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"LAMDA: LA grangrian Model of Pollutant Diffusion in the Atmosphere"

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

LAMDA

LAgrangian Model of Pollutant Diffusion in Atmosphere

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LAMDA computer code has been developed to simulate airborne pollutant dispersion with Lagrangian statistical (Monte Carlo) model.
In the Monte Carlo models (which are called particle models or random walk models as well) the diffusion of a plume is simulated following in a Lagrangian frame the trajectories of a large number of particles whose movements is assigned according to the Eulerian wind statistics. These models allow to make maximum use of available observational data. This, in particular, states the reason for which they are so interesting and appealing in air pollution modeling.
It is possible to simulate complex situations which are frequently occurring (wind shear, vertical inversion of temperature, calm contitions, etc.), using directly the meteorological measurements; in particular, data giving by remote sensing sensors (like Sodar Doppler which yields the vertical profiles of the 3 wind velocity components and their variances and the RASS which measures the vertical profile of the air temperature), can be properly and easily used by these models.

THE MODEL

Particle motion is obtained by the finite difference integration of the Langevin equation for the particle velocity. This is a stochastic differential equation in which the acceleration of a single particle is the sum of two terms. The first one, proportional to the particle velocity, is a friction term while the second is a random term that describes the interaction with the other fluid particles.
Each component of the particle velocity is splitted into two terms: the first one, which is the value of considered variable averaged over a certain time interval, represents the transport due to the average flow conditions, whereas the second term simulates the diffusion and it is computed according to the vertical distribution of the turbulent parameters in the atmosphere. The meteorological input is made of vertical profiles, horizontally homogeneous, of the transport wind and turbulent parameters. The model is three-dimensional and can be used for simulations over flat terrains.
All the particles are horizontally moved according to the following scheme:

$$X(t + \Delta t) = X(t) + \left(u_x + u_x'(t)\right) \Delta t$$

$$Y(t + \Delta t) = Y(t) + \left(u_y + u_y'(t)\right) \Delta t$$

where u_x , u_y and u_x', u_y' are the components of the mean wind and their fluctuations computed with respect to a fixed coordinate system in which x-axis points towards the east and the y-axis towards the north. u_x', u_y' are not directly computed, but are derived from their values (u', v') estimated in a mobile coordinate system in which the x-axis is aligned along the mean wind direction. u' and v' are evaluated according to the following scheme:

$$u'(t + \Delta t) = u'(t)\ r_{u'} + u''(t + \Delta t)\ \sigma_{u'} \sqrt{1 - r_{u'}^2}$$

$$v'(t + \Delta t) = v'(t)\ r_{v'} + v''(t + \Delta t)\ \sigma_{v'} \sqrt{1 - r_{v'}^2}$$

where u" and v" are random velocities with zero mean and unit standard deviation; $r_i = \exp(-(\Delta t/T_{L_i}))$ is the Lagrangian autocorrelation function (with i=u' and v'); σ_i and T_{L_i} are the standard deviations and Lagrangian time scales of the horizontal wind.
This scheme comes from Brusasca et al. (1987).
Two kinds of vertical computational scheme can be chosen depending on the input data availability.
The first one needs vertical profiles for the first three moments of vertical wind speed.
The vertical particle positions are computed at each time step Δt as follows:

$$Z(t + \Delta t) = Z(t) + 0.5\big(w'(t+\Delta t) + w'(t)\big)\ \Delta t$$

and w' is evaluated according to the following scheme:

$$w'(t+\Delta t)=w'(t) \left(1 - \frac{\Delta t}{2T_{L_w}}\right)\left(1 + \frac{\Delta t}{2\ T_{L_w}}\right)^{-1} + \mu \left(1 + \frac{\Delta t}{2\ T_{L_w}}\right)^{-1}$$

where T_{L_w} is the Lagrangian time scale of the vertical wind and μ is picked at random from a probability density function whose first three moments are:

$$\overline{\mu} = \frac{\Delta t}{\rho} \frac{\partial}{\partial z} \left(\rho\ \overline{u_3^2(z)}\right)$$

$$\overline{\mu^2} = 2 \frac{\Delta t}{T_{L_w}}\ \overline{u_3^2(z)} + \frac{\Delta t}{\rho} \frac{\partial}{\partial z} \left(\rho\ \overline{u_3^3(z)}\right)$$

$$\overline{\mu^3} = 3 \frac{\Delta t}{T_{L_w}}\ \overline{u_3^3(z)} + \frac{\Delta t}{\rho}\frac{\partial}{\partial z}\left(\rho\ \overline{u_3^4(z)}\right) - 3 \frac{\Delta t}{\rho}\ \overline{u_3^2(z)}\ \frac{\partial}{\partial z}\left(\rho\ \overline{u_3^2(z)}\right)$$

and, according to De Baas et al. (1986) we set:

$$\overline{u_3^4(z)} = 3\left(\overline{u_3^2(z)}\right)^2$$

where $\overline{u_3^i(z)}$ (with i=2,3,4) are the highest order moments of vertical wind velocity distribution. The theoretical derivation of this scheme comes from Thomson (1984).

In the second scheme the vertical particle positions are computed at each time step Δt as follows:

$$Z(t + \Delta t) = Z(t) + \left(w_z + w_z'(t)\right) \Delta t$$

where w_z and w_z' are the vertical mean wind and fluctuations
w' is evaluated according to the following scheme:

$$w'(t + \Delta t) = w'(t)\ r_{w'} + w''(t + \Delta t)\ \sigma_{w'} \sqrt{1 - r_{w'}^2} + d$$

where w" are random velocities with zero mean and unit standard deviation; $r_{w'} = \exp(-(\Delta t/T_{L_w}))$ is the Lagrangian autocorrelation function, $\sigma_{w'}$ and T_{L_w} are the standard deviations and Lagrangian time scales of the vertical wind.

$$d = \partial\sigma_{w'}^2/\partial z\ \left((\sigma_{w'}^2 + w'^2) / 2\sigma_{w'}^2 \right)\ T_{L_w}\ (1 - r_{w'})$$

is the drift velocity (Sawford, 1985). It is a correction term introduced to avoid unrealistic particle accumulation in regions where $\sigma_{w'}$ is small.

In homogeneous turbulence $\partial\sigma_{w'}^2/\partial z = 0$ and d = 0.

For homogeneous and slightly inhomogeneous turbulence w_z is set to zero while in convective unstable conditions is set to a constant value (upward or downward) to simulate the effects of the thermal plumes due to the heat convection. This semi-empirical approach allows the simulation of an asymmetric vertical wind velocity distribution in the absence of direct high order moments measurement.
This scheme comes from Brusasca et al. (1987).

