On-line integrated modelling: feedbacks, deposition and PBL

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NetFAM-DMI Practical Course
"Environment - HIgh Resolution Limited Area Model (**Enviro-HIRLAM**)"
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Lectures Outline:

- Main focus on further development of Enviro-HIRLAM
- Possible feedbacks in integrated NWP-ACP models
- Missing feedback mechanisms in the model
- Deposition mechanism improvements
- PBL feedbacks in integrated NWP-ACP models
- Requirements and recommendations for further research

Atmosphere Interactions:

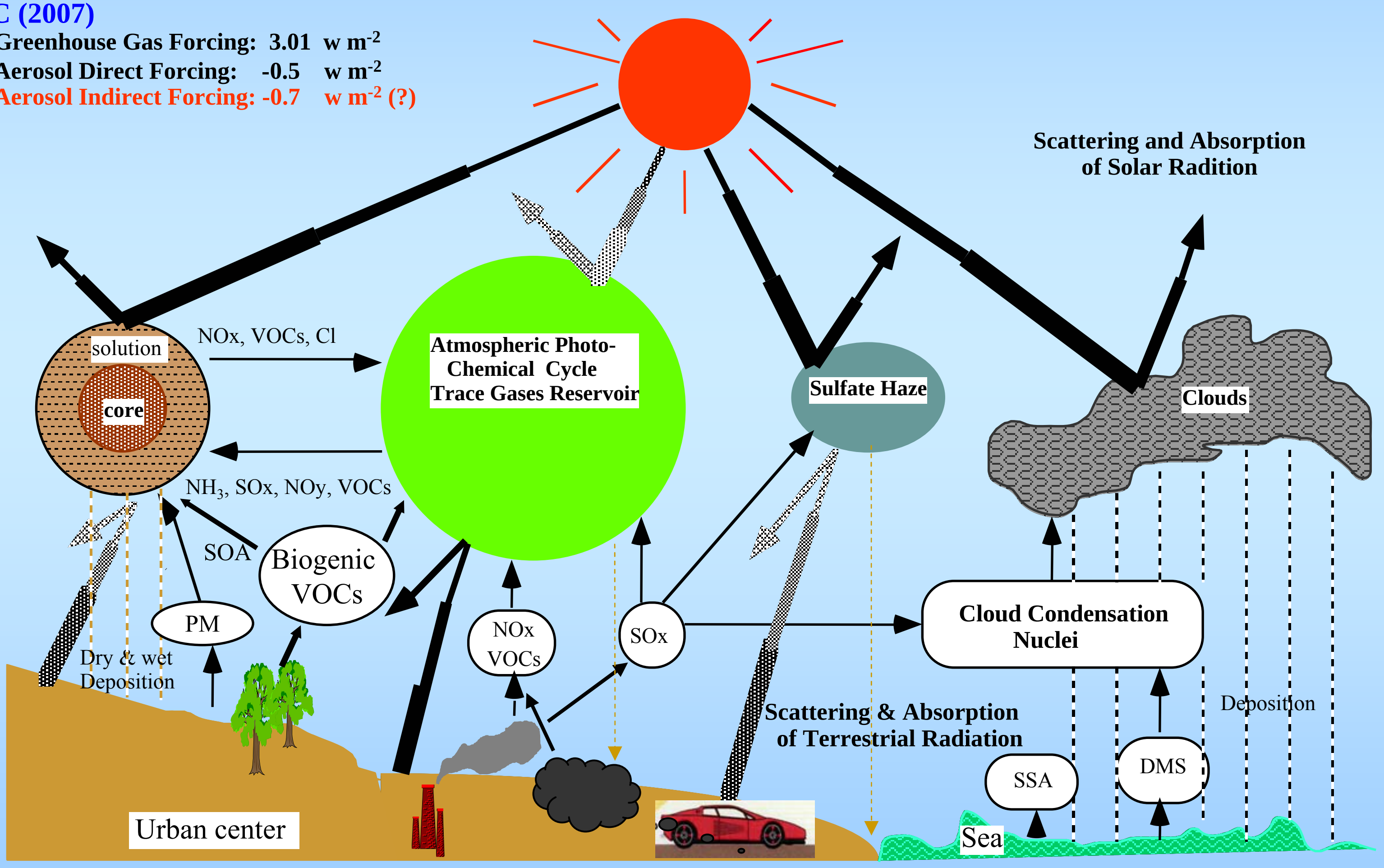
Gases, Aerosols, Chemistry, Transport, Radiation, Climate

IPCC (2007)

Greenhouse Gas Forcing: 3.01 w m^{-2}

Aerosol Direct Forcing: -0.5 w m^{-2}

Aerosol Indirect Forcing: -0.7 w m^{-2} (?)



