Optimal forecasting of atmospheric quality in industrial regions: risk and uncertainty assessment

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Goal

Development of theoretical background and computational technology
for environmental and ecological applications

CONCEPT
OF ENVIRONMENTAL MODELING

The methodology is based on:

- **control theory,**
- **sensitivity theory,**
- **risk and vulnerability theory,**
  - variational principles,
  - combined use of models and observed data,
  - forward and inverse modeling procedures,
  - methodology for description of links between regional and global processes (including climatic changes) by means of orthogonal decomposition of functional spaces for analysis of data bases and phase spaces of dynamical systems

Basic elements for concept implementation:

- models of processes
- data and models of measurements
- adjoint problems
- constraints on parameters and state functions
- functionals: objective, quality, control, restrictions etc.
- sensitivity relations for target functionals and constraints
- feedback equations for inverse problems

Statement of the problem

- **Mathematical model**

$$B\frac{\partial\vec{\varphi}}{\partial t}+G(\vec{\varphi},\vec{Y})-\vec{f}-\vec{r}=0,$$

$$\vec{\varphi}^{0}=\vec{\varphi}_{0}^{0}+\vec{\xi},\quad \vec{Y}=\vec{Y}_{0}+\vec{\varsigma};$$

$\vec{\varphi}\in\Im(D_t)$ is the state function,

$\vec{Y}\in\Re(D_t)$ is the parameter vector.

G is the “space” operator of the model

- **A set of measured data $\vec{\varphi}_m,\vec{\Psi}_m$ on D_t^m**

$$\vec{\Psi}_m=[H(\vec{\varphi})]_m+\vec{\eta},$$

$[H(\vec{\varphi})]_m$ **is the model of observations**.

- $\vec{r},\vec{\xi},\vec{\varsigma},\vec{\eta}$ **are the terms describing uncertainties and errors of the corresponding objects.**

Desired!

Transport and transformation model

$$L\varphi \equiv \frac{\partial \pi c_i}{\partial t} + \mathrm{div}\pi(c_i\,\mathbf{u} - \mu_{c_i}\mathrm{grad}c_i) + (S\varphi)_i - f_i(\mathbf{x},t) - r_i = 0$$

$$\frac{\partial \pi}{\partial t} + \mathrm{div}\pi\,\mathrm{u} = 0$$ continuity equation

$\varphi = \{c_{i,}\ i = \overline{1,m}\}$ state function

f_i source term, $D_t = \{0 \le t \le \bar{t};\ \vec{x} \in D\}$,

$(S\varphi)_i \equiv \left(\Gamma(\varphi)\right)_i \varphi_i - \left(\Pi(\varphi)\right)_i$ transformation operators,

$\left(\Gamma(\varphi)\right)_i \varphi_i \ge 0,\ \left(\Pi(\varphi)\right)_i \ge 0,\ \ \varphi \ge \mathbf{0}$

Граничные и начальные условия

$$(R\varphi)_i = q_i,\ \ (\mathbf{x},t \in \Omega_t)$$

$$\varphi(\mathbf{x},0) = \varphi^0(\mathbf{x}).$$

General form of functionals

$$\Phi_k(\vec{\varphi}) = \int_{D_t} F_k(\vec{\varphi})\chi_k(\vec{x},t)dDdt \equiv \left(F_k, \chi_k\right), \quad k = 1,...,K$$

F_k are the **Lipschitz's** functions of the given form, differentiable, bounded

$\chi_k dDdt$ are **Radon's or Dirac's** measures on D_t, $\chi_k \in \Im^*(D_t)$.

Quality functionals

$$\Phi_k(\vec{\varphi}) = \int_{D_t} (\Psi - H(\vec{\varphi}))_m^T M(\Psi - H(\vec{\varphi}))_m \chi_k(\vec{x},t)dDdt,$$

"Measurement" functionals

$$\Phi(\vec{\varphi}) = \sum_{k=1}^{K} \int_{D_t} \left[H(\vec{\varphi})\right]_{mk} \delta(\vec{x} - \vec{x}_{mk})dDdt, \quad \vec{x}_{mk} \in D_t^m$$

Restriction functionals

$\vec{\varphi}(\vec{x},t) \le N, \quad \vartheta_k(\vec{\varphi}(\vec{x},t) \le 0$ distributive constraints

$$\Phi_k(\vec{\varphi}) = \int_{D_t} (\vartheta_k(\vec{\varphi}) + |\vartheta_k(\vec{\varphi})|)\chi_k(\vec{x},t)dDdt$$

