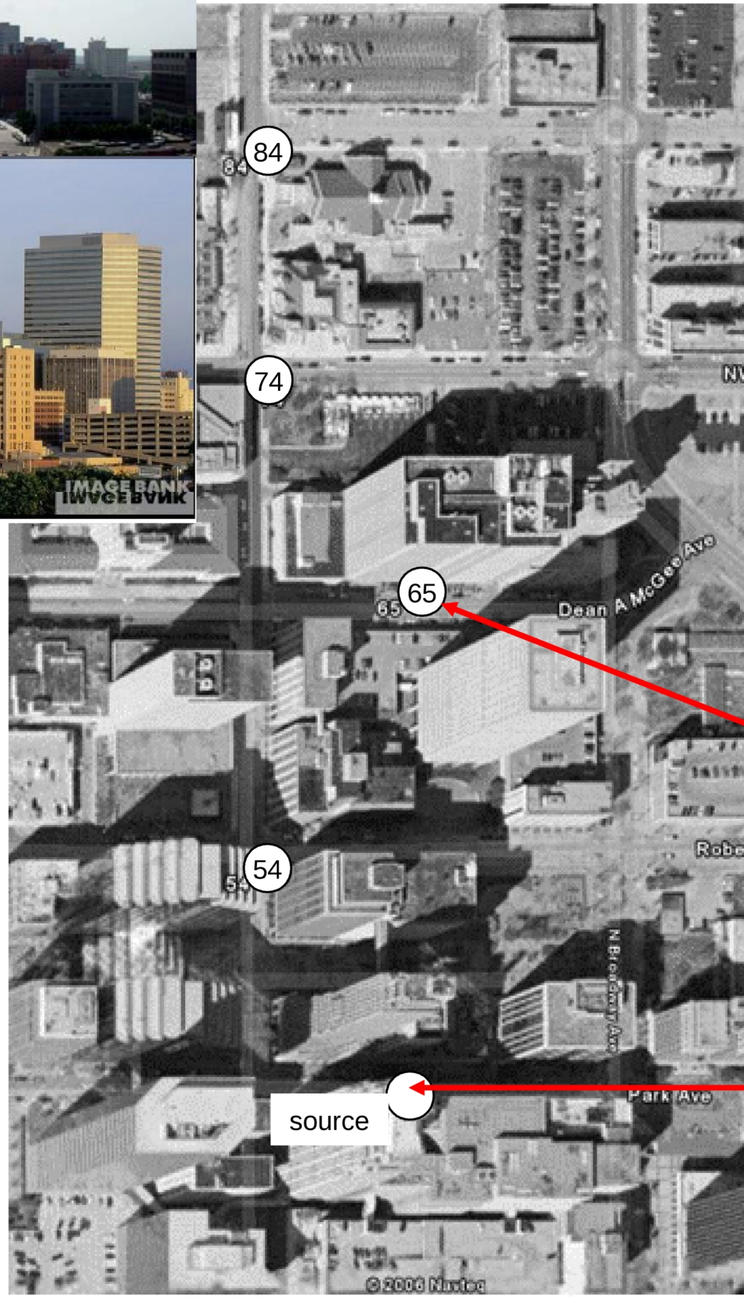
Thomson LS trajectory model to compute paths in urban flow – modifications:

- when particle moves out of cell (I,J,K), check for encounter with building wall: perform perfect reflection off walls

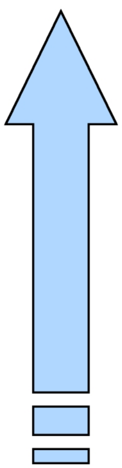
- prohibit particle velocities that differ from the local mean by more than (arbitrarily) 6 standard deviations



