



INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE CENTRATOM TRIESTE



UNITED NATIONS INDUSTRIAL DEVELOPMENT ORGANIZATION



INTERNATIONAL CENTRE FOR SCIENCE AND HIGH TECHNOLOGY

c/o INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS - 34100 TRIESTE (ITALY) VIA GIULIANO F. RABUATTO 10 P.O. BOX 586 TELEPHONE (0432) 701 TELEFAX (0432) 701111 TELEX 66000 ICPH

SMR/760-47

**"College on Atmospheric Boundary Layer
and Air Pollution Modelling"
16 May - 3 June 1994**

"Lagrangian Particle Models"

F. DESIATO
Agenzia Nazionale per la Protezione dell'Ambiente
A.N.P.A. (EX-ENEA/DISP)
Rome, Italy

Please note: These notes are intended for internal distribution only.

LAGRANGIAN PARTICLE MODELS

$$U = U_A + U'$$

$$U' \quad \kappa\text{-theory: } U' = -\frac{\kappa}{\epsilon} \nabla C$$

Monte-Carlo:

$$U'(t + \Delta t) = U'(t) R(\Delta t) + U''(t)$$

$$R(\Delta t) = \overline{U'(t) U'(t + \Delta t)} / \overline{U'^2}$$

$$T_L = \lim_{t \rightarrow \infty} \int_0^t R(t) dt$$

$$\sigma_{U''} = \sigma_{U'} [1 - R^2(\Delta t)]^{1/2}$$

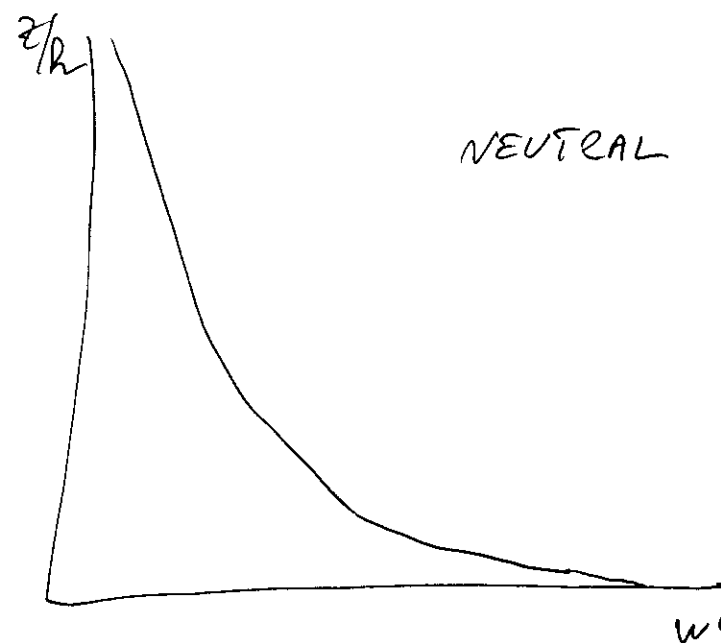
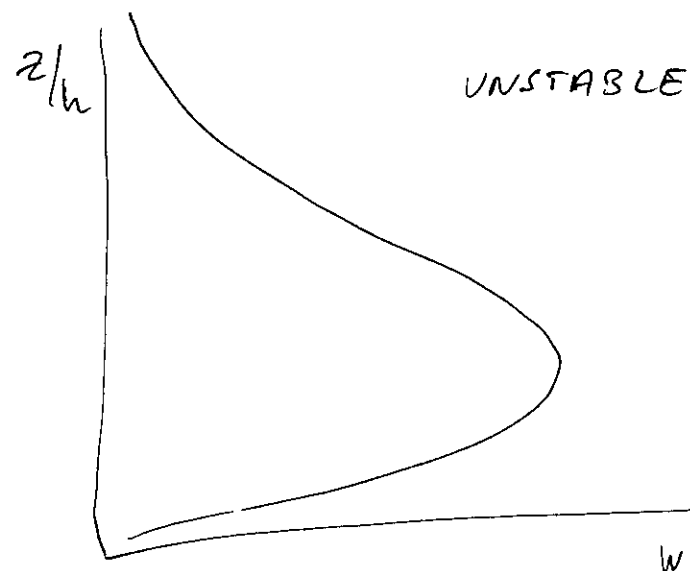
$$R(\Delta t) = \exp(-\Delta t / T_L)$$

$$U'(t + \Delta t) = e^{-\Delta t / T_L} U' + (1 - R^2)^{1/2} \sigma_{U'} r$$

DRIFT VELOCITY (additional term for w')

$$(1 - e^{-\frac{\Delta t}{T_L}}) T_L \partial \sigma_{U'}^2 / \partial z$$

$$\sigma_U, T_L \quad f(z, h, L, U_*, w_*, z_0)$$



ARIES

(Atmospheric Release Impact Evaluation System)

is an integrated hardware/software system for the evaluation of atmospheric dispersion at different space and time scales.

Two versions of ARIES have been realized:

ARIES-I for the real-time evaluation of the consequences of accidental releases.

Platform: cluster of VAX 6300 and 6400 - VMS
Telephone link with the Italian Weather Service

ARIES-W for the previsional or post-facto analysis concerning routine emissions.

Platform: ALPHA 3000 Workstation - OSF.

The two systems share several components:
models, environmental data banks, user interface.

ARIES-I (Atmospheric Release Impact Evaluation System-Improved)

AIM:

to provide a technical support for real-time evaluation of the consequences of accidental releases in the atmosphere.

BY MEANS OF:

integration of atmospheric dispersion modelling techniques with environmental data base.

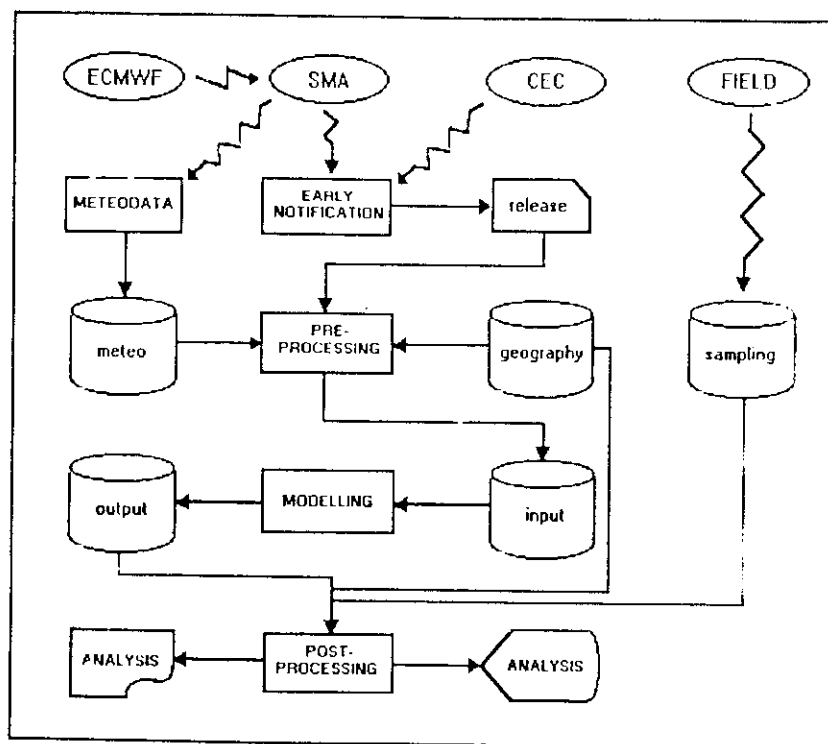


Fig. 1 - Functional model evaluation scheme in ARIES-I

ARIES-I

FEATURES

- Pollution episodes everywhere on the European territory, with different space and time scales, can be considered.
- Flexibility with respect to the type and the number of data available in real-time.
- Several functions of input and output processing can be carried out automatically.
- Model components and data banks can be updated or implemented without altering the system structure.

