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

"Lagrangian Particle Dispersion Modeling in Mesoscale Applications"

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College on Atmospheric Boundary Layer and Air Pollution Modelling

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LAGRANGIAN PARTICLE DISPERSION MODELING IN MESOSCALE APPLICATIONS

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OUTLINE

1. Introduction
   - short overview of Lagrangian particle dispersion (LPD) modeling
   - advances in computer technology
   - advances in meteorological mesoscale modeling
2. Mesoscale atmospheric dispersion
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   - examples
3. Implementation of LPD models for mesoscale applications
   - simplifications: Markov chain & fully random walk
   - hybrid models
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     - particle model ⟹particle model
     - particle/puff model
   - source- and receptor-oriented modeling
   - benchmark tests
4. Meteorological input
   - turbulence parameterization

5. Concentration calculations
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   - demonstration of a simple uniform kernel
   - effect of grid resolution and smoothing
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   - transformations and removal processes
   - dry deposion
   - heavy particles
   - buoyancy
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   - operational systems (RAMS-ERDAS, PROWESS)

LAGRANGIAN PARTICLE DISPERSION MODELS

◇

EXAMPLES

(Obukhov, 1959)	atmospheric dispersion as
(Smith, 1968)	a Markov chain process
(Hall, 1975)	surface layer &
(Reid, 1979)	vegetation canopies
(Wilson et al., 1981)	
(Legg and Raupach, 1982)	
(Ley and Thomson, 1983)	
(Davis, 1983)	neutral boundary layer
(Lamb, 1978)	convective boundary layer
(Bærentsen and Berkowicz, 1984)	
(De Baas et al., 1986)	
(Luhar and Britter, 1990)	
(Hurley and Physick, 1993)	
(McNider, 1981)	mesoscale systems
(Pielke et al., 1983)	
(Ettling et al., 1986)	
(Segal et al., 1988)	
(Yamada and Bunker, 1988)	
(Pielke et al., 1991)	
(Uliasz, 1994)	

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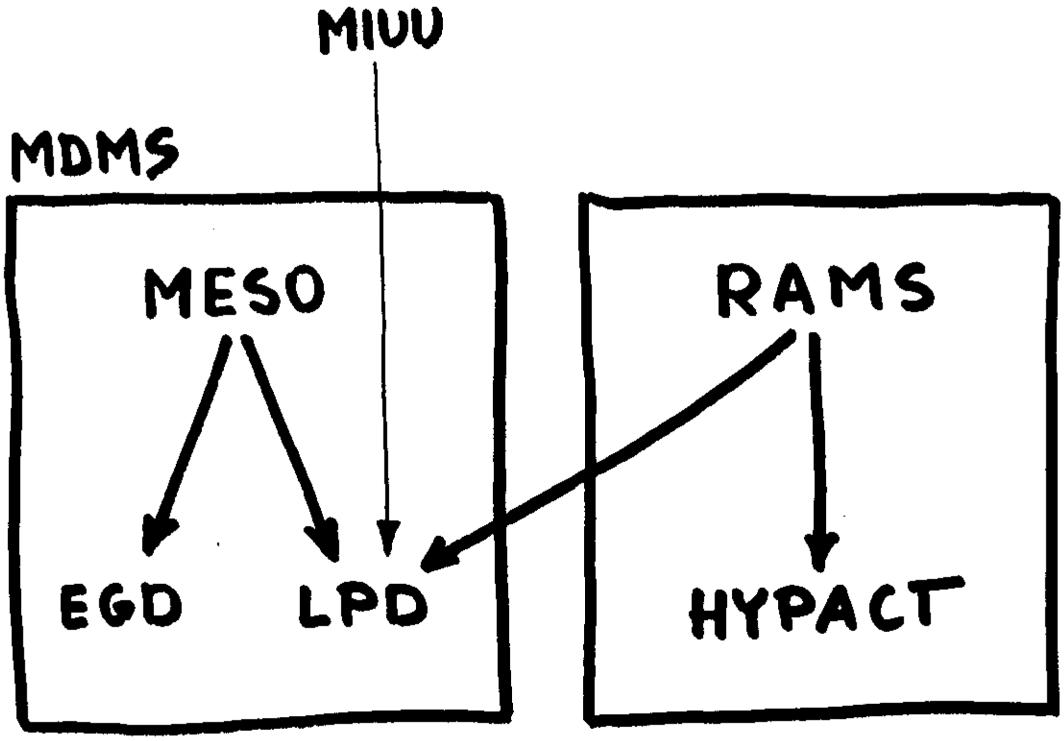


MDMS - Mesoscale Dispersion Modelling System

RAMS - Regional Atmospheric Modelling System

LPD - Lagrangian Particle Dispersion model

HYPACT - Hybrid Particle and Concentration Transport

EGD - Eulerian Grid Dispersion model

MESO - 3D mesoscale meteor. model

MIUU - Uppsala University mesoscale model

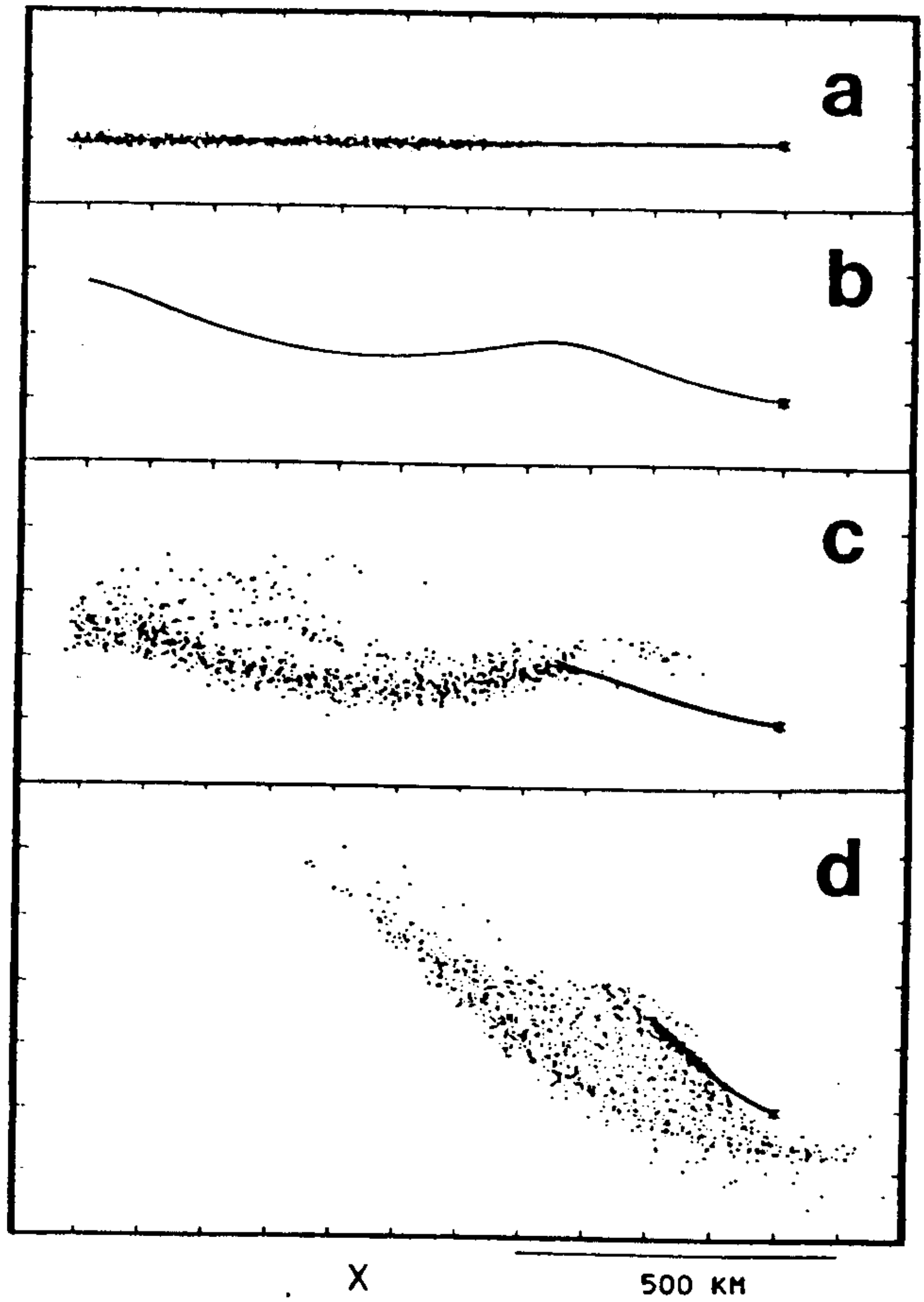


Figure 1.10: Instantaneous depiction of Mt. Isa plume simulation after 42 h for four increasingly realistic flow fields: (a) PBL turbulence but no PBL shear, Coriolis force, or horizontal temperature gradient; (b) Coriolis force and PBL shear but no PBL turbulence or horizontal temperature gradient; (c) PBL turbulence, PBL shear, and Coriolis force but no horizontal temperature gradient; (d) same as (c) except with a north-south horizontal temperature gradient (from McNider et al., 1988).