After Y. Zhang, DMI, Copenhagen, 2007

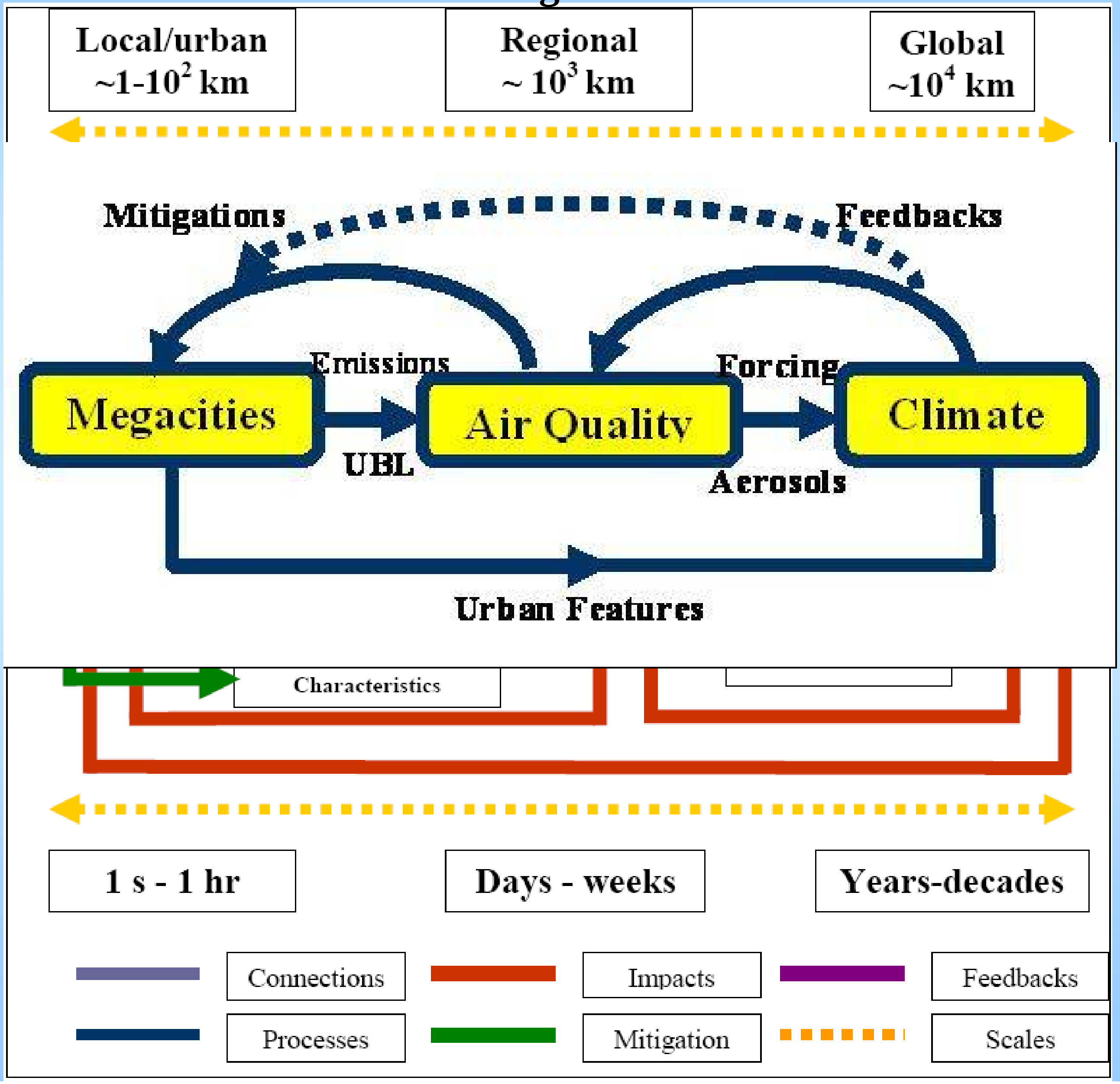
Examples of Important Feedbacks

- Effects of Meteorology and Climate on Gases and Aerosols
    - Meteorology is responsible for atmospheric transport and diffusion of pollutants
    - Changes in temperature, humidity, and precipitation directly affect species conc.
    - The cooling of the stratosphere due to the accumulation of GHGs affects lifetimes
    - Changes in tropospheric vertical temperature structure affect transport of species
    - Changes in vegetation alter dry deposition and emission rates of biogenic species
    - Climate changes alter biological sources and sinks of radiatively active species
- Effects of Gases and Aerosols on Meteorology and Climate
    - Decrease net downward solar/thermal-IR radiation and photolysis (direct effect)
    - Affect PBL meteorology (decrease near-surface air temperature, wind speed, and cloud cover and increase RH and atmospheric stability) (semi-indirect effect)
    - Aerosols serve as CCN, reduce drop size and increase drop number, reflectivity, and optical depth of low level clouds (LLC) (the Twomey or first indirect effect)
    - Aerosols increase liquid water content, fractional cloudiness, and lifetime of LLC but suppress precipitation (the second indirect effect)

(after Round Table of Copenhagen COST-NetFAM workshop, 2007)

Connections between megacities, air quality and climate:

main feedbacks, ecosystem, health and weather impact pathways, and mitigation routes



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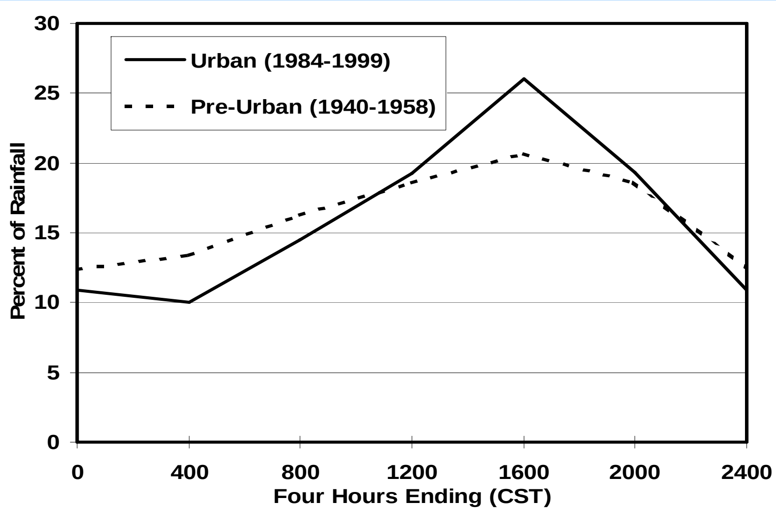
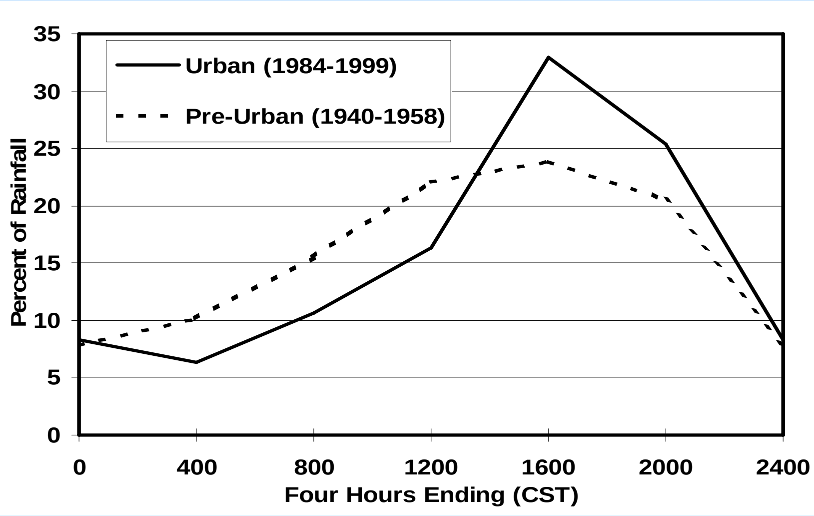
Do Cities Affect the Diurnal Cycle of Rainfall?



Average annual diurnal rainfall distributions at gage 4311 (UA) for the urban (1984-1999) and pre-urban (1940-1958) time periods



Average warm season diurnal rainfall distribution at gage 4311 for the urban (1984-1999) and pre-urban (1940-1958) time periods

(NASA, Shepherd, 2004)

The peak fraction of daily rainfall is more pronounced for the 12-16 and 16-20 4-hr time increments for the urban time period compared to the pre-urban time period; The warm season experiences a greater diurnal modification

Aerosol feedbacks to be considered

<u>Direct effect</u> - Decrease solar/thermal-infrared radiation and visibility:

- **Processes involved: radiation (scattering, absorption, refraction, etc.);**
- **Key variables: refractive indices, extinction coefficient, single-scattering albedo, asymmetry factor, aerosol optical depth, visual range;**
- **Key species: - cooling: water, sulphate, nitrate, most OC;**
  - warming: BC, OC, Fe, Al, polycyclic/nitrated aromatic compounds;

<u>Semi-direct effect</u> - Via PBL meteorology and photochemistry, photolysis and aerosol emission/ blowing changes:

- **Processes involved: PBL, surface layer, photolysis, meteorology-dependent processes;**
- **Key variables: temperature, pressure, relative and water vapour specific humidity, wind speed and direction, clouds fraction, stability, PBL height, photolysis rates, emission rates of meteorology-dependent primary species (dust, sea-salt, pollen and other biogenic);**

<u>First indirect effect</u> (so called the Twomey effect) – Affect clouds drop size, number, reflectivity, and optical depth via CCN or ice nuclei:

- **Processes involved: aerodynamic activation / resuspension, clouds microphysics, hydrometeor dynamics;**
- **Key variables: int./act. fractions, CCN size/compound, clouds drop size / number / liquid water content, cloud optical depth, updraft velocity;**

<u>Second indirect effect</u> (also called as the lifetime or suppression effect) - Affect cloud liquid water content, lifetime and precipitation:

