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ADE as the basis for CTM

- Advection Diffusion Equation (ADE) is formally "derived" (Reinolds) using the ensemble averaging; usually, however, it is either spatial or temporal averaging;
- When averaging, the spectrum is split into the turbulence and mean motion with a cut-off at 20 min to 1 hour;
- The meso-meteorological gap is characterized with very high uncertainty.

Van der Hoven's spectrum of atmospheric turbulence

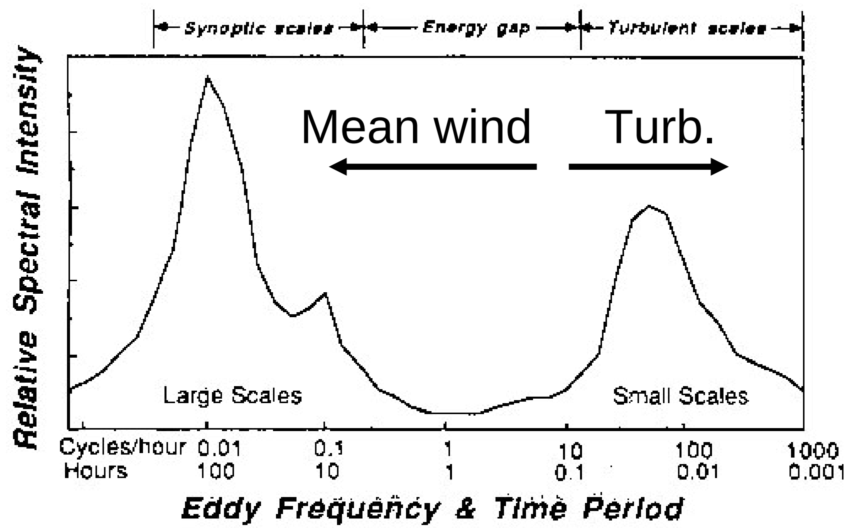


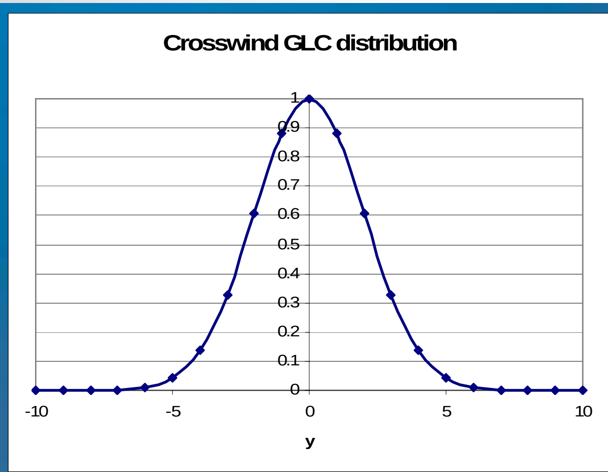
Fig. 2.2 Schematic spectrum of wind speed near the ground estimated from a study of Van der Hoven (1957).

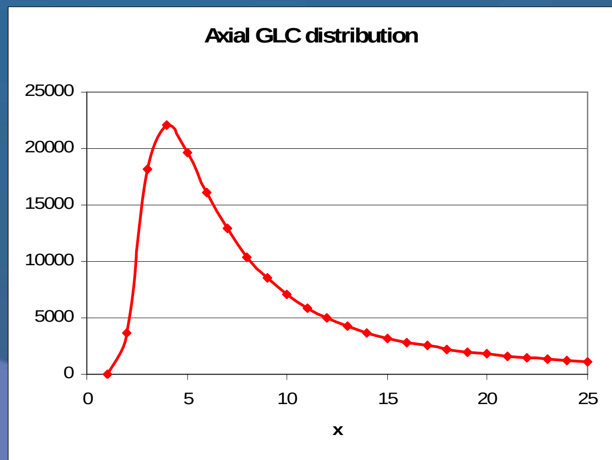
$$\frac{\partial C}{\partial t}+\frac{\partial (U_i C)}{\partial x_i}=\frac{\partial}{\partial x_i}(-<u_i' c'>)+S$$

$$-<u'_i c'> = K_{ij}\frac{\partial C}{\partial x_j}$$

Characteristic features of the steady-state ADE solution for a point source (from the Gaussian model)

