PROPOSAL OF A NEW LAGRANGIAN PARTICLE MODEL FOR THE SIMULATION OF DENSE GAS DISPERSION

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We study the accidental releases of hazardous materials denser than ambient air.

The emitted cloud begins to disperse under the action of its own momentum and buoyancy.

Its excess of density reduces as ambient air is entrained until, at some distance downwind, transition to passive dispersion behaviour takes place.

An important issue is the spread at the ground due to gravity.

Dispersion simulation in these cases is mostly done by empirical or integral models or, in some specific cases, by computational fluid dynamics (CFD) models.

Another way, here proposed, is offered by Lagrangian particle dispersion (LPD) models.

The LPD approach is a compromise between the complexity and CPU time demanding of CFD models and the simpler integral models.

Here we describe a new version of the LPD **MicroSpray** model, especially oriented to deal with dense gas dispersion in urban environment.

Model system **MSS** includes **MicroSWIFT** and **MicroSpray**

MicroSWIFT is a prognostic (mass consistent) wind interpolator over complex terrain accounting for complex terrain and buildings.

MicroSpray is a LPD model directly derived from SPRAY which may accounts for the presence of buildings, other obstacles, complex terrain, and possible occurrence of low wind speed and stable conditions.

Thus, the new version of **MicroSpray** model is especially oriented to deal with dense gas dispersion in urban environment and industrial sites.

Initial phase

Five conservation equations

mass

energy

vertical momentum

x-horizontal

y-horizontal momentum

are integrated for each particle

based on:

Glendening, J.W., J.A. Businger, and R.J. Farber, (1984), “Improving plume rise prediction accuracy for stable atmospheres with complex vertical structure”. *J. Air Pollut. Control Ass.*, 34 : 1128–1133

and following the work of

Hurley, P.J., and P.C. Manins (1995) “Plume rise and enhanced dispersion in LADM.”, *CSIRO Division of Atmospheric Research*, ECRU Technical Note No.4

and

Hurley P.J. (2005) “The Air Pollution Model (TAPM) Version 3. Part1: Technical Description”. *CSIRO Atmospheric Research Technical Paper* No. 71

Equations

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a} u_s b^2\right] = E u_s$$

Entrainment flux (mass conservation)

$$\frac{d}{dt}\left[u_s b^2 B\right] = -\frac{\rho_p}{\rho_a} N^2 u_s w_p b^2$$

Buoyancy flux (energy conservation)

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a} u_s w_p b^2\right] = B b^2 u_s$$

vertical momentum conservation

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a} u_s b^2 u_p\right] = E u_s u_a$$

X horizontal momenta conservation

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a} u_s b^2 v_p\right] = E u_s v_a$$

Y horizontal momenta conservation

five unknowns ρ_p, u_p, v_p, w_p, b

where:

$$N^2 = \frac{g}{\vartheta_a}\frac{\partial \vartheta_a}{\partial z}$$

Brunt-Vaisala

$$E = 2\, b\, u_e$$

entrainment

Plume spread at ground

When a dense plume reaches the ground an horizontal momentum is generated by the weight of the plume itself that tends to spread the plume

A hybrid algorithm used

the movement of each particle depends on the characteristics of the 'ensemble'

To each particle is assigned an horizontal speed $U_g = 1.41\sqrt{g\,\Delta_a\,H}$

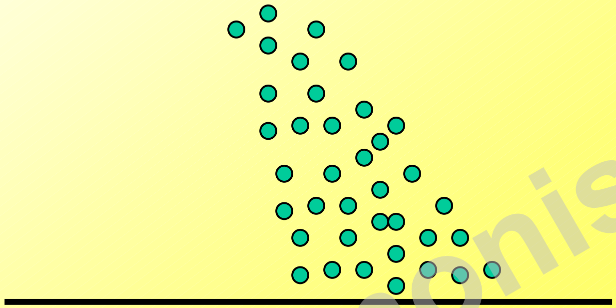
with: $\Delta_a = \dfrac{\rho_{bulk} - \rho_a}{\rho_a}$

ρ_{bulk}= 'bulk' density of the plume above the particle

H = 'bulk' height of the plume above the particle

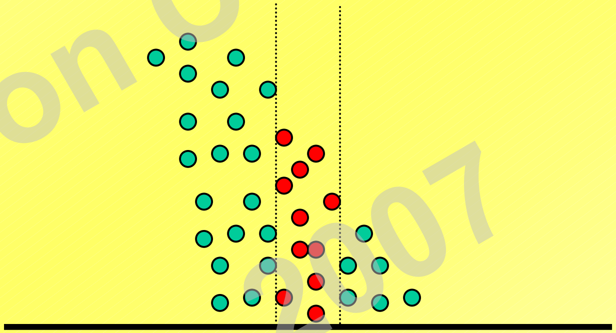
How to compute *H and* ρ_{bulk} ?