CASE STUDIES

Our steps to validate the particle model were the following:

- It has been tested in homogeneous and stationary turbulence against analytical solution assuming an exponential Lagrangian correlation function. (Brusasca et al., 1987)
- Its simulation in convective contitions have been compared to the Willis and Deardorff (1981) water tank experiments (Anfossi et al. 1988)
- In order to ascertain whether our model is able to simulate airborne pollutant dispersion in the real atmosphere, our model were compared to a series of tracer experiments performed in the Rhine valley, F.R.G. (Brusasca et al. 1989)
- It has proved in strong stable and low windspeed meandering conditions, comparing the model results with the tracer data obtained by the Idaho National Engineering Laboratory in U.S.A. (Anfossi et al. 1990).

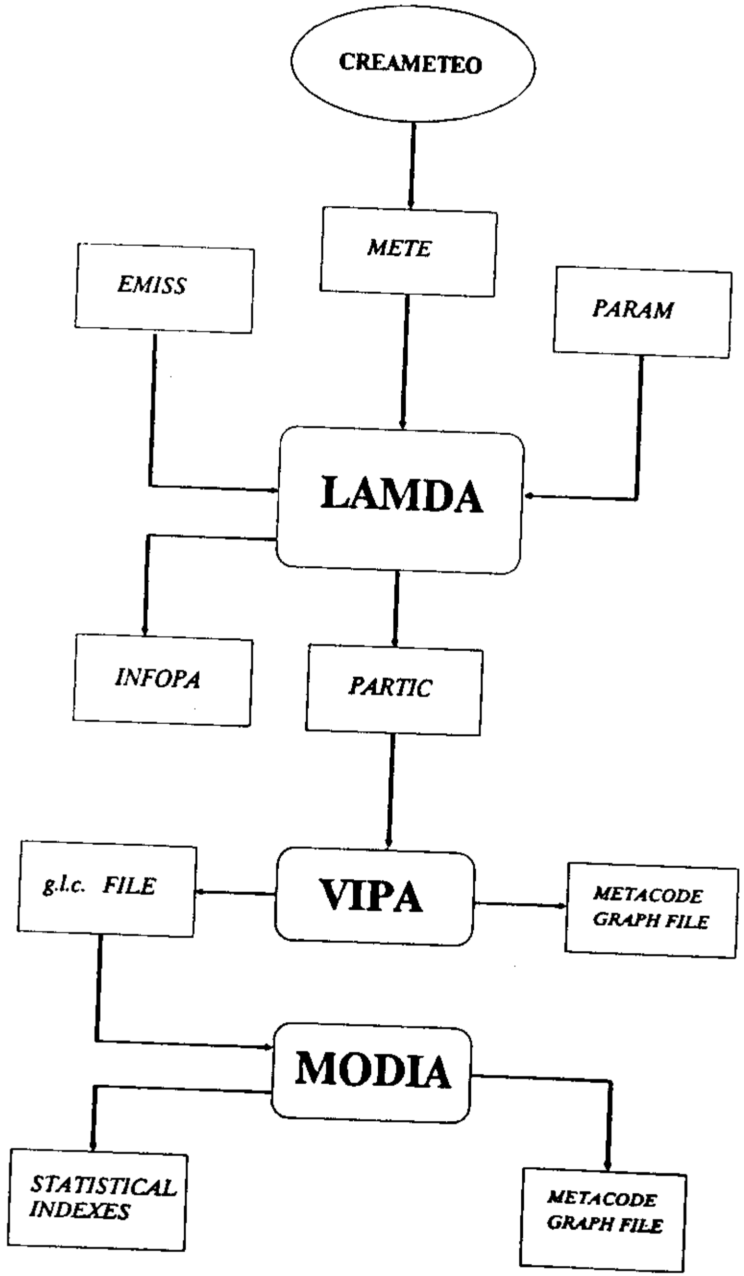
All these text gave satisfactory and incouraging results.

SOFTWARE STRUCTURE

LAMDA computer code is written in FORTRAN 77 and runs on Digital computers (VAX and MicroVax series) with VMS operating system. The following is a flow-chart of the structure of LAMDA software, including pre and post-processing modules.

The main input of the code is made of emission parameters like number of particles, source position and characteristics, meteorological parameters and run parameters like computational domain dimensions and time step duration.

The main output is a file containing the coordinates (x,y,z) of each particle at each time step. Concentrations are computed dividing the computational domain in cells of volume $\Delta x \Delta y \Delta z$ and counting how many particles are present in each cell at a certain time. By using the interactive graphic post-processor VIPA is possible to display the "puff" of particles to plot the isoconcentration lines on the x-y or x-z planes, to determine the standard deviations and centerline of the plume, and so on. Some examples of these possibilities are showed in the following figures 1 and 2.



Finally, by using our package MODIA is possible to compare g.l.c. predicted by the model with observed data.

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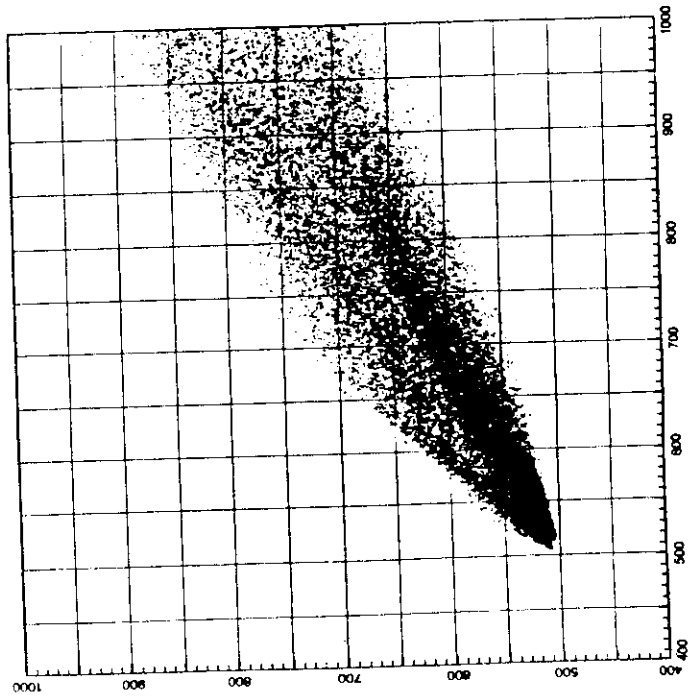

Fig 1

x-y view of a particle plume from the simulation of test n. 4 of the tracer experiment held by the Idaho National Engineering Laboratory (INEL) in low windspeed stable conditions.