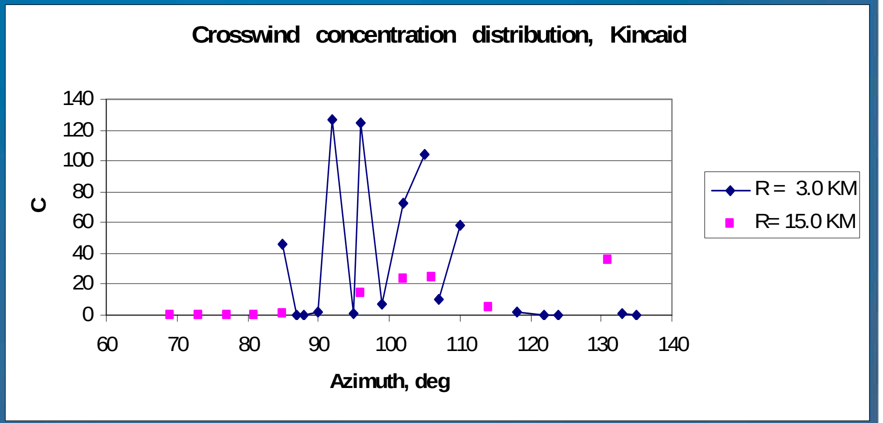
- Plume axis is a straight line;
- Cross-wind GLC distribution is the Gaussian;
- Along-wind GLC distribution is a smooth curve with only one maximum.

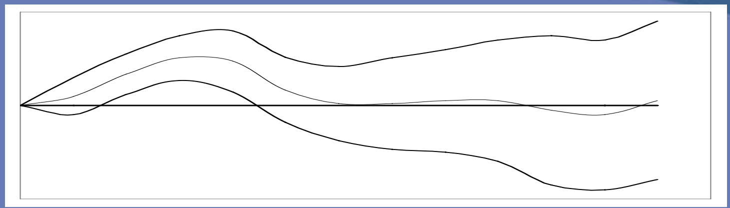




Why the measured concentrations with the same averaging time look differently?

- Multi-scale atmospheric turbulence couldn't be filtered out with an averaging;
- It results in fluctuations of properties to be simulated;
- The most visible feature is the plume meandering, i.e., directional variations in vertical and horizontal planes;
- More than one GLC maxima have been registered, especially in convective conditions .



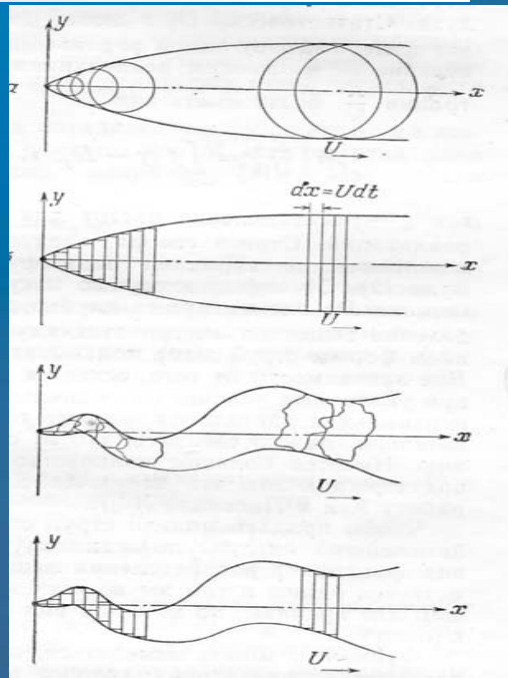


The larger gradients and curvature of the simulated fields the stronger the fluctuations of concentrations.

Statistical plume model (F. Gifford, 1959) - 1

Assumptions:

- A plume is represented as superposition of "flat and thin" discs; coordinates of their center of mass, Dy and Dz, are distributed normally with identical dispersions $\overline{D}^2$ relative to the location of the source, (0,0);
- Mean concentration distribution (MCD) is a convolution of distribution of the center of mass and distribution of concentrations relative to the center of mass.
- MCD in the resulting plume is Gaussian (it implies that the distribution of concentrations in discs is Gaussian either).



Plume as superposition of puffs (a) or discs (b); meandering plume as superposition of "elementary parcels" (c) or discs (d).