1) when a particles 'reaches' the ground



$$H = \frac{1}{np}\sum_{i=1}^{np} z_{p_i}$$

2) all the particles p_i belonging to a dx dy column are accounted



$$\rho_{bulk} = \frac{1}{np}\sum_{i=1}^{np} \rho_{p_i}$$

Direction of the spread

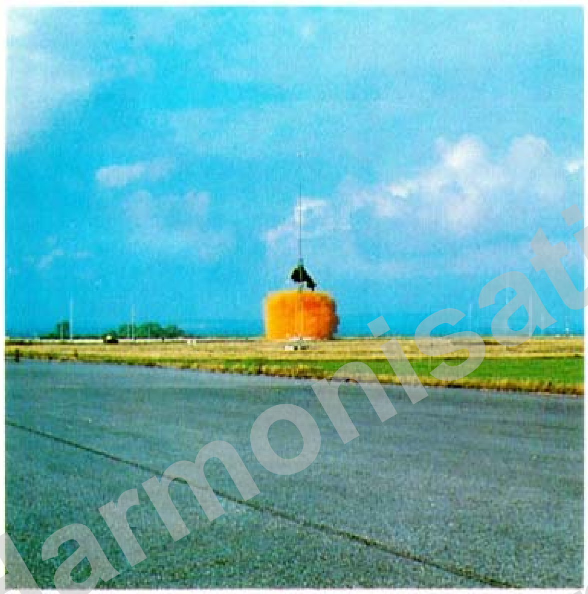
$$\begin{cases} V_{gs} = U_g \sin(\gamma) \\ U_{gs} = U_g \cos(\gamma) \end{cases}$$

where γ is randomly picked from a uniform [0°-360°] distribution

γ is chosen at emission time and kept by the particle

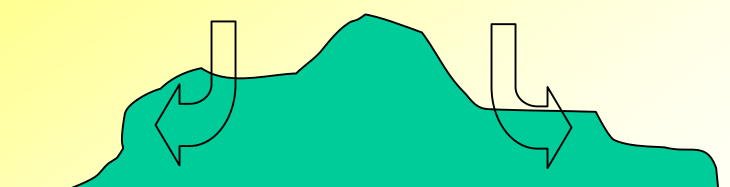
Thorney Island, instantaneous release, exp. 8

