

On-line integrated Enviro-HIRLAM system: strategy, current status and further developments

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Zelenogorsk (St. Petersburg), Russia, 14-15 July 2008



Enviro-HIRLAM development team:

Currently 4 institutions are working:

- Danish Meteorological Institute,
- University of Copenhagen,
- Tomsk State University,
- Russian State Hydro-Meteorological University.

Teams willing to join the development team:

- University of Tartu, Estonia,
- Ukrainian State Ecological University,
- Belgium Meteorological Institute,
- Vilnius University, Lithuania.

There is an initial working group (under COST728 and HIRLAM-A) for HIRLAM-ACTM integration work and a sub-program for the Enviro-HIRLAM/HARMONIE development cooperation. Any HIRLAM and other teams are also welcome to join the team!

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2 different tasks in HIRLAM-ACTM:

- (i) improvement of HIRLAM outputs for ACT modelling applications and correspondingly improvement of ACT models (for different off-line ACT models, like MATCH, SILAM, EMEP, CAC, DERMA; DACFOS),
- (ii) improvement of NWP itself by implementation of ACTMs and aerosol/gases forcing/feedback mechanisms into HIRLAM (mostly by on-line integration, like in EnviroHIRLAM).

Integrated Atmospheric System Model Structure



<u>One-way:</u> 1. Meteo-fields as a driver for ACTM; 2. Chemical composition fields as a driver for R/GCM (or for NWP)

<u>Two-way:</u> 1. Driver + partly feedback (data exchange); 2. Full feedbacks included on each time step (on-line coupling)



Advantages of On-line & Off-line modeling

On-line coupling

- Only one grid;
- No interpolation in space
- No time interpolation
- Physical parameterizations are the same; No inconsistencies
- Harmonised advection schemes for all variables (meteo and chemical)
- Possibility to consider aerosol forcing mechanisms
- All 3D met. variables are available at the right time (each time step); No restriction in variability of met. fields
- Possibility of feedbacks from meteorology to emission and chemical composition
- Does not need meteo- pre/postprocessors

Off-line

- Possibility of independent parameterizations;
- Low computational cost (if NWP data are already available and no need to run meteorological model);
- More suitable for ensembles and operational activities;
- Easier to use for the inverse modelling and adjoint problem;
- Independence of atmospheric pollution model runs on meteorological model computations;
- More flexible grid construction and generation for ACT models,
- Suitable for emission scenarios analysis and air quality management.

On-line integrated meso-scale models

- At the current stage most of the online coupled models do not consider feedback mechanisms or include only direct effects of aerosols on meteorological processes (like COSMO LM-ART and MCCM).
- Only two meso-scale on-line integrated modelling systems (WRF-Chem and Enviro-HIRLAM) consider feedbacks with indirect effects of aerosols.



Numerical Weather Prediction Model

Ecosystem

models

Ocean

dynamics

model

Integrated Assessment Model

Applications of Enviro-HIRLAM for:

- (i) chemical weather forecasting
- (ii) air quality and chemical composition longer-term assessment
- (iii) weather forecast (e.g., in urban areas, severe weather events, etc.),
- (iv) pollen forecasting,
- (v) climate change modelling (Enviro-HIRHAM),
- (vi) volcano eruptions, nuclear explosion consequences(vii) Other emergency preparedness

Processes/feedbacks to be considered

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

• Direct effect - Decrease solar/thermal-IR radiation and visibility

- Processes needed: radiation (scattering, absorption, refraction, etc.)
- Key variables: refractive indices, ext. coeff., SSA, asymmetry factor, AOD, visual range
- Key species: cooling: water, sulfate, nitrate, most OC