ARIES-I models

Forecasting

- * Long range

APOLLO

(Atmospheric POLLutant LONG range dispersion)

Nowcasting

- * Local scale, flat terrain

SPADE

(Sequential Puff for Atmospheric Dispersion Evaluation)

- * Local and meso scale, complex terrain

CONDOR

(3-d mass-consistent diagnostic wind field model, by
Moussiopoulos and Flassak)

ARCO

(Atmospheric Release in COMplex Terrain)

APOLLO (Atmospheric POLLutant LONG range dispersion)

AIM:

Real time estimate of the atmospheric dispersion of stable or first order decaying pollutants at distances up to some thousands of km from one point source.

METHOD:

Lagrangian particle
Particles are tracked by a three-dimensional wind field to which turbulent motions are superimposed.

INPUT:

- . topography
- . roughness
- . 3-D wind field
- . geopotential
- . precipitation
- . vertical temperature profiles

OUTPUT:

- . instantaneous air concentration
- . time-integrated air concentration
- . dry deposition
- . wet deposition

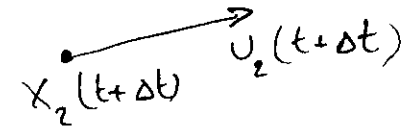
Time and space resolution of all input and output data are flexible.

Particle trajectory

(Reap)



U_1, U_2 interpolated in space and time from gridded data.



first guess:

$$X_2(t+\Delta t) = X_1(t) + U_1(t)\Delta t$$

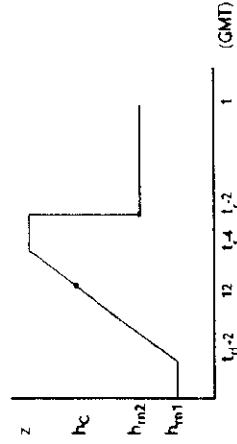
$$X_2^i(t+\Delta t) = X_1(t) + 0.5[U_1(t) + U_2^i(t+\Delta t)]\Delta t$$

iterated until

$$|X_2^i - X_2^{i-1}| < \epsilon$$

Mixing Layer

- Mechanical mixing depth
 $h_m = .25u_* / f$
- Convective mixing depth h_c computed from
 $u_* = kV_s / \ln(z_s/z_0)$
- 12 GMT temperature soundings.



t_d = local dawn GMT time
 t_s = local sunset GMT time

u_* , L

are derived from

u , z_0 , T , cloud cover
 with the 'energy budget'
 method (Van Ulden and Holtslag)

$$T_{Lg} = 10^4 s \text{ (Gifford)}$$

$$T_{Lz} = f(u_*, h, L)$$

$$\sigma_v, \sigma_w = f(u_*, h, z)$$

GRID-FREE CONCENTRATION CALCULATION

('kernel' method)

$$c(r, t) = \frac{\Delta(r)}{\ell^3} \sum_{i=1}^n m_i W(r_i - r, \ell)$$

$r_i - r$ = vector distance of particle i
from receptor

m_i = particle mass

ℓ = smoothing length

$\Delta(r)$ = boundary correction

Gaussian kernel:

$$W = \frac{1}{(2\pi)^{3/2}} \exp\left(-\frac{1}{2} \frac{|r_i - r|^2}{\ell^2}\right)$$

ℓ should be a function of the
mean interparticle separation
around r .

AIR CONCENTRATION
For particle with

$z_m(x, y) < z_s(x, y) + h(x, y)$

$$C_n(i, j) = \sum_m \frac{q_{nm}}{2\pi h(i, j) \sigma_m^2} \cdot \exp\left[\frac{-(x_m - x_i)^2}{2\sigma_m^2}\right] \cdot \exp\left[\frac{-(y_m - y_i)^2}{2\sigma_m^2}\right]$$

· DRY DEPOSITION

$$D_{\Delta t}(i,j) = C(i,j) \cdot V_d \cdot \Delta t$$

· WET DEPOSITION

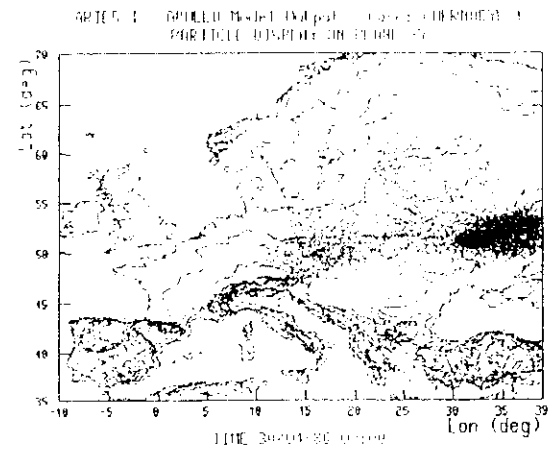
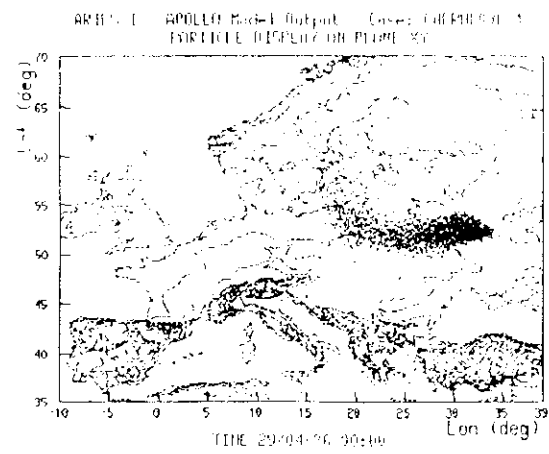
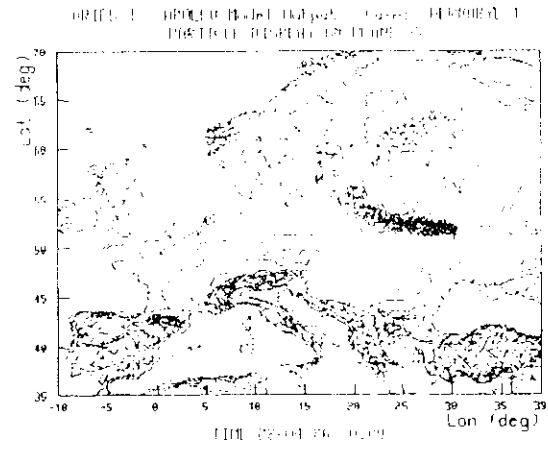
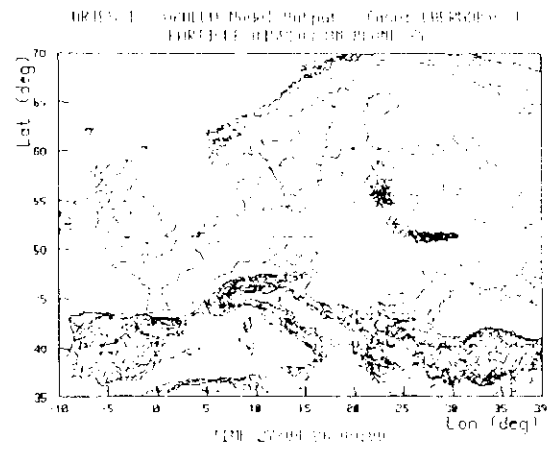
$$w_{\Delta t}(i,j) = \sum_m \frac{\wedge q_m}{2 \pi \sigma_m^2} \exp \left[\frac{-(x_m - x_i)^2}{2 \sigma_m^2} \right] \cdot$$

$$\cdot \exp \left[\frac{-(y_m - y_i)^2}{2 \sigma_m^2} \right] \cdot \Delta t$$

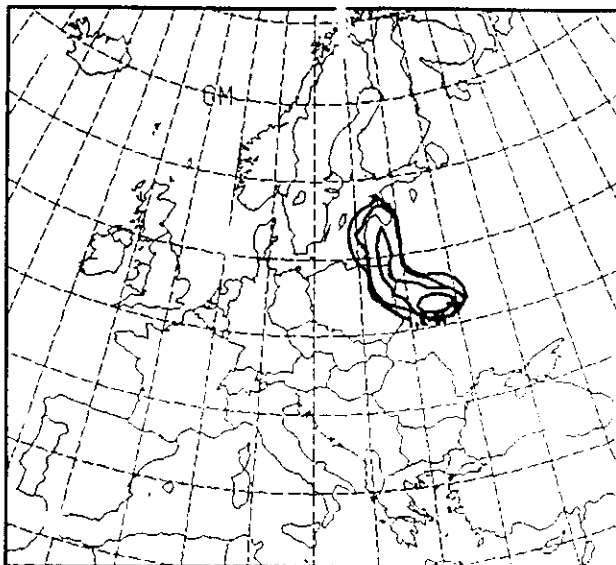
$$\wedge = WP^{-8}(i,j)$$

. PARTICLE DEPLETION BY:

- Radioactive decay or first order chemical reaction
- Scavenging by dry deposition
- Scavenging by wet deposition

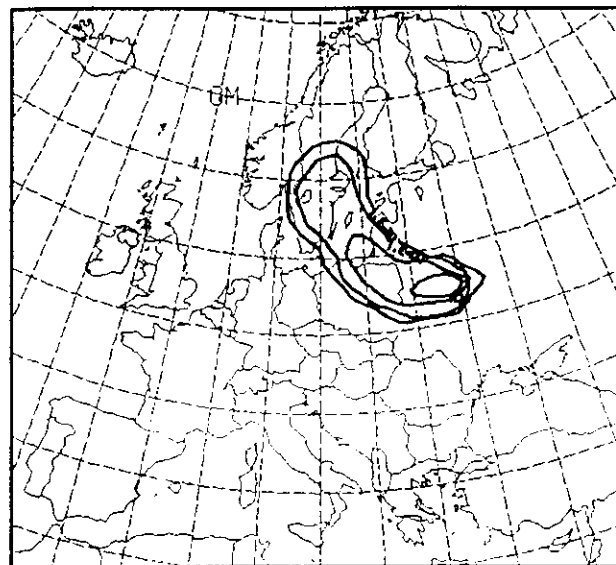


ARIES-I - APOLLO Model Output - Case: CHERNOBYL_1
C137 AIR CONCENTRATION (BQ/MC)



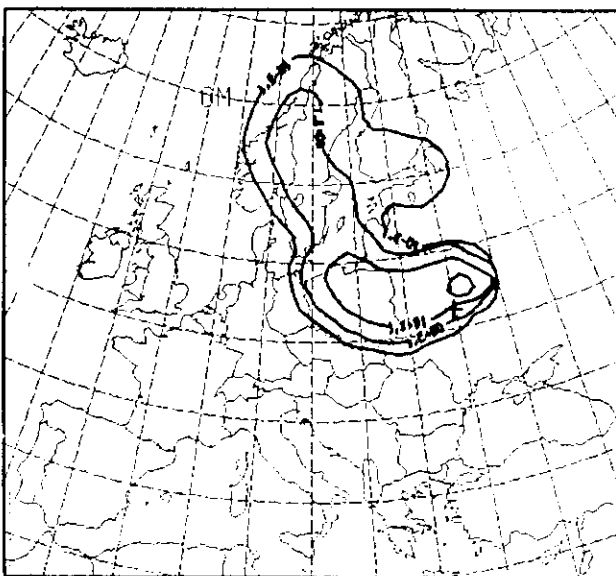
TIME 27/04/86 00:00

ARIES-I - APOLLO Model Output - Case: CHERNOBYL_1
C137 AIR CONCENTRATION (BQ/MC)



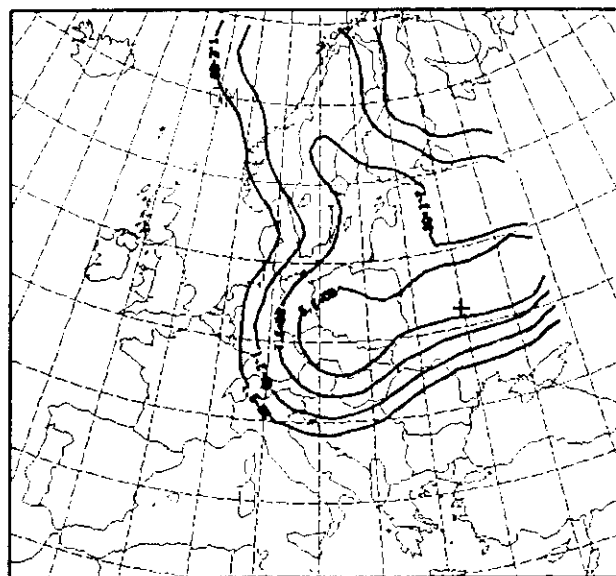
TIME 28/04/86 00:00

ARIES-I - APOLLO Model Output - Case: CHERNOBYL_1
C137 AIR CONCENTRATION (BQ/MC)



TIME 29/04/86 00:00

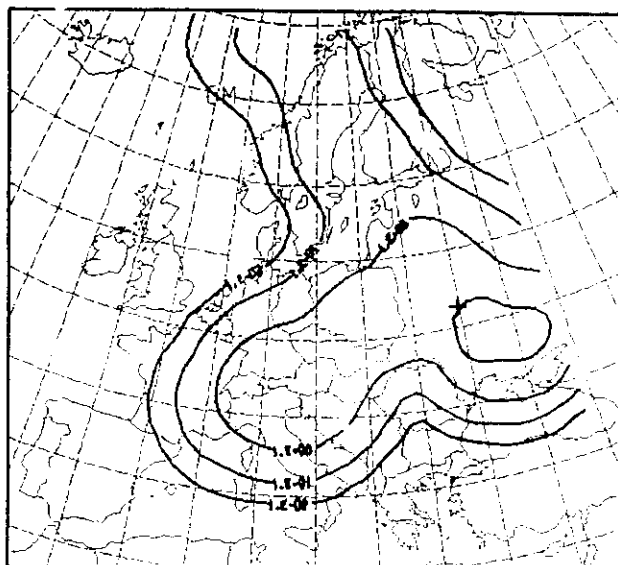
ARIES-I - APOLLO Model Output - Case: CHERNOBYL_1
C137 AIR CONCENTRATION (BQ/MC)



TIME 30/04/86 00:00

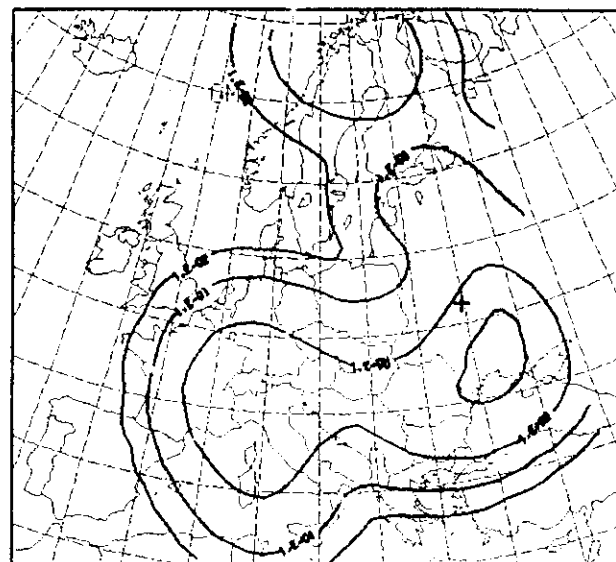
11

ARIES-I - APOLLO Model Output - Case: CHERNOBYL_1
C137 AIR CONCENTRATION (BQ/MC)