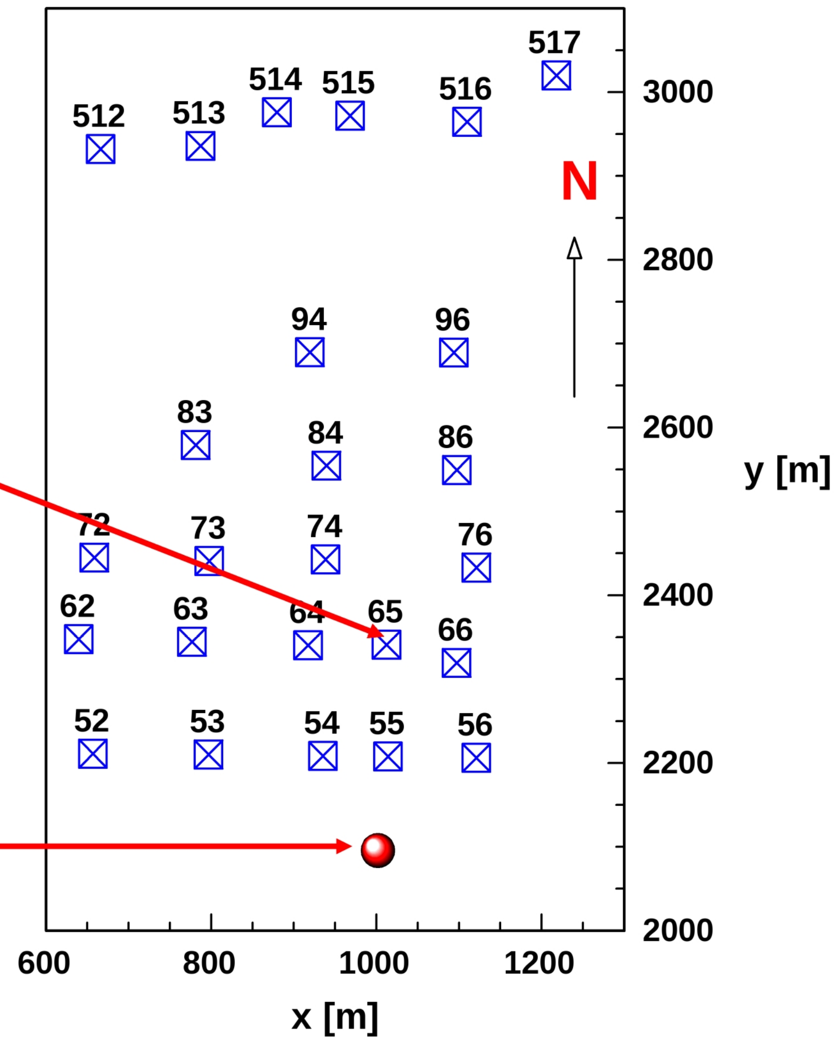
Joint Urban 2003 – tracer expt. in Oklahoma City