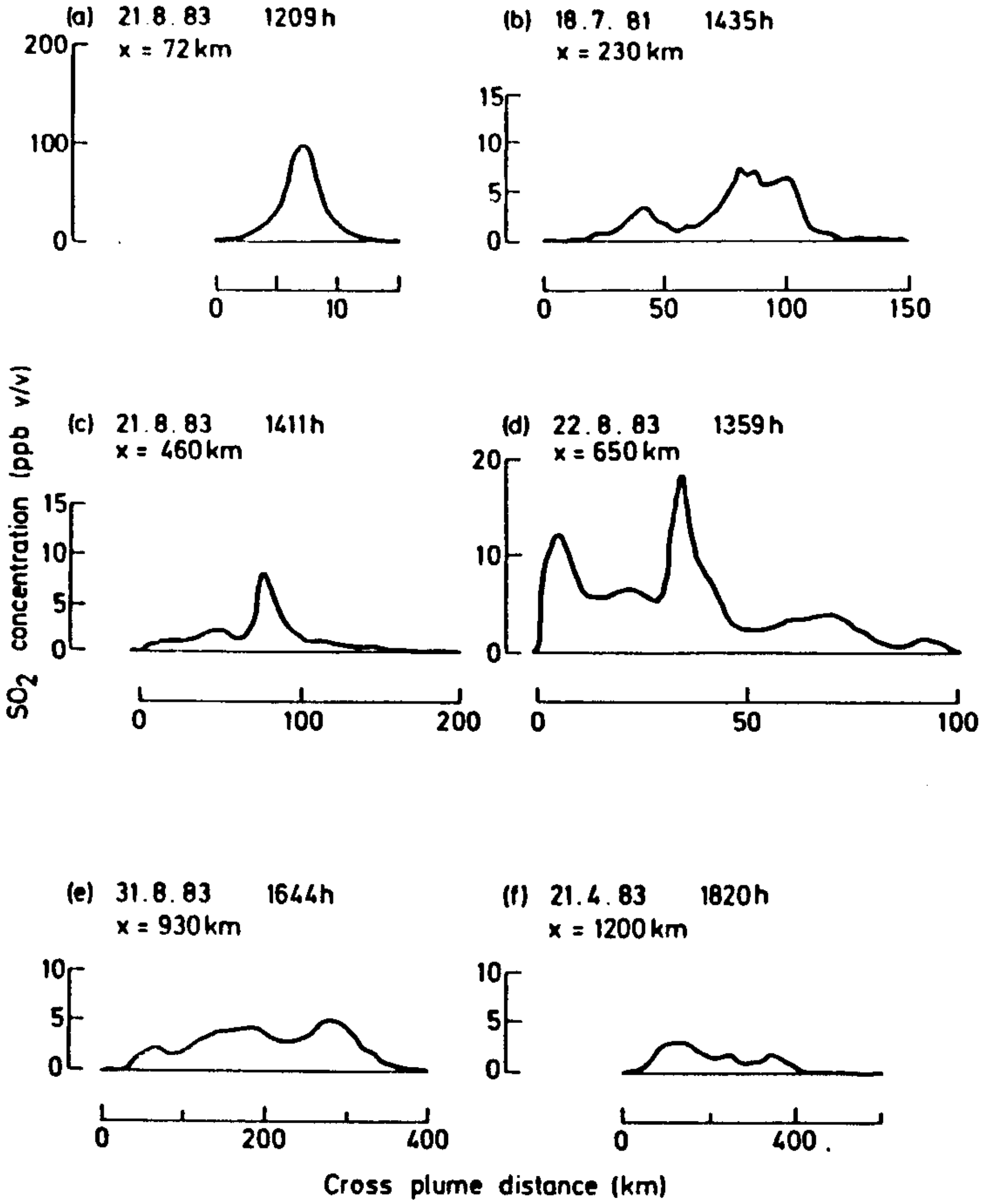


Figure 1.2: Variations of Mt. Isa plume SO_2 crosswind concentration distributions with distance from source as measured by aircraft (from Carras and Williams, 1988).

SAMPLE RESULTS:
AIR POLLUTION IN SHENANDOAH NATIONAL PARK
(complex terrain in the eastern United States)

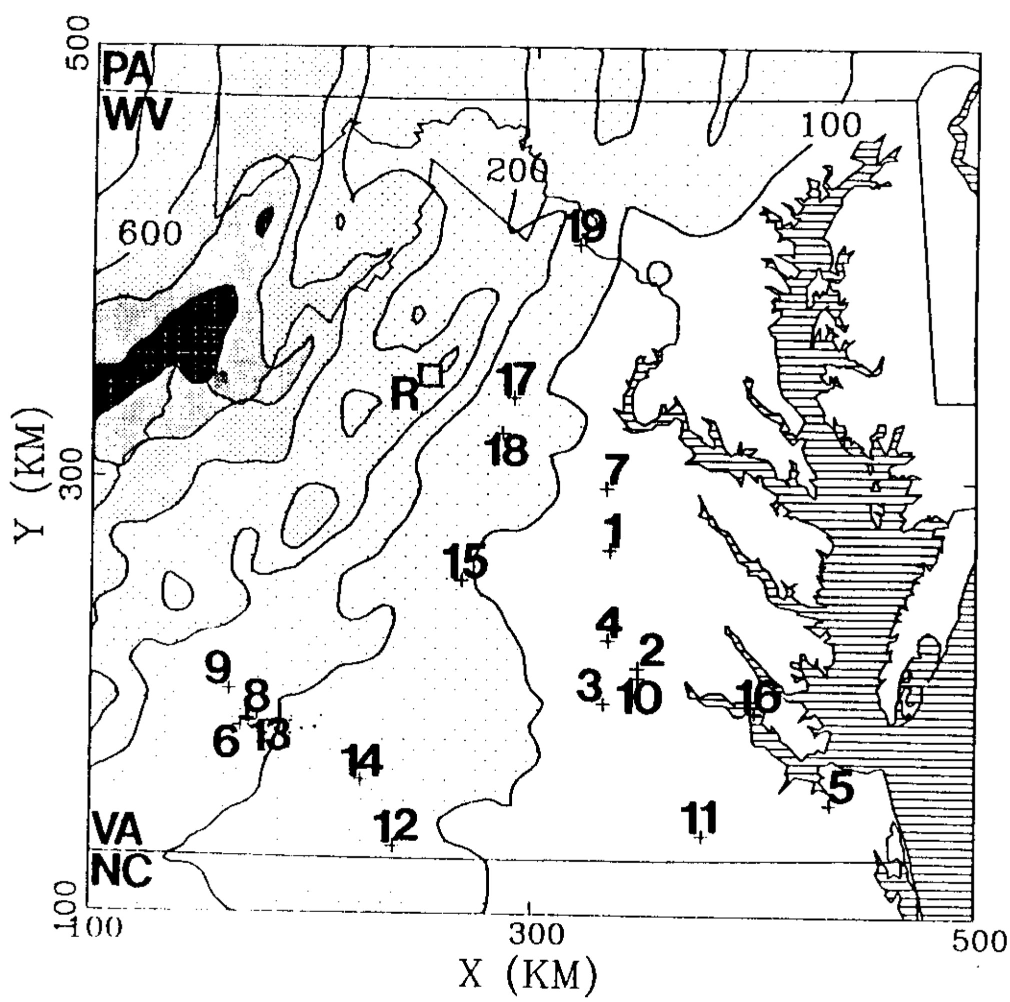


Figure 2. Central part of the modeling domain with terrain topography and locations of the emission sources (crosses - numbers) and the receptor in Shenandoah National Park (square - R). Water surfaces are indicated by horizontal hatching. Terrain height contours are 100, 200, 400, 600, 800, 1000 m.

Shenandoah simulation

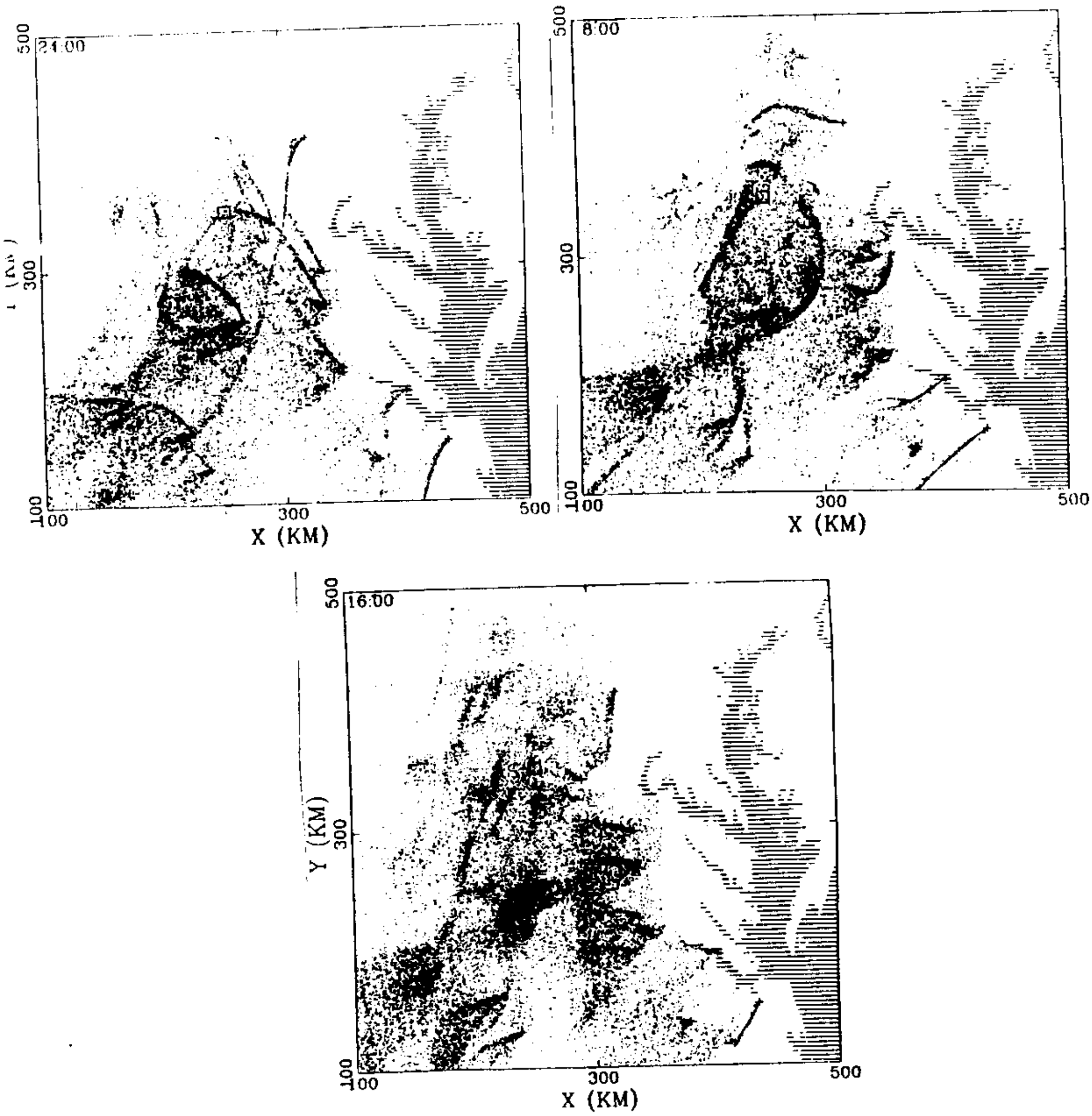
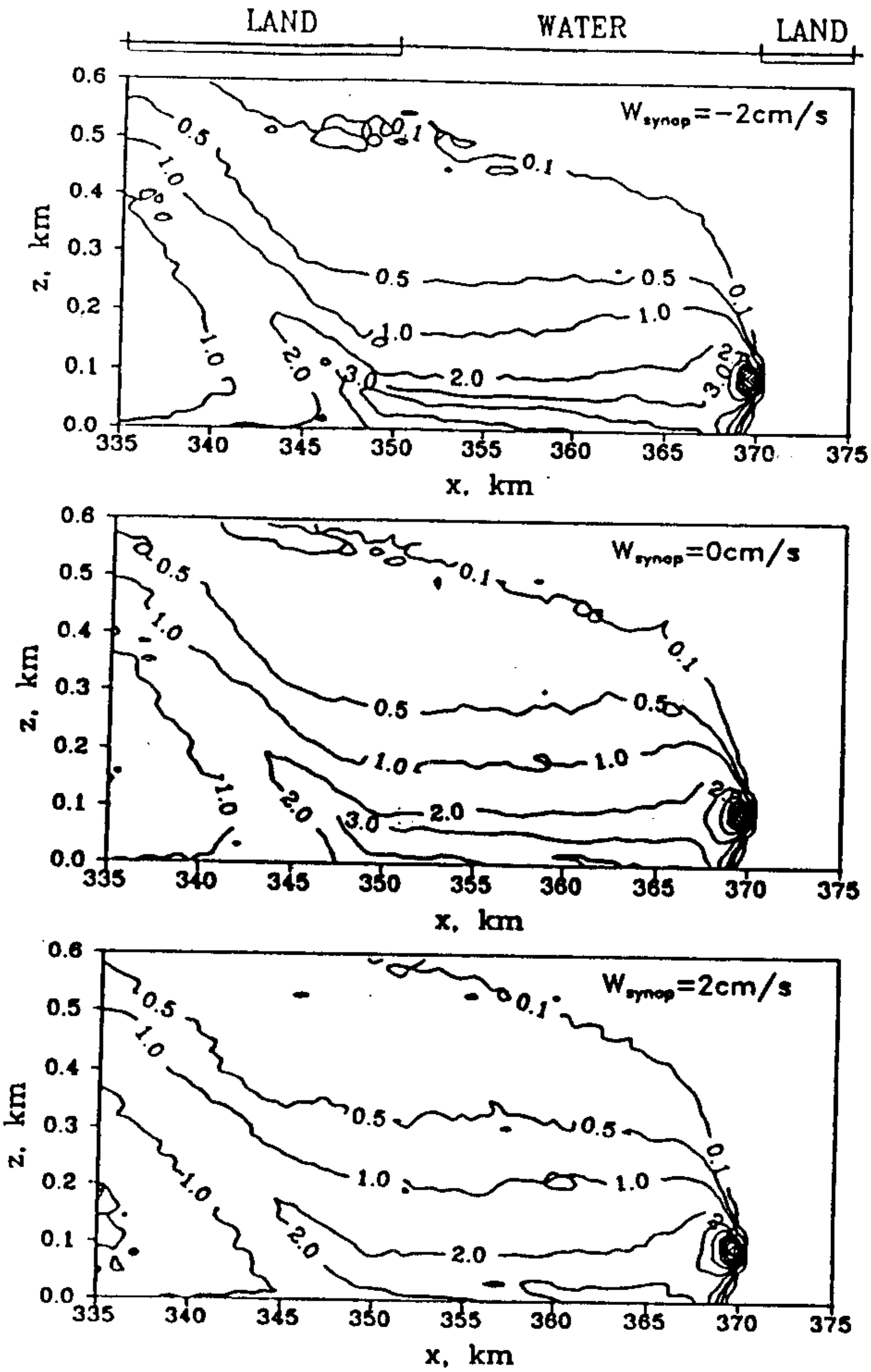