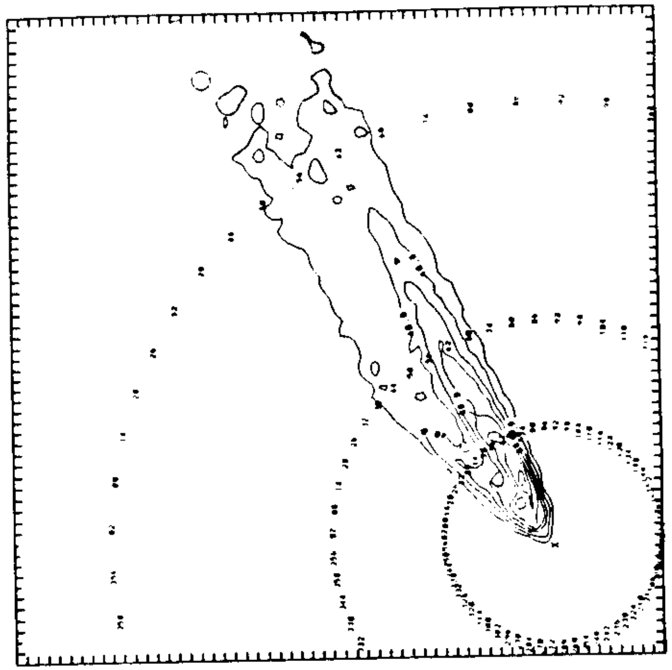

Fig 2

Ground level concentration isolines from the simulation of test n. 4 of INEL experiment. Source position is located in the center of the inner circle. Sampler position (marked by angular position in degree) are indicated on the 100, 200 and 400 m arcs respectively; concentration contours are labelled in $\mu g/m^3$ (contour interval of 20 $\mu g/m^3$).

PARTICLE DIFFUSION MODEL EVALUATION AGAINST TRACER EXPERIMENT

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MODEL EVALUATION

A Monte Carlo particle model for simulating pollutant dispersion in the atmosphere has been developed by our team. Its ability to predict ground level concentrations (g.l.c.'s) is verified against experimental data from the Karlsruhe Nuclear Research Center (F.R.G.).

Numerical schemes and parametrizations of the particle model are described in Brusasca et al.(1989) where two of the above mentioned KNRC tracer experiments are examined in details; meteorological and emission data are presented in Thomas et al. (1983) and are summarized in Table 1. The eight exercises considered in this model evaluation were performing during daytime with a wide range of meteorological conditions ranging from strong instability and low wind speed to neutrality and strong wind speed.

For all the exercises (except one) two consecutively half an hour periods have been simulated; two different non buoyant tracers were simultaneously emitted at 160 and 195 m thus giving rise to 30 tests. Air was sampled at 33 to 64 locations downwind of the source on 4-5 concentric arcs ranging from 200 to 9000 m.

To estimate the goodness of fit between observed and predicted g.l.c.'s, we use our package (MODIA - Morselli and Brusasca 1989) to calculate various statistical indexes and to display several comparative graphs.

The following indexes are computed:

Normalized Bias

$$NBIAS = \frac{\overline{(C_p - C_o)}}{\overline{C_o}}$$

Normalized Gross Error

$$NGRER = \frac{\overline{|C_p - C_o|}}{\overline{C_o}}$$

Normalized Noise

$$NNOIS = \frac{\overline{\left[(C_p - C_o) - \overline{(C_p - C_o)} \right]^2}}{\overline{C_o}^2}$$

Normalized Mean Square Error

$$NMSE = \frac{\overline{(C_p - C_o)^2}}{(\overline{C_p}\;\overline{C_o})}$$

Root Mean Square of the Fractional Deviation

$$RMSFD = \exp\left\{ \left[\overline{\left(\ln \frac{C_o + b}{C_p + b} \right)^2} \right]^{1/2} \right\}$$

Correlation coefficient

$$CORRE = \frac{\overline{(C_p - \overline{C_p})(C_o - \overline{C_o})}}{\sigma_o \sigma_p}$$

where C_o and C_p refer to the observed and predicted concentrations at each sampling point and b is the experimental background.
NBIAS indicates underprediction or overprediction of the models, NMSE and RMSFD refer the scatter, respectively, of the differences and quotients between observed and predicted g.l.c.'s
Furthermore it's possible to display the scatter diagram and the cumulative frequency distribution (c.f.d.) of the g.l.c.'s (Fig. 1 and 2); besides these curves we also calculate c.f.d. of the index $R = (C_o+b)/(C_p+b)$, with the convention that R=1/R if R<1. From the R-c.f.d. (Fig. 3) the percentage of data which are simulated within a specified error factor can be estimated.

The model evaluation was carried out on our particle model and on 10 Gaussian models which differed from one another for the choice of sigma curves and wind speed and direction (Table 2). The first five refer to the Gaussian models with vertically averaged wind speed and direction and with the dispersion sigmas given according to, respectively, Pasquill-Gifford (1), Briggs open-country (2), Briggs urban (3), Brookhaven (4) and Karlsruhe (5); the following five (from 6 to 10) still refer to the Gaussian model with the above mentioned dispersion sigma but with wind speed and direction measured at emission height; the last one (11) refers to our particle model.

RESULTS

Statistical indexes for the 11 models computed on the eight KNRC exercises are shown in Table 3.
Particle model exhibits the best performances for all the indexes; among the Gaussian models, model 8 is the best for NBIAS and NMSE, but has bad scores for NGRER, NNOIS and RMSFD indexes; totally the model 5 is the best and model 6 is the worst.
By using a "bootstrap resampling" procedure suggested by Hanna (1988), we can define the statistical confidence interval for the aforesaid indexes (Fig. 4); for example, in Fig. 4a, it is concluded with better than 95 percent confidence that NBIAS is not zero for all models except number 11; models 3 and 8 (Briggs urban sigmas) overpredict significantly and other Gaussian models underpredict significantly.
The application of the bootstrap technique to the different model predictions provides a clearer discrimination among models: we obtain that the particle model indexes are significantly (better than 99 percent confidence) different from all the indexes obtained by Gaussian models, on the contrary the performances among the best Gaussian models are not significantly different one to another. (Fig. 5).
The foregoing comparisons were repeated taking into account only the higher g.l.c.'s (either observed or calculated); this serves to emphasise the model performance evaluation over the high ranges of concentration. The results are shown in Table 4.
These figures confirm the remarkable performance of our particle model and Fig. 6 strengthens the difference with the Gaussian model performances.

CONCLUSION

The results presented in the previous section show that our particle model is able to predict g.l.c.'s with a high degree of accuracy: the point-by-point comparisons between observed and calculated data yielded very good statistical indexes.
Data were also compared to the simulations of 10 different Gaussian models in order to prove the particle model performances against simple and widely used models. A rather complete "model evaluation" was carried out: particle model yields satisfactory results and shows performances which are significantly better than all the Gaussian models.