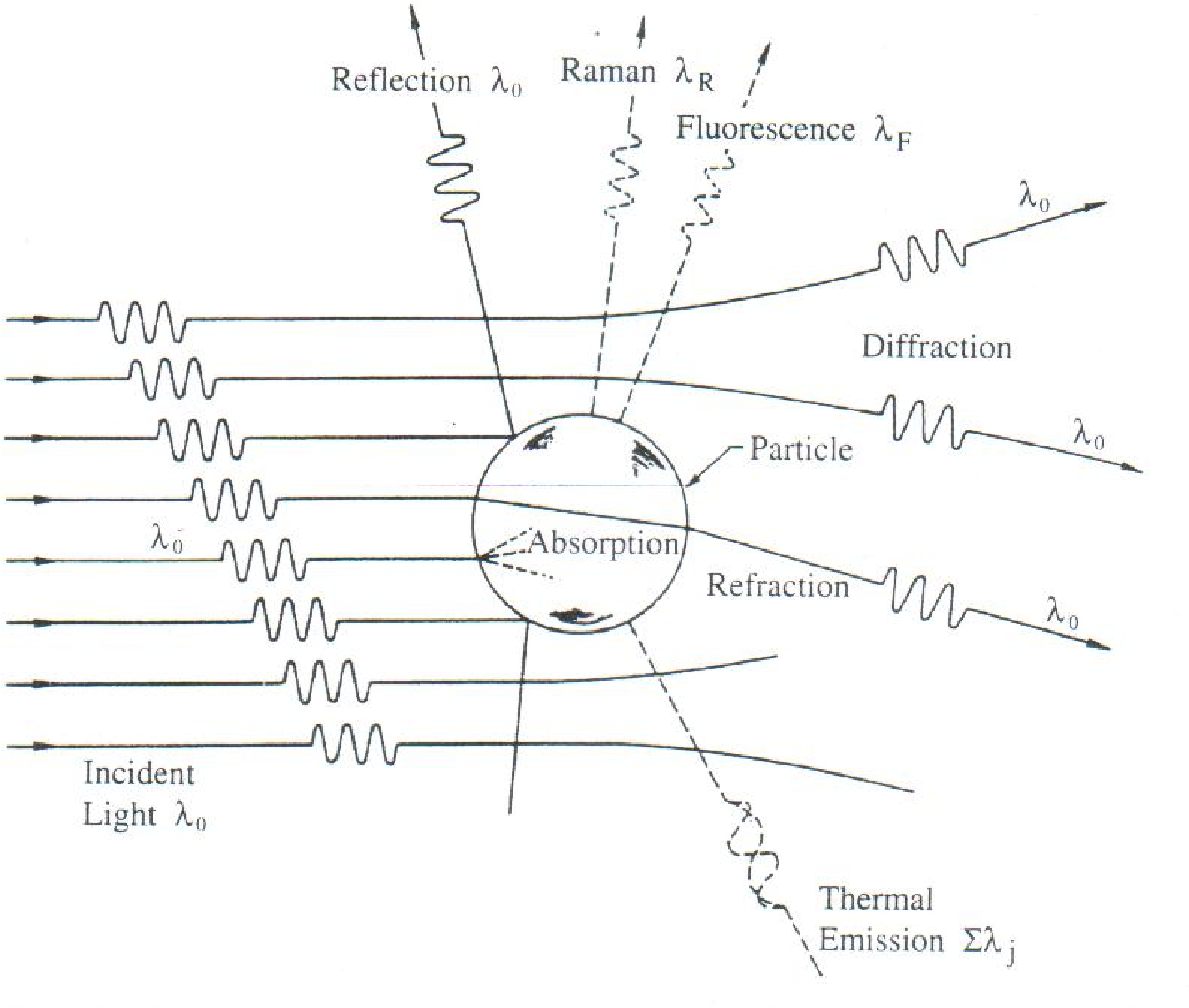
- **Processes involved: clouds microphysics, washout, rainout, droplet sedimentation;**
- **Key variables: scavenging efficiency, precipitation rate, sedimentation rate.**

Direct Aerosol Forcing

Despite big similarities with gases the particle scattering absorption is more complex due to variety of size and composition aerosols.

(i) warm the air by absorbing solar and thermal-IR radiation (black carbon, iron, aluminium, polycyclic and nitrated aromatic compounds),

(ii) cool the air by backscattering incident short wave radiation to space (water, sulphate, nitrate, most of organic compounds)



Direct aerosol effect in models

- Realisation depends on the radiation scheme used in the model.
- The presence of aerosols in the atmosphere may absorb, scatter and re-emit incoming shortwave radiation.
- These effects have not been implemented into the model yet and the radiation scheme used in HIRLAM (Savijärvi, 1990) is to simplified to account for these effects (only via empirical coeffeicients, but it could also be tested with Li et al (2001) parameterisation).
- Following (Seinfeld and Pandis, 1998) it is possible to estimate the effect of a layer of scattering aerosol accounting for surface reflections, by modifying the surface albedo accordingly.
- Another approach would be to use look-up tables for the complex index of refraction for various aerosol compositions, assuming that the aerosol is in the Rayleigh scattering regime.

Feedbacks classification is not complete

- Combined/overal effect of different aerosol feedbacks is very difficult to predict due to non-linearity and non-additivity of different interacting mechanisms.
- Aerosols affect the meteorology by changing cloud characteristics in many ways (and different directions).
- They act as cloud condensation and ice nuclei, they may inhibit freezing and they could have an influence on the hydrological cycle.
- While the cloud albedo enhancement (Twomey effect) of warm clouds received most attention so far and traditionally is the only indirect aerosol forcing considered in transient climate simulations, the multitude of effects should be considered.

Different chain aerosol effects on water clouds

- **Cloud albedo effect (pure forcing)**

– for a constant cloud water content, more aerosols lead to more and smaller cloud droplets ⇒ larger cross sectional area ⇒ more reflection of solar radiation

- **Cloud lifetime effect (involves feedbacks)**

– the more and smaller cloud droplets will not collide as efficiently ⇒ decrease drizzle formation ⇒ increase cloud lifetime ⇒ more reflection of solar radiation

- **Semi-direct effect (involves feedbacks)**

– absorption of solar radiation by black carbon within a cloud increases the temperature ⇒ decreases relative humidity ⇒ evaporation of cloud droplets ⇒ more absorption of solar radiation (opposite sign)

=> Online integrated models are necessary to simulate correctly these effects involved 2nd feedbacks

Carbonaceous Aerosols

•Carbonaceous aerosols are divided into two categories: black carbon (BC) and **organic carbon** (OC). BC is a strong absorber of visible and near-IR light; OC mostly scatters radiation.

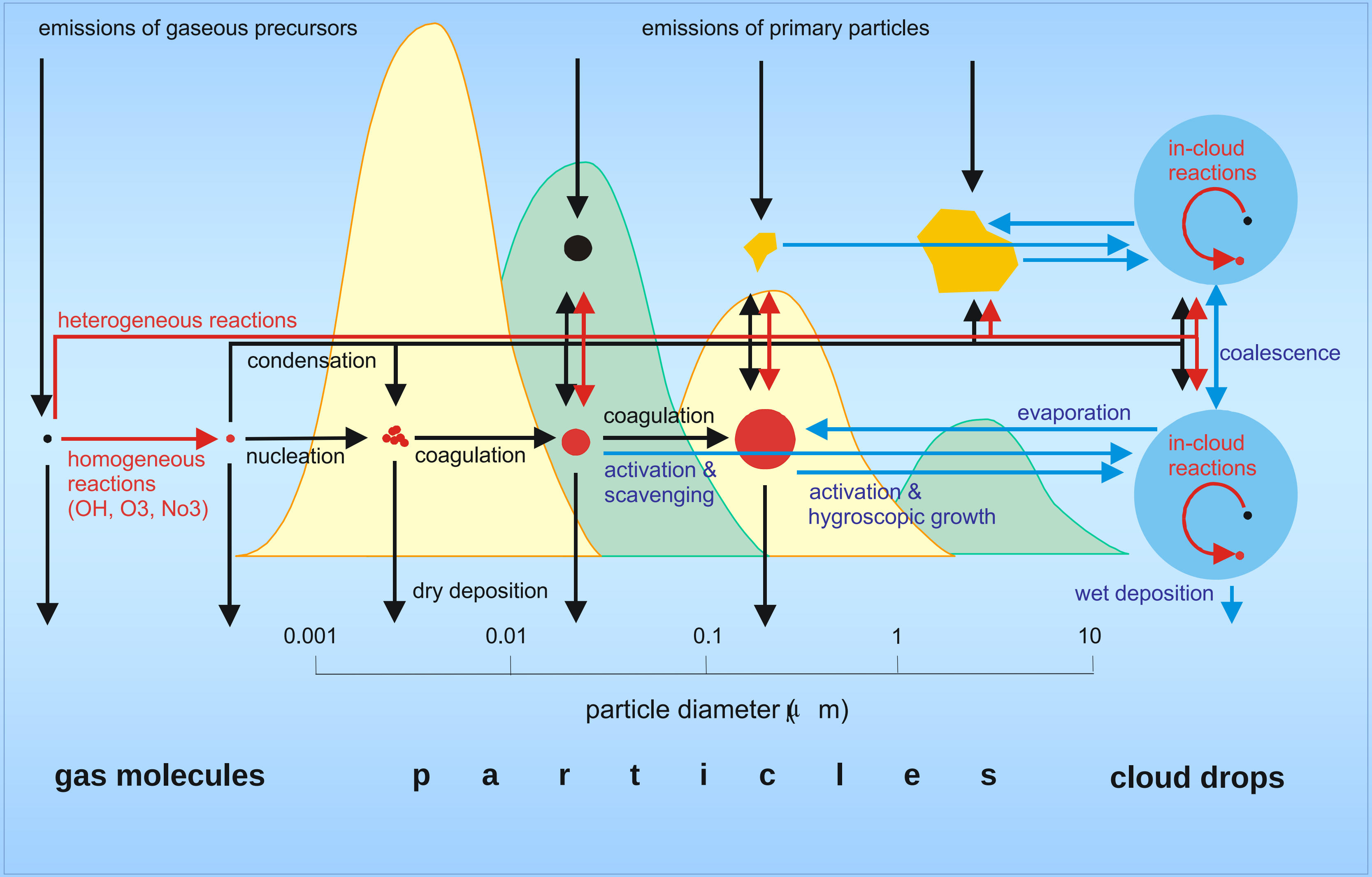
•OC is further divided into primary organic aerosol (POA) and **secondary organic aerosol** (SOA).