Plume without initial momentum



t=0

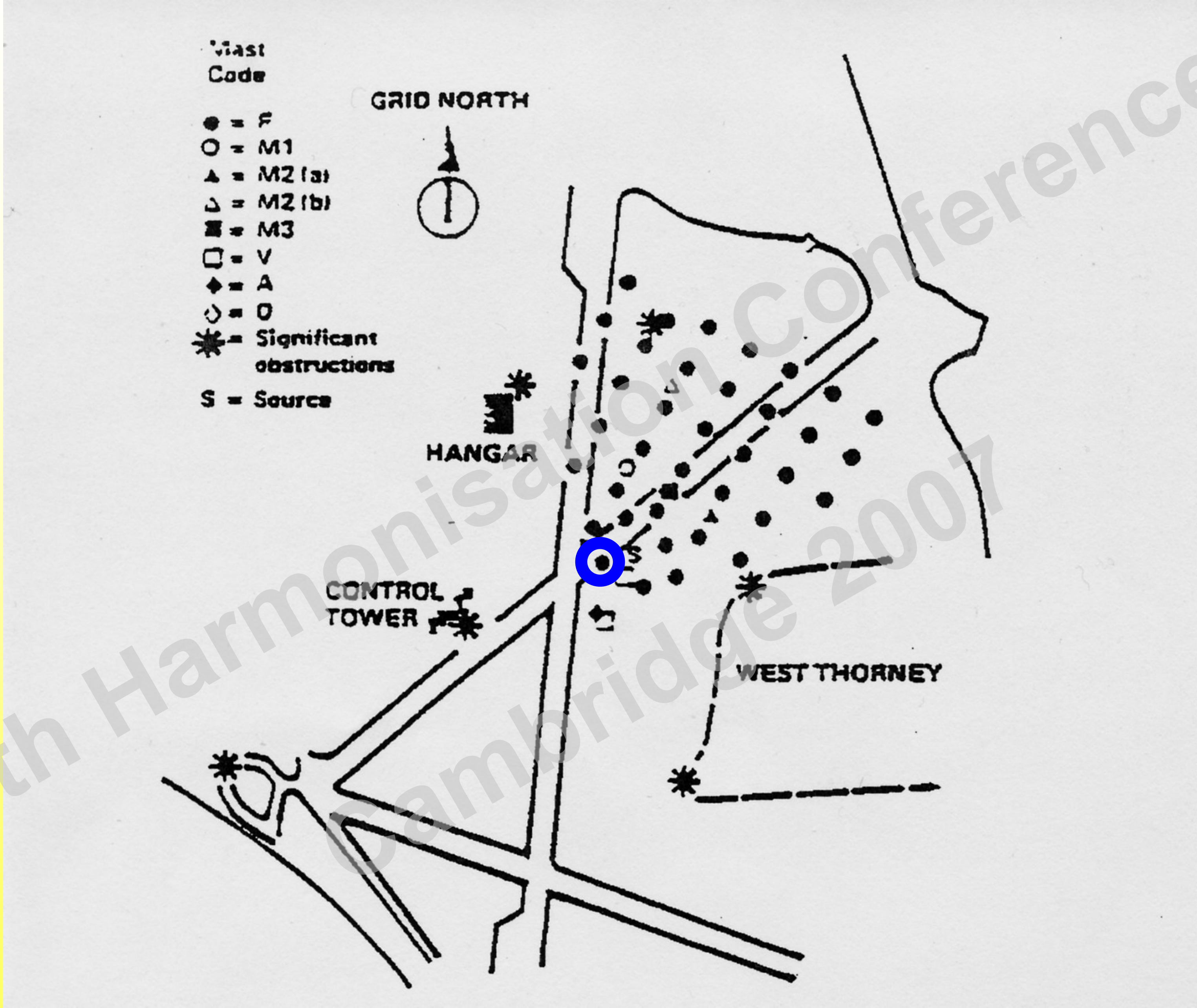
t=T



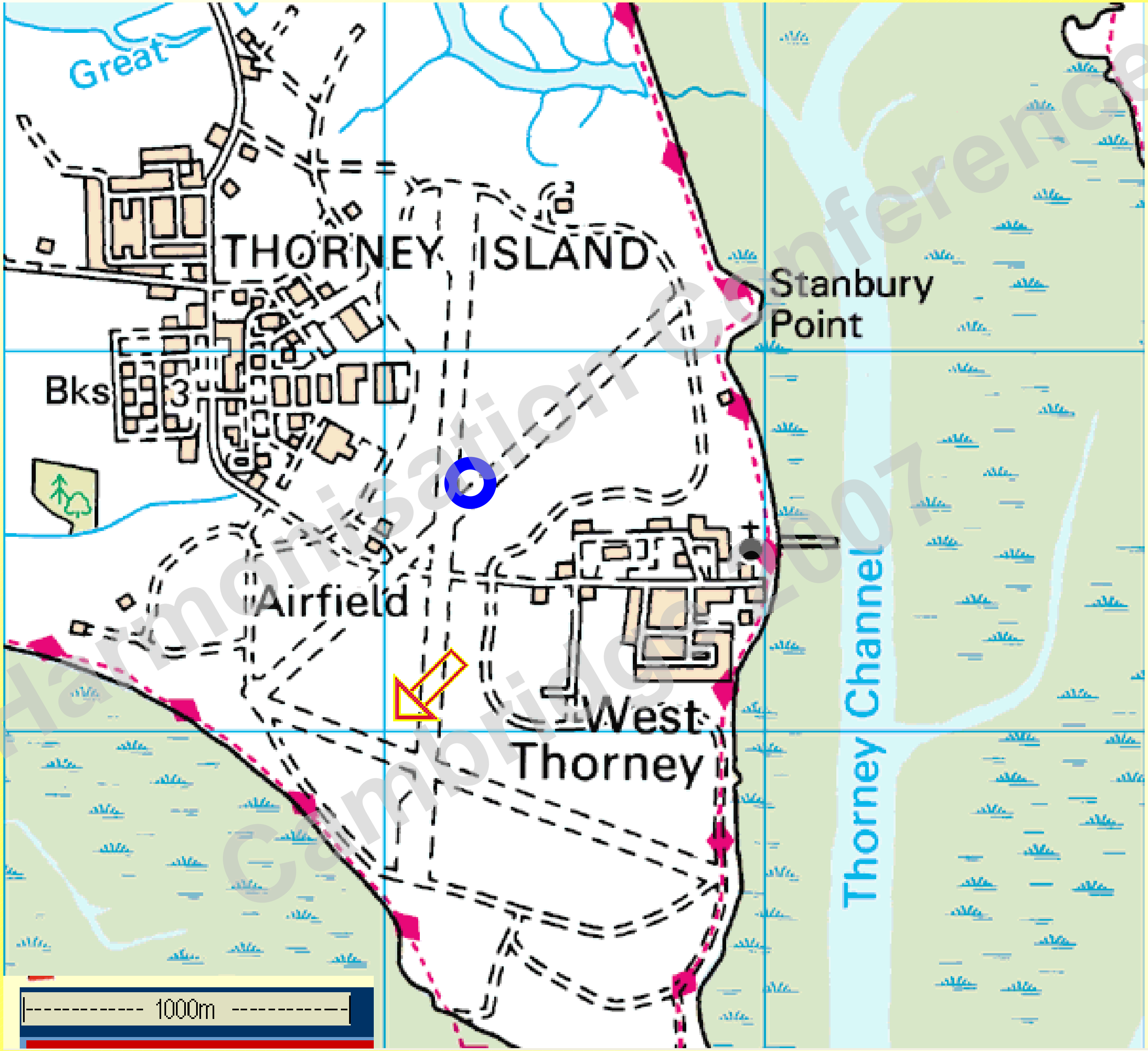
Thorney Island Exp. 8

(plume without initial momentum)

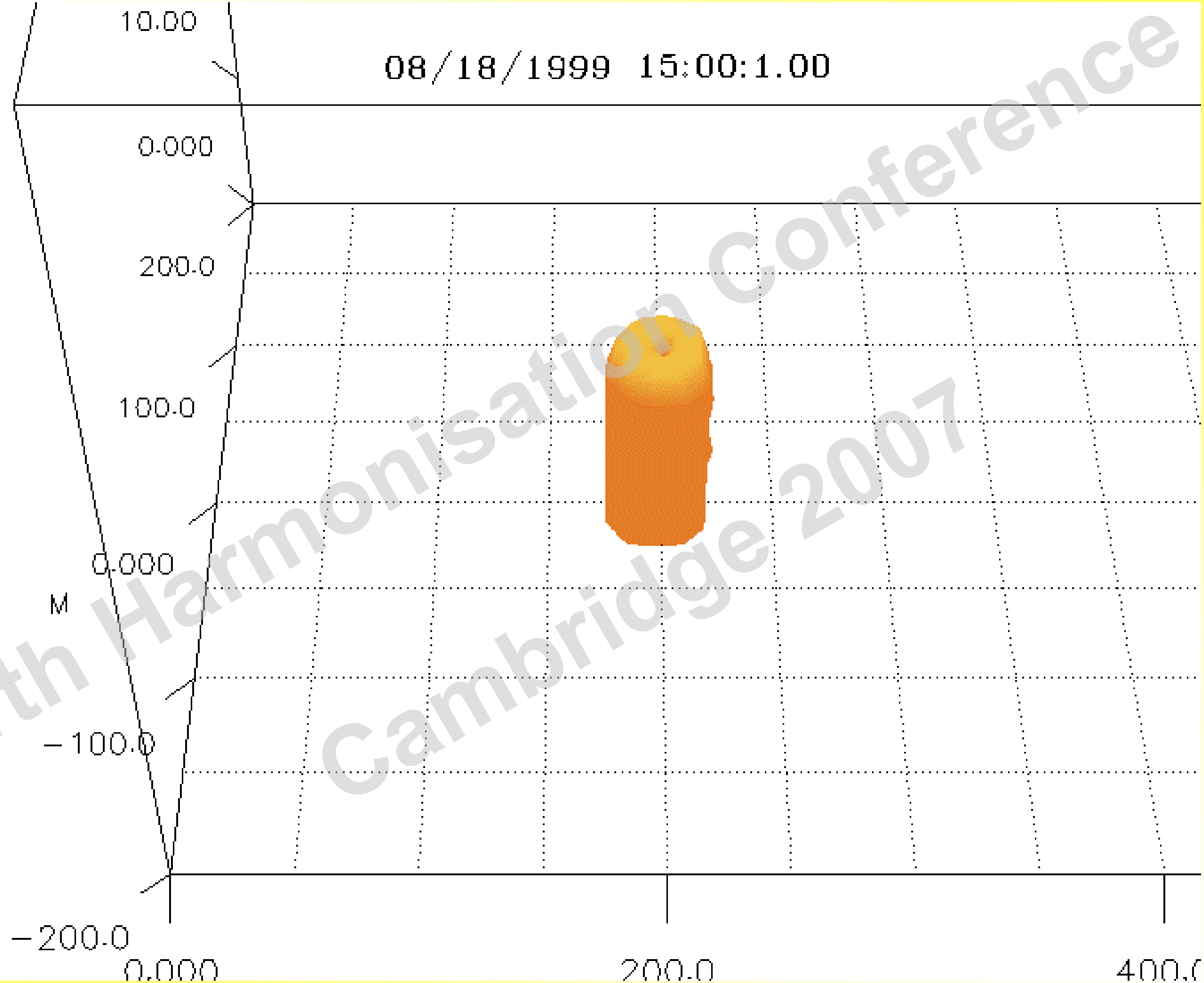
- emission = cylinder (d=14 m, h=13 m)
- neutral stratification
- wind at 10 m (2.4 m/s)
- relative emission density ρ_e/ρ_a equal to 1.63
- 3958 kg of a mixture of Freon-12 and Nitrogen
- 46 samplers in the range 70 – 550 m
  at different heights (0.4, 2.4, 4.4, 6.4 m)