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Statistical plume model (F. Gifford, 1959) - 2

Results:

- Concentrations in the plume are stochastic variables;
- Frequency distribution of their logarithms is :

$$p(s) = A\frac{e^{m^2/\sigma^2}}{\pi\sigma^2}e^{-s^2/\sigma^2}I_0\left(\frac{m\sqrt{2s}}{\sigma^2}\right);$$

where

$$s = -\ln(\alpha_1 C/M);$$

$$\alpha_1 = 2\pi U\overline{Y}^2;$$

$$m = \sqrt{\frac{y^2+z^2}{4\overline{Y}^2}}$$

C is the concentration; M is the emission rate; A – normalizing factor; I_0 – modified Bessel function.

$$p(C/M) = A\frac{\alpha_1 e^{m^2/\sigma^2}}{\pi\sigma^2}(\alpha_1 C/M)^{0.5/\sigma^2-1}I_0\left(\frac{m}{\sigma^2}\sqrt{-2\ln(\alpha_1 C/M)}\right)$$

FINAL FREQUENCY DISTRIBUTION OF CONCENTRATIONS IN THE PLUME

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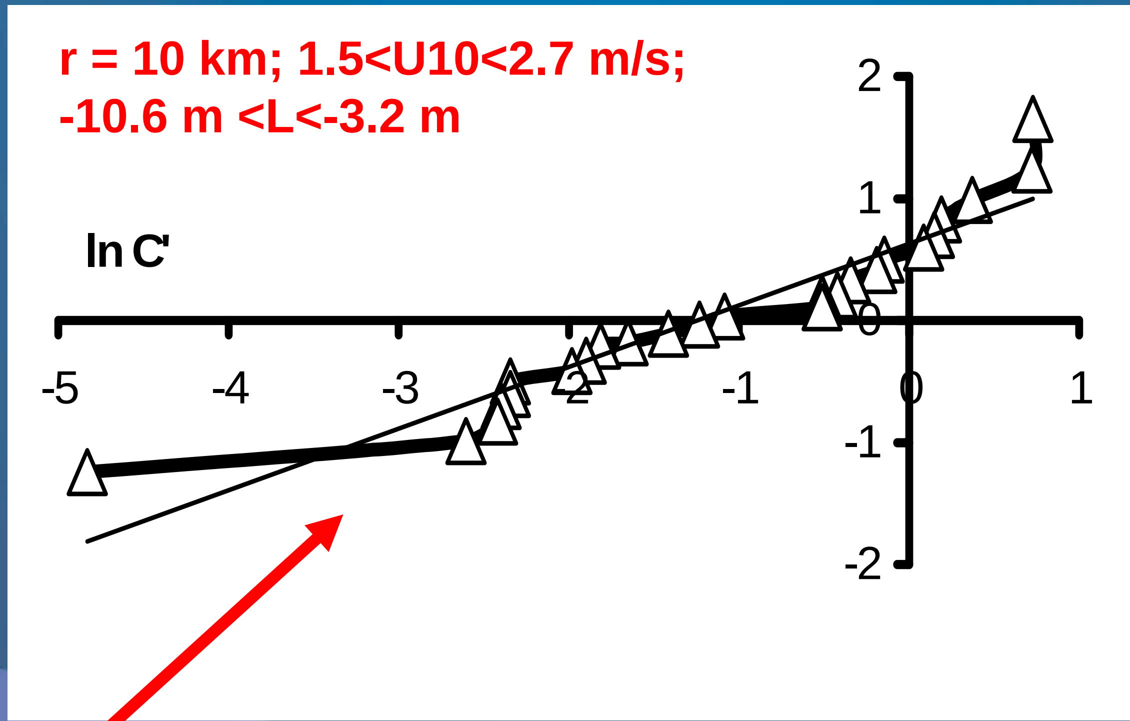
Statistical plume model - 3

- Except tails, the Gifford's distribution is close to log-normal:

$$p(c)=\frac{1}{\sqrt{2\pi}\,s\,c}e^{-\frac{[\ln(c/m)]^2}{2s^2}}$$



PDF of Kincaid data correspond to s varying between 0.6 and 1.2 (Genikhovich & Filatova, 2001)

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Consequences for validation of dispersion models - 1

- The "traditional" model validations starts with stratifying the measurements into groups (gradations) with "insignificant scatter" of governing parameters;
- Indicators of performance of dispersion models (left-hand panel) are estimated for each group;
- It means comparison of deterministic model predictions with stochastic measurements