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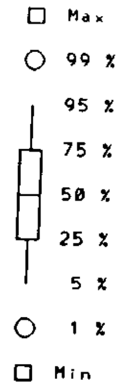
KNRC exerc.	date	stab. cat.	wind average 0-200m speed(m/s)	dir(°)	height PBL(m)	number of samplers	range of down-wind distance(m)
52	28/09/77 14.00-15.00	C-B	3.5-3.0	234-231	600-600	36	200-2000
55	05/04/78 14.00-15.00	C-C	7.0-7.6	59-55	1200-1300	33	300-5000
59	27/07/78 14.30-15.00	A-A	2.3	305	1000	36	200-3000
63	14/12/78 14.00-15.00	D-D	9.5-9.4	228-222	1600-1500	64	700-9000
64	15/05/79 14.00-15.00	B-B	3.9-4.1	96-88	900-900	46	300-5000
66	26/06/79 14.00-15.00	B-C	4.6-4.4	276-251	900-900	33	250-4000
72	02/07/80 13.00-14.00	D-D	10.1-10.1	247-245	1800-1700	44	500-8000
73	04/09/80 14.00-15.00	C-C	5.7-5.6	223-224	700-700	59	200-2500

Tab. 1 - Main characteristics of the 8 KNRC tracer experiments

MODEL NUMBER	SIGMA CURVES	WIND
1	Pasquill-Gifford	vertically averaged
2	Briggs Open-country	" "
3	Briggs Urban	" "
4	Brookhaven	" "
5	Karlsruhe	" "
6	Pasquill-Gifford	at the emission height
7	Briggs Open-country	" " "
8	Briggs Urban	" " "
9	Brookhaven	" " "
10	Karlsruhe	" " "
11	Monte Carlo Particle	

Tab. 2 - Characteristics of the 11 diffusion models



Whisker plots

Model	N.data	NBIAS	NGRER	NNOIS	NMSE	RMSFD	CORRE
1	1211	-0.6439	0.9339	6.0787	18.2229	5.2207	0.2900
2	1211	-0.5555	0.9033	5.7897	13.7091	4.7825	0.3612
3	1211	0.3112	1.1626	7.1472	5.5202	5.1186	0.4548
4	1211	-0.3997	0.8910	5.6435	9.6593	4.3075	0.4379
5	1211	-0.2647	0.8142	4.7187	6.5074	3.7359	0.5428
6	1211	-0.6898	0.9532	6.1564	21.3650	5.4411	0.2583
7	1211	-0.6144	0.9245	5.9006	16.2684	5.0324	0.3252
8	1211	0.1178	1.0737	5.9274	5.3107	5.0128	0.4696
9	1211	-0.4852	0.9008	5.5350	11.1991	4.5239	0.4148
10	1211	-0.2457	0.8812	5.1231	6.8665	3.9330	0.5076
11	1211	0.0164	0.7643	3.8918	3.8262	3.0494	0.6791

"RANKING" of MODELS

NBIAS	NGRER	NNOIS	NMSE	RMSFD	CORRE
11	11	11	11	11	11
8	5	5	8	5	5
10	10	10	3	10	10
5	4	9	5	4	8
3	9	4	10	9	3
4	2	2	4	2	4
9	7	7	9	8	9
2	1	8	2	7	2
7	6	1	7	3	7
1	8	6	1	1	1
6	3	3	6	6	6

Tab. 3 - Statistical indexes for the 11 models (entire sample)

Model	N.data	NBIAS	NGRER	NNOIS	NMSE	RMSFD	CORRE
1	255	-0.6350	0.9159	1.4117	4.9566	20.0490	-0.0969
2	259	-0.5404	0.8774	1.4222	3.7178	15.7010	-0.0085
3	372	0.3059	1.1205	2.6335	2.0828	9.7208	0.1946
4	260	-0.3649	0.8654	1.4940	2.5531	11.8430	0.1033
5	272	-0.2587	0.7621	1.3245	1.8705	7.2017	0.2341
6	252	-0.6904	0.9291	1.3507	5.8856	21.0622	-0.1386
7	258	-0.6092	0.8990	1.3972	4.5107	17.0178	-0.0567
8	355	0.0934	1.0177	2.1441	1.9634	9.7585	0.1961
9	267	-0.4553	0.8733	1.4472	3.0273	12.4858	0.0632
10	277	-0.2477	0.8361	1.4664	2.0239	7.9567	0.2053
11	273	0.0307	0.6932	1.0965	1.0608	3.6000	0.4499

"RANKING" of MODELS

NBIAS	NGRER	NNOIS	NMSE	RMSFD	CORRE
11	11	11	11	11	11
8	5	5	5	5	5
10	10	6	8	10	10
5	4	7	10	3	8
3	9	1	3	8	3
4	2	2	4	4	4
9	7	9	9	9	9
2	1	10	2	2	2
7	6	4	7	7	7
1	8	8	1	1	1
6	3	3	6	6	6

Tab. 4 - Statistical indexes for the 11 models (higher g.l.c.'s)