•The dominant emissions of BC and POA are fossil fuel and biomass burning.

•SOAs are formed when volatile organic compounds (VOCs) are oxidized to form semi-volatile products.

•Biogenic VOCs, especially monoterpenes ($C_{10}H_{16}$), are the most important VOCs for SOA formation.

Scheme of Aerosol-CCN/IN dynamics modelling



Raes et al., AE, 2000

How are aerosol effects on clouds simulated in meteorology/climate models?

- **Predict aerosol mass concentrations:**

– *sources* (aerosol emissions of the major aerosol species: sulfate, black carbon, organic carbon, sea salt, dust)

– *transformation* (aerosol formation and dynamics, dry and wet deposition, chemical transformation and transport)

- **Need a good description of cloud properties:**

– *precipitation formation* (collision/coalescence of cloud droplets and ice crystals, riming of snow flakes)

- **Need to parameterize aerosol-cloud interactions:**

– *cloud droplet nucleation* (activation of hygroscopic aerosol particles)

– *ice crystal formation* (contact and immersion freezing, homogeneous freezing in cirrus clouds)

Scientific hypotheses/questions still to be tested/addressed

(formulated on COST-NetFAM workshop in Copenhagen, May 2007)

- **Hypothesis**
  - **Feedback mechanisms are important in accurate modeling of NWP/MM-ACT and quantifying direct and indirect effects of aerosols.**

  => *the answer is 'Yes, they can be very important'*

- **Key questions** ***(still waiting for answers)***
  - **What are the effects of climate/meteorology on the abundance and properties (chemical, microphysical, and radiative) of aerosols on urban/regional scales?**
  - **What are the effects of aerosols on urban/regional climate/meteorology and their relative importance (e.g., anthropogenic vs. natural)?**
  - **How important the two-way/chain feedbacks among meteorology, climate, and air quality are in the estimated effects?**
  - **What is the relative importance of aerosol direct and indirect effects in the estimates on different time and space scales?**
  - **What are the key uncertainties associated with model predictions of those effects?**
  - **How can simulated feedbacks be verified with available datasets?**

DEPOSITION MECHANISMS

- **Particle size dependend parameterisations for dry and wet deposition,**
- **Resistance approach for dry deposition,**
- **Terminal settling velocity in different regimes:**

  - Stockes low,

  - non-stacionary turbulence regime,

  - correction for small particles,
- **Different scavenging of particles and gases,**
- **Depending on classification of land/sea surface,**
- **Below-cloud scavenging (washout)**
- **Rainout between the cloud base & top (scavenging into cloud):**

  - *convective* precipitation,

  - *stratiform* precipitation,
- **Scavenging by snow.**
- **3D cloud water and humidity available for deposition simulation**

Wet deposition processes

- Below-cloud scavenging (washout) coefficient for aerosol particles of radius *rp*

$$\Lambda = -\pi N_r \int a^2 w_r(a) E(r_p, a) f_a(a) da,$$

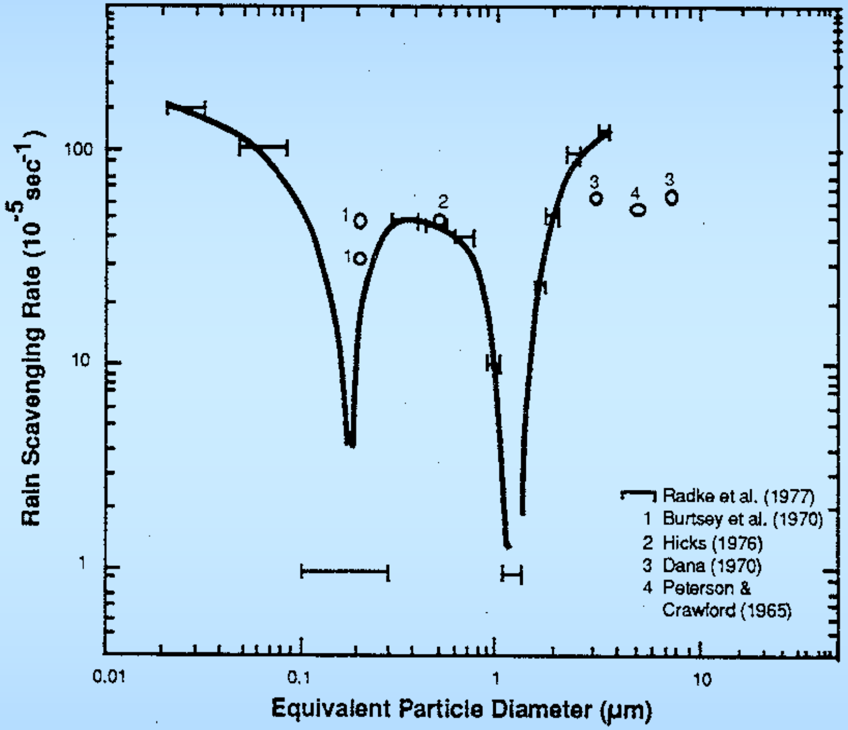
- the 'Greenfield gap',

- Rainout between the cloud base & top (scavenging into the cloud):

- *convective* precipitation,

- *stratiform* precipitation,

- Scavenging by snow,
- Orographic effects (seeder-feeder effect),
- Deposition caused by surface fog.



Measured Values of Scavenging Coefficient vs. Particle Size (McMahon and Dennison, 1979))

Two formulations for the washout coefficient, Λ' (s-1)

1) as <u>empirical function of particle radius</u> r (μm) & <u>rainrate</u> q (mm/h):

$\Lambda'(r,q) = a_0\, q^{0.79}$, $\quad r < 1.4\ \mu m$

$\Lambda'(r,q) = (b_0 + b_1 r + b_2 r^2 + b_3 r^3)\, f(q)$, $\quad 1.4\ \mu m < r < 10\ \mu m$

$\Lambda'(r,q) = f(q)$, $\quad r > 10\ \mu m$

where $f(q) = a_1 q + a_2 q^2$, $a_0 = 8.4\cdot10^{-5}$, $a_1 = 2.7\cdot10^{-4}$, $a_2 = -3.618\cdot10^{-6}$, $b_0 = -0.1483$, $b_1 = 0.3220133$, $b_2 = -3.0062\cdot10^{-2}$, and $b_3 = 9.34458\cdot10^{-4}$.