Indicators of performance (IP)

$$\mathrm{FBM} = \frac{<\mathrm{M}> - <\mathrm{P}>}{<\mathrm{M}> + <\mathrm{P}>};$$

$$\mathrm{MFB} = <\frac{\mathrm{M}-\mathrm{P}}{\mathrm{M}+\mathrm{P}}>;$$

$$\mathrm{FAa} = \mathrm{Prob}\{\frac{\mathrm{P}}{a} < \mathrm{M} < a\mathrm{P}\};$$

$$\mathrm{NMSE} = \frac{<(\mathrm{M}-\mathrm{P})^2>}{<\mathrm{P}> \cdot <\mathrm{M}>};$$

$$\mathrm{Corr} = \frac{<(\mathrm{P}-<\mathrm{P}>)(\mathrm{M}-<\mathrm{M}>)>}{\sqrt{<(\mathrm{P}-<\mathrm{P}>)^2> \cdot <(\mathrm{M}-<\mathrm{M}>)^2>}}.$$

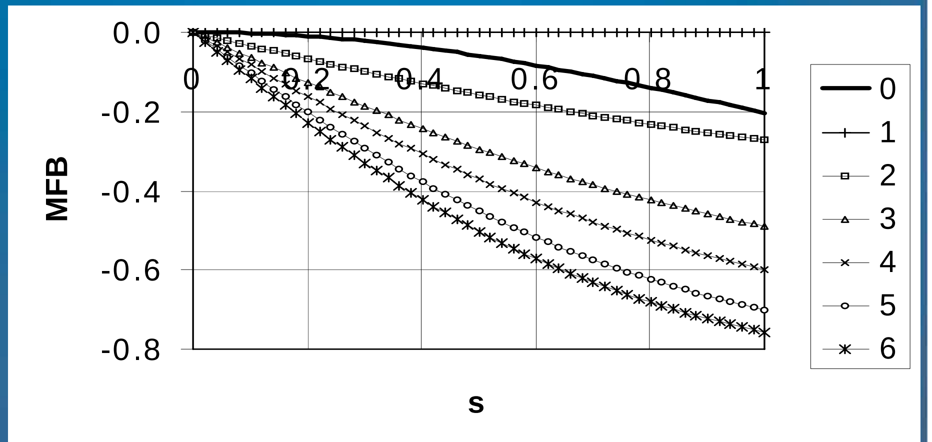
P is "prediction" (deterministic); M is "measurement" (stochastic); < > - symbol of averaging.

Consequences for validation of dispersion models - 2

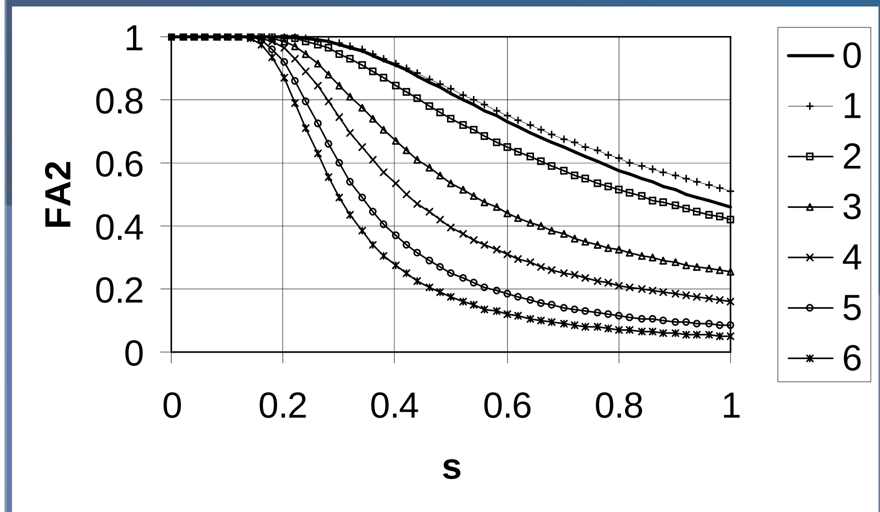
- The best ("ideal") values of IP correspond to an "ideal model" that exactly predicts for each gradation the characteristics of interest (e.g., mean value or upper percentile);
  - but only mean value can be reproduced exactly and only if the model is “perfectly” tuned to predict it.