Differentiability in extended sense

Extended functional for construction of optimal algorithms and uncertainties assessment

$$\tilde{\Phi}^h(\vec{\varphi}) = \Phi_k^h(\vec{\varphi}) + 0.5\Big\{\alpha_1(\vec{\eta}^T M_1 \vec{\eta})_{D_t^m} + \alpha_2(\vec{r}^T M_2 \vec{r})_{D_t^h}$$

$$+\alpha_3(\vec{\xi}^T M_3 \vec{\xi})_{D^h} + \alpha_4(\vec{\zeta}^T M_4 \vec{\zeta})_{R^h(D_t^h)}\Big\}^h + \Big[\mathbf{I}^h(\vec{\varphi},\vec{Y},\vec{\varphi}^*)\Big]_{D_t^h}$$

$M_i, (i = \overline{1,4})$ are the weight matrices,

$\alpha_i \geq 0, \ \sum_{i=1}^{4} \alpha_i = 1$ are the weight coefficients,

$\vec{\varphi}, \vec{\varphi}^*$ are the solutions of the direct and adjoint problems generated from

$$\mathbf{I}^h(\vec{\varphi},\vec{Y},\vec{\varphi}^*) = 0$$

Additive aggregation of the functionals for decomposition

Optimal forecasting and design

Optimality is meant in the sense that estimations of the goal functionals do not depend on the variations :

- of the sought functions in the phase spaces of the dynamics of the physical system under study
- of the solutions of corresponding adjoint problems that generated by variational principles
- of the uncertainty functions of different kinds which explicitly included into the extended functionals

The universal algorithm of forward & inverse modeling

$$\frac{\partial \tilde{\Phi}_k^h}{\partial \vec{\varphi}^*} \equiv B\Lambda_t \vec{\varphi} + G^h(\vec{\varphi}, \vec{Y}) - \vec{f} - \vec{r} = 0$$

$$\frac{\partial \tilde{\Phi}_k^h}{\partial \vec{\varphi}} \equiv (B\Lambda_t)^T \vec{\varphi}_k^* + A^T(\vec{\varphi}, \vec{Y})\vec{\varphi}_k^* + d_k = 0, \qquad \vec{\varphi}_k^*(\vec{x})\Big|_{t=\bar{t}} = 0$$

$$d_k = \frac{\partial}{\partial \overline{\varphi}}(\Phi_k^h(\vec{\varphi}) + 0.5\alpha_1(\vec{\eta}^T M_1 \vec{\eta})), \quad \vec{\varphi}^0 = \vec{\varphi}_a^0 + M_3^{-1}\vec{\varphi}_k^*(\vec{x}, 0), \quad t = 0$$

$$\vec{r}(\vec{x}, t) = M_2^{-1}\varphi_k^*(\vec{x}, t), \qquad \vec{Y} = \vec{Y}_a - M_4^{-1}\vec{\Gamma}_k$$

$$\vec{\Gamma}_k = \frac{\partial}{\partial \vec{Y}} I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}_k^*)$$

$$A(\vec{\varphi}, \vec{Y})\delta\vec{\varphi} \equiv \frac{\partial}{\partial \alpha}\left[G^h(\vec{\varphi} + \alpha\,\delta\vec{\varphi}, \vec{Y})\right]_{\alpha=0}$$

$\Lambda_t \varphi$ is the approximation of time derivatives

Initial guess: $\vec{r}^{(0)} = 0$, $\vec{\varphi}^{0(0)} = \vec{\varphi}_a^0$, $\vec{Y}^{(0)} = \vec{Y}_a$

Some elements
of optimal forecasting and design

The main sensitivity relations

$$\delta\Phi_k^h(\varphi) \equiv (\Gamma_k, \delta \mathrm{Y}) \equiv \frac{\partial}{\partial\alpha} I^h(\varphi, \mathrm{Y}+\alpha\ \ \delta\mathrm{Y},\ \varphi_k^*)\Big|_{\alpha=0}$$

Algorithm for calculation
of sensitivity functions

$$\Gamma_k = \frac{\partial}{\partial\delta\mathrm{Y}}\left(\frac{\partial}{\partial\alpha} I^h(\varphi, \mathrm{Y}+\alpha\ \ \delta\mathrm{Y}, \varphi_k^*)\Big|_{\alpha=0}\right)$$