Figure 3. Plan-view projections of distribution of airborne particles at 2100 LST on day 2, and 0800 and 1600 LST on day 3.



Simulated crosswind integrated concentration in the Øresund tracer experiment on June 4, 1984 for various synoptic vertical motions

CONCENTRATION CALCULATIONS

- **counting particles in a sampling volume**

$$c(x,y,z,t) = \frac{1}{\Delta x_s \Delta y_s \Delta z_s} \sum_{i=1}^{N} m_{pi} I \qquad (1)$$

where

$$I = \begin{cases} 1 & for\ |X_i - x| < \Delta x_s/2\ and\ |Y_i - y| < \Delta y_s/2\ and\ |Z_i - z| < \Delta z_s/2 \\ 0 & otherwise \end{cases},$$

- **kernel density estimator**

$$c(x,y,z) = \sum_{i=1}^{N} \frac{m_{pi}}{h_{xi} h_{yi} h_{zi}} [K(r_x, r_y, r_z) + K(r_x, r_y, r'_z)] \qquad (2)$$

where the kernel K satisfies the condition

$$\frac{1}{h_{xi} h_{yi} h_{zi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} K dx dy dz = 1 \qquad (3)$$

and

$r_x = (X_i - x)/h_{xi}$, $r_y = (Y_i - y)/h_{yi}$, $r_z = (Z_i - z)/h_{zi}$, $r'_z = (Z_i + z)/h_{zi}$.

- **Gaussian kernel**

$$K(r_x, r_y, r_z) = \frac{1}{(2\pi)^{3/2}} \exp\left(-\frac{r_x^2}{2}\right) \exp\left(-\frac{r_y^2}{2}\right) \exp\left(-\frac{r_z^2}{2}\right) \qquad (4)$$

- **parabolic kernel**

$$K(r_x, r_y, r_z) = \frac{15}{8\pi}(1 - r^2) I, \quad I = \begin{cases} 1 & for\ r^2 = r_x^2 + r_y^2 + r_z^2 < 1 \\ 0 & otherwise \end{cases} \qquad (5)$$

- **uniform kernel:**

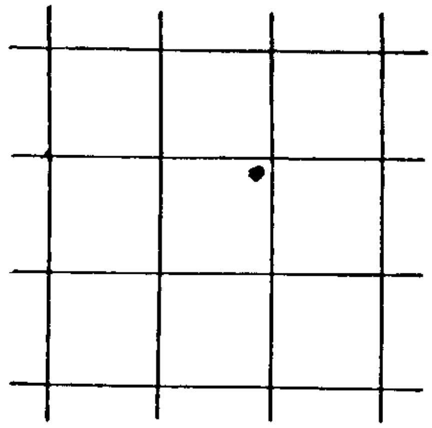
$$K(r_x, r_y, r_z) = \frac{1}{8} I_x I_y I_z, \quad I_\alpha = \begin{cases} 1 & for\ r_\alpha^2 < 1 \\ 0 & otherwise \end{cases}, \qquad \alpha = x, y, z \qquad (6)$$

$h_x << \Delta x$

particle position: .4 .4 .5
bandwidths hx,hz: .0 .0

Z= .5

Y/X	-2.0	-1.0	.0	1.0	2.0
2.0	.0	.0	.0	.0	.0
1.0	.0	.0	.0	.0	.0
.0	.0	.0	100.0	.0	.0
-1.0	.0	.0	.0	.0	.0
-2.0	.0	.0	.0	.0	.0

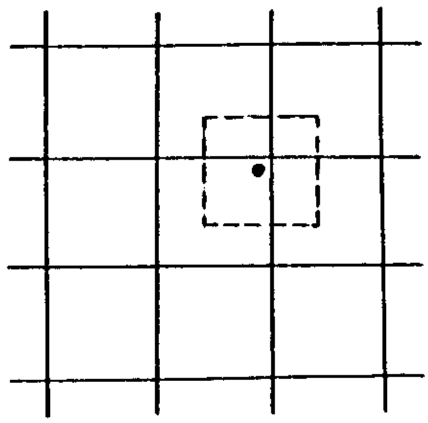


$h_x = 0.5 \Delta x$

particle position: .4 .4 .5
bandwidths hx,hz: 1.0 .0

Z= .5

Y/X	-2.0	-1.0	.0	1.0	2.0
2.0	.0	.0	.0	.0	.0
1.0	.0	.0	24.0	16.0	.0
.0	.0	.0	36.0	24.0	.0
-1.0	.0	.0	.0	.0	.0
-2.0	.0	.0	.0	.0	.0