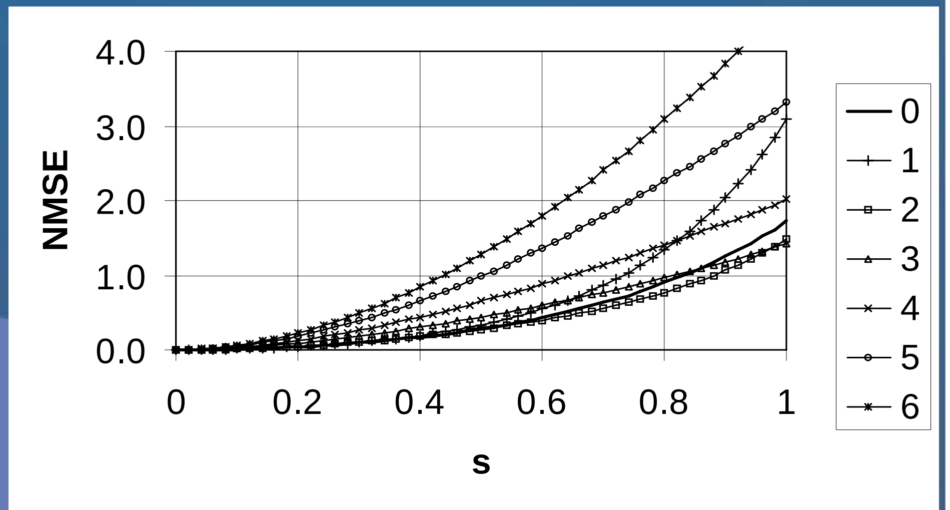
Consequences for validation of dispersion models - 3

Ind	Me-an	50 %	75 %	90 %	95 %	98 %	99 %
No	0	1	2	3	4	5	6



PDF of Kincaid data correspond to s varying between 0.6 and 1.2





Ensemble modeling of the regional dispersion (project PREVIEW, Robertson et al., 2007) - 1

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- Hypothetical accident at the nuclear power station;
- Ensemble weather predictions using the ECMWF products (51 ensemble members);
- Dispersion modeled using MATCH (Multi-scale Atmospheric Transport and Chemistry Model, SMHI).

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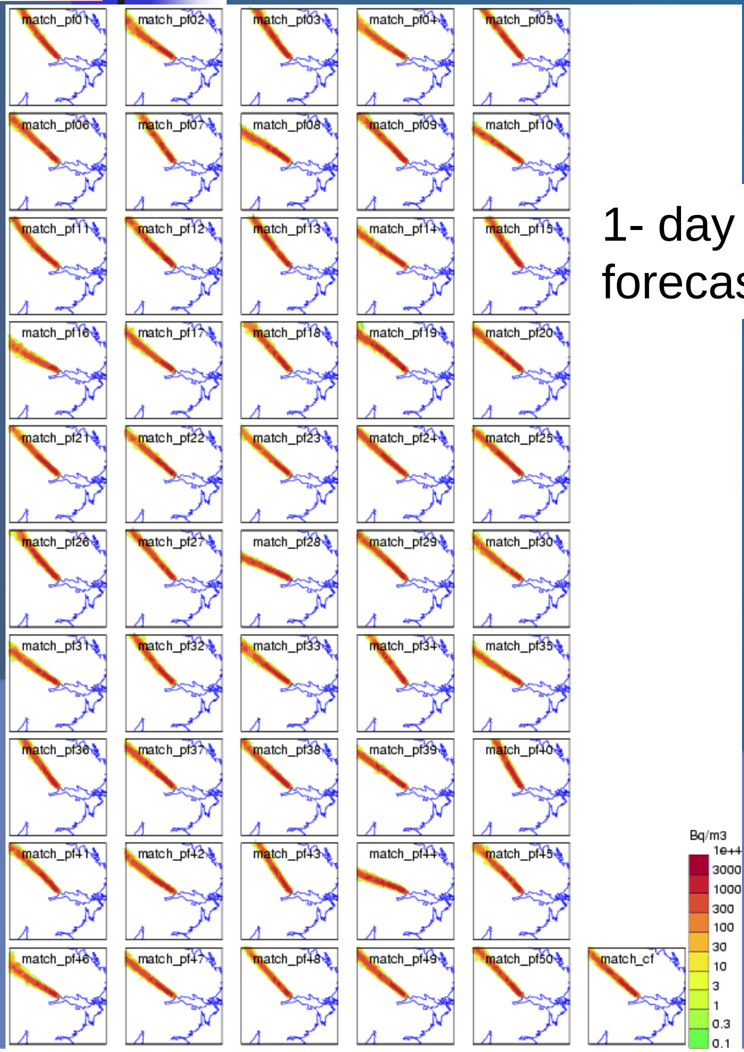
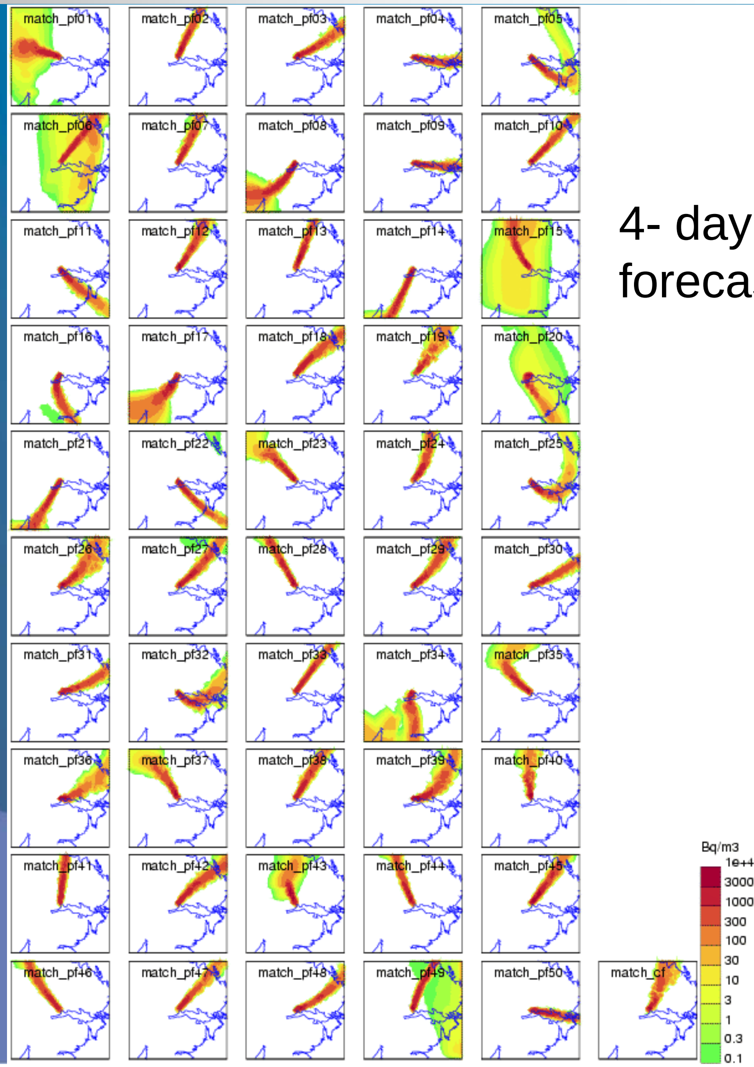
Ensemble modeling of the regional dispersion (PREVIEW) - 2