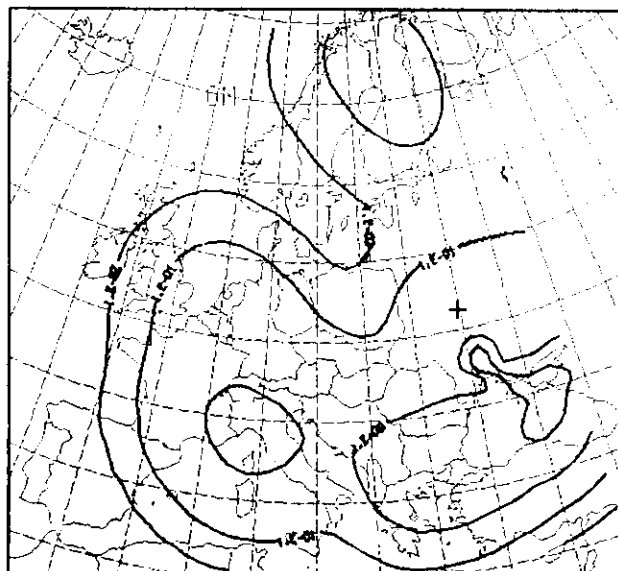
TIME 01/05/86 00:00

ARIES-I - APOLLO Model Output - Case: CHERNOBYL_1
C137 AIR CONCENTRATION (BQ/MC)



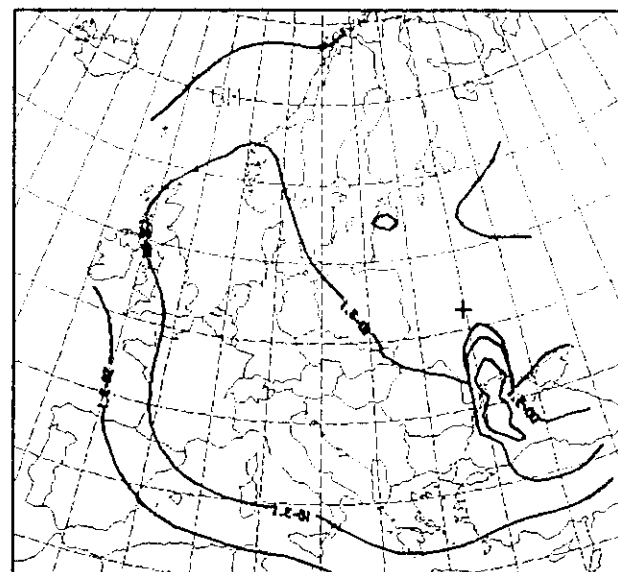
TIME 02/05/86 00:00

ARIES-I - APOLLO Model Output - Case: CHERNOBYL_1
C137 AIR CONCENTRATION (BQ/MC)



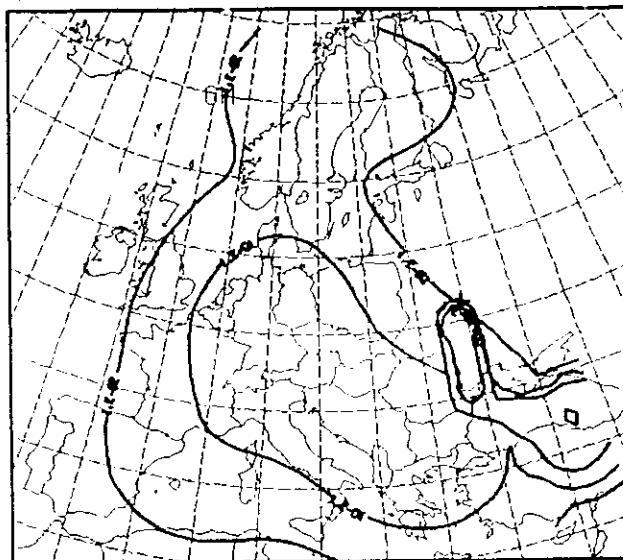
TIME 03/05/86 00:00

ARIES-I - APOLLO Model Output - Case: CHERNOBYL_1
C137 AIR CONCENTRATION (BQ/MC)



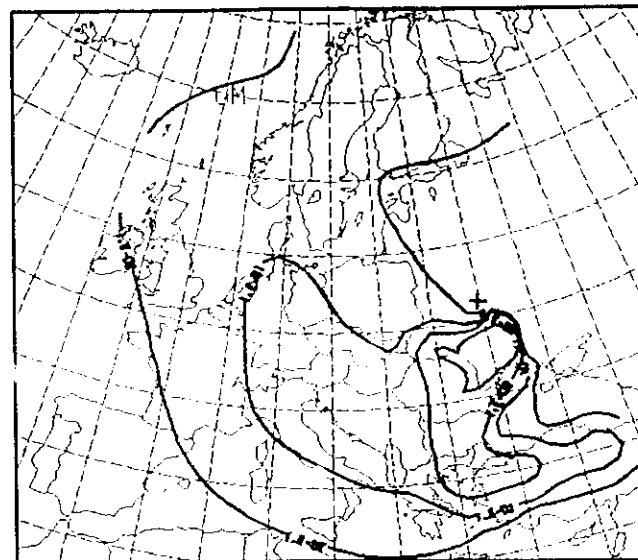
TIME 04/05/86 00:00

ARIES-I - APOLLO Model Output - Case: CHERNOBYL_1
C137 AIR CONCENTRATION (Bq/mC)



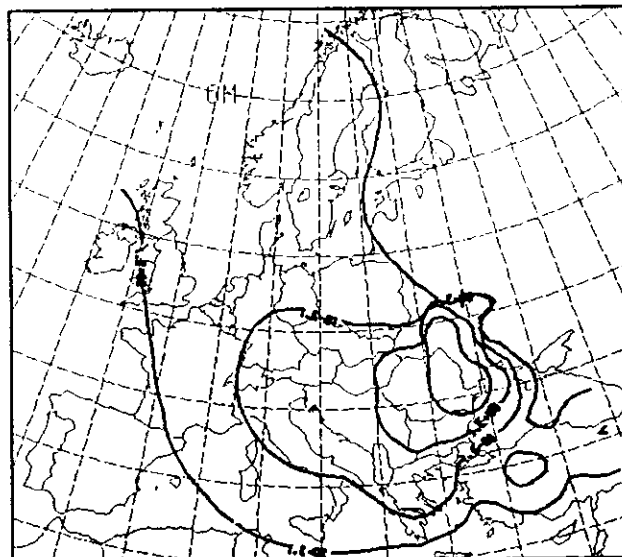
TIME 05/05/86 00:00

ARIES-I - APOLLO Model Output - Case: CHERNOBYL_1
C137 AIR CONCENTRATION (Bq/mC)



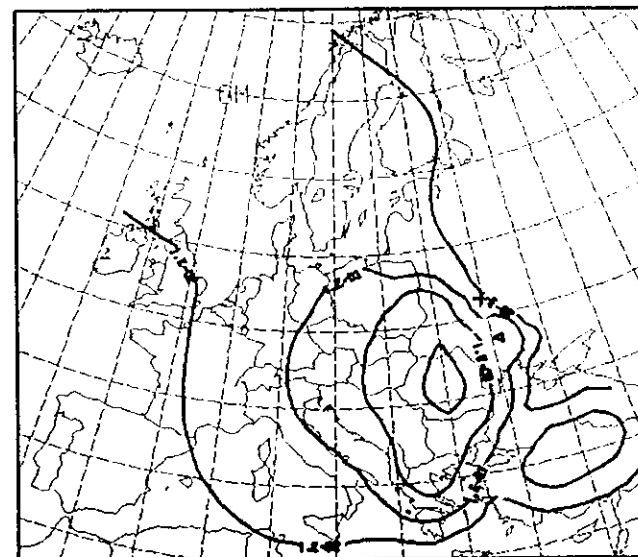
TIME 06/05/86 00:00

ARIES-I - APOLLO Model Output - Case: CHERNOBYL_1
C137 AIR CONCENTRATION (Bq/mC)