warming: BC, OC, Fe, Al, polycyclic/nitrated aromatic compounds

• Semi-direct effect - Affect PBL meteorology and photochemistry

- Processes needed: PBL/LS, photolysis, met-dependent processes
- Key variables: T, P, RH, Qv, WSP, WDR, Cld Frac, stability, PBL height, photolysis rates, emission rates of met-dependent primary species (dust, sea-salt, biogenic)
- First indirect effect Affect cld drop size, number, reflectivity, and optical depth via CCN
 - Processes needed: aero. activation/resuspension, cld. microphysics, hydrometeor dynamics
 - Key variables: int./act. frac, CCN size/comp., cld drop size/number/LWC, COD, updraft vel.
- Second indirect effect Affect cloud LWC, lifetime, and precipitation
 - Processes needed: in-/below-cloud scavenging, droplet sedimentation
 - Key variables: scavenging efficiency, precip. rate, sedimentation rate
- All aerosol effects
 - Processes needed: aero. thermodynamics/dynamics, aq. chem., precursor emi., water uptake
 - Key variables: aerosol mass, number, size, comp., hygroscopicity, mixing state

Implementation Priorities

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

• 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, DMRH
- Other
 - Subgrid variability, multiple size distributions

Enviro-HIRLAM on-line system realisation steps:

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- (i) nesting of models for high resolutions,
- (ii) improved resolution of boundary and surface layer characteristics and structures,
- (ii) 'urbanisation' of the model,
- (iii) improvement of advection schemes,
- (iv) implementation of chemical mechanisms,
- (v) implementation of aerosol dynamics,
- (vi) realisation of feedback mechanisms,
- (vii) assimilation of monitoring data.

First version of Enviro-HIRLAM modelling systems, showing the components of a forecast



Korsholm, Baklanov, Gross, Mahura (2007)

Improvements of Advection Schemes for Tracers

- Default Eulerian central-different (CD) scheme
- Semi-Lagrangian (SL) scheme in HIRLAM
- Original Bott scheme (*Bott, 1989*): 4th order polynomials in x and y; 2nd order polynomials in z
- Modified Bott-Easter scheme (*Easter, 1993*)
- Cell Integrated Semi-Lagrangian (CISL) scheme (*Machenhauer and Kaas, 2004*)
- New Cell Integrated Semi-Lagrangian scheme (Kaas, 2008)



Mass conservation test for ETEX release

Convection

- The Tiedtke mass-flux scheme may be used to convect aerosols and gases.
- The mass-flux calculation is the same as for air, hence, the density difference between air and the gases is not accounted for and it is assumed that the settling velocity is negligible compared to the convective updraught velocity.
- Another option is to use the STRACO convection and condensation scheme. This scheme is currently being modified to account for the convection of extra tracers.

Aerosol models in Enviro-HIRLAM



- The formation and transformations of atmospheric aerosols are known to be influenced by the dissolution of trace gases (if wetted), nucleation, condensation, evaporation and coagulation.
- Therefore, the aerosol module in Enviro-HIRLAM comprises two parts:
 a thermodynamic equilibrium model (NWP-Chem-Liquid) and
 an aerosol dynamics model.
- For simulating aerosol dynamics 3 models has been implemented, covering both sectional and modal approaches:

- the modal aerosol module from the Chemistry-Aerosol-Cloud (CAC) model developed at DMI (Gross and Baklanov, 2002),

- the sectional Model for Simulating Aerosol Interactions and Chemistry (MOSAIC) (Zaveri et al., 2007) and

- the Modal Aerosol Dynamics Model for Europe (MADE) (Ackermann et al., 1998) with the secondary organic aerosol model (SORGAM) (Schell et al., 2001) (referred to as MADE/SORGAM).

• Note that only the implementation of the CAC aerosol model has been tested so far.

Aerosol Dynamics Modelling (CAC)

The following aerosol physical processes are solved

- 1. Nuclei mode (i):
 - •nucleation, N(i),
 - •condensation growth, G(i),
 - •intramodal coagulation, C(i->i),
 - •intermodal transfer of moment from nuclei mode, C(i->j),

d M(i)/dt = N(i) + G(i) + C(i-i)

- 2. Accumulation mode (j):
 - •condensation growth, G(j),
 - intramodal coagulation C(j->j)
 - •intermodal transfer of moment to accumulation mode, C(i->j),
 - primary emission, E(k,j)

d M(k,j)/dt = G(j) - C(j->j) + C(i->j) + E(j)