2) theoretical <u>formulae</u> for the <u>Brownian capture mechanism</u>, the <u>aerosol capture efficiency</u> due to the <u>impaction</u> of aerosol particles on the rain drop and <u>interception</u> of particles by the rain drop:

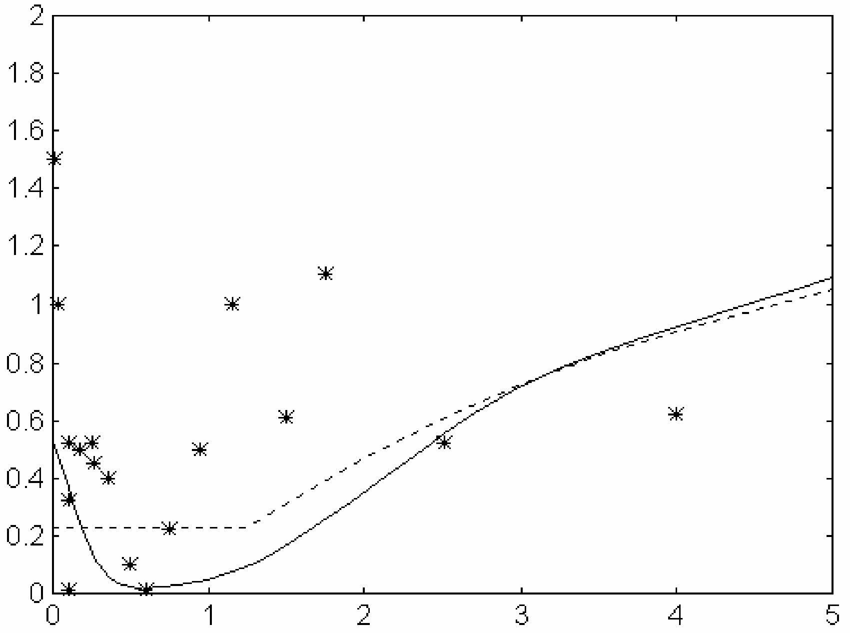
$$\Lambda = \frac{q}{2a_m}\left[\frac{4}{Pe}\left(1+0.4\,\mathrm{Re}^{1/2}\,Sc^{1/3}\right)+\right.$$

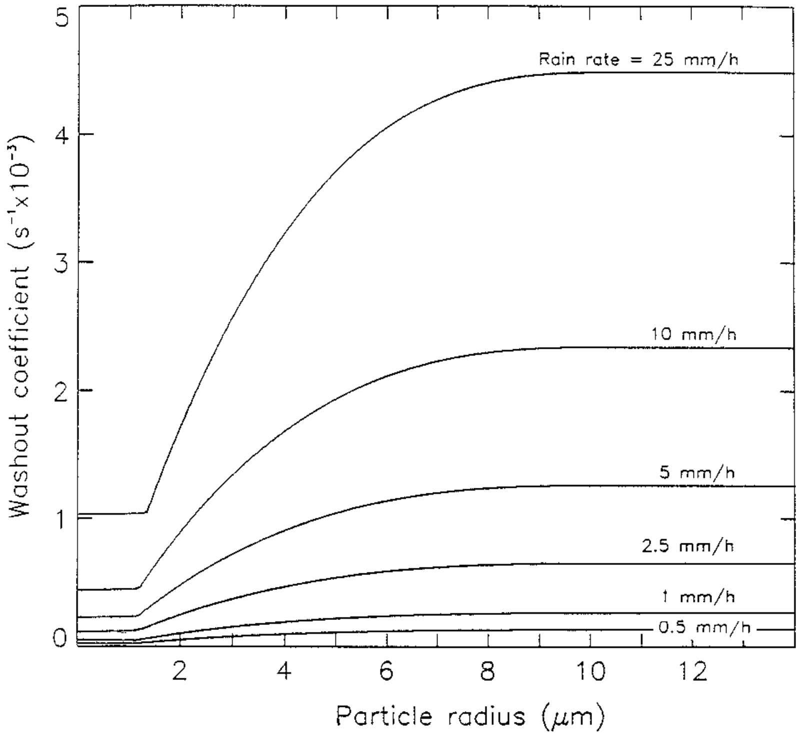
$$\left.\frac{4r_p}{a_m}\left(\frac{r_p}{a_m}+\frac{(1+2\,\mu_w r_p/\mu_a a_m)}{\left(1+\mathrm{Re}^{-1/2}\,\mu_w/\mu_a\right)}\right)+\left(\frac{\rho_w}{\rho_a}\right)^{\frac{1}{2}}\left(\frac{St-St_*}{St-St_*+2/3}\right)^{\frac{3}{2}}\right]$$

where a_m is the volume-mean raindrop projected radius, St - the Stokes number ($-2r_p^2\rho_p w_r/9$♋$\rho_a\nu$), St_* - the critical Stokes number ($1.2+\ln(1+Re)/12)/(1+\ln(1+Re)$), μ_w and μ_a - the dynamic viscosities of water and air, respectively, and ρ_p, ρ_w and ρ_a - the density of particles, water and air, respectively, Pe - the Peclet number (aw_r/D), Sc -the Schmidt number (ν/D), Re - the Reynolds number (aw_r/ν), ν - the kinematic viscosity of the air (μ_a/ρ_a), and D - the Brownian diffusivity of particles.

Baklanov and Sørensen, 2001

Wet deposition processes





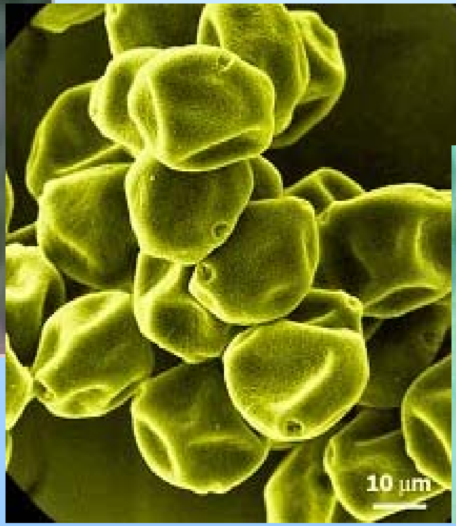
Dependence of the washout coefficient on particle radius for a rain intensity of 5 mm/h.

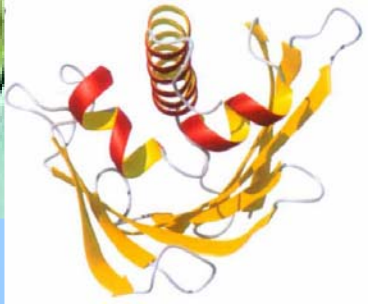
Dependence of the washout coefficient on particle radius and rain intensity.

Baklanov and Sørensen, 2001

Specific Aerosols: Birch Pollen Forecasting:

1. Specific meteorology-dependent emission,
2. Resuspension and blowing changes
3. Specific deposition mechanism
4. Chemically active as well,
5. Synergy health effects together with other pollutants
6. Special version of Enviro-HIRLAM





Improving PBL parameterisations and feedbacks of PBL

Are we satisfied with PBL resolution, parameterization schemes of the PBL height, and turbulence fluxes?

