

# Introduction to atmospheric dispersion modelling

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- Main parts of the atmosphere
- Basic terms
  - > atmospheric tracer
  - temporal and spatial scales
  - > life time in the atmosphere
  - life cycle of atmospheric tracers
- Dispersion equation
- Langrangian and Eulerian dispersion models
- Parts of a dispersion model
- Model Quality Assurance
- Summary



#### Major layers of the atmosphere

- Troposphere (tropos=mixing): interaction with surface
- Stratosphere: ozone-uv heating
- Mesosphere: mixing again
- Thermosphere: O<sub>2</sub>, N<sub>2</sub> solar radiation heating
- Ionosphere: ions
- Exosphere: fast molecules escape to the open space





#### Pollution cycle in the troposphere





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### **Dispersion equation**

- Mass conservation
  - ➤ transport
  - > sources
  - ➤ sinks
- Scale separation
  - ➤ mean flow
  - > turbulence
- Closure problem





 $\succ$  K-theory  $\rightarrow$  turbulent diffusion coefficient

$$LC = \frac{\partial C}{\partial t} + \frac{\partial}{\partial x_i} (U_i C) - \frac{\partial}{\partial x_i} \rho K_{ii} \frac{\partial (C / \rho)}{\partial x_i} + R(C) = E$$



#### From concentration to load

$$M = \int_{0}^{T} dt \int_{-\infty}^{\infty} \int \int C p \, dx = (C, p) - \text{load functional}$$

p is a weight (sensitivity) function of the load:

- Population exposure p(
- Ecosystem damage
- Observational site

 $p(\mathbf{x}, \mathbf{t}) = \delta(\mathbf{x} - \mathbf{x}_{city})$   $p(\mathbf{x}, \mathbf{t}) = p(\mathbf{t}) \ \mathbf{1}(\mathbf{A}_{ecosystem})$   $p(\mathbf{x}, \mathbf{t}) = \delta(\mathbf{x} - \mathbf{x}_{site}) \ \mathbf{1}(\mathbf{t}, \mathbf{t}_{beg}, \mathbf{t}_{end})$ 

#### Alternative way to get the load function

Consider some function  $C^*$  satisfying  $L^*C^* = p$ , where  $L^*$  is adjoint to L.

#### Then

$$M = (C^*, E) = (C^*, LC) = (L^*C^*, C) = (p, C)$$
  
L<sup>\*</sup>C<sup>\*</sup> = p - adjoint dispersion equation  
$$\partial_{x} = \partial_{x} = \partial_{x} = \partial_{x} = \partial_{x} = C = C^* \xrightarrow{x \to \infty} 0$$

$$L^* = -\frac{\partial}{\partial t} - \frac{\partial}{\partial x_i} (U_i) - \frac{\partial}{\partial x_i} K_{ii} \frac{\partial}{\partial x_i} + R(C) \qquad \begin{array}{c} C, C^* \to 0\\ C^*(t=T) = 0 \end{array}$$

#### Forward problem:

$$\mathbf{L} = \frac{\partial}{\partial t} + \frac{\partial}{\partial x_i} (\mathbf{U}_i) - \frac{\partial}{\partial x_i} \rho \mathbf{K}_{ii} \frac{\partial (1/\rho)}{\partial x_i} + \mathbf{R}; \quad \mathbf{L}\mathbf{C} = \mathbf{E}; \ \mathbf{M} = (\mathbf{p}, \mathbf{C})$$

Inverse (adjoint) problem

$$L^* = -\frac{\partial}{\partial t} - \frac{\partial}{\partial x_i} (U_i) - \frac{\partial}{\partial x_i} K_{ii} \frac{\partial}{\partial x_i} + R; \quad L^* C^* = p; \ M = (E, C^*)$$



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### Classifications of models

- Model principles
  - Eulerian
  - Lagrangian
  - Gaussian
  - statistical Monte-Carlo
- Scales
  - global
  - continental
  - regional
  - local/urban

#### Classifications of models.2



#### > Chemicals

- acid
- ozone
- greenhouse gas
- inert aerosol/dust
- radio-activity
- toxic
- persistent pollutants
- Model media
  - atmospheric
  - multi-media
  - integrated models

### Classifications of models.3

- Input data
  - climatological
  - real-time data
- Time dimension: direction, horizon
  - re-analysis
  - now-casting
  - forecasting
- Problem to solve
  - forward
  - inverse



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## SILAM v.5: outlook

- Modules
  - 8 chemical and physical transformation modules (6 open for operational use),
  - ➢ 6 source terms (all open),
  - 2 aerosol dynamics (one open)
  - > 3D- and 4D- Var
- Domains: from global to betameso scale (~1km resolution)
- Meteo input:
  - > ECMWF
  - HIRLAM, AROME, HIRHAM, ECHAM, and any other who can write GRIB-1 or GRIB-2

> WRF



# FMI regional AQ assessment and forecasting platform



#### **SILAM scales**







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#### Model vs reality

- Model is never a copy of reality
  - It represents only those features, which are deemed to be important for a specific application
- The extent of their similarity is to be established in each specific case



I.Repin. Zaporozhje Cossacks are writing a letter to Turkish sultan

W.Kandinski. Cossacks



### Model Quality Assurance (QA)

- Tests of individual modules (development stage)
- Sensitivity runs
- Model-measurement comparison
- Model-model comparison



#### Model-measurement comparison

- The only connection between model and reality
- Data sets from different origin
  - > point observations vs grid-mean model results
  - representativeness error
  - instrumental errors
- Observations are expensive => sparse
- Limited number of observed variables
- Specific statistical methods are required to obtain nontrivial conclusions

#### Model inter-comparison

- Useful if lacking measurements
- Similar features of data
- Large data sets => high accuracy
- Wide variety of analytical methods
- Ensemble model
- Possibly, no connection to reality



## Summary



- Distribution of an atmospheric pollutant is described via dispersion equation, which is a representation of the mass conservation law
- Duality of dispersion problem allows for usage of forward and adjoint dispersion equations
  - ➢ identical final results the load
  - > choice depends on specific task
- Model quality assurance implies several actions and covers ALL stages of the model development