3. Mechanical generation mode (k): emission, condensation growth, coagulation

<u>Realisation:</u> 3 versions, incl CAC, MOSAIC, MADE/SORGAM

- 1. Sectional numerical approach,
- 2. Analytical solutions using the modal approach => 8 times faster

Deposition Mechanisms in Enviro-HIRLAM

- Emissions -> Eulerian point sources
- Particle size dependent parameterizations for dry and wet deposition
- Resistance approach for dry deposition (Wesley, 1989; Zanetti, 1990)
- Terminal settling velocity in different regimes:
 - Stokes' law
 - non-stationary turbulence regime
 - correction for small particles
- Dependent on land use classification
- Below-cloud scavenging (washout); precipitation rates (*Baklanov & Sørensen, 2001*)
- Scavenging by snow (Maryon et al., 1996)
- Different scavenging of particles and gases
- Rainout into 3D clouds (based on on-line coupling):
 - convective precipitation
 - stratiform precipitation



Enviro-HIRLAM evaluation – ETEX-1



Tracer concentration (ng/m³) at 12, 24, 36, 48 hours after start of release. Top panel: simulation, bottom panel: measurements.



Enviro-HIRLAM evaluation – ETEX-1

Station ->	B05	CR03	D05	D4 4	DK02	DK05	H02	D42	NL01	NL05	PL03
Bias (ngm ⁻³)	0.76	-0.08	0.02	0.4 5	-0.01	-0.11	-0.02	-0.14	0.48	0.65	-0.06
NMSE	12.9	7.95	2.0	4.5 4	0.93	4.77	1.05	2.25	4.46	14.8	1.95
Correlation	0.80	0.92	0.29	0.6 4	0.68	0.08	0.86	0.46	-0.05	0.29	0.43
FMT (%)	12.9	26.1	29.6	32. 1	51.4	15.4	49.3	32.7	15.9	19.1	38.4

Averages: bias 0.18 ngm⁻³; correlation 0.49; NMSE 5.25; FMT 29.4% **Global:** bias 0.39 ngm⁻³; correlation 0.57; NMSE 104.59; FMT 18.4 %

• Transport and dispersion performs satisfactory when compared to ETEX-1

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Enviro-HIRLAM evaluation – Chernobyl





Enviro-HIRLAM evaluation – Chernobyl



Dry and wet deposition perform satisfactory when compared to Chernobyl accident data



Top: concentration as function of time at F15 and DK02 for different coupling intervals: 30, 60, 120, 240, 360 minutes. Bottom: concentration after 36 hours with the same coupling intervals

Online vs. offline experiments.



Enviro-HIRLAM: On-line versus off-line for ETEX-1 experiment

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<= Normalized mean square difference

Measured and modelled time development of concentration (ngm-3) at ETEX stations F15 (left) and DK02 (right) for coupling intervals 10 (online), 30, 60, 120, 240 and 360 minutes



Enviro-HIRLAM: Feedbacks of urban aerosols First indirect effect

Second indirect effect will be considered in the next presentation

For water clouds: $r_{eff}^{3} = kr_{v}^{3}$ $r_{eff}^{3} = 3L/(4\pi\rho_{l}kN)$ (*Wyser et al. 1999*)

L : Cloud condensate content

N: Number concentration of cloud droplets

 $\Delta N_{cont} = 10^{8.06} \text{ conc}^{0.48}$ $\Delta N_{marine} = 10^{2.24} \text{ conc}^{0.26}$ (*Boucher & Lohmann, 1995*)

Emission rate: 7.95 gs⁻¹; ETEX Diameter: 1 µm

	k	N [m ⁻³]		
Marine	0.81	108		
Cont	0.69	4x10 ⁸		



Urban fractions [%; dark green – dark red]



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Reference concentration (μ g/m³) at surface (left) and at app. 400 m (right). Time: 06 UTC, date: 13-04-2007

Enviro-HIRLAM: Feedbacks of urban aerosols First indirect effect

600 400

400

200



Boundary layer height (m) at 06 UTC on 13-04-2007 (left) and 12 UTC on 12-04-2007 (right)

Enviro-HIRLAM: Feedbacks of urban aerosols First indirect effect

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PBLH (m) average from 06 UTC 11-04-2007 to 06 UTC 13-04-2007

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 (Δ h is about 100-200 m for stable boundary layer).