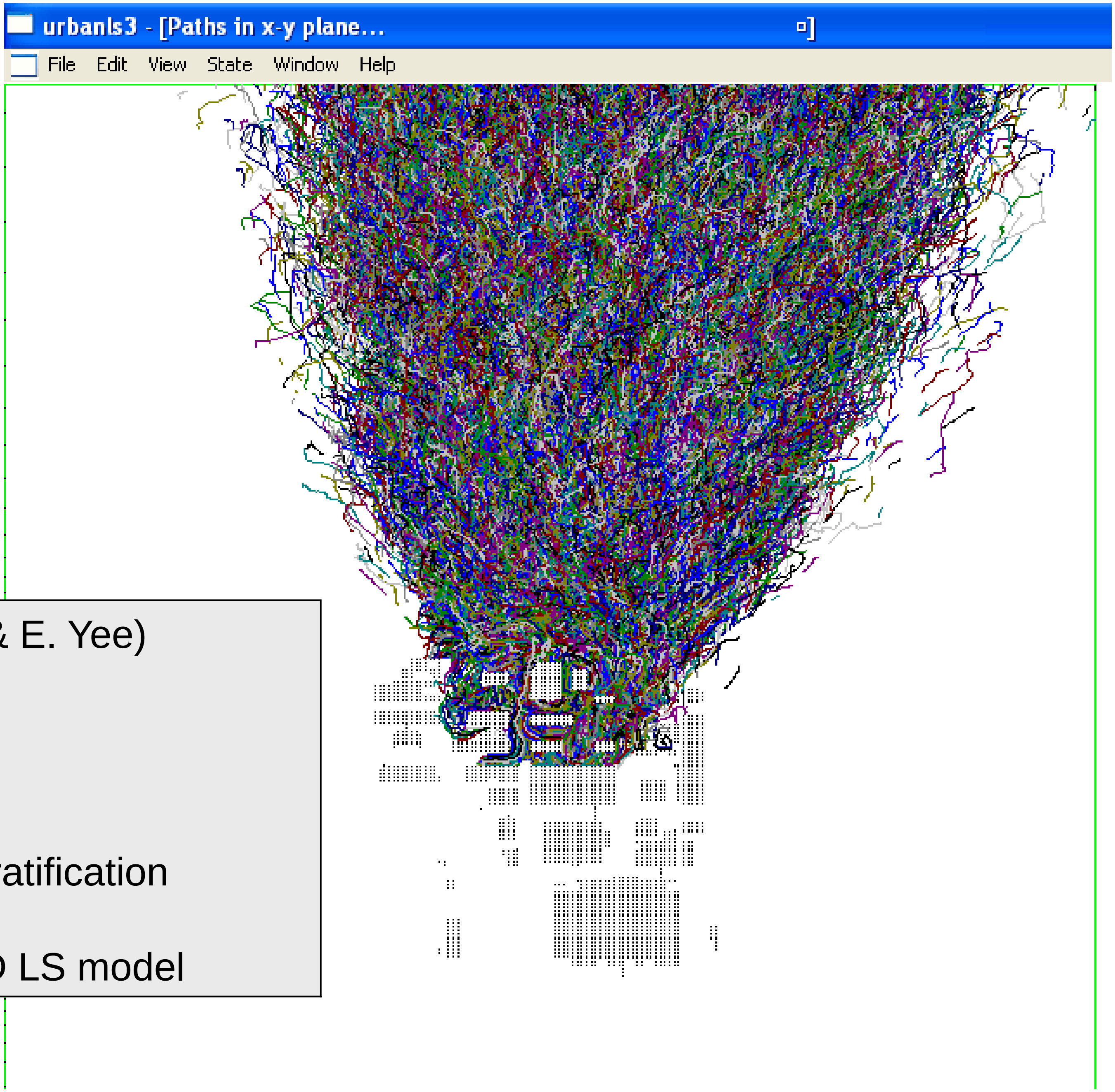
wind



Run IOP9r2: source on 0600-0630 LST; observations are avg. 0615-0630

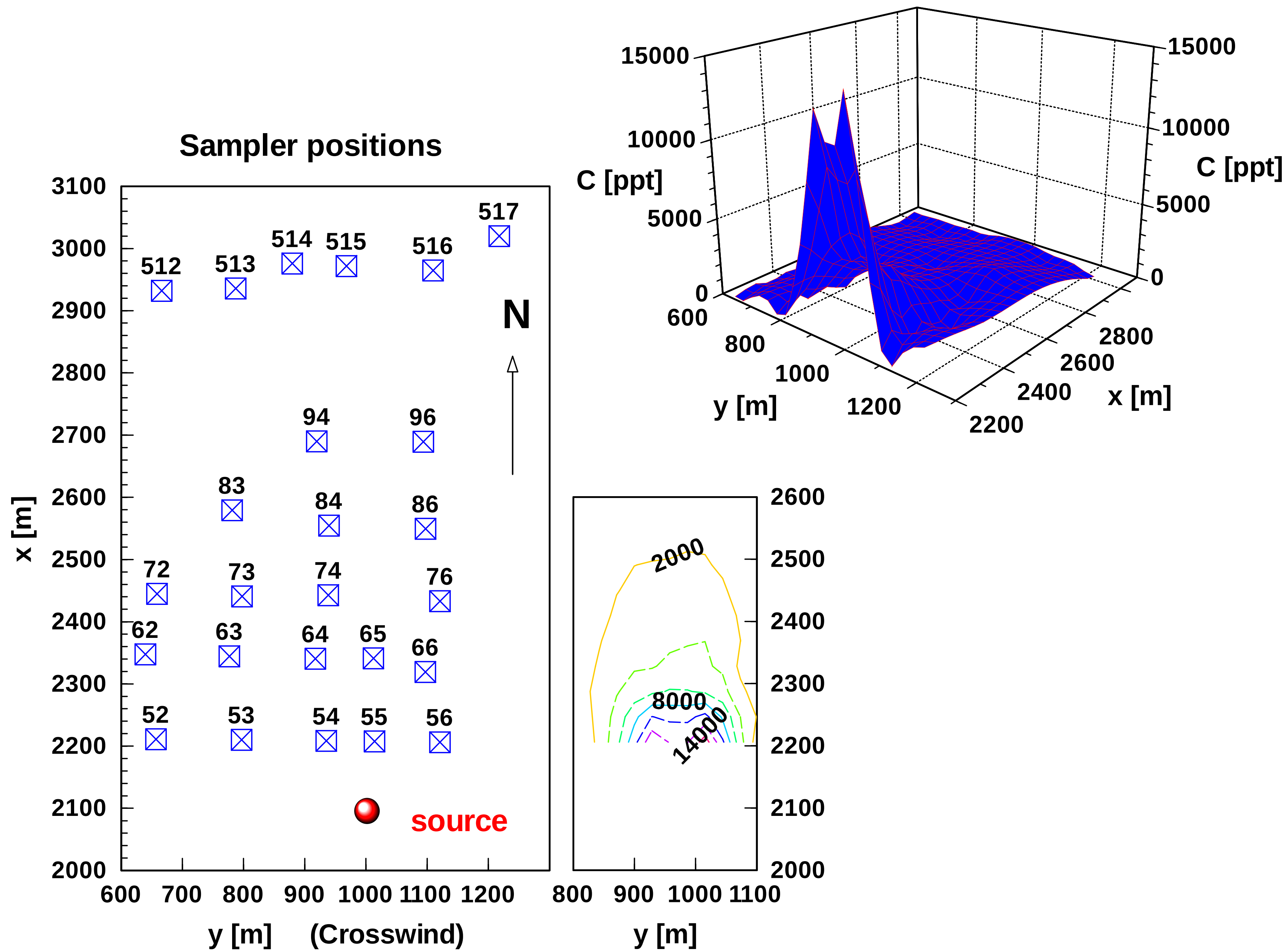


Forward paths from the (point) source, computed for run IOP9r2



- *k*-epsilon model (F.-S. Lien & E. Yee) provides hi-res flow