Mast
Code
= F
= M1
= M2 (a)
= M2 (b)
= M3
= V
= A
= O
= Significant obstructions
S = Source
GRID NORTH
HANGAR
CONTROL TOWER
WEST THORNEY
S


Great
THORNEY ISLAND
Stanbury Point
Bks
Airfield
West Thorney
Thorney Channel
1000m

Thorney Island Exp 8
Plume without initial momentum



08/18/1999 15:00:1.00
10.00
0.000
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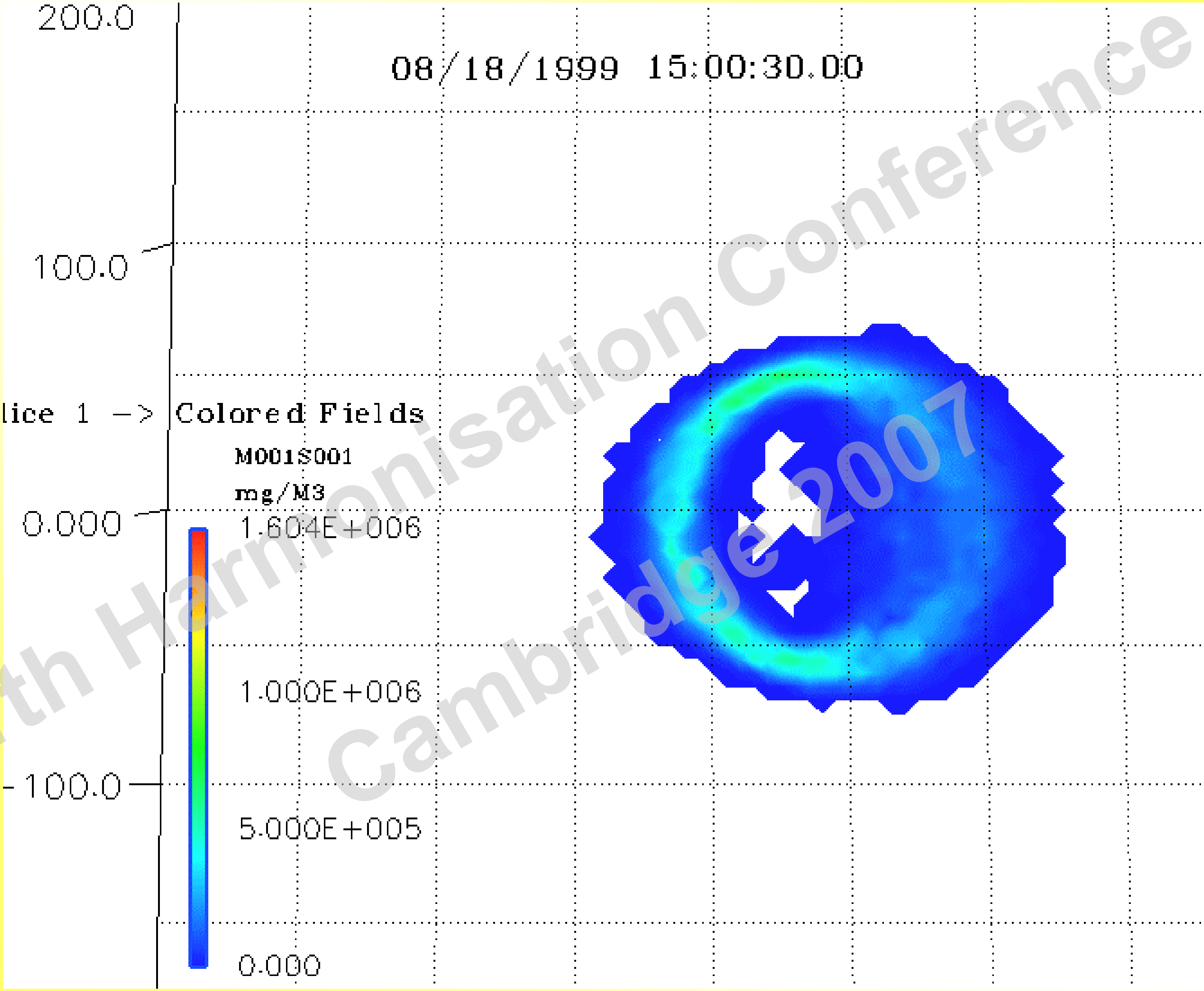
100.0
0.000
M
-100.0
-200.0
0.000
200.0