1- day forecast



4- day forecast

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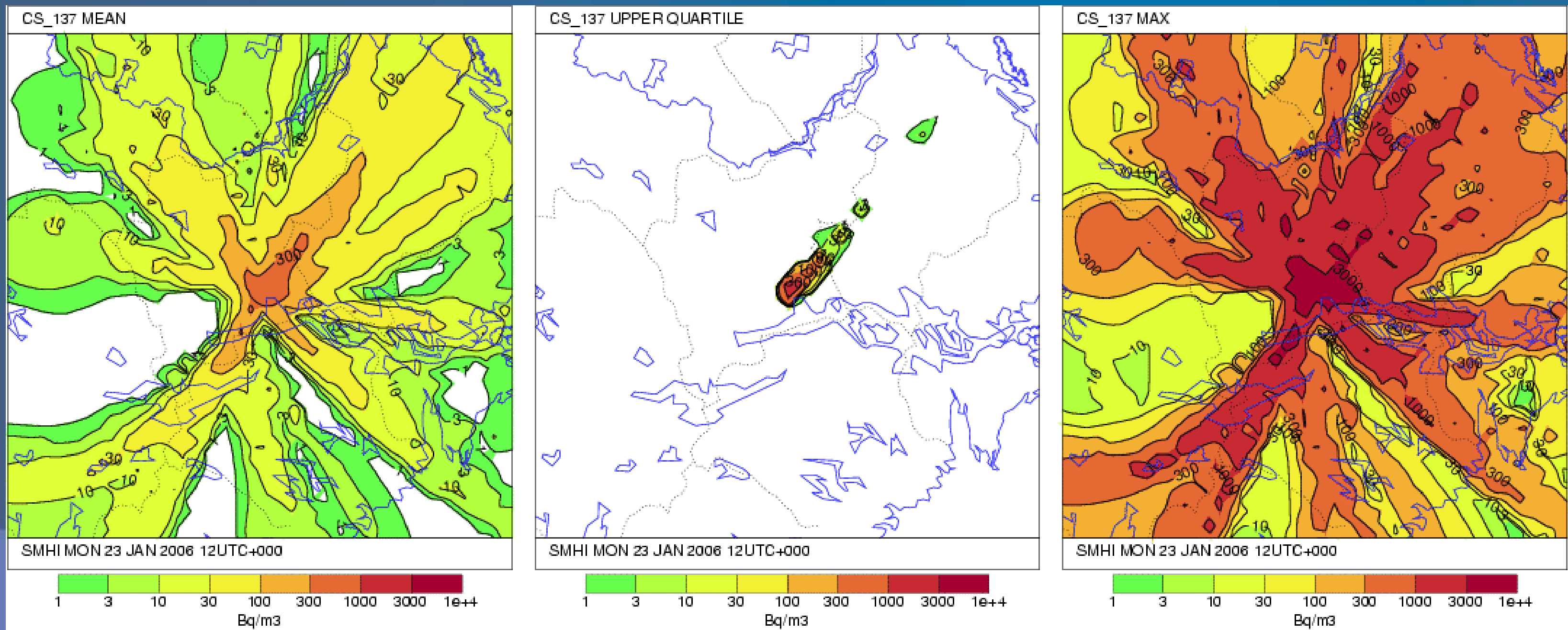
Ensemble modeling of the regional dispersion (PREVIEW) - 3