- gridlength ~ 10 x 10 x 3 m
- resolve buildings, neglect stratification
- trajectories by well-mixed 3D LS model

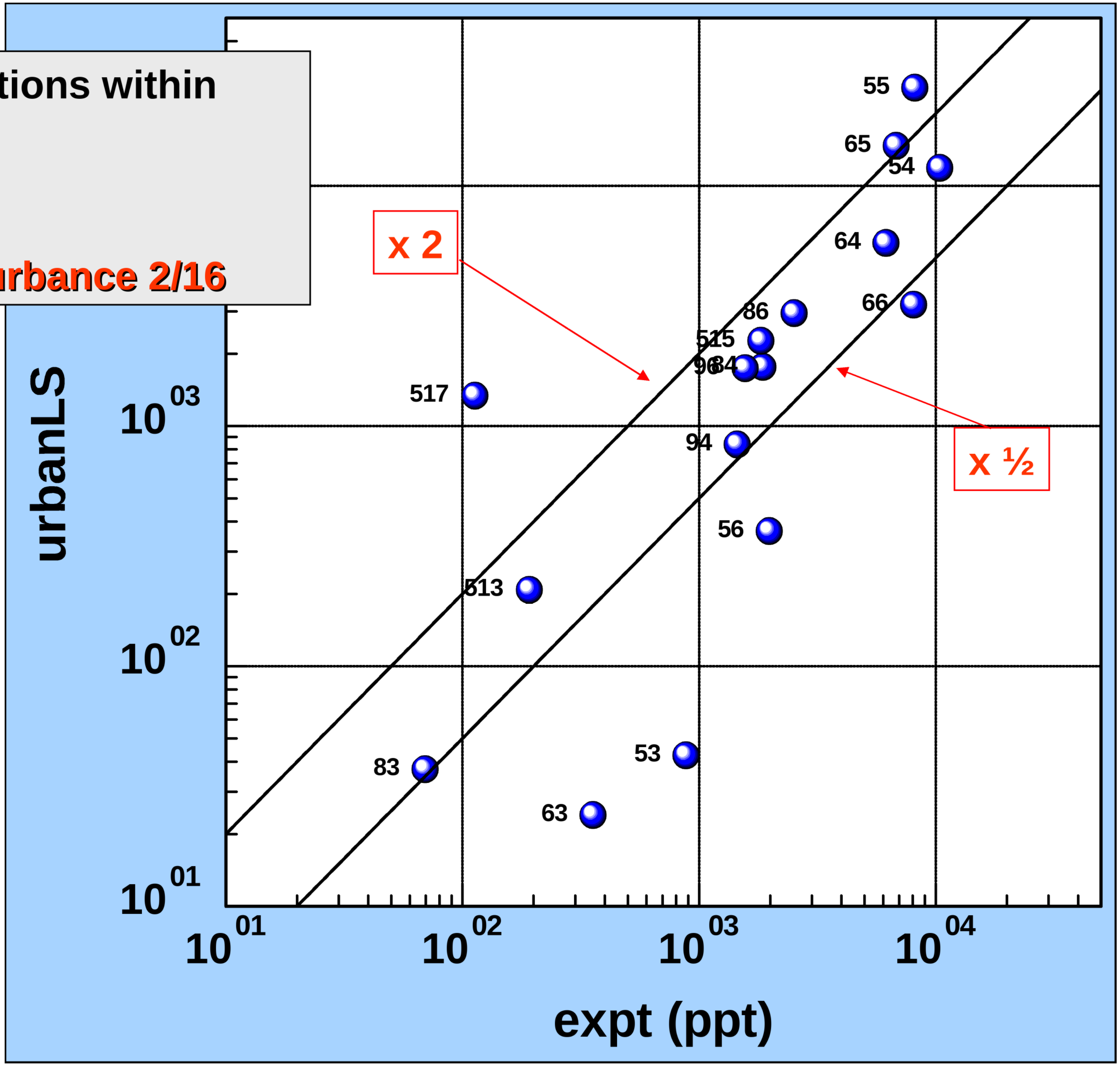
Mean ground-level concentration [parts per trillion] from forward LS simulation