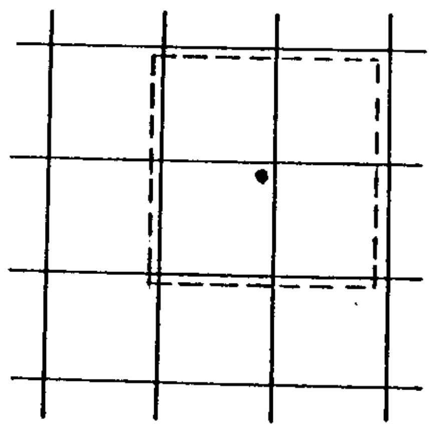


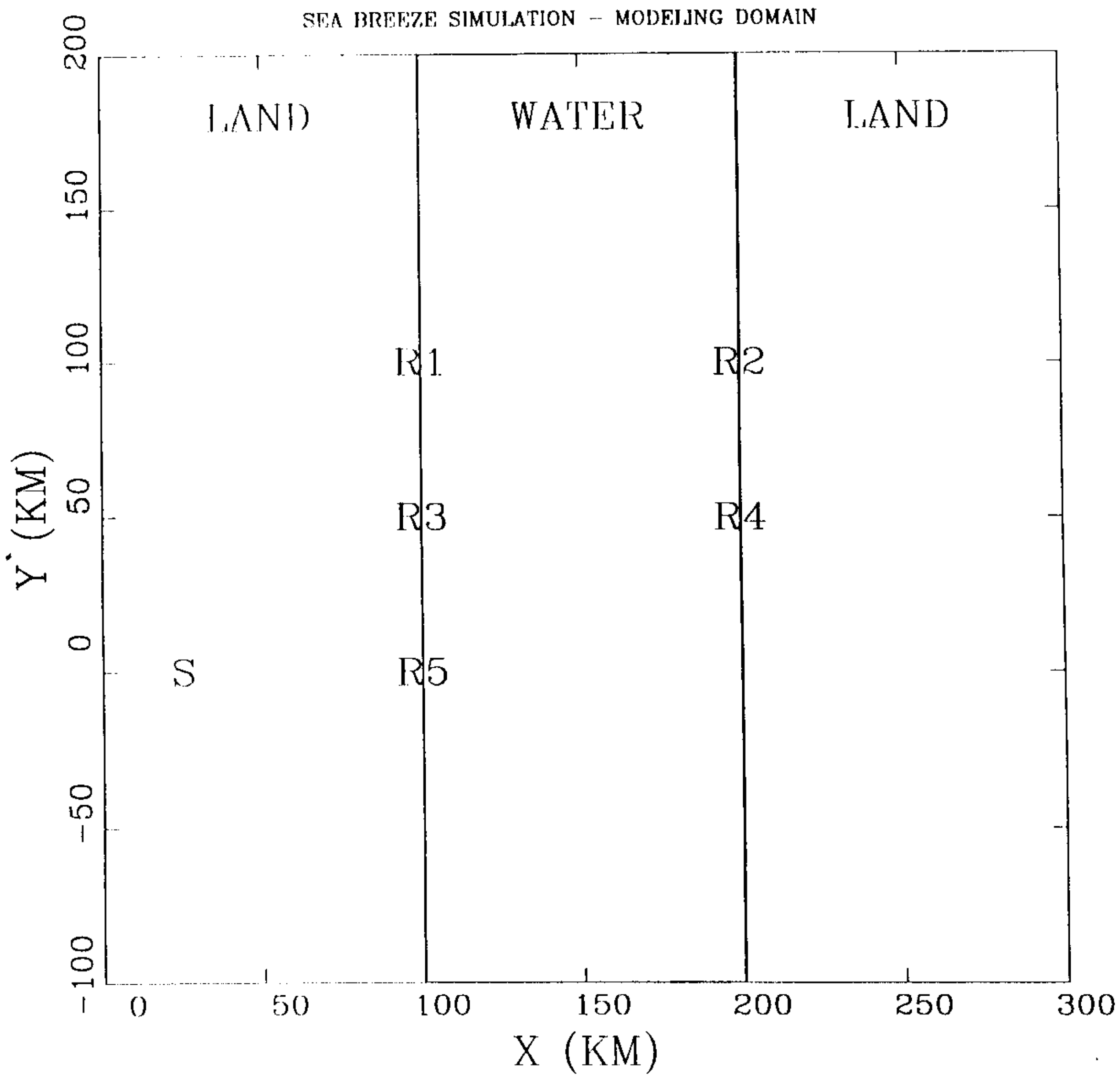
$h_x = \Delta x$

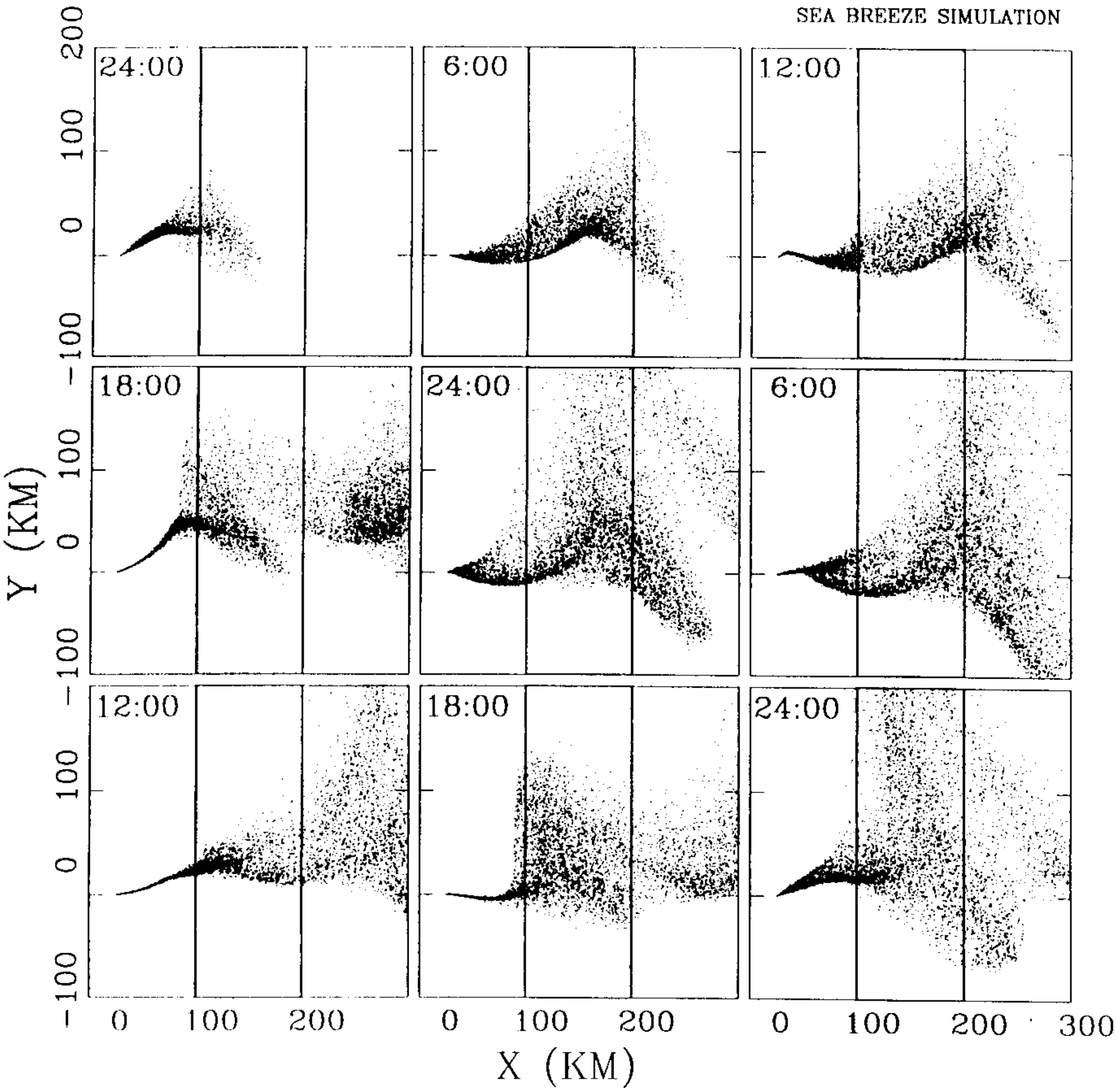
particle position: .4 .4 .5
bandwidths hx,hz: 2.0 .0

Z= .5

Y/X	-2.0	-1.0	.0	1.0	2.0
2.0	.0	.0	.0	.0	.0
1.0	.0	2.3	22.5	20.3	.0
.0	.0	2.5	25.0	22.5	.0
-1.0	.0	.3	2.5	2.3	.0
-2.0	.0	.0	.0	.0	.0