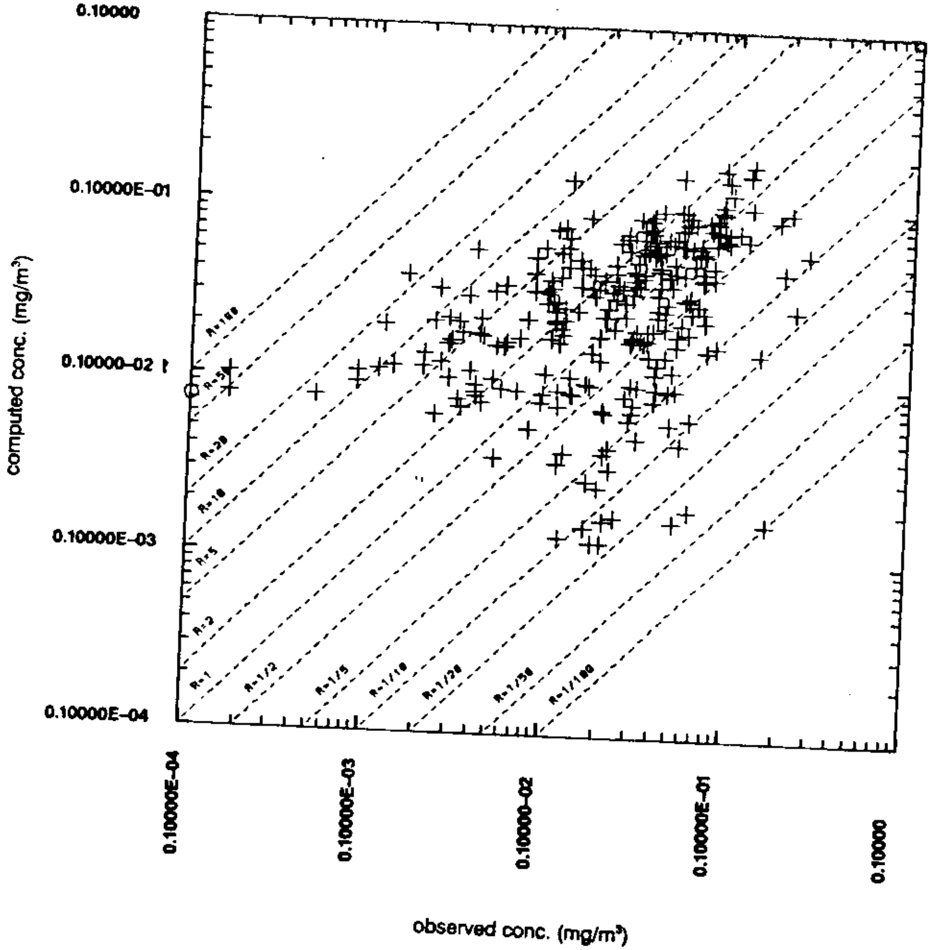


Fig.1 Scatter diagram between observed and computed (by particle model) g.l.c.'s for the 8 KNRC exercises: highest values.
R = Computed/Observed

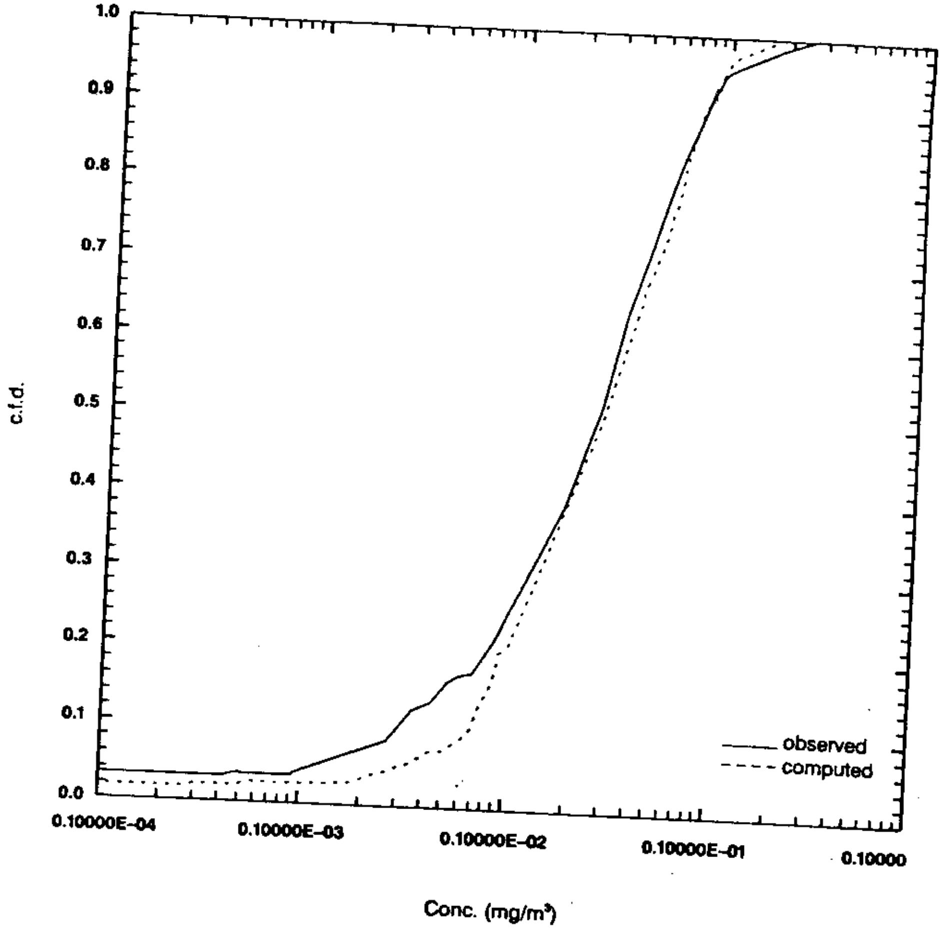


Fig.2 Cumulative frequency distrubution (c.f.d.) of the g.l.c.'s for the 8 KNRC exercises: highest values.

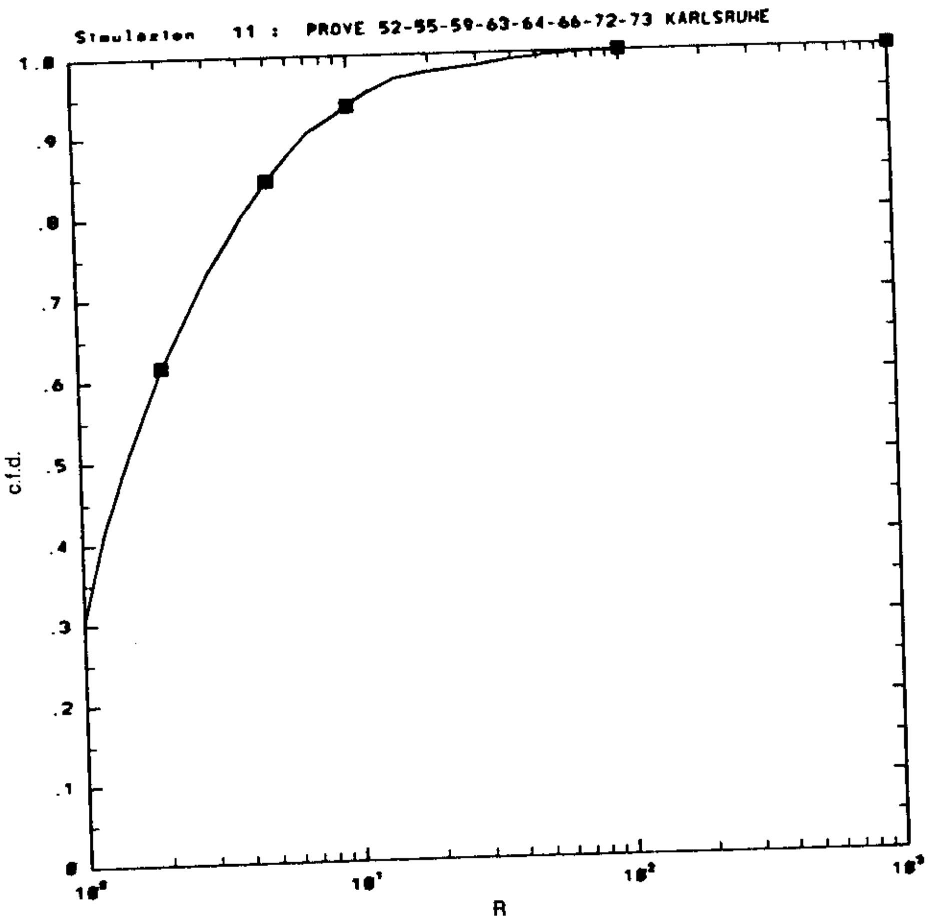


Fig.3 Cumulative frequency distribution (c.f.d.) of index R for the 8 KNRC exercises.The black squares indicate an error factor of 2,5,10,100,1000 between computed and observed data.