Special focus on SBL cases (most important for air pollution applications)

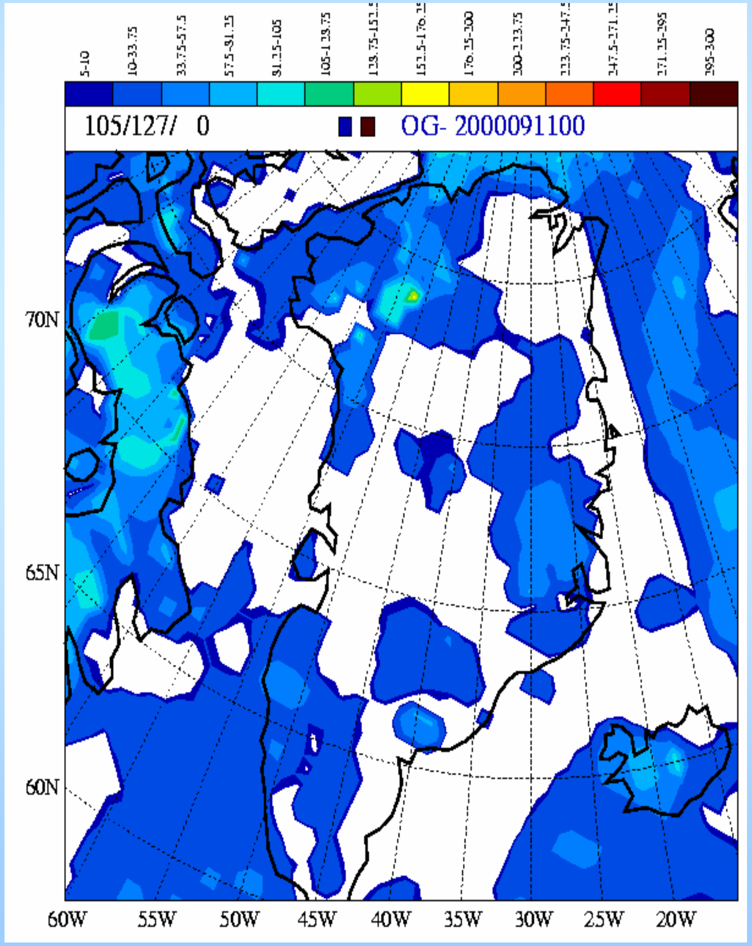
High-resolution models with a detailed description of the PBL structure are necessary to simulate accurately aerosol effects

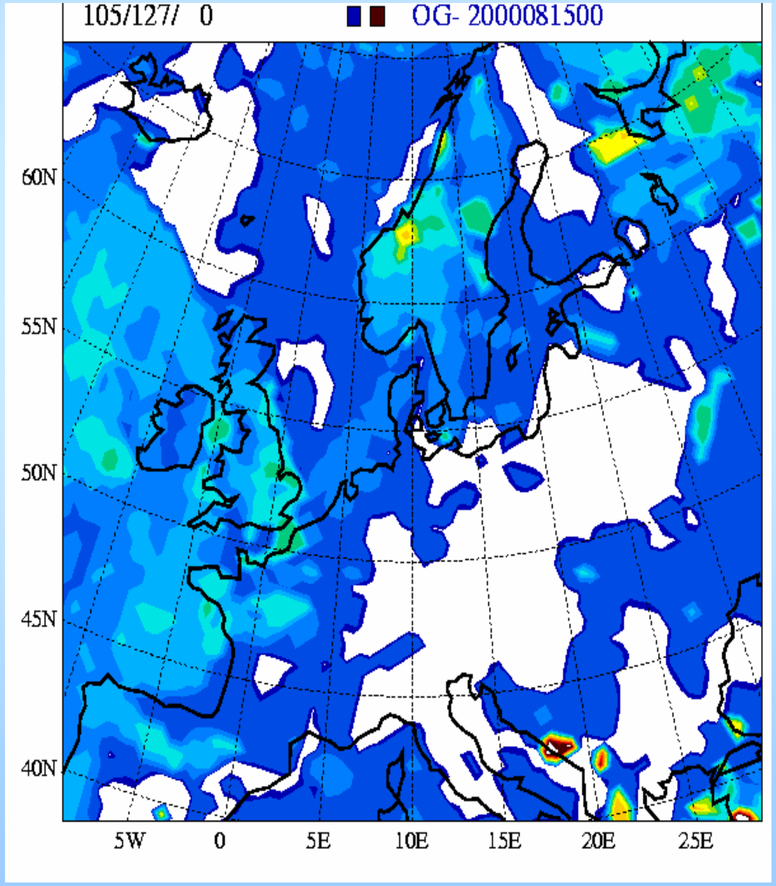
What are two-way feedbacks between aerosols and the PBL structures and turbulence characteristics ?

Peculiarities of SBLs in Northern regions:

- long lived and very shallow SBLs,
- thoroughly stable stratification (without the residual layer),
- vertical wave propagation is not blocked,
- SBL turbulence becomes essentially non-local,
- traditional local theory predicts an insufficient turbulence mixing.

The nocturnal PBL height forecasted by the DMI-HIRLAM model with the CBR scheme and the TKE decay approach for the PBL height for Greenland (left) and Europe (right)





Basic types of the stable ABL

- Until recently ABLs were distinguished accounting only for $F_{bs}=F_*$:

  neutral at $F_* = 0$
  stable at $F_* < 0$
  convective at $F_* > 0$

- Now more detailed classification distinguish between

  truly neutral (TN) ABL: $F_* = 0$, $N = 0$
  conventionally neutral (CN) ABL: $F_* = 0$, $N > 0$
  nocturnal stable (NS) ABL: $F_* < 0$, $N = 0$
  long-lived stable (LS) ABL: $F_* < 0$, $N > 0$

- Realistic models should cover all types; current models – only TN and NS

Zilitinkevich, Esau, Baklanov (2007)

Ri-number methods for SBL height estimation

Following Zilitinkevich & Baklanov (2002), we can distinguish four different Ri methods.

1. Gradient Richardson number. Infinitesimal disturbances in a steady-state homogeneous stably stratified sheared flow decay if the gradient Richardson number Ri exceeds a critical value Ri*c*,

$$\mathrm{Ri} \equiv \frac{\beta(\partial\theta_v/\partial z)}{(\partial u/\partial z)^2 + (\partial v/\partial z)^2} > \mathrm{Ri}_c = 0.25$$

2. Bulk Richardson number. An alternative, widely used method of estimating *h* employs, instead of the gradient Richardson number Ri, the boundary-layer bulk Richardson number, Ri*b*, specified as

$$\mathrm{Ri}_B \equiv \frac{\beta \Delta\theta_v h}{U^2}$$

through the wind velocity at the upper boundary of the layer and the virtual potential temperature increment across the layer.

3. Finite-difference Richardson number. The idea is to exclude the lower portion of the SBL and to determine a “finite-difference Richardson number”, Ri*F*

$$h_E \approx \frac{(h_E - z_2)^2}{h_E - z_1} = \frac{\mathrm{Ri}_{Fc}(\delta U)^2}{\beta\delta\theta_v}$$

4. Modified Richardson number method. The SBL critical bulk Richardson number, Ri*Bc*, is not a constant and evidently increases with increasing free flow stability and very probably depends on the surface roughness length, the Coriolis parameter and the geostrophic wind shear in baroclinic flows. For practical use Zilitinkevich and Baklanov (2002) recommended:

$$\mathrm{Ri}_{Bc} \approx 0.1371 + 0.0024\frac{N}{|f|}$$

where N is the Brunt-Väisälä frequency in the adjacent layer of the free atmosphere.

Formulations based on equation of TKE budget

Zilitinkevich *et al*. (2002), Zilitinkevich & Baklanov (2002) and Zilitinkevich & Esau (2003) suggested new diagnostic and prognostic parameterisations for SBL height, including effects of the free-flow stability and baroclinity:

$$\frac{\partial h}{\partial t} + \mathbf{V} \cdot \nabla h = -C_E \,|\, f \,|\, (h - h_{CQE}) + K_h \nabla^2 h$$

$$h_E = C_R \frac{u_*}{|\, f \,|} \left[1 - \left(\frac{\mathrm{Ri}_c}{\mathrm{Ri}} \right)^{1/2} \right]^{-1/2}$$

$$\left(1 + \frac{C_R^2 C_{uN}}{C_S^2} \mu_N + \frac{C_R^2}{C_S^2} \mu \left[1 - \left(\frac{\mathrm{Ri}_c}{\mathrm{Ri}} \right)^{1/2} \right] \right)^{-1/2}$$

Stability parameters: $\mu = \frac{u_*}{|\, f \,|\, L}$ internal, $\mu_N = \frac{N}{|\, f \,|}$ external.