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0.000
-100.0
lice 1 -> Colored Fields
M001S001
mg/M3
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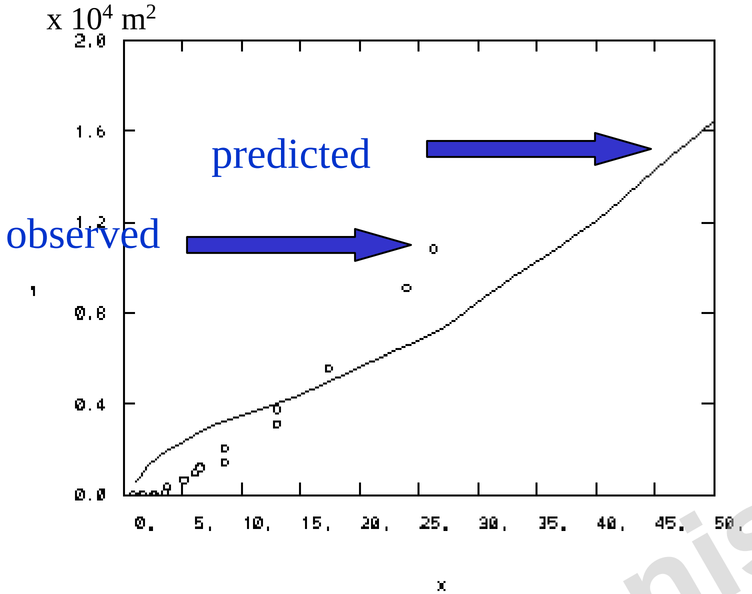
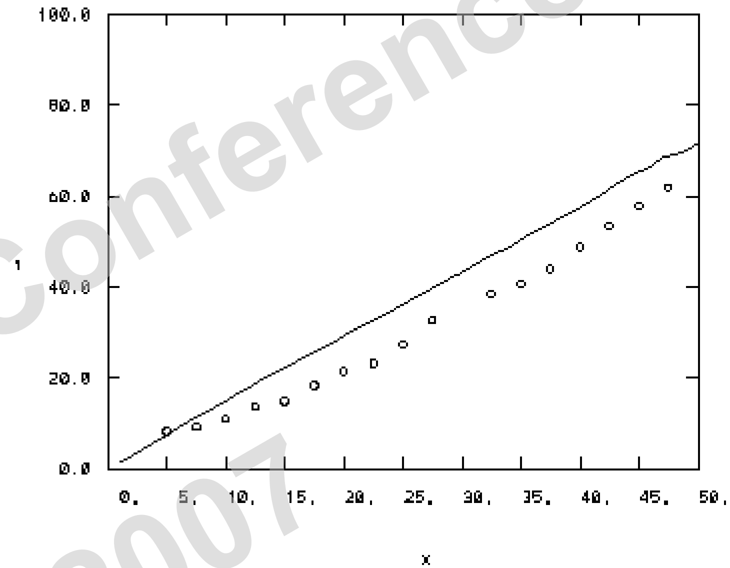
1.000E+006
5.000E+005
0.000