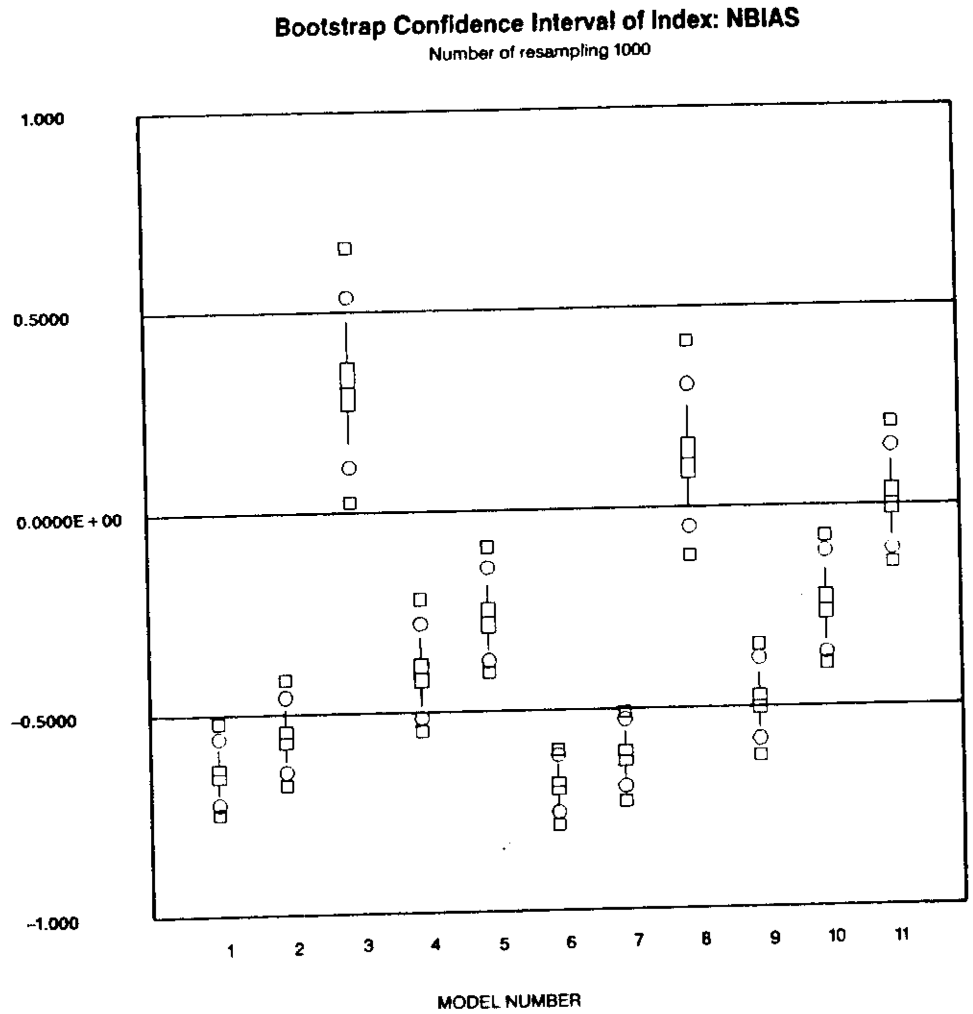


Fig.4a Whisker plots of cumulative distribution funtions of NBIAS for the 11 models as determined by bootstrap resampling; all data are considered.

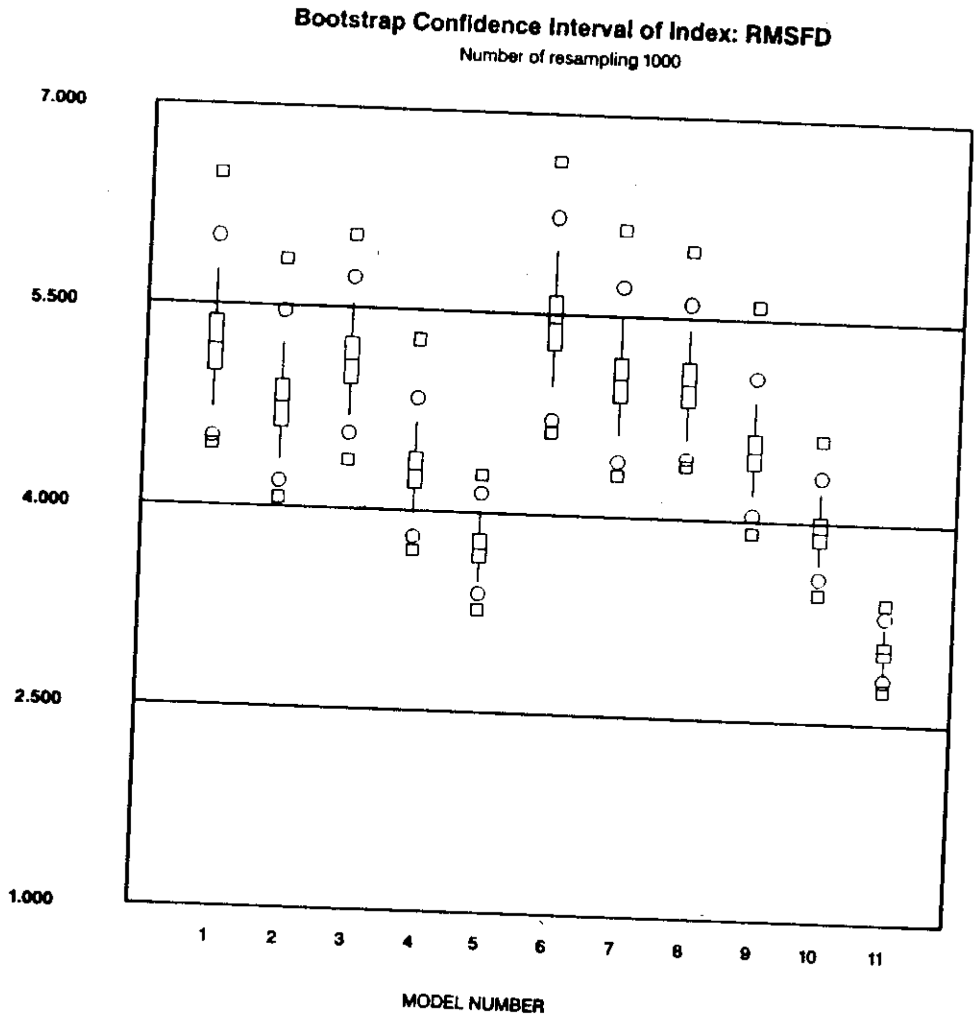


Fig.4b Whisker plots of cumulative distribution funtions of RMSFD for the 11 models as determined by bootstrap resampling; all data are considered.