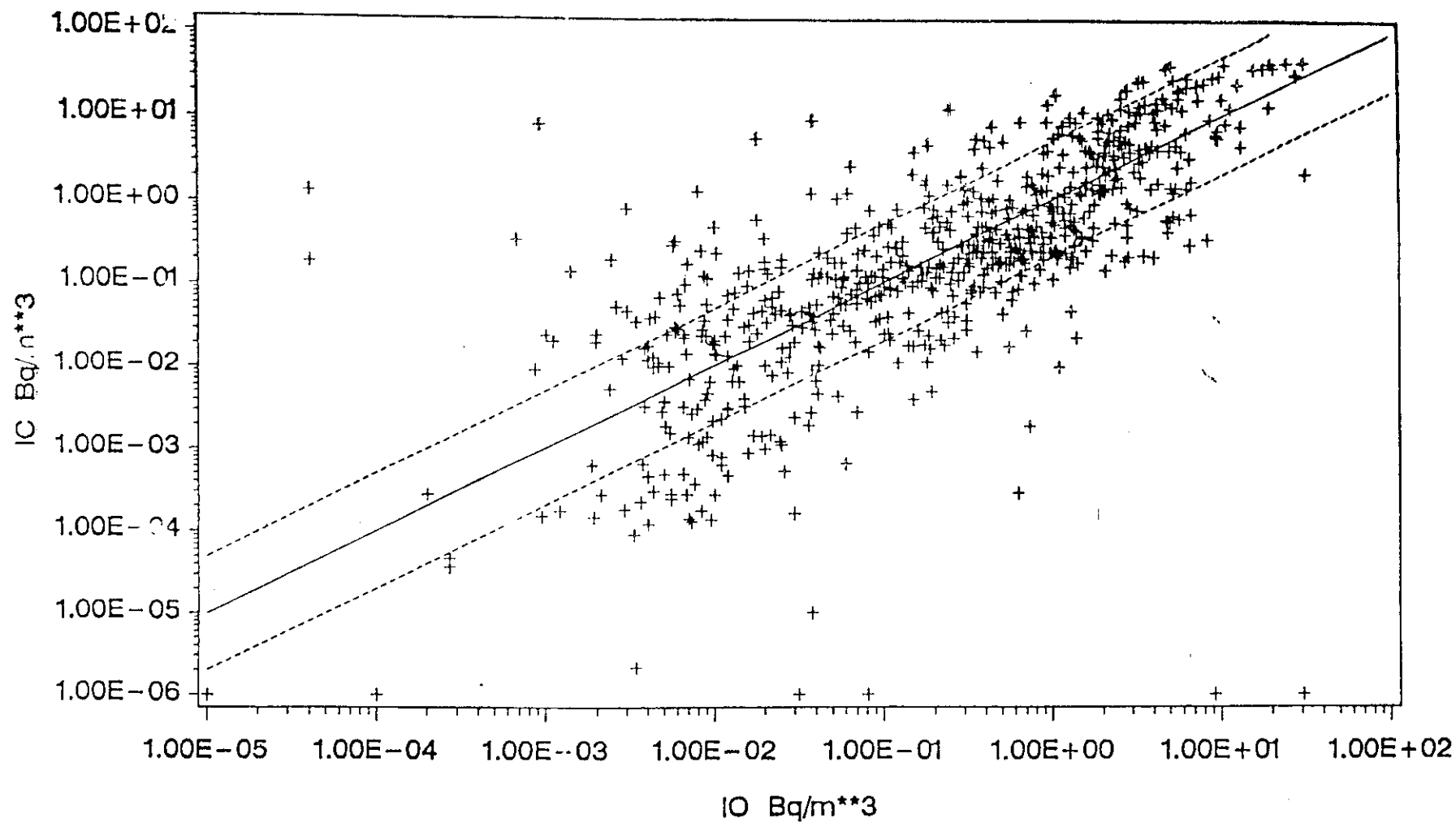
TIME 07/05/86 00:00

ARIES-I - APOLLO Model Output - Case: CHERNOBYL_1
C137 AIR CONCENTRATION (Bq/mC)



TIME 08/05/86 00:00

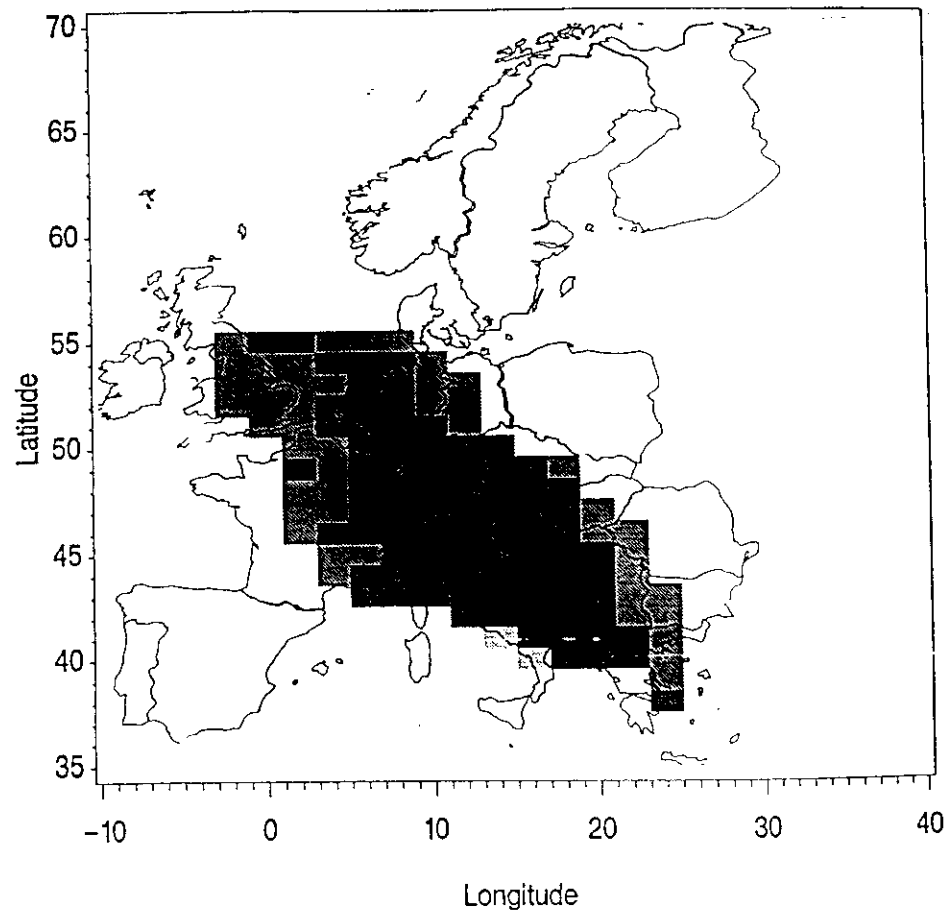
– Global Scatter Diagram – (model = mod5)
IO vs. IC (area A air concentration)



FA2 = 34 % FA5 = 69 % FOEX = 46 %

-Space Figure of Merit- (Model=mod5)

, -131 day = 86/05/02 (area A air concentration)



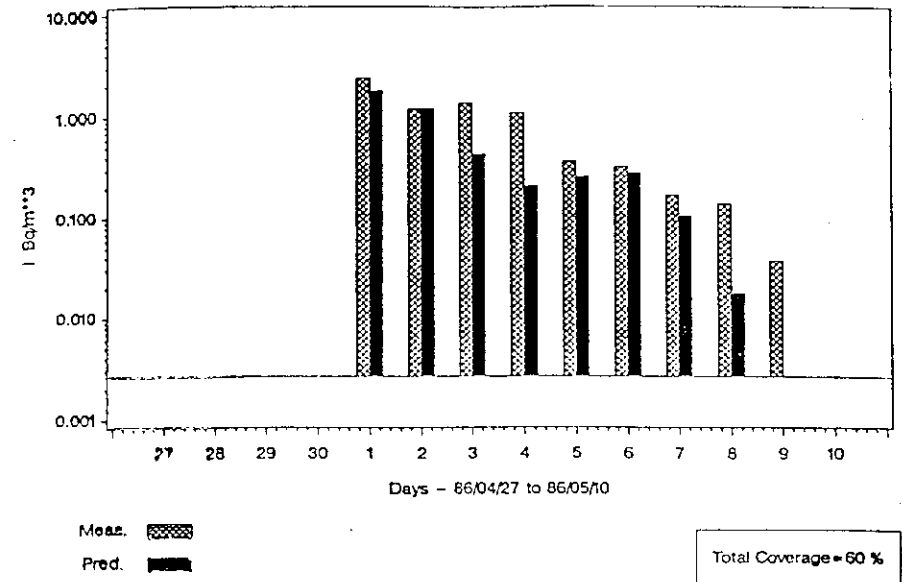
Coverage = 64 %

Significant level = 1 Bq/m³

Light gray=meas. Medium gray=pred. Dark gray=overlap.