Zilitinkevich et al. SBL height formulation (Continuation)

The MO length scale L and the internal-stability parameter

$\mu = u_* |f| L$ are modified $L_{baroclinic} = \dfrac{u_T^3}{-F_{bs}} = L\left[1 - \left(\dfrac{\mathrm{Ri}_c}{\mathrm{Ri}}\right)^{1/2}\right]^{-3/2}$

$$u_T^2 = \frac{u_*^2}{1 - (\mathrm{Ri}_c/\mathrm{Ri})^{1/2}}$$

Free-atmosphere parameters:

baroclinic shear $\Gamma = \dfrac{g}{|f|T}\left[\left(\dfrac{\partial T}{\partial y}\right)^2 + \left(\dfrac{\partial T}{\partial x}\right)^2\right]^{1/2}$

Brunt-Väisälä frequency $N \equiv \left(\dfrac{g}{T}\dfrac{\partial \theta_v}{\partial z}\right)^{1/2}$

Richardson number $1 < \mathrm{Ri} = \left(\dfrac{N}{\Gamma}\right)^2 < 10$

Urban boundary layer (UBL) height

Compared to homogeneous rural PBLs, UBL shows

(i) <u>greatly enhanced mixing</u> due to <u>large surface roughness</u> and <u>increased surface heating</u>

(ii) <u>horizontal heterogeneity</u> due to <u>variations in roughness and heating from rural area to city-centre</u>.

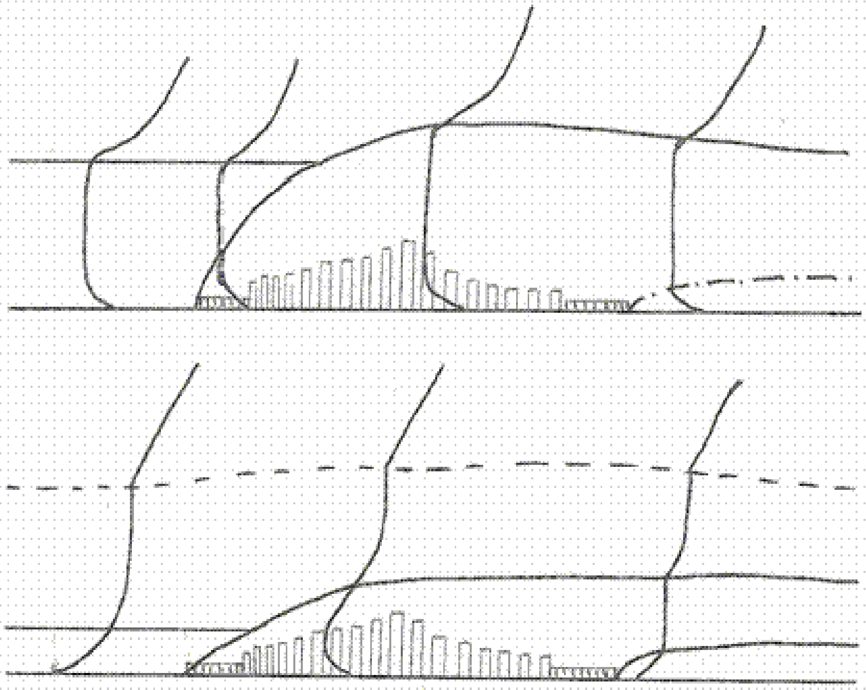
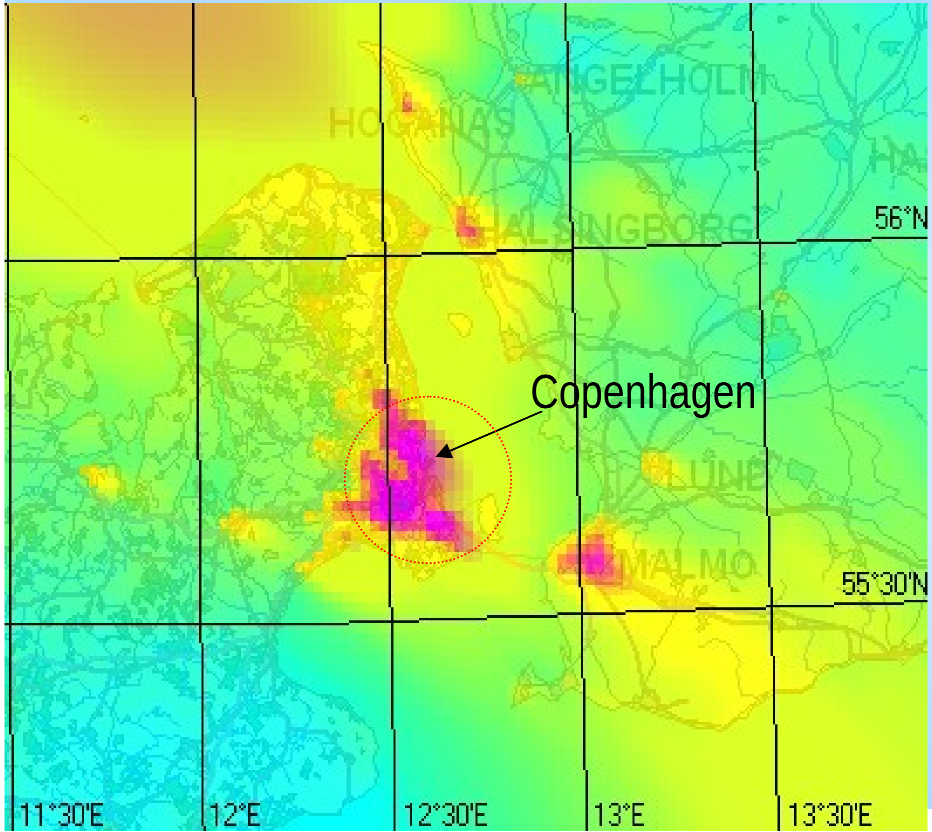


Figure 1: The simplified scheme of vertical structure of the urban boundary layer and typical potential temperature profiles: a) daytime UBL, b) nocturnal UBL.