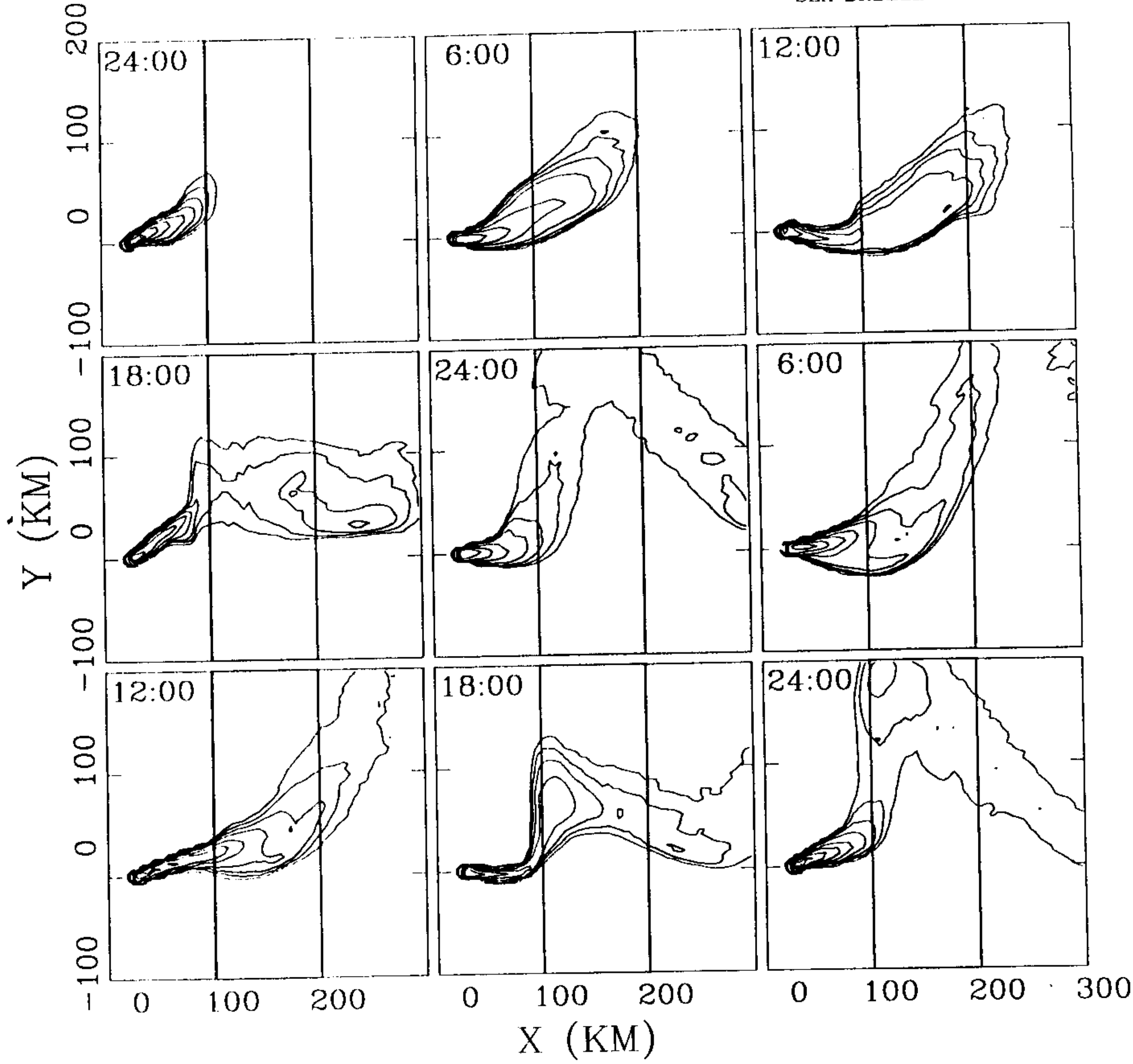


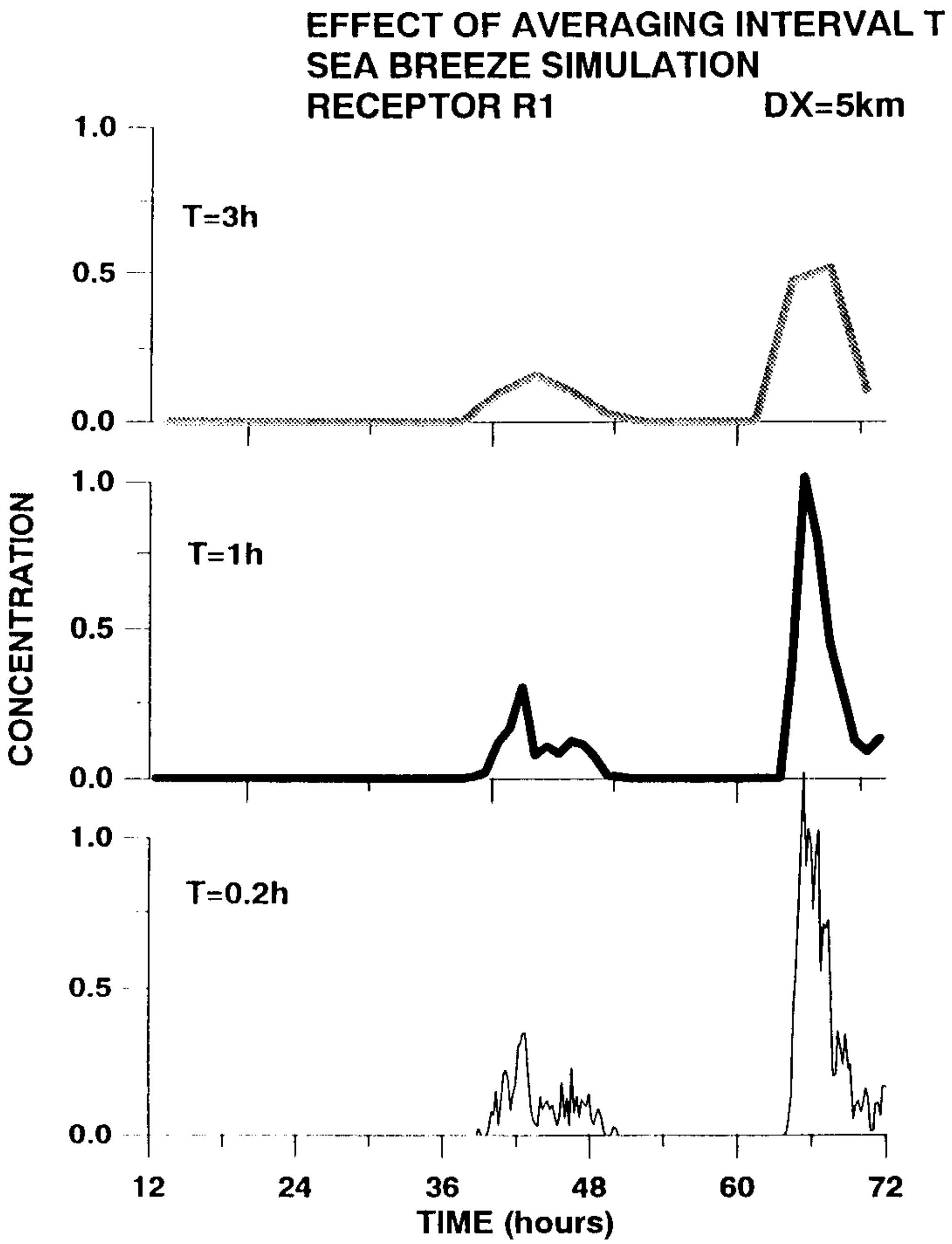

SEA BREEZE SIMULATION – MODELING DOMAIN
LAND
WATER
LAND
R1
R2
R3
R4
S
R5
Y (KM)
X (KM)
200
150
100
50
0
-50
-100
0
50
100
150
200
250
300

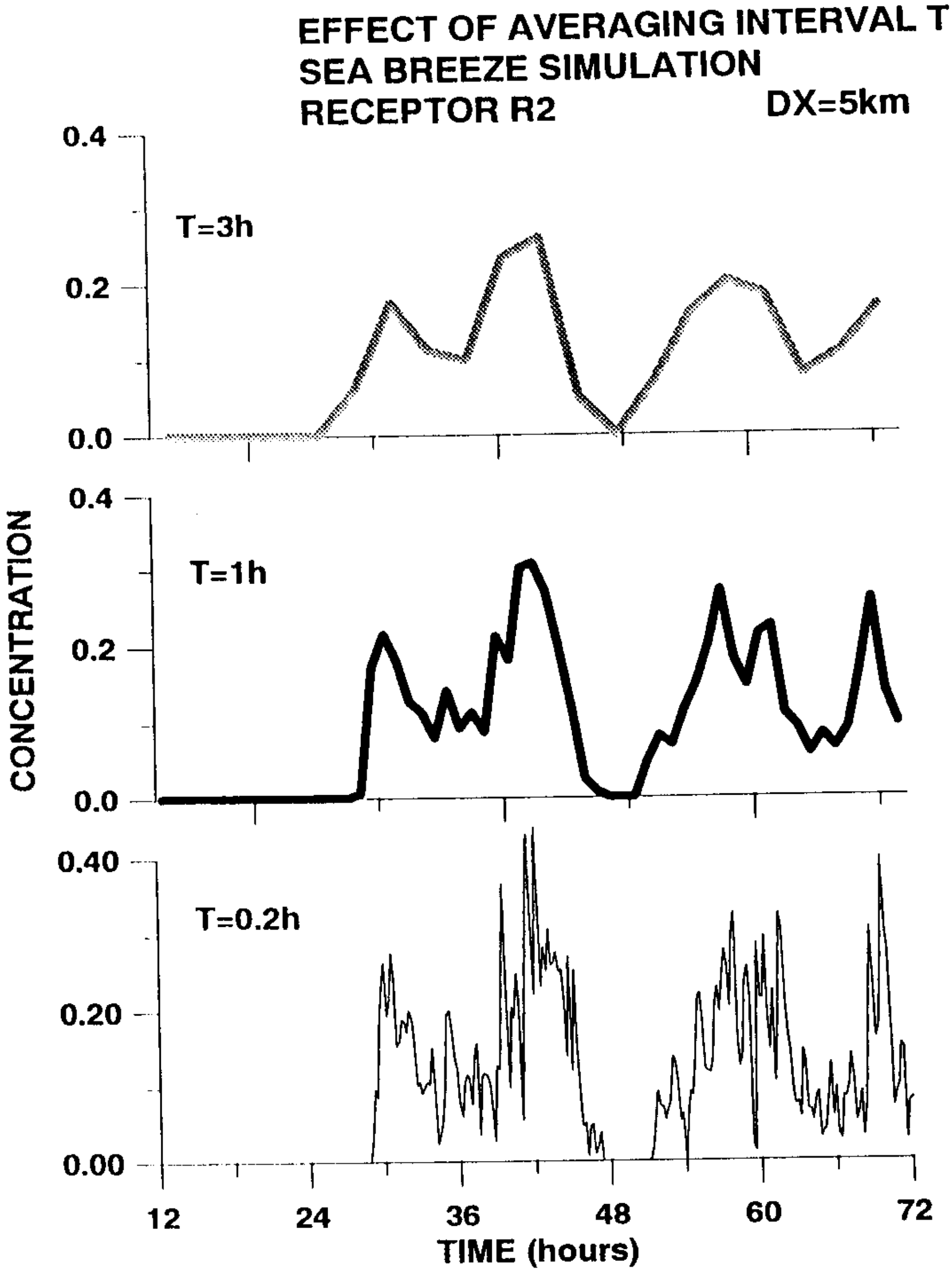


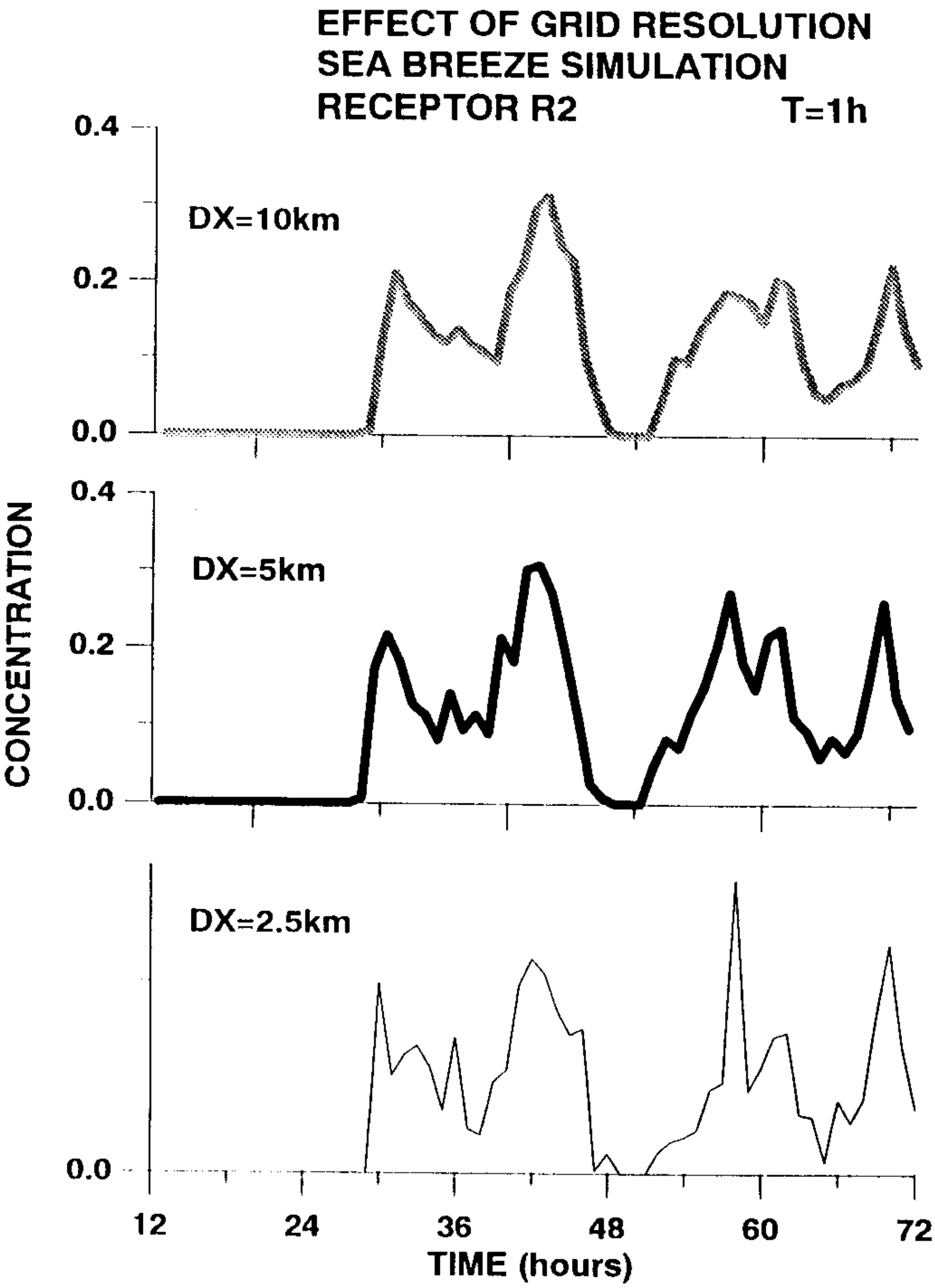
SEA BREEZE SIMULATION
24:00
6:00
12:00
18:00
24:00
6:00
12:00
18:00
24:00
Y (KM)
X (KM)
-100
0
100
200
0
100
200
300