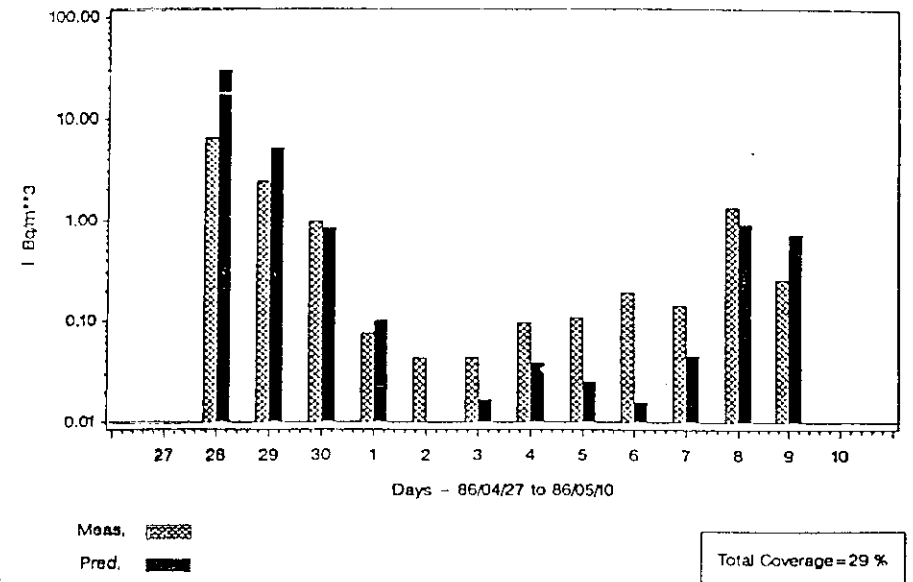
- Time evolution of daily average concentration -

1-131 locality = CASACCIA (Model = mod5)



- Time evolution of daily average concentration -

1-131 locality = STOCKHOLM (Model = mod5)



ARCO

Run a) $\sigma_v(z) = \sigma_v^m(z_i) \exp(-1/2(z-z_i)/h)$

T_L Hanna (1982)

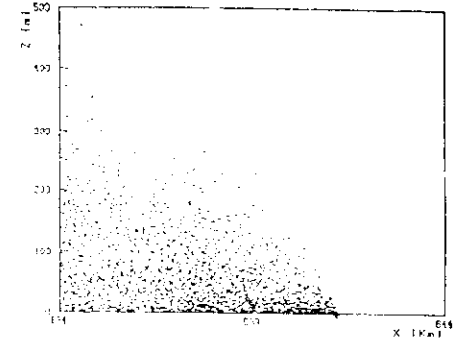
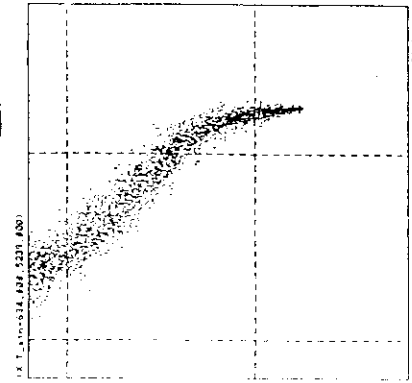
Run b) σ_v as Run a)

$T_L = 750$ s (Neumann, 1978)

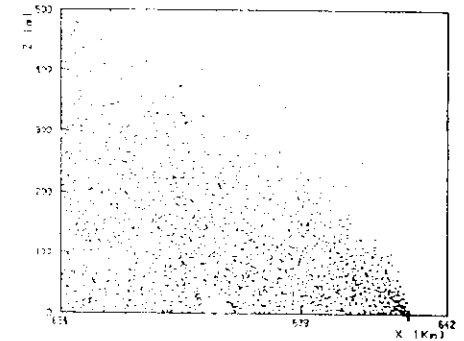
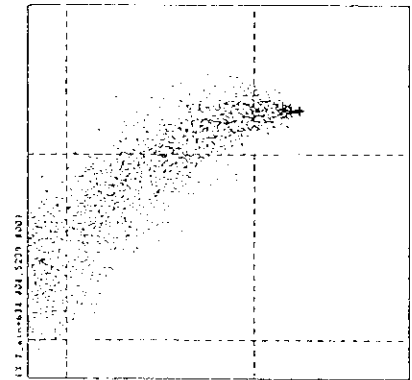
Run c) σ_v Hanna (1982)

$T_L = 750$ s

	CIC/Q		σ_y	
	Bias	NMSE	Bias	NMSE
Run a)	5.7	3.3	-1005	1.35
Run b)	0.5	0.6	-607	0.50
Run c)	1.8	1.4	-972	1.15



Run b



Run c

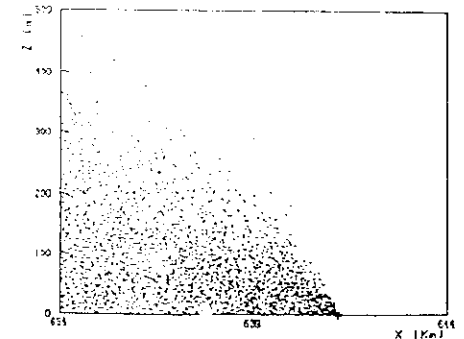
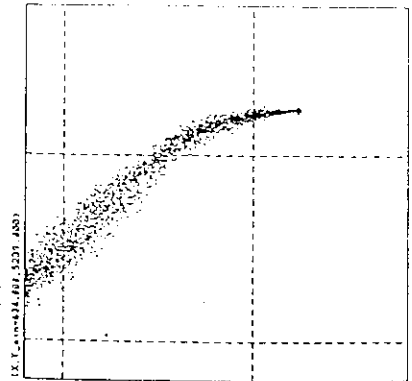


Fig. 2. Particle display on x-y (left) and x-z (right) planes, SIESTA experiment no. 1, 15/11/85, 12:00.