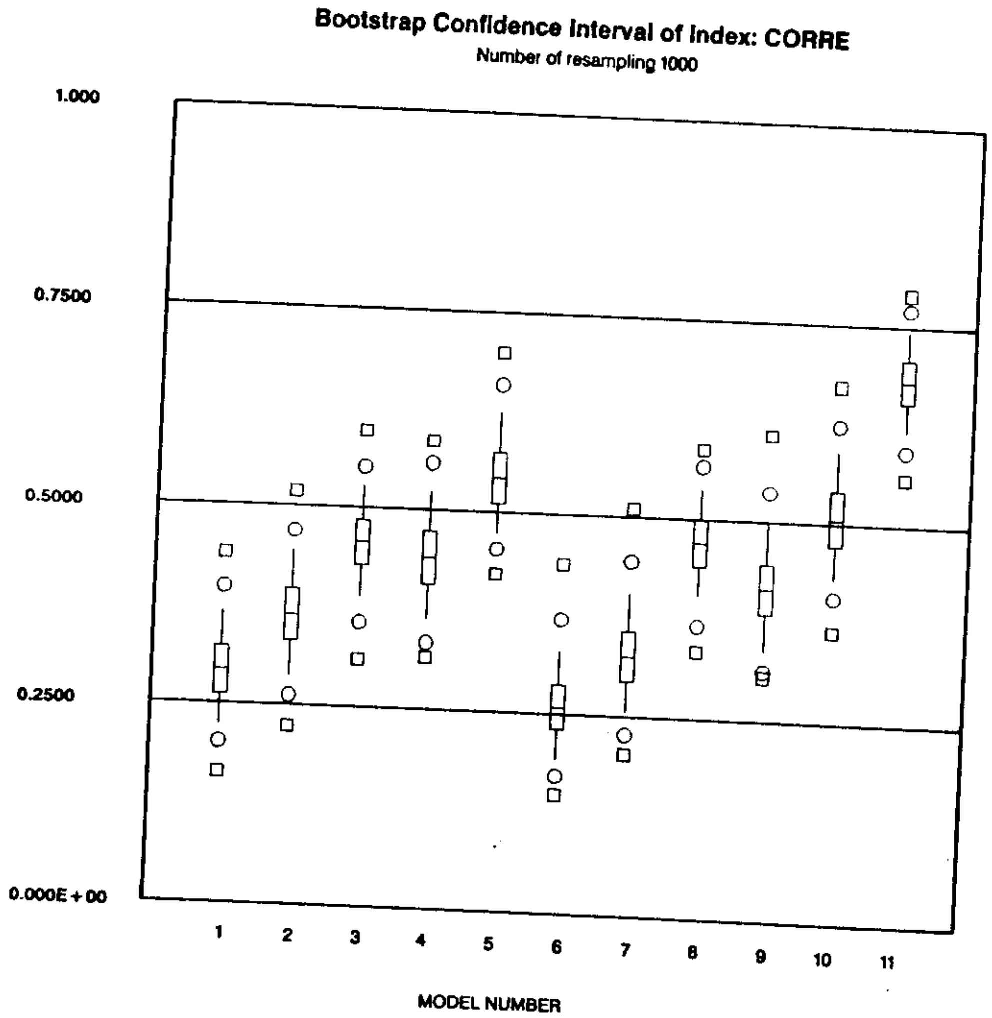


Fig.4c Whisker plots of cumulative distribution funtions of CORRE for the 11 models as determined by bootstrap resampling; all data are considered.

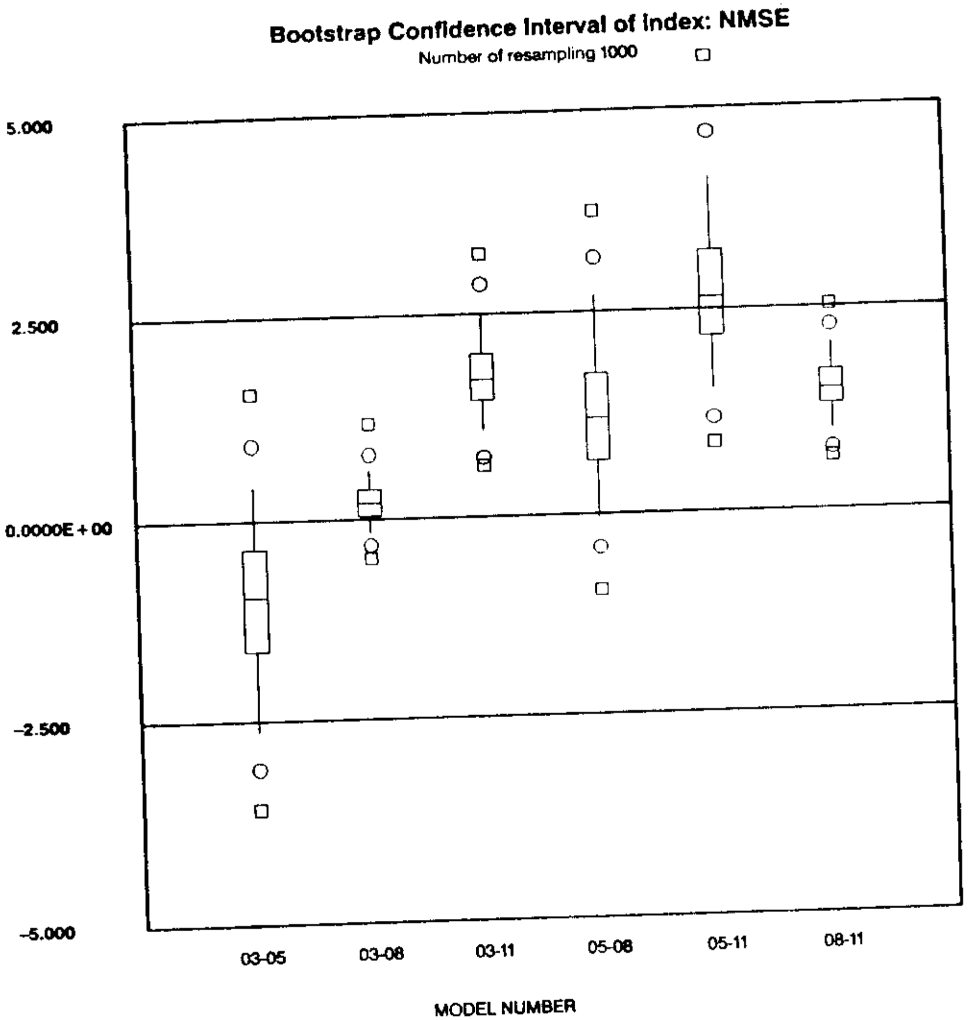


Fig.5a Expected distribution of NMSE(model i) - NMSE(model j) costructed using 1000 bootstrap resamples; the 4 models have the best performance for NMSE (see Tab. 3); all data are considered.