SEA BREEZE SIMULATION

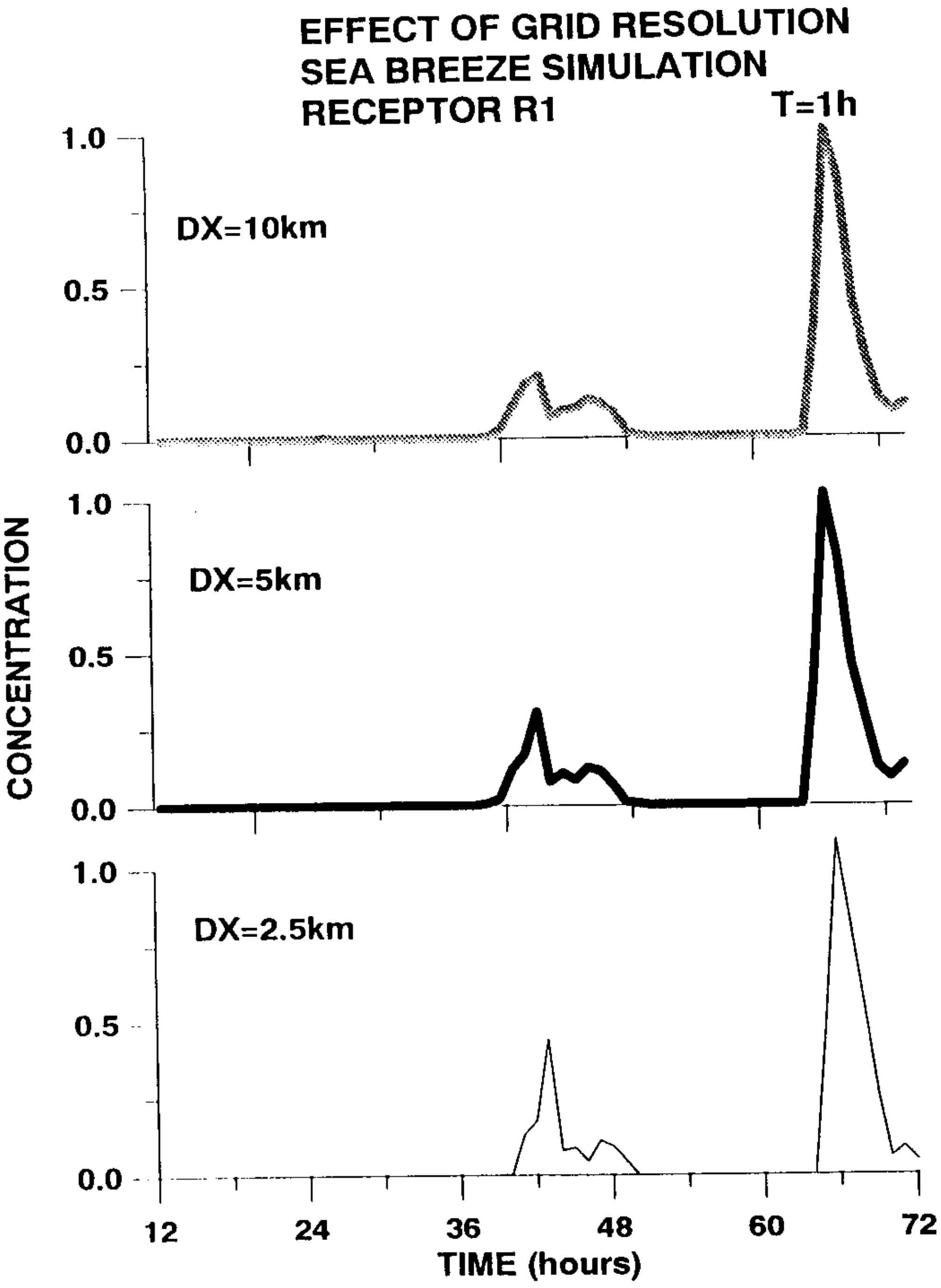



EFFECT OF AVERAGING INTERVAL T
SEA BREEZE SIMULATION
RECEPTOR R1
DX=5km
T=3h
T=1h
T=0.2h
CONCENTRATION
1.0
0.5
0.0
12
24
36
48
60
72
TIME (hours)

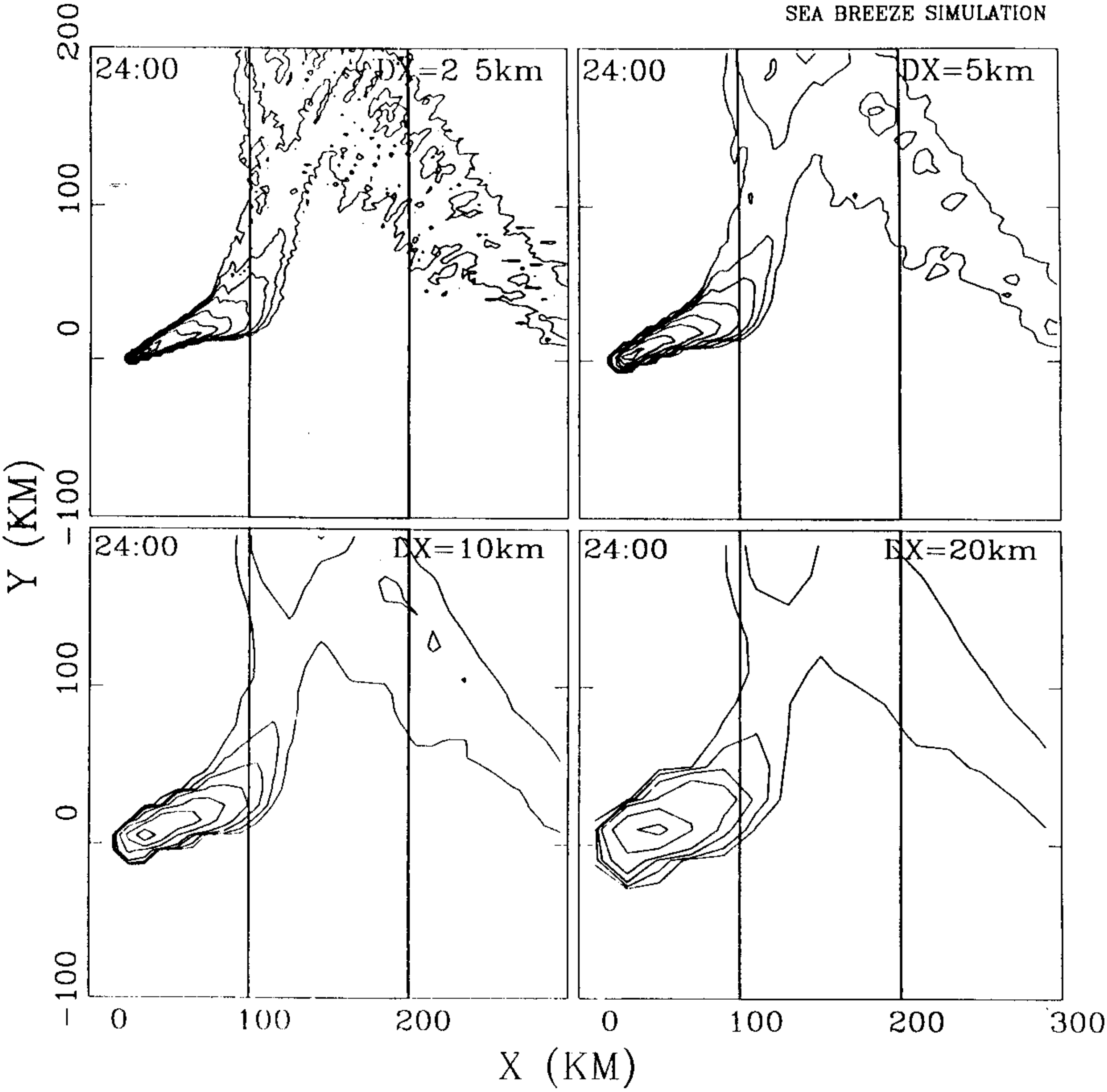

EFFECT OF AVERAGING INTERVAL T
SEA BREEZE SIMULATION
RECEPTOR R2
DX=5km
T=3h
T=1h
T=0.2h
CONCENTRATION
0.4
0.2
0.0
0.40
0.20
0.00
12
24
36
48
60
72
TIME (hours)