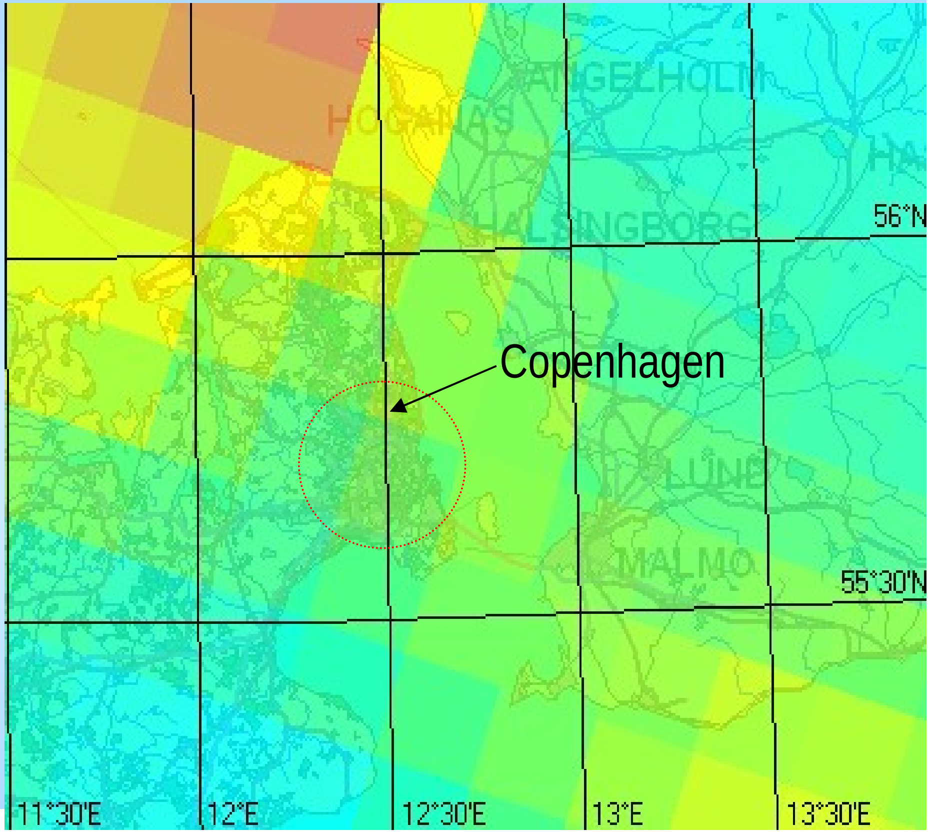
Methods for estimation of UBL height

- with only local correction to the heat fluxes and roughness length
- accounting for the growth of the internal boundary layer (IBL)
- using direct simulation of the vertical profiles of TKE or turbulent fluxes in 3D meteorological models

PBL height from different versions of DMI-HIRLAM



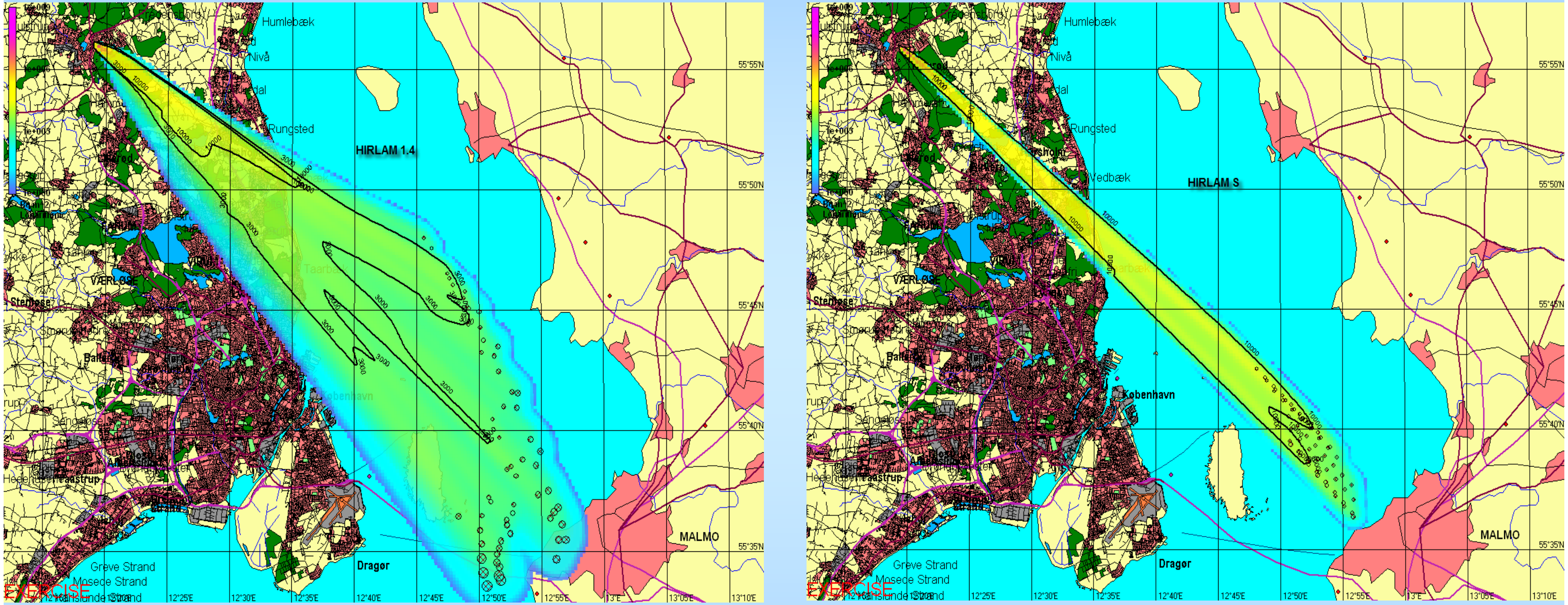
urbanised 1.4 km



operational 15 km

The effects of urban aerosols on the urban boundary layer height, h, could be of the same order of magnitude as the effects of the urban heat island (Δh is about 100-200 m for stable boundary layer).

Sensitivity of ARGOS dispersion simulations to urbanized DMI-HIRLAM NWP data



urbanised U01, 1.4 km resolution

operational S05, 5 km resolution

Cs-137 air concentration for different DMI-HIRLAM data
A local-scale plume from the ^{137}Cs hypothetical atmospheric release in Hillerød at 00 UTC, 19 June 2005 as calculated with RIMPUFF using DMI-HIRLAM and visualised in ARGOS for the Copenhagen Metropolitan Area.

Applicability of 'rural' PBL-height formulations to urban areas

- In the daytime common methods perform better than at night
- Convective UBL: slab model OK (Gryning & Batchvarova, 2001)
- Stable (nocturnal) UBL; counteraction between negative 'non-urban' and positive urban (anthropogenic) surface heat fluxes → common methods need to be improved
- Prospective: prognostic equation for the stable ABL height – Zilitinkevich *et al*. (2002), (Zilitinkevich and Baklanov, 2002)
- Meso-meteorological and NWP models with high-order, non-local turbulence closures give promising results (especially for the CBL), however urban effects need to be included

Coupling Air Quality and Meteorology/Climate Modeling
Rationale and Motivation

- Common deficiencies of a global climate-aerosol model
  - Coarse spatial resolution cannot explicitly capture the fine-scale structure that characterizes climatic changes (e.g., clouds, precipitation, mesoscale circulation, sub-grid convective system, etc.) and air quality responses
  - Coarse time resolution cannot replicate variations at smaller scales (e.g., hourly, daily, diurnal)
  - Simplified treatments (e.g., simple met. schemes and chem./aero. treatments) cannot represent intricate relationships among meteorology/climate/AQ variables
  - Most models simulate climate and aerosols offline with inconsistencies in transport and no climate-chemistry-aerosol-cloud-radiation feedbacks
- Common deficiencies of a urban/regional climate or AQ model
  - Most AQMs do not treat aerosol direct and indirect effects
  - Most AQMs use offline meteorological fields without feedbacks
  - Some AQMs are driven by a global model with inconsistent model physics
  - Most regional climate models use prescribed aerosols or simple modules without detailed chemistry and microphysics

(after Round Table of Copenhagen COST-NetFAM workshop, 2007)

Implementation Priorities

- Highest priority (urgent)
  - Aerosol thermodynamics/dynamics, aq. chem., precursor emi., water uptake
  - Radiation, emission, PBL/LS schemes, photolysis, aerosol-CCN relation
  - Coding standard and users' guide for parameterizations
- High priority (pressing)
  - Aero. activation/resuspension, Brownian diffusion, drop nucleation scavenging
  - Other in-/below-cloud scavenging (collection, autoconversion, interception, impaction)
- Important
  - Hydrometeor dynamics, size representation, hysteresis effect
- Other
  - Subgrid variability, multiple size distributions

(after Round Table of Copenhagen COST-NetFAM workshop, 2007)

Recommended literature:

- Baklanov A., 2008: Integrated Meteorological and Atmospheric Chemical Transport Modeling: Perspectives and Strategy for HIRLAM/HARMONIE. HIRLAM Newsletter, 53.
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