Enviro-HIRLAM: Feedbacks of urban aerosols



Difference (ref - perturbation) in accumulated wet deposition [ng/m²] Difference (ref - perturbation) in accumulated dry deposition [ng/m²]



Feedbacks through the first indirect effect lead to modifications of the order 7 % in dry and wet deposition patterns over major polluted areas in Europe.

Enviro-HIRLAM partial call-tree displaying the main routines which have been modified as well as new additions (in green) with a short description









Effects of aerosol particles on climate: Jacobson (2002) classification and Some examples

- Self-Feedback Effect
- Photochemistry Effect
- Smudge-Pot Effect
- Daytime Stability Effect
- Particle Effect Through Surface Albedo
- Particle Effect Through Large-Scale Meteorology
- Indirect Effect
- Semidirect Effect
- BC-Low-Cloud-Positive Feedback Loop



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=> High-resolution on-line integrated models with a detailed description of the PBL structure are necessary to simulate such effects

Different 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 \Rightarrow larger cross sectional area \Rightarrow more reflection of solar radiation

Cloud lifetime effect (involves feedbacks)

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

Semi-direct effect (involves feedbacks)

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

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

HIRLAM-ACTM integration: e.g. Enviro-HIRLAM New integrated (on-line coupled) modeling system structure for predicting the atmospheric composition

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Particle Scattering and Absorption Extinction Coefficients

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

Aerosol particle absorption and scattering extinction coefficients (in cm⁻¹) at a given wavelength can be estimated as:

$$\sigma_{a,p} = \sum_{i=1}^{N_b} n_i \pi r_i^2 Q_{a,i} \qquad \sigma_{s,p} = \sum_{i=1}^{N_b} n_i \pi r_i^2 Q_{s,i}$$

Where the summations are over N_b particle sizes, ni is the number concentration (part. per cm3 of air) of particles of raius ri (cm), πr_i^2 is the actual cross-section of a particle (cm² per part.), Q_{ai} and Q_{si} are single-particle absorption and scattering efficiencies (dimensionless).

Direct aerosol effect in the model

- Realisation depends on the radiation scheme used in the model.
- The first simple version of implementation into the Enviro-HIRLAM model with the radiation scheme of Savijärvi (1990) is realised based on 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.

First indirect aerosol effect in Enviro-HIRLAM (Korsholm et al., 2008)

As anthropogenic aerosols enter cloud environments the number concentration of cloud condensation nuclei (CCN) is modified, generally, resulting in more numerous and smaller CCN (decreased mean diameter). The cloud radiation characteristics depend on bulk cloud properties and a decrease in droplet mean diameter results in a modification (whitening) of the cloud albedo. The HIRLAM radiation scheme is based on (Savijärvi, 1990) and all water cloud radiation is parameterized via the cloud droplet effective radius, r_e , which may be written as:

$$r_e = \left(\frac{3L_c}{4\pi\rho_w kN}\right)_{1/3}$$

where L_c is the cloud condensate content, ρ_w is the density of water, k is a fitting parameter which distinguishes between land and water surfaces and N is the cloud droplet number concentration (Wyser, et al., 1999). N may be decomposed into a natural background and an anthropogenic contribution: $N = N_{back} + N_{anthr}$, where N_{back} is a constant for clean air supplied in HIRLAM depending only on the surface type (land or water), while N_{anthr} is calculated in the aerosol module assuming that all accumulation mode aerosols may act as CCN.

The new ALADIN/HARMONIE cloud scheme (*Pinty and Jabouille, 1998; Caniaux et al., 1994*) is more suitable for implementation of more comprehensive aerosol dynamics and indirect effects of aerosols (CCN/IN) models, but will be more expensive computationally.