In 4 days:



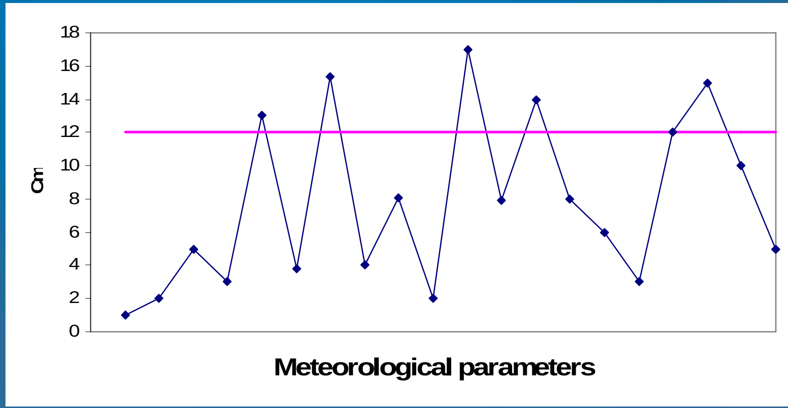
Mean — 75th percentile — Max

What's the way out?

- Do not try to predict unpredictable
- Dispersion models should be mainly used to predict statistically stable ("robust") characteristics of the air pollution (e.g., PDFs or their certain percentiles);
- Mean values could be used only if they are "good representatives" of the sample, i.e., if the standard deviations are small;
- Predictions of "individual concentrations" should be given in probabilistic form (e.g., accompanied with confidence intervals);

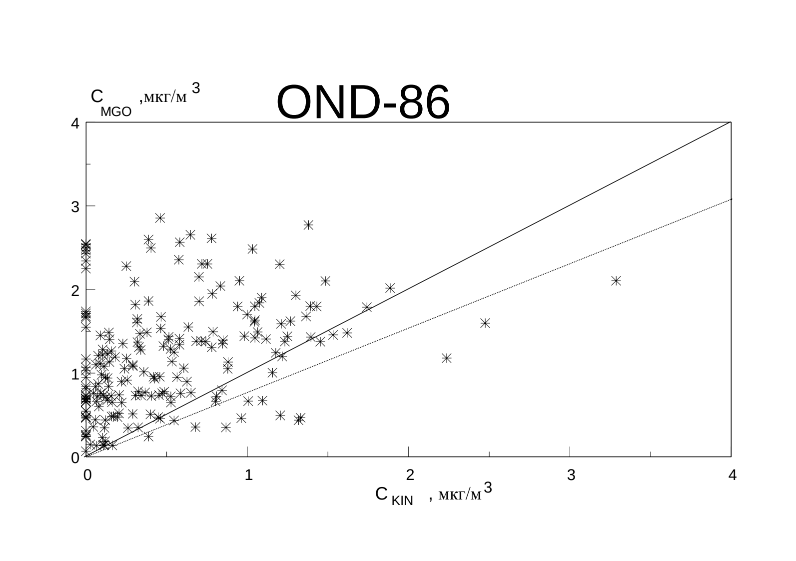
OND-86 (Russian regulatory dispersion model)