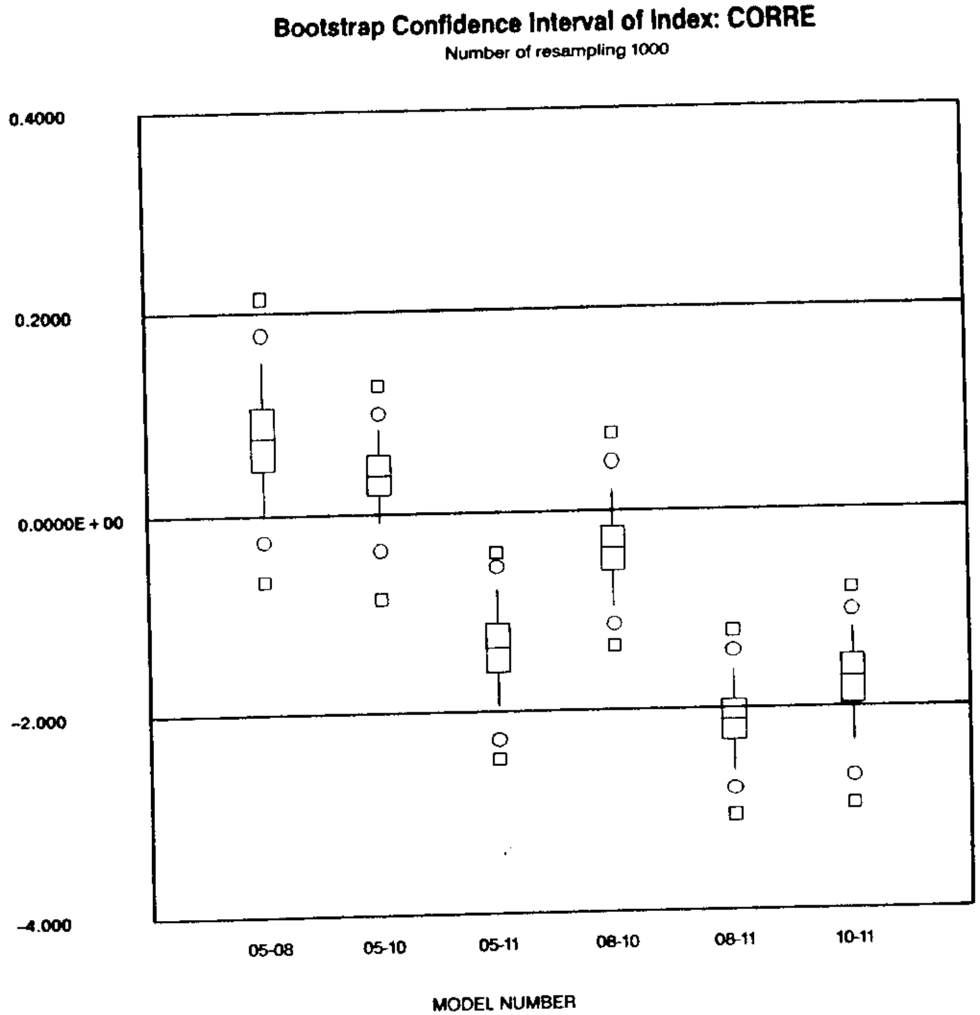


Fig.5b Expected distribution of CORRE(model i) - CORRE(model j) costructed using 1000 bootstrap resamples; the 4 models have the best performance for CORRE (see Tab. 3); all data are considered.

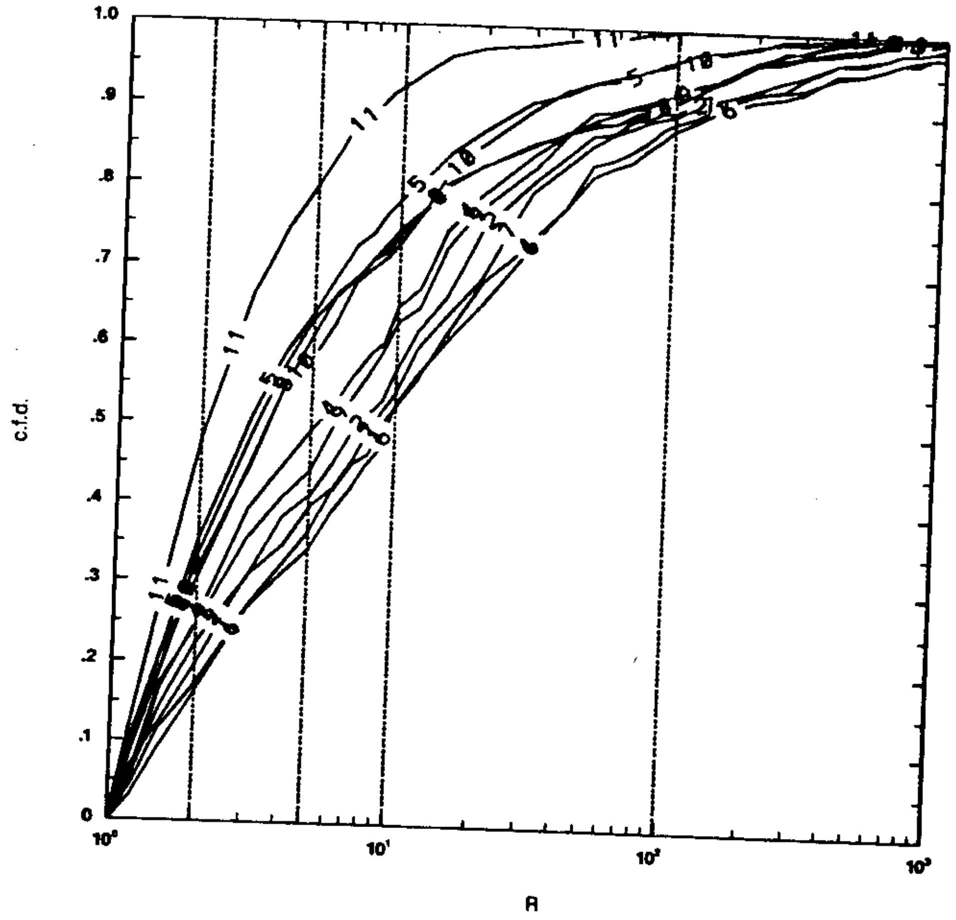


Fig.6 The cumulative frequency distribution (c.f.d.) of index R for the 11 models; only the high values are included.