The feed-back relations

$$\frac{dY_\alpha}{dt} = -\eta_\alpha \Gamma_{k\alpha},\ \ \alpha = \overline{1, N_\alpha},\ \ N_\alpha \le N$$

$\Gamma_k = \{\Gamma_{ki}\}$ are the sensitivity functions

$\delta\mathbf{Y} = \{\delta Y_i\}$ are the parameter variations

$$k = \overline{1,K},\ i = \overline{1,N}$$

Real time equations of back relations

$$\Phi_k(\varphi,\mathbf{Y}) = \Phi_{ks}(\varphi) + \Phi_{kp}(\mathbf{Y})$$

$$\Phi_{kp}(\mathbf{Y}) = 0.5\int_{D_t}\left\{\sum_{i=1}^{N}\left(\gamma_1\Gamma_{ip}^{(1)}\left|\mathrm{grad}\left(Y_i-\tilde{Y}_i\right)\right|^2+\gamma_2\Gamma_{ip}^{(2)}\left(Y_i-\tilde{Y}_i\right)^2\right)\right\}dDdt$$

$$\frac{\partial Y_i}{\partial t} = -\kappa\frac{\partial\Phi_k(\varphi,\mathbf{Y})}{\partial Y_i},\quad i=\overline{1,N};\quad \kappa\cong\Phi_k(\varphi,\mathbf{Y})\Big/\left(\frac{\partial\Phi_k}{\partial\mathbf{Y}},\frac{\partial\Phi_k}{\partial\mathbf{Y}}\right)$$

$$\frac{\partial Y_i}{\partial t} = -\kappa\left\{\frac{\partial I^h(\varphi,\mathbf{Y},\varphi^*)}{\partial Y_i}-\gamma_1\,\mathrm{div}\,\Gamma_{ip}^{(1)}\,\mathrm{grad}\left(Y_i-\tilde{Y}_i\right)+\gamma_2\Gamma_{ip}^{(2)}\left(Y_i-\tilde{Y}_i\right)\right\}$$

$\tilde{Y}$ - a priori parameter values

$\gamma_1,\gamma_2 \geq 0$ - weight coefficients

$\Gamma_{ip}^{(\alpha)}$ - matrices of scale coefficients and weights

Algorithms of uncertainty calculation based on sensitivity analysis and data assimilation:

in model

$$\vec{r}(\vec{x},t) = M_2^{-1}\varphi_k^*(\vec{x},t),$$

in initial state

$$\vec{\xi} = M_3^{-1} \quad \vec{\varphi}_k^*(\vec{x},0), \qquad t = 0$$

in model parameters and sources

$$\vec{\zeta} = M_4^{-1}\vec{\Gamma}_k = M_4^{-1}\frac{\partial}{\partial \vec{Y}} I^h(\vec{\varphi},\vec{Y},\vec{\varphi}_k^*)$$

$M_i,(i=\overline{2,4})$ are the weight matrices

Risk assessment
with the help of sensitivity functions

Threshold of safety intervals

$$\Delta_k^s,\ k = \overline{1, K}$$

safe ecological conditions

$$\left|\delta\Phi_k\right| \le \Delta_k^s$$

Estimations for deterministic case

$$\left|\delta\Phi_k\right| \le \sum_{i=1}^{N} \left|\Gamma_{ki}\right| \left|\delta Y_i\right|$$

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Risk estimates
for deterministic-stochastic case

$$\mathrm{E}(\delta \mathbf{Y}) = \{\mathrm{E}_i \equiv \mathrm{E}(\delta Y_i), \quad (i = \overline{1, N})\}$$

$$\mathrm{E}(\delta\Phi) = \sum_{i=1}^{N} \Gamma_i \mathrm{E}(\delta Y_i)$$

$$\mathrm{D}(\delta\Phi) = (\mathrm{D}(\delta \mathbf{Y})\Gamma, \Gamma)$$

$$P(\delta\Phi \in \Delta) = \int_{\Delta} f(x)dx, \qquad x \equiv \delta\Phi$$

$$f(x) = \frac{1}{\sqrt{2\pi \mathrm{D}(x)}} \quad e^{-\frac{(x-\mathrm{E}(x))^2}{2\mathrm{D}(x)}},$$