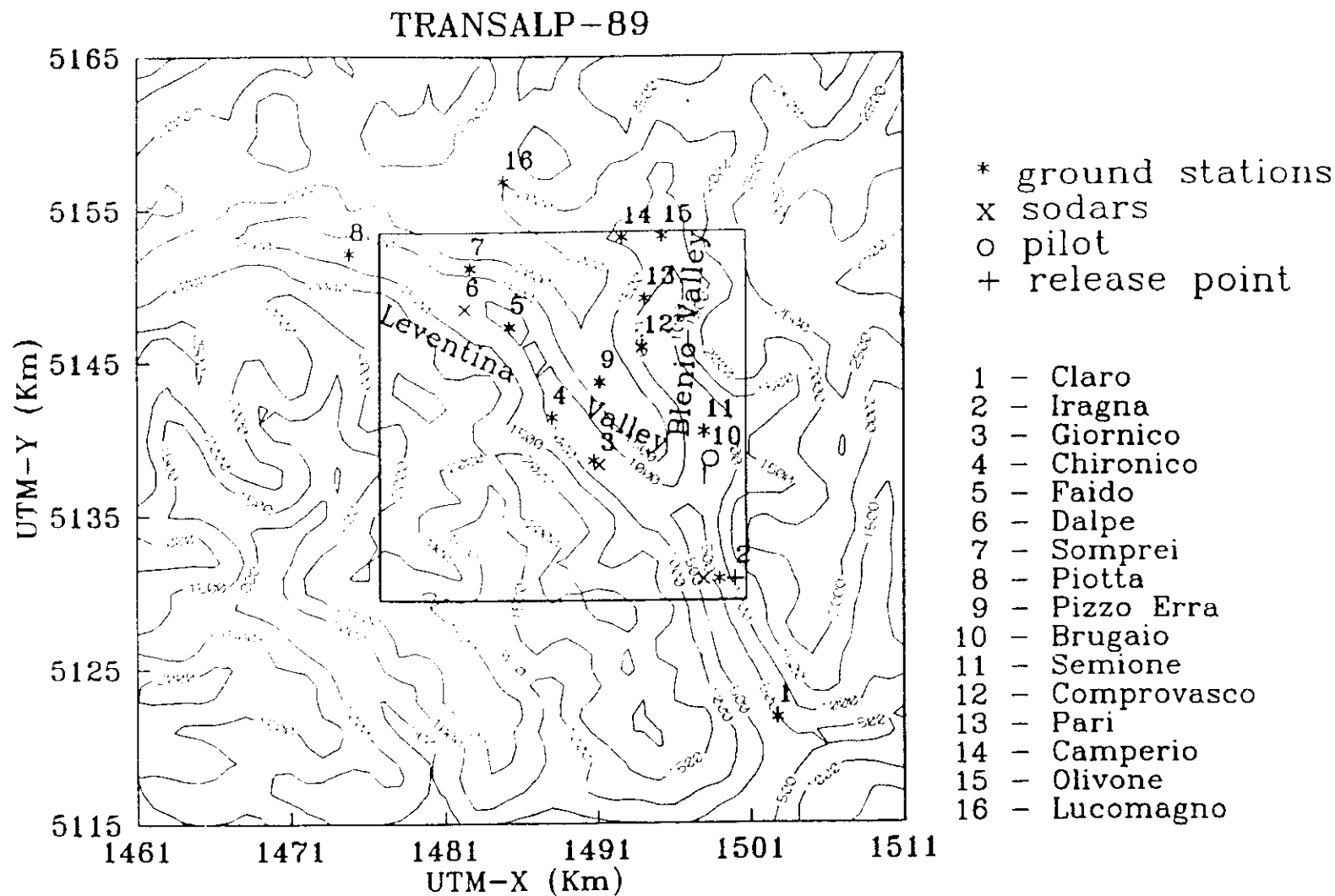
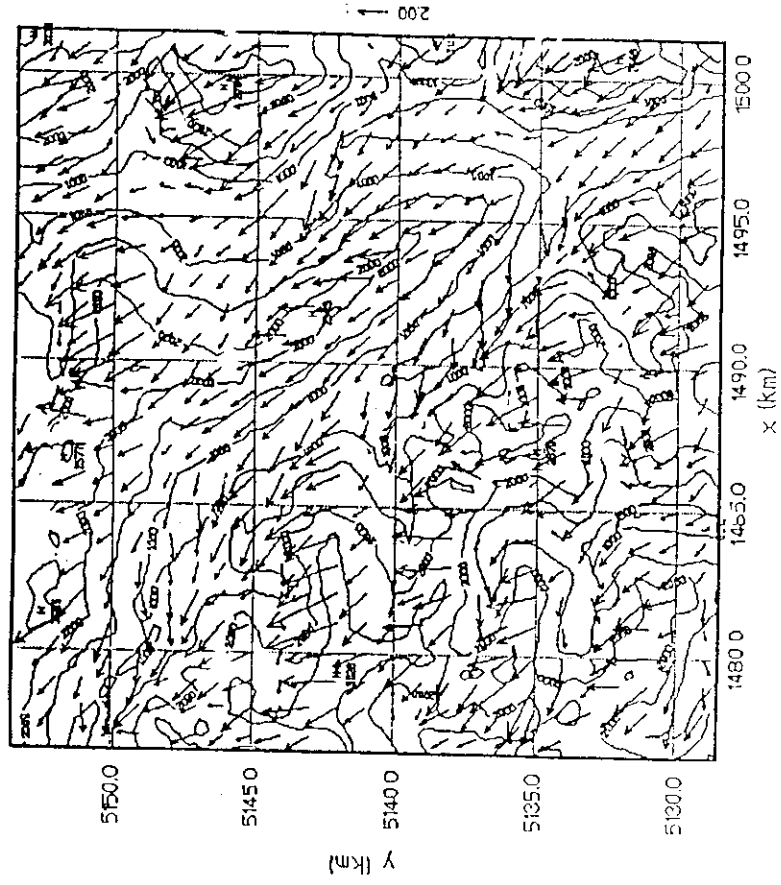
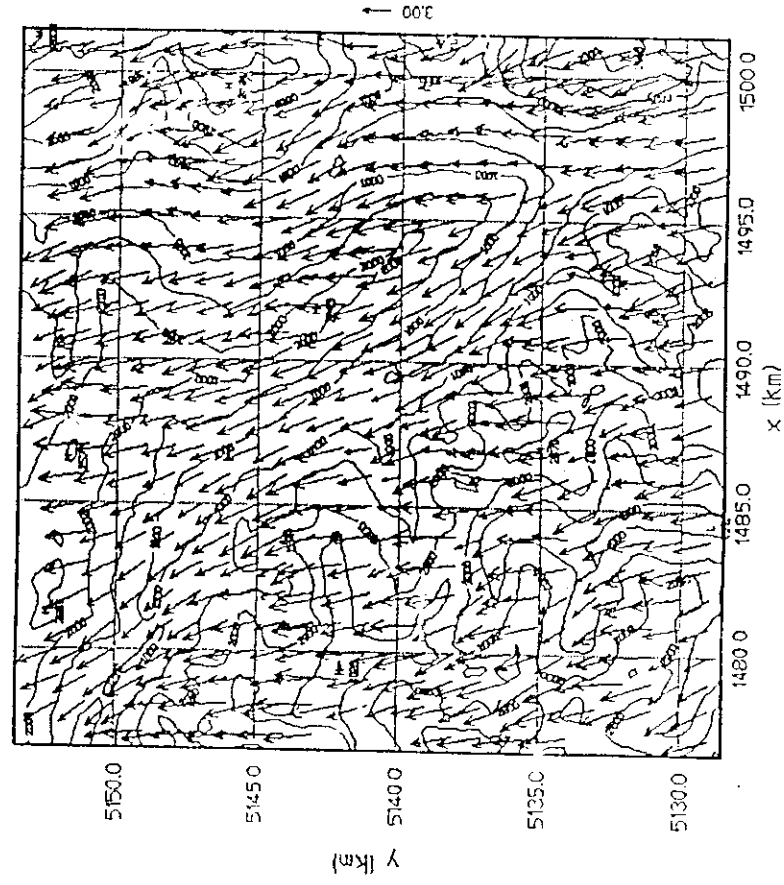