Second indirect aerosol effect in Enviro-HIRLAM *(Korsholm et al., 2008)*

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The description of cloud microphysics in the STRACO scheme is based on the Sundqvist parameterization (Sundqvist, 1988, Sundqvist, et al., 1989, Sundqvist, 1993). STRACO has been extended to include the effects of cloud drop number concentration and characteristic droplet radius r, by combining the autoconversion term for cloud water from (Rasch and Kristjansson, 1998) with the existing formulation in the STRACO scheme (Sass, 2002). In STRACO precipitation release is written $G_p = \Phi q_c (1 - \exp(-X^2))$ where q_c is the cloud condensate, $X = \hat{q}_c/\mu$ where $\hat{q}_c = q_c/f$ is the in-cloud specific cloud condensate and f is the grid box fractional cloud cover. The Φ term is defined as: $\Phi = \Phi_1 \Phi_2 \Phi_3 \Phi_4$ where Φ_2 describes the effect of collision/coalescense and the Bergeron-Findeisen mechanism, Φ_3 expresses a temperature dependency at cold temperatures, Φ_4 is height dependent and describes an enhanced sedimentation of cloud droplets from fog (clouds at very low levels) and Φ_1 is the autoconversion term which is now defined as:

$$\Phi_1 = C_{l,out} \widehat{q}_c \frac{\rho_a}{\rho_w} \left(\widehat{q}_c \frac{\rho_a}{\rho_w} N \right)^{\frac{1}{3}} H(r - r_0)$$

Here ρ_a represents air density, H is the Heavy-side step function, $C_{l,aut}$ is a constant (Rasch and Kristjansson, 1998), $r = [(3\rho_a q_c)/(4\pi N \rho_w)]^{1/3}$ is the mean cloud droplet radius and r_0 is a constant threshold drop radius (5µm).

As before $N = N_{back} + N_{anthr}$ where N_{back} depends only on surface type and N_{anthr} is calculated in the aerosol module. The modifications made to the STRACO scheme is currently being tested, but preliminary runs show that it gives results similar to the latest STRACO version.

Further work with Enviro-HIRLAM development

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There are a number of outstanding issues which will be dealt with in the future, e.g.:

- Enviro-HIRLAM currently runs on the NEC-SX6 super-computer at DMI, but will be ported and optimized to the new CRAY-XT5 at DMI (this work is going),
- the model will be updated to HIRLAM version 7.1,
- will be implemented and available on the chemical branch of HIRLAM,
- improvement and validation of the direct and indirect aerosol effects,
- implementation of the gas feedback mechanisms,
- implementation and parallelization of a new advection scheme,
- updates for the gas-phase chemistry and aerosol modules,
- in MEGAPOLI it is planed to test EnviroHIRLAM with the aerosol model from University of Helsinki,
- improved representation of PBL and SL, further 'urbanization' of the model,
- a new mass conservative horizontal diffusion scheme will be implemented,
- heterogeneous chemistry will be expanded and implemented,
- data assimilation for the chemical compounds to be implemented,
- expansion of the HARMONIE system to include the Enviro-HIRLAM chemistry and aerosol features and feedbacks,
- Climate version of the Enviro-HIRLAM => Enviro-HIRHAM (based on newest HIRLAM version)

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These would be a joint effort for the Enviro-HIRLAM developers and the HIRLAM consortium.

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.

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• Key questions

- 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?
- What are the key uncertainties associated with model predictions of those effects?
- How can simulated feedbacks be verified with available datasets?



Megacities: Emissions, Impact on Air Quality and Climate, and Improved Tools for Mitigation Assessments (MEGAPOLI)

New EC 7FP project for: ENV.2007.1.1.2.1. Megacities and regional hot-spots air quality and climate

Project duration: 2008 - 2011 years 28 European research organisations from 12 countries are involved. Coordinator: A. Baklanov (DMI) Vice-coordinators: M. Lawrence (MPIC) and S. Pandis (FRTHUP)



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