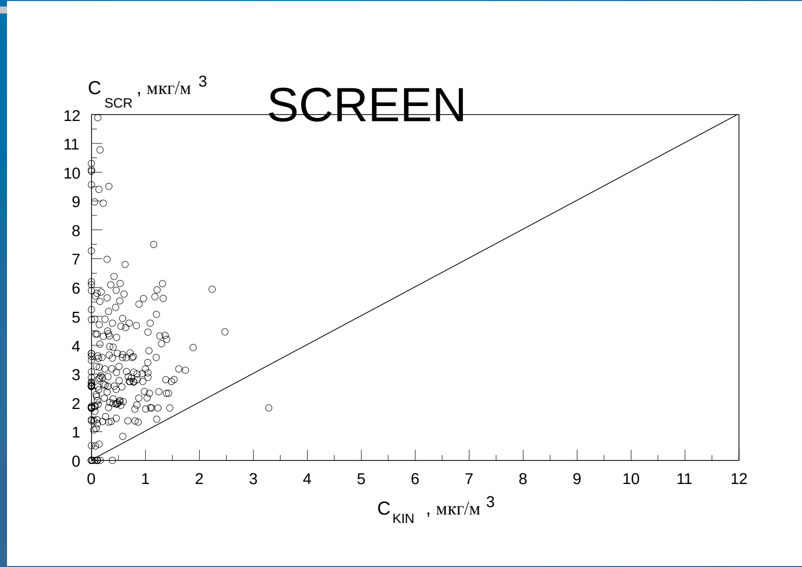
- Developed at MGO, direct ADE solution;
- Governing parameters: surface wind speed, wind direction, and stratification parameter $\lambda = K_z/(zU(z))$;
- 2% of possible meteo parameters with highest concentrations is removed from the phase space
- Hence, the model predicts the annual 98th percentiles of PDF ("majorant" concentration).



- Approach was later adopted by SCREEN model (US EPA)

Comparison OND-86 (left panel) and SCREEN-3 (right panel) axial concentrations with Kincaid data





- Bisectrix corresponds to the perfect agreement between measurements and calculations; dots above it indicate on overestimation; the dotted line has a slope of 1.25;

- For OND-86, 98% of dots are above the dotted line (i.e., it predicts the 98th percentile with an error of 25%); the predicted maximum of 3 $\mu g/m^3$ is close to the measured one of 3.3 $\mu g/m^3$;

-For SCREEN-3 practically all dots are above the bisectrix, and predicted maximum is about 12 $\mu g/m^3$.

Dispersion modeling using simulated PDF

- Based on the joint solution of ADE and equations for turbulent fluxes of pollutants;
- PDF is assumed to have a certain functional form depending from a few parameters (like mean and dispersion) reconstructed from the above mentioned solution.

Lagrangian puff models SKIPUFF (a core diffusion solver in HPAC)

- SKIPUFF (Second Order Closure Integrated Puff model) was developed by R. Sykes et al.;
- Assumes the clipped normal distribution of concentrations;
- Equations are solved separately for the moments corresponding to individual puffs;
- Turbulent second-order closure - after Donaldson (1973) and Lewellen (1977);
- Includes the procedure of merging the puffs;
- Validated upon Kincaid – and other widely used data sets;
- Could be used in the "standard" and "ensemble" modes;
- Built-in into the operational model HPAC developed by the US DTRA (Defense Threat Reduction Agency) intended for the emergency response applications.

Ensemble simulations

- ADE is solved using a set ("ensemble") of alternative meteorological forecasts generated with either one or several meteo drivers;
  - the scatter of these forecast is believed to characterize uncertainties of atmospheric fields;
- When using several CTMs, a "hyper-ensemble" is generated.

What's good and bad with ensemble modeling?

- \+ No assumptions about the properties of atmospheric fluctuations are needed;
- \+ The approach is universally applicable for solution of stationary and/or non-stationary problems at different temporal – and spatial scales;
- \+ Experience shows that ensemble predictions are routinely better than any individual ones
- \- No objective algorithms have been developed yet for attaching probabilities of occurrence to the ensemble members;
- \- As a result, the formal proof for applicability of the ensemble modeling is still to be developed.