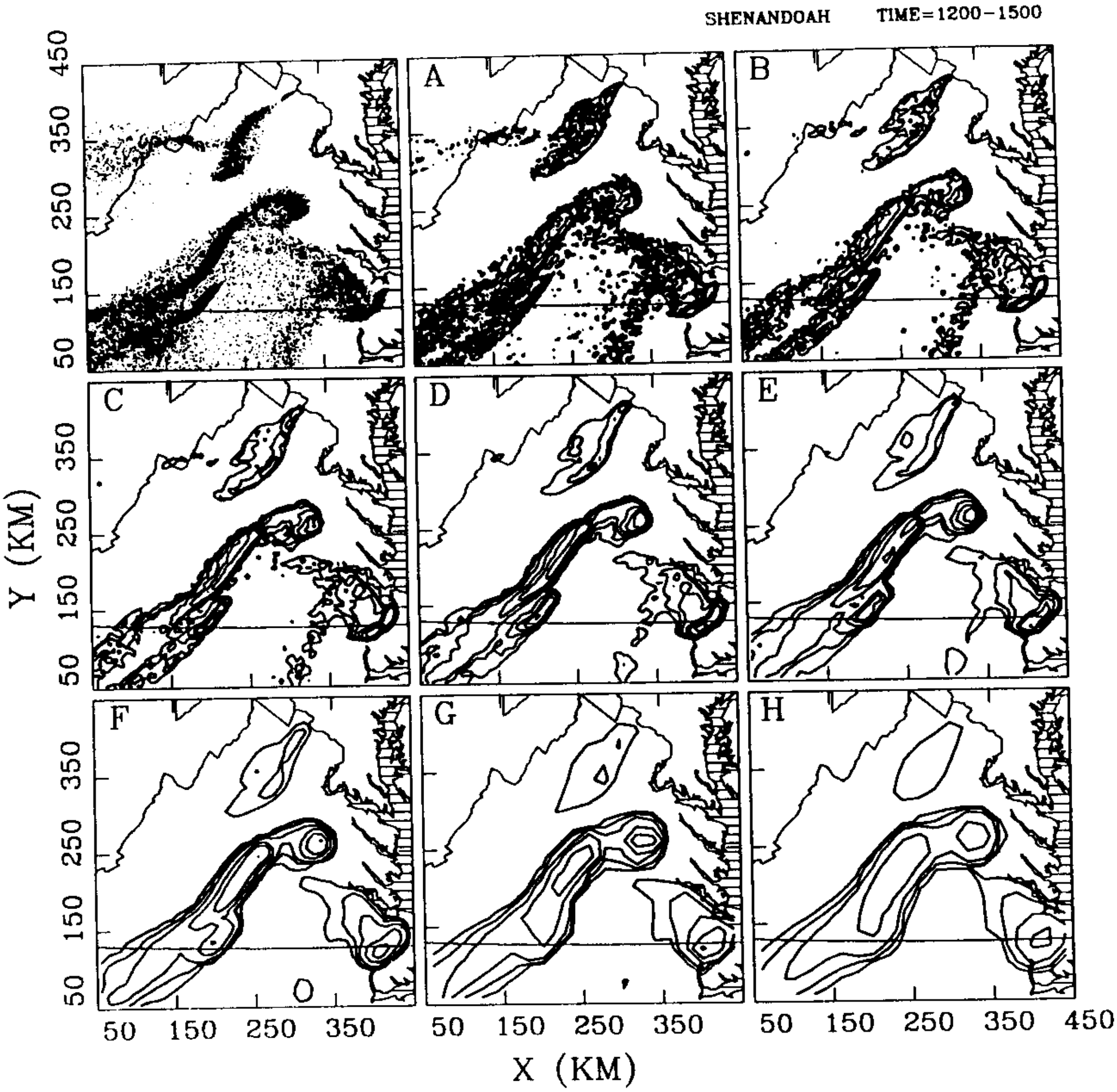


EFFECT OF GRID RESOLUTION
SEA BREEZE SIMULATION
RECEPTOR R2
T=1h
DX=10km
DX=5km
DX=2.5km
CONCENTRATION
0.4
0.2
0.0
12
24
36
48
60
72
TIME (hours)



EFFECT OF GRID RESOLUTION
SEA BREEZE SIMULATION
RECEPTOR R1
T=1h
DX=10km
DX=5km
DX=2.5km
CONCENTRATION
1.0
0.5
0.0
12
24
36
48
60
72
TIME (hours)


SEA BREEZE SIMULATION
24:00
DX=2 5km
24:00
DX=5km
24:00
DX=10km
24:00
DX=20km
Y (KM)
X (KM)
200
100
0
-100
0
100
200
300


SHENANDOAH TIME=1200-1500
A
B
C
D
E
F
G
H
Y (KM)
X (KM)
50
150
250
350
450

2c

RECEPTOR-ORIENTED DISPERSION MODELING

AIR POLLUTION AT THE RECEPTOR

$$\Phi[C] = \int\int R(\underline{x}, t)C(\underline{x}, t)d\underline{x}dt \tag{1}$$

$C(\underline{x}, t)$ - pollution concentration
$R(\underline{x}, t)$ - receptor function (location and geometry of the receptor, sampling time)

EXAMPLE: 2-D K-THEORY DIFFUSION EQUATION

MODEL EQUATION

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + w\frac{\partial C}{\partial z} - \frac{\partial}{\partial z}K\frac{\partial C}{\partial z} = Q \tag{2}$$

$$t = 0, \quad C = C_0 \tag{3}$$

$$x = 0, \quad C = 0 \tag{4}$$

$$z = 0, H, \quad \frac{\partial C}{\partial z} = 0 \tag{5}$$

period of simulation: $0 \leq t \leq T$
modeling domain: $0 \leq x \leq L, 0 \leq z \leq H$

DERIVATION OF AN ADJOINT EQUATION

- multiply equation (2) by the function C^* to be defined later

$$\left(\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + w\frac{\partial C}{\partial z} - \frac{\partial}{\partial z}K\frac{\partial C}{\partial z}\right) C^* = QC^* \tag{6}$$

- integrate over modeling domain and period of simulation

$$\int_0^T \int_0^L \int_0^H \left(\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + w\frac{\partial C}{\partial z} - \frac{\partial}{\partial z}K\frac{\partial C}{\partial z}\right) C^* dz dx dt = \int_0^T \int_0^L \int_0^H QC^* dz dx dt \tag{7}$$

- integrate by parts and introduce initial (3) and boundary conditions (4-5)

$$\int_0^T \frac{\partial C}{\partial t} C_* dt = CC^*|_0^T - \int_0^T C\frac{\partial C^*}{\partial t} dt = CC^*|_T - C_0\, C^*|_0 - \int_0^T C\frac{\partial C^*}{\partial t} dt \tag{8}$$

$$\int_0^L u\frac{\partial C}{\partial x} C_* dx = uCC^*|_0^L - \int_0^L Cu\frac{\partial C^*}{\partial x} dx = uCC^*|_L - \int_0^L Cu\frac{\partial C^*}{\partial x} dx \tag{9}$$

$$\begin{aligned}&\int_0^H \left(w\frac{\partial C}{\partial z} - \frac{\partial}{\partial z}K\frac{\partial C}{\partial z}\right) C^* dz = \\ &C\left(wC^* + K\frac{\partial C^*}{\partial z}\right) - K\frac{\partial C}{\partial z}C^*\Big|_0^H - \int_0^H C\left(-w\frac{\partial C^*}{\partial z} - \frac{\partial}{\partial z}K\frac{\partial C^*}{\partial z}\right) dz = \\ &C\left(wC^* + K\frac{\partial C^*}{\partial z}\right)\Big|_0^H - \int_0^H C\left(-w\frac{\partial C^*}{\partial z} - \frac{\partial}{\partial z}K\frac{\partial C^*}{\partial z}\right) dz\end{aligned} \tag{10}$$

• rewrite equation (10)

$$\int_0^T \int_0^L \int_0^H \left(\underbrace{-\frac{\partial C^*}{\partial t} - u\frac{\partial C^*}{\partial x} - w\frac{\partial C^*}{\partial z} - \frac{\partial}{\partial z}K\frac{\partial C^*}{\partial z}}_{R} \right) C dz dx dt +$$

$$\int_0^L \int_0^H (CC^*|_T - C_0\, C^*|_0)\, dz dx +$$

$$\int_0^T \int_0^H uCC^*|_L\, dz dt + \int_0 \int_0^L C \left(wC^* + K\frac{\partial C^*}{\partial z} \right)\Big|_0^H dx dt =$$

$$\int_0^T \int_0^L \int_0^H QC^* dz dx dt \qquad (11)$$

• formulate equation for C^*

$$-\frac{\partial C^*}{\partial t} - u\frac{\partial C^*}{\partial x} - w\frac{\partial C^*}{\partial z} - \frac{\partial}{\partial z}K\frac{\partial C^*}{\partial z} = R \qquad (12)$$

$$t = T, \quad C^* = 0 \qquad (13)$$

$$x = L, \quad C^* = 0 \qquad (14)$$

$$z = 0, H, \quad K\frac{\partial C^*}{\partial z} = 0, \quad (w = 0) \qquad (15)$$

• rewrite equation (11)

$$\underbrace{\int_0^T \int_0^L \int_0^H RC dz dx dt}_{\Phi[C]} - \int_0^L \int_0^H C_0\, C^*|_0\, dz dx =$$

$$\int_0^T \int_0^L \int_0^H QC^* dz dx dt \qquad (16)$$

AIR POLLUTION AT THE RECEPTOR

source- and receptor-oriented approach

$$\Phi[C] = \underbrace{\int_0^T \int_0^L \int_0^H RC\,dz\,dx\,dt}_{source-oriented}$$
$$= \underbrace{\int_0^T \int_0^L \int_0^H QC^* dz\,dx\,dt + \int_0^L \int_0^H C_0\, C^*|_0\, dz\,dx}_{receptor-oriented}$$

LAGRANGIAN FRAMEWORK

$$C\left\langle \underline{x}, t\right\rangle = \int_{-\infty}^{t} \int p(\underline{x}, t|\underline{x}', t')Q(\underline{x}', t')d\underline{x}'dt' \tag{17}$$

$$C\left\langle \underline{x}, t\right\rangle = \int_0^t \int p(\underline{x}, t|\underline{x}', t')Q(\underline{x}', t')d\underline{x}'dt' + \int p(\underline{x}, t|\underline{x}', 0)\left\langle C(\underline{x}', 0)\right\rangle d\underline{x}' \tag{18}$$

MODEL EQUATIONS

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + w\frac{\partial C}{\partial z} - \frac{\partial}{\partial z}K\frac{\partial C}{\partial z} = Q \tag{19}$$

$$t = 0, \quad C = C_0 \tag{20}$$

$$x = 0, \quad C = 0 \tag{21}$$

$$z = 0, H, \quad \frac{\partial C}{\partial z} = 0 \tag{22}$$

AND ADJOINT EQUATIONS

$$-\frac{\partial C^*}{\partial t} - u\frac{\partial C^*}{\partial x} - w\frac{\partial C^*}{\partial z} - \frac{\partial}{\partial z}K\frac{\partial C^*}{\partial z} = R \tag{23}$$