Comparing LS model with observed concentration

Fraction of predictions within factor of two:

- **forwards 9/16**
- **backwards 8/16**
- **ignoring flow disturbance 2/16**

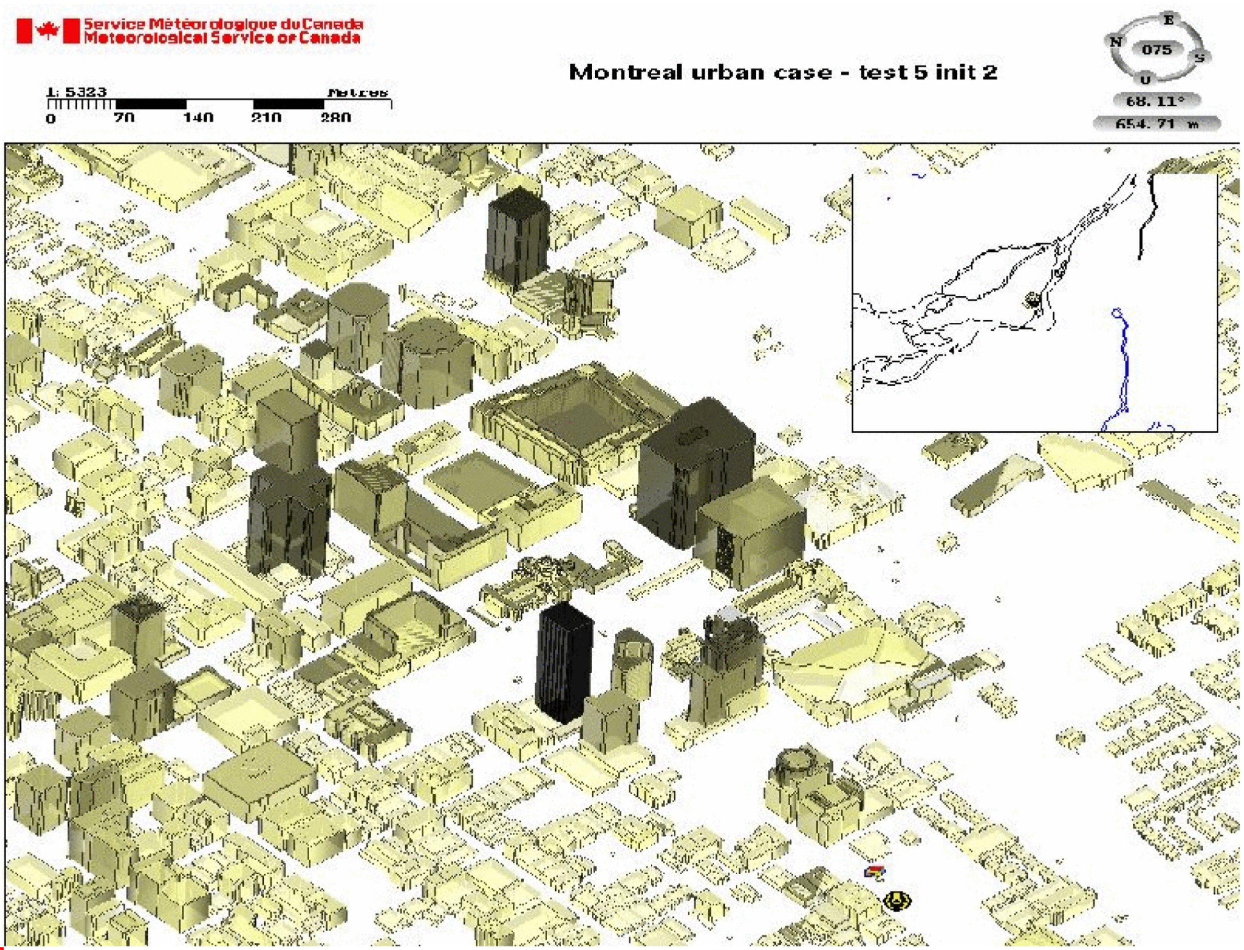


accounting for flow disturbance yields a major improvement in model accuracy

Conclusion

• CRTI urban dispersion project hinges on wind modelling from the global down to street scale

• modelling system runs at CMC - more realistic than, say, re-tuning Gaussian puff/plume model



Lecture ended here 7 April 2016