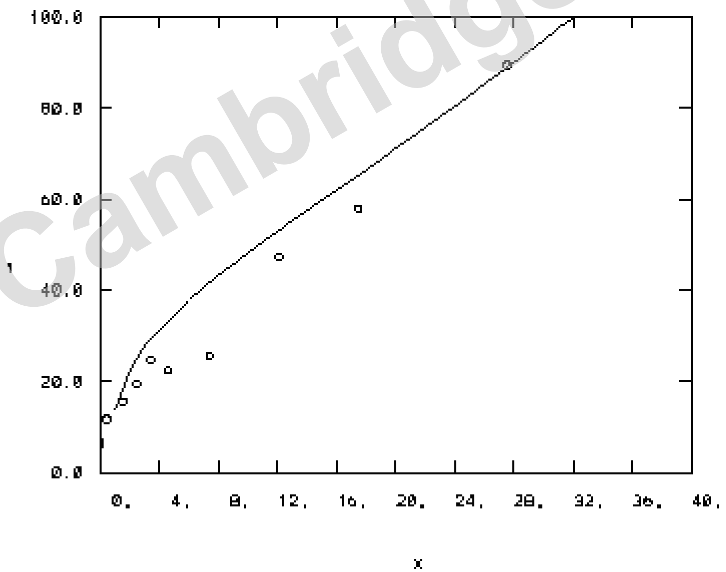
area vs time

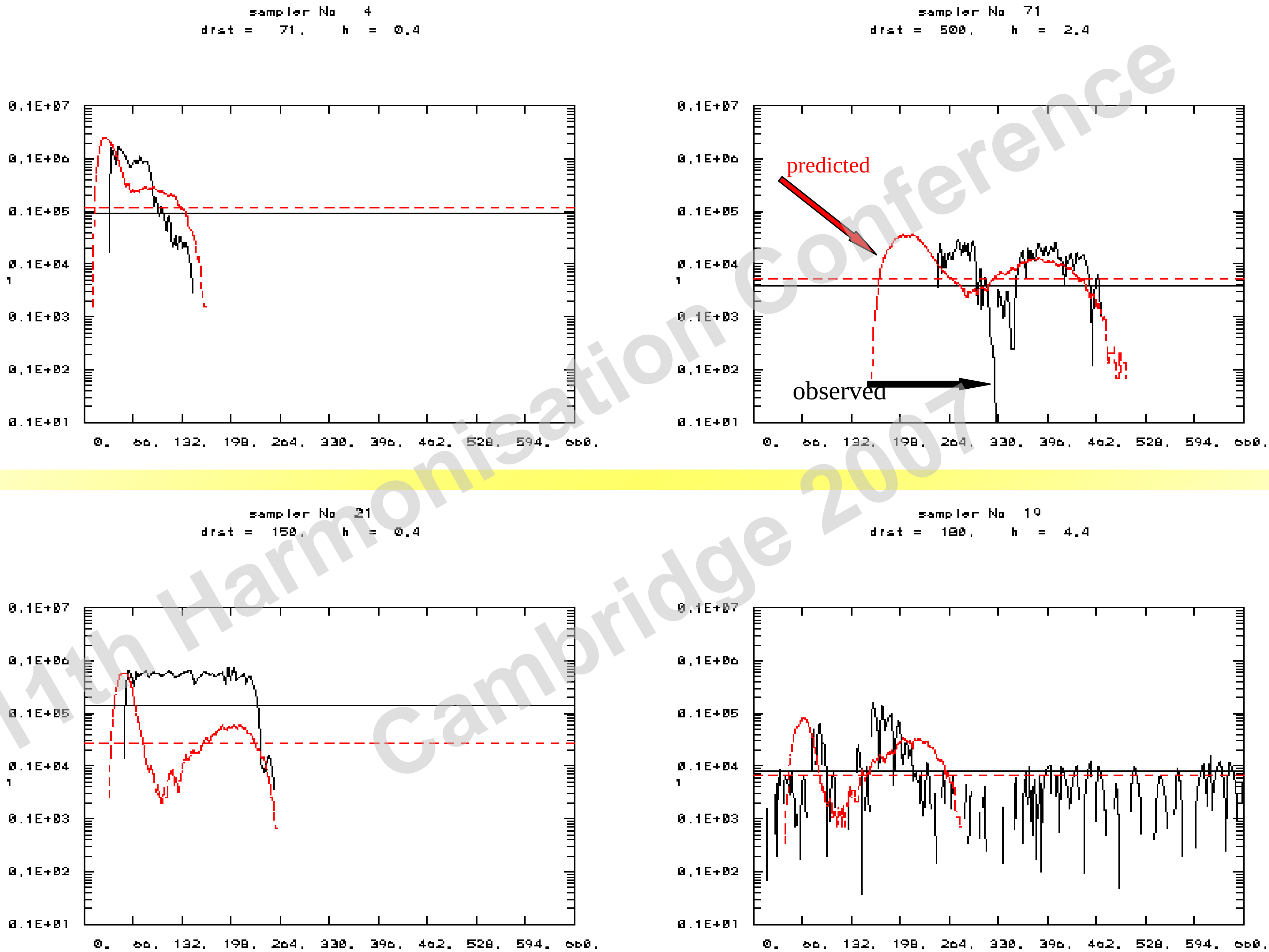


cloud centroid vs time



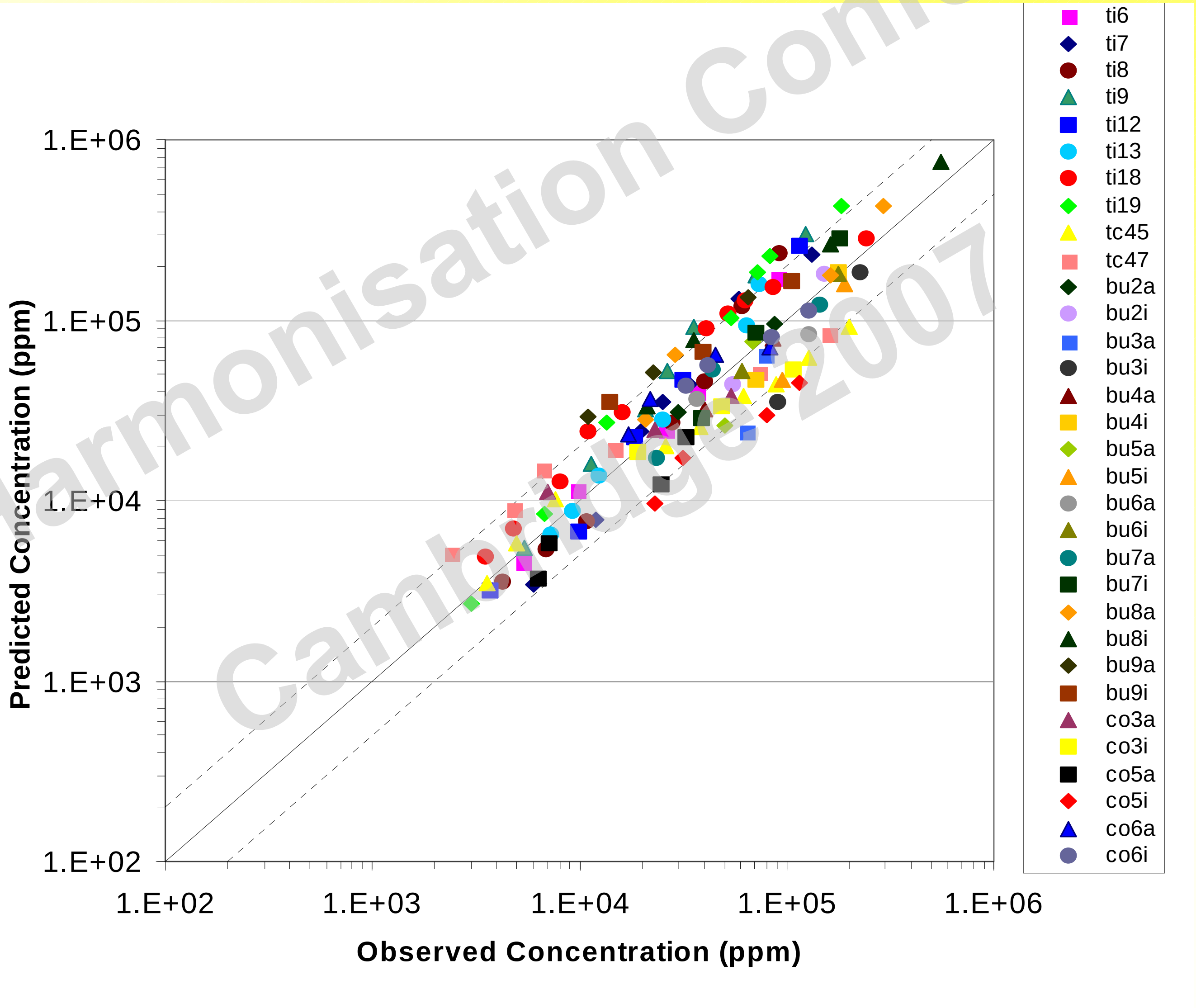
Downwind front vs time





sampler No 4
dist = 71. h = 0.4
sampler No 71
dist = 500. h = 2.4
predicted
observed
sampler No 21
dist = 150. h = 0.4
sampler No 19
dist = 100. h = 4.4
0.1E+07
0.1E+06
0.1E+05
0.1E+04
0.1E+03
0.1E+02
0.1E+01
0. 66. 132. 198. 264. 330. 396. 462. 528. 594. 660.

MicroSpray dense-gas model evaluation with MDA dataset
(TIsland-Ist + TIsland-Cont + Burro+Coyote)



CONCLUSIONS

We presented a new version of the LPD model **MicroSpray** devoted to simulate the dense gas dispersion.

We compared its prediction with a tracer experiment (**Thorney Island Exp.8**).

Preliminary results suggest that **MicroSpray** is able to perform correct simulations of dense gas dispersion in real field situations.

questions?