Figure 1



Wind direction and speed at $z=10.0$ m

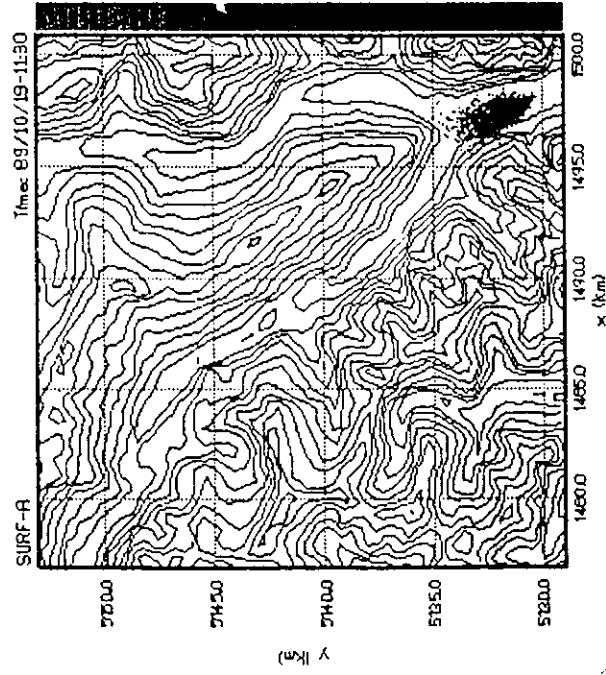
Figure 5a



Wind direction and speed at $z=190.1$ m

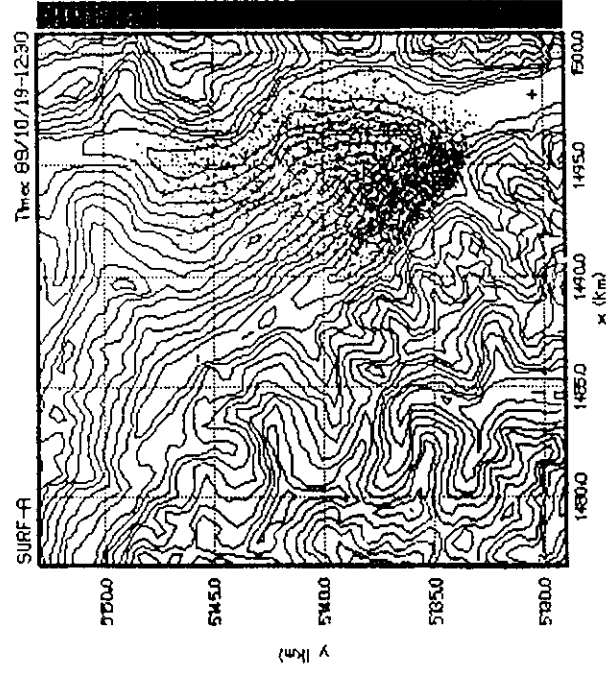
Figure 5b

ARIES-W - Arco



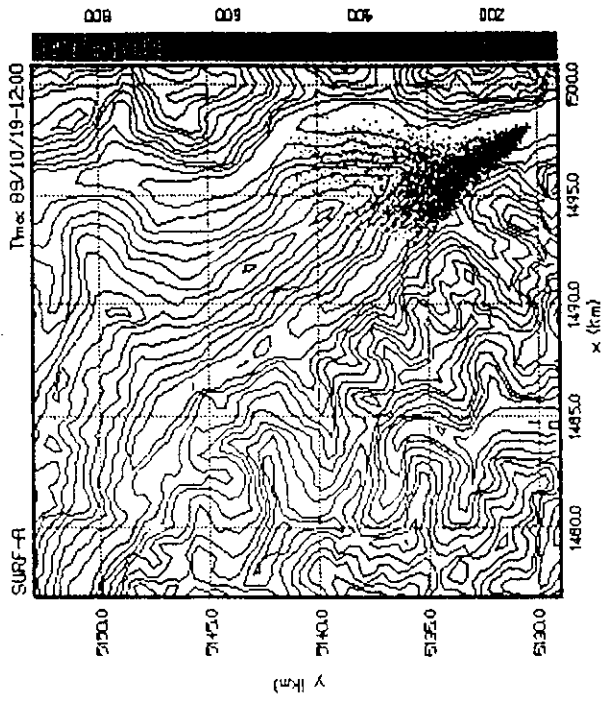
Particle display on plane XY

ARIES-W - Arco



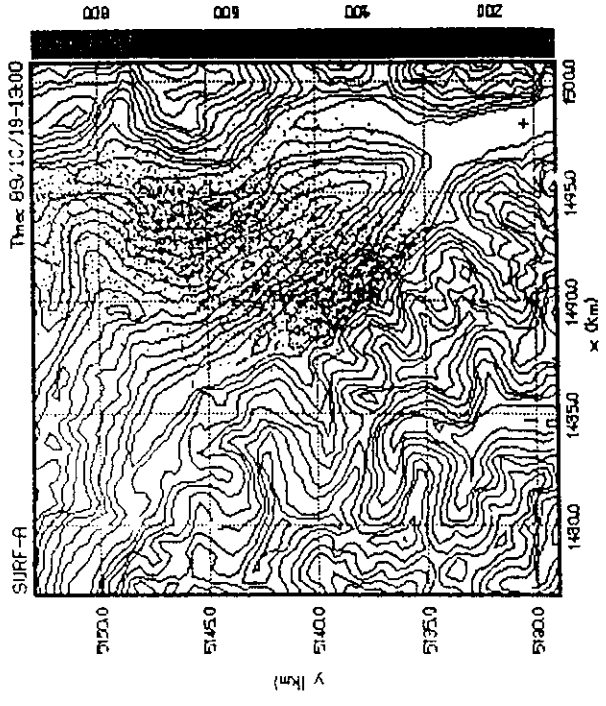
Particle display on plane XY

ARIES-W - Arco



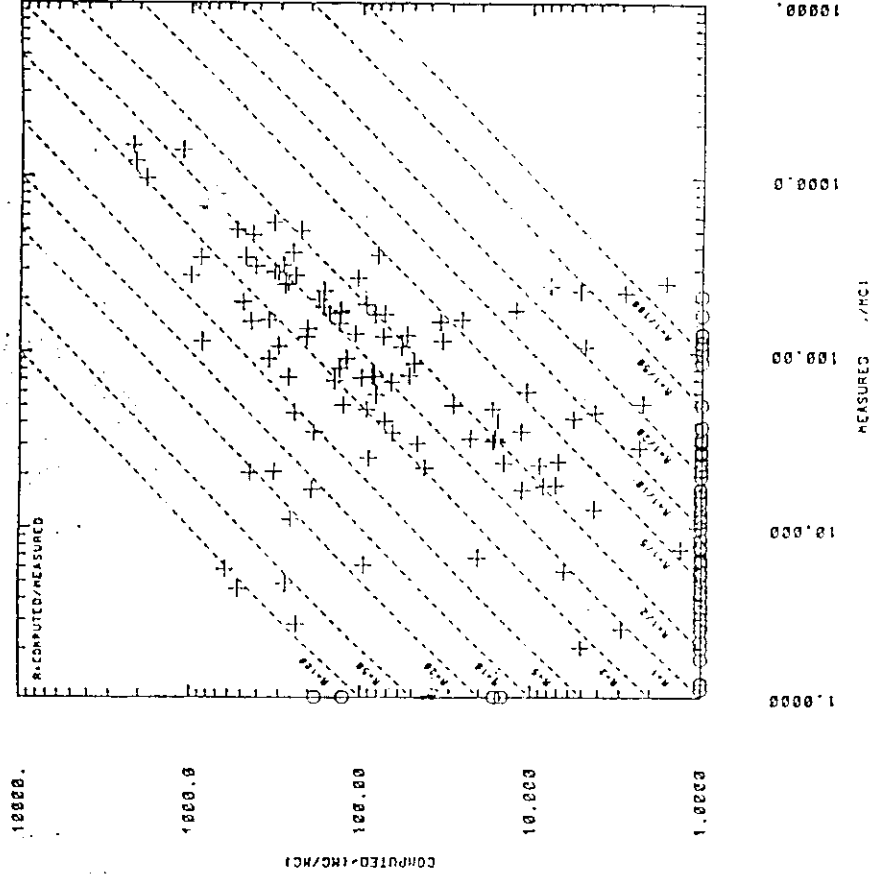
Particle display on plane XY

ARIES-W - Arco



Particle display on plane XY

1/2 hour concentr.



time-integrated concentr.

	Mean (ng/m ³)	St.Dev. (ng/m ³)	Max (ng/m ³)	Top_10 (ng/m ³)	FB	NNR	CORRE
CBS.	564.5	733.0	3066.5	1511.6	-	-	-
ARCO	809.3	918.2	4672.4	1801.6	-0.127	0.381	0.87
SPRAY	633.7	679.3	3452.0	1425.2	0.048	0.795	0.57

maximum concentr.

	Mean (ng/m ³)	St.Dev. (ng/m ³)	Max (ng/m ³)	Top_10 (ng/m ³)	FB	NNR	CORRE
CBS.	303.7	347.5	1502.3	684.5	-	-	-
ARCO	458.0	480.3	2221.1	998.6	-0.405	0.370	0.88
SPRAY	303.8	298.8	1553.3	646.3	0.0002	0.855	0.70

