UDC 550.34.01:551.509.313.43

A.A. Baklanov, *Prof., Sc.D.*
Danish Meteorological Institute, Copenhagen, Denmark

CHEMICAL WEATHER FORECASTING: A NEW CONCEPT AND METHODOLOGY OF TWO-WAY INTEGRATED MESO-SCALE MODELLING

Abstract. *During the last decade a new field of atmospheric modelling – the chemical weather forecasting (CWF) – is quickly developing and growing. However, in the most of the current studies and publications this field is considered in a simplified concept of the off-line running chemical transport models with operational NWP data as a driver. A new concept and methodology considering the chemical weather as two-way interacted meteorological weather and chemical composition of the atmosphere is suggested and discussed. The on-line integration of mesometeorological models and atmospheric aerosol and chemical transport models gives a possibility to utilize all meteorological 3D fields in the chemical transport model at each time step and to consider feedbacks of air pollution (e.g. urban aerosols) on meteorological processes/climate forcing and further on the chemical composition. This very promising way for future atmospheric simulation systems (as a part of and a step to Earth System Modelling) will lead to a new generation of models for meteorological, environmental and chemical weather forecasting. The methodology how to realise the suggested integrated CWF concept is demonstrated on example of the European Enviro–HIRLAM integrated system. Importance of different feedback mechanisms for CWF is also discussed in the paper.*

Keywords: *chemical weather forecasting, off-line and on-line chemical transport modeling, feedbacks mechanisms, two-way interacted meso-scale modelling*

1 Introduction

During the last decade a new field of atmospheric modelling – the chemical weather forecasting (CWF) – is quickly developing and growing [22]. This was possible mostly due to quick growing supercomputer capability and operationally available high-resolution numerical weather prediction (NWP) data for atmospheric chemical transport models (ACTMs). However, in the most of current systems, studies and publications this new direction is considered in a simplified concept. It includes only operational air quality forecast for the main pollutants significant for health effects and uses numerical ACTMs with operational NWP data as a driver (see e.g. the COST Action ES0602: Towards a European Network on Chemical Weather Forecasting and Information Systems, web-site: http://www.chemicalweather.eu/).

However, such a way is very limited due to the off-line coupling the ACTMs with NWP or mesometeorological models (MMMs) (which are running completely independently and NWP does not get any benefits from the ACTM) without a possibility to consider any feedback mechanisms. Many experimental studies and numerical research simulations show that atmospheric processes (meteorological weather, including the precipitation, thunderstorms, radiation budget, cloud processes and planetary boundary layer (PBL) structure) depend on concentrations of chemical components (especially aerosols) in the atmosphere. Therefore ACTMs have to be run together at the same time steps using on-line coupling and considering two-way interaction between the meteorological processes, from one side, and chemical transformation and aerosol dynamics, from other side.

Proceeding from the above mentioned limitations, a new concept and methodology considering the chemical weather as two-way interacted meteorological weather and chemical composition of the atmosphere is suggested and discussed. The CWF should include not only health-effecting pollutants (air quality components), but also green-house gases and aerosols effecting climate, meteorological processes, etc. Such the concept of CWF requests a strategy of new generation integrated meteorology and ACT modelling systems for predicting atmospheric composition, meteorology and climate change. The on-line integration of