$$t = T, \quad C^* = 0 \tag{24}$$

$$x = L, \quad C^* = 0 \tag{25}$$

$$z = 0, H, \quad K\frac{\partial C^*}{\partial z} = 0 \tag{26}$$

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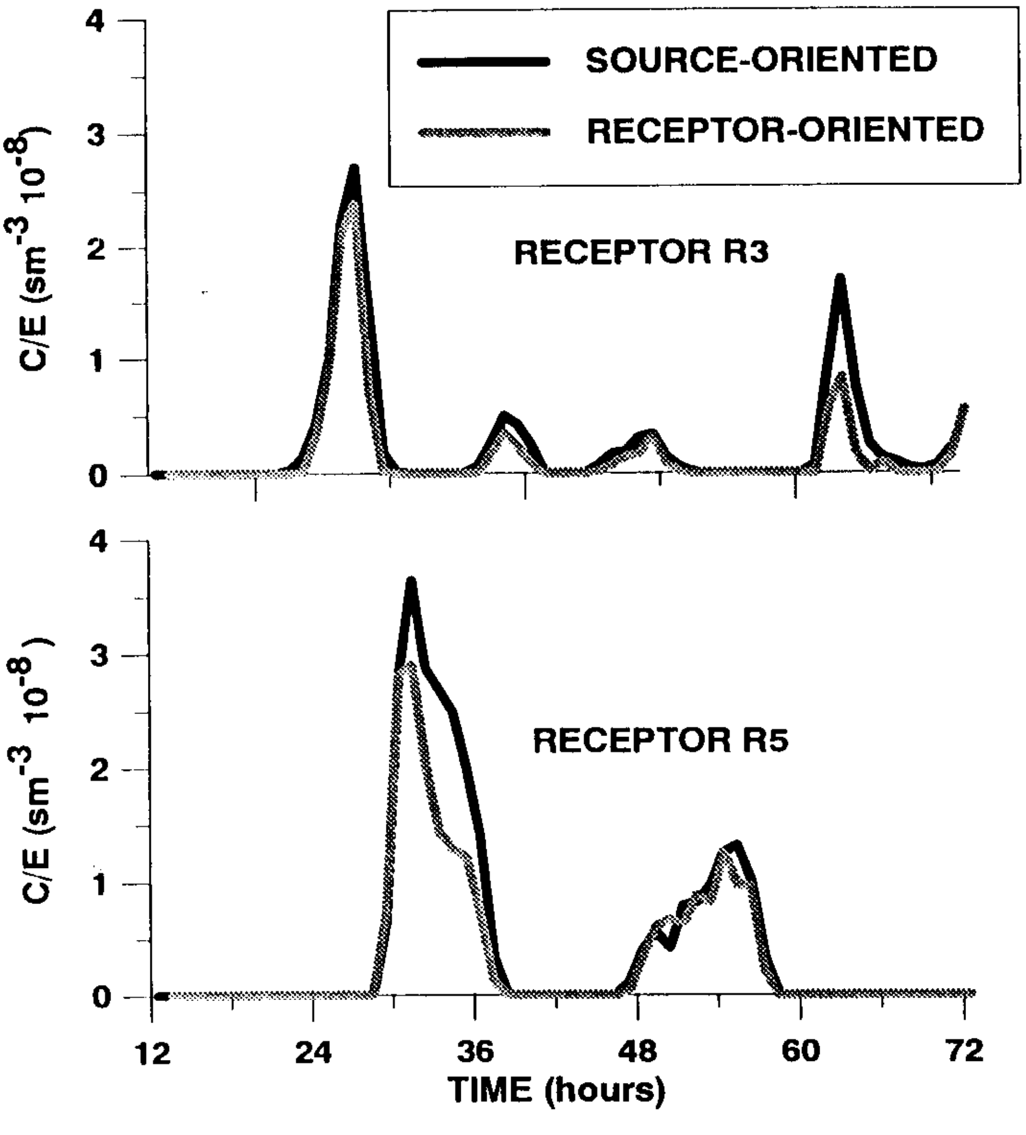
SOURCE- AND RECEPTOR-ORIENTED APPROACH
SEA BREEZE SIMULATION
DX=5km T=1h



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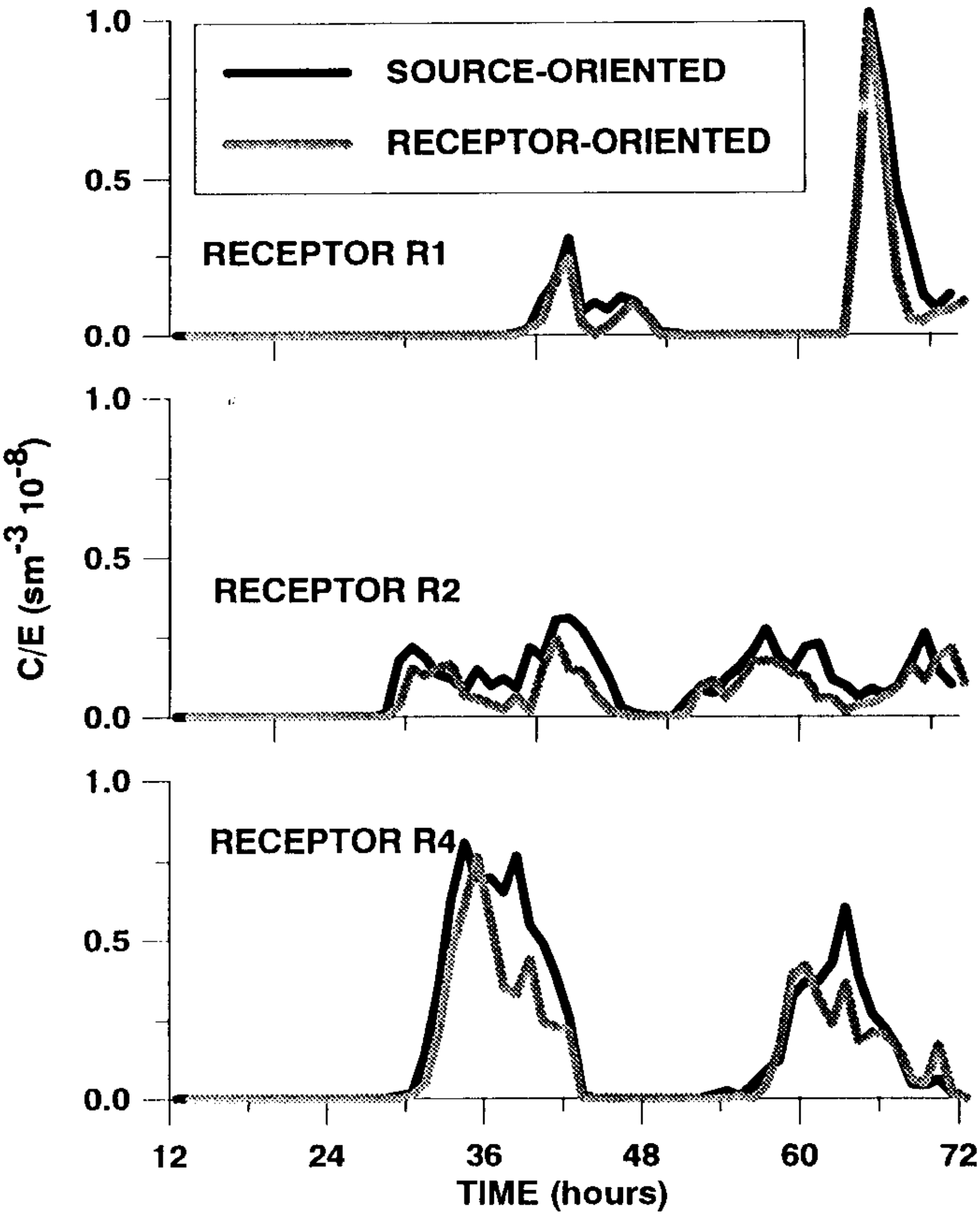

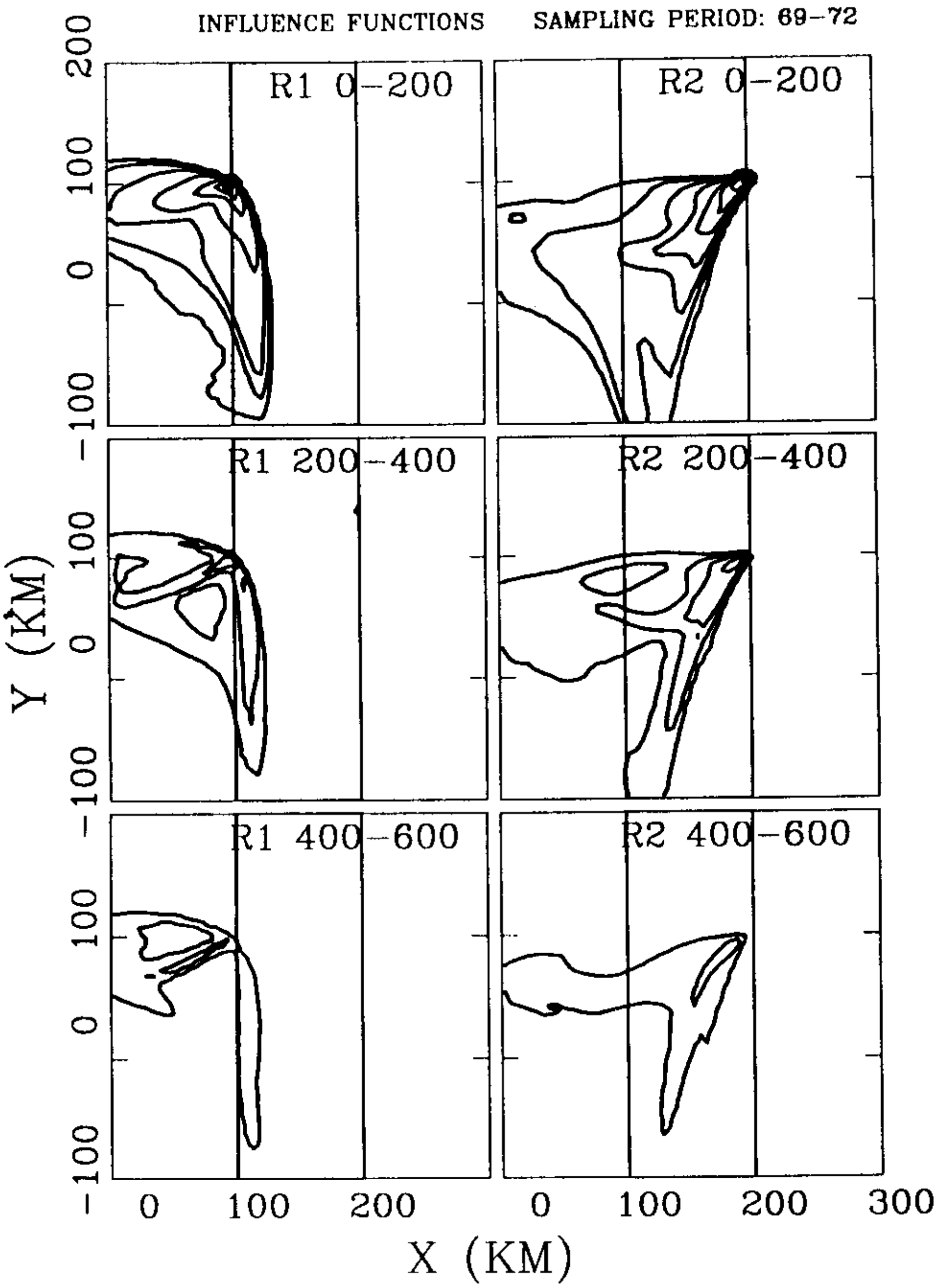

INFLUENCE FUNCTIONS SAMPLING PERIOD: 69-72
R1 0-200
R2 0-200
R1 200-400
R2 200-400
R1 400-600
R2 400-600
Y (KM)
X (KM)
-100
0
100
200
300