$$R^s = P(|\delta\Phi| \le \Delta^s)$$

Probability risk assessment

$$R^s = \frac{1}{\sqrt{2\pi \mathrm{D}(x)}} \int_0^{\Delta^s} e^{-\frac{(x-\mathrm{E}(x))^2}{2\mathrm{D}(x)}} dx = \frac{2}{\sqrt{2\pi}} \int_0^{\lambda} e^{-\frac{t^2}{2}} dt = \Psi(\lambda) \ ,$$

$$\lambda = \lambda(R^s) = (\Delta^s - \mathrm{E}(x)) / \sqrt{\mathrm{D(x)}}$$

Risk domain

$$R^r = 1 - R^s \equiv P\{\delta\Phi > \Delta^s\}$$

Safe range

$$\left|\Delta^s - \mathrm{E}(\delta\Phi)\right| = \lambda \sqrt{\mathrm{D}(\delta\Phi)}$$

Fundamental role
of uncertainty functions

- integration of all technology components
- bringing control into the system
- regularization of inverse methods
- targeting of adaptive monitoring
- cost effective data assimilation

From risk assessment to design of sustainable development strategy

- Risk/vulnerability assessment

Models of processes &

data bases

+

environment quality functionals

- Strategy of sustainable development

Models of processes &

data bases

+

superposition of different

multi-criteria functionals:

environment quality,

objective, control, restrictions, etc.

Advantage of the approach

- Consistency of all technology elements
- Optimality of numerical schemes based on discrete-analytical approximations(without flux-correction procedures)
- Cost-effectiveness of computational technology

Idea and basic approximations

Differential operators of common kind in the models

$$0 = \int_{x_{i-1}}^{x_i} \left(L\varphi - f \right) \varphi^* dx = \int_{x_{i-1}}^{x_i} L^* \varphi^* \varphi dx +$$

$$\left(A\varphi, \varphi^* \right)\Big|_{x_{i-1}}^{x_i} - \int_{x_{i-1}}^{x_i} f(x) \varphi^*(x) dx = 0$$

If $L^* \varphi^* = 0,$ then

$$\left(A\varphi, \varphi^* \right)\Big|_{x_{i-1}}^{x_i} - \int_{x_{i-1}}^{x_i} f(x) \varphi^*(x) dx = 0, \;\; i = \overline{2, n_x}$$

$\varphi^{*(\alpha)}(x), \;\; x_{i-1} \le x \le x_i, \;\; \alpha = 1, 2$ integrating multipliers

Fundamental **analytical** solutions of local adjoint problems

$$\left\{ \varphi_i^{*(1)} = 1, \quad \varphi_{i+1}^{*(1)} = 0 \right\}, \quad \left\{ \varphi_i^{*(2)} = 0, \quad \varphi_{i+1}^{*(2)} = 1 \right\}, \; i = \overline{1, n_x - 1}$$

Variational principle for successive schemes

$$\sum_{j=2}^{J}\left\{\Phi^{j}(\varphi^{j},Y)+\sum_{\alpha=1}^{r}\left\{\left[\left(\psi_{\alpha}^{j}-\varphi_{\alpha}^{j}\right)+\Delta\tau_{\alpha j}\left(L_{\alpha}^{j}\psi_{\alpha}^{j}-f_{\alpha}^{j}\right)\right]\psi_{\alpha}^{*j}\right.\right.$$

$$\left.+\left[\psi_{\alpha}^{j}-\left(\sigma_{\alpha}\varphi_{\alpha}^{j}+(1-\sigma_{\alpha})\varphi_{\alpha}^{j-1}\right)\right]\varphi_{\alpha}^{*j}\delta t_{j}\right\}$$

$$\left.+\left[\left(\varphi_{1}^{j-1}-\varphi^{j-1}\right)\varphi_{1}^{*j}+\sum_{\alpha=2}^{r}\left(\varphi_{\alpha}^{j-1}-\varphi_{\alpha-1}^{j}\right)\varphi_{\alpha}^{*j}+\left(\varphi^{j}-\varphi_{r}^{j}\right)\varphi^{*j}\right]\delta t_{j}\right\}$$

$$\psi_{\alpha}^{j}=\sigma_{\alpha}\varphi_{\alpha}^{j}+(1-\sigma_{\alpha})\varphi_{\alpha}^{j-1}$$

$$0.5\le\sigma_{\alpha}\le 1,\quad \Delta\tau_{\alpha j}=\sigma_{\alpha}\Delta t_{j}$$

Variational principle for parallel schemes

$$\sum_{j=2}^{J}\left\{\sum_{\alpha=1}^{r}\left\{\left[\left(\psi_\alpha^j-\varphi^{j-1}\right)+\Delta\tau_{\alpha j}\left(L_\alpha^j\psi_\alpha^j-f_\alpha^j\right)\right]\psi_\alpha^{*j}\right.\right.$$

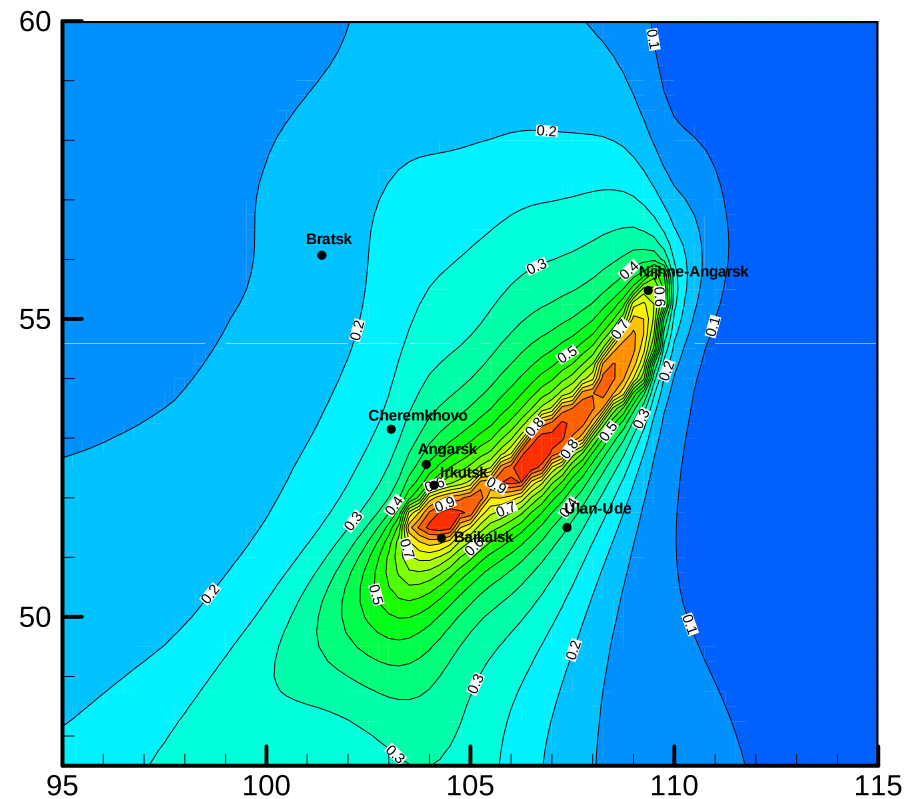
$$\left.+\left[\psi_\alpha^j-\left(\sigma_\alpha\varphi_\alpha^j+(1-\sigma_\alpha)\varphi_\alpha^{j-1}\right)\right]\varphi_\alpha^{*j}\delta t_j\right\}$$

$$\left.+\left[\varphi^j-\frac{1}{r}\sum_{\alpha=1}^{r}\varphi_\alpha^j\right]\varphi^{*j}\delta t_j\right\}+\sum_{j=2}^{J}\sum_{\alpha=1}^{r}\Phi_{k\alpha}^j(\vec{\varphi},\vec{Y})$$

$$\Phi_k^h=\sum_{j=2}^{J}\sum_{\alpha=1}^{r}\Phi_{k\alpha}^j(\vec{\varphi},\vec{Y})=\sum_{j=2}^{J}\sum_{\alpha=1}^{r}\left(\int_D F_{k\alpha}^j(\vec{\varphi},\vec{Y})\chi_{k\alpha}^j(\vec{x},t)dD\right)\delta t_j$$

$\varphi^1(\vec{x},t_0)$ given

Long-term forecast of environmental risk for Lake Baikal region



Surface layer, October

Conclusion

Algorithms for optimal environmental forecasting and design are proposed:

- uncertainty calculations
- risk assessment
- feed-back relations

The fundamental role of uncertainty is highlighted

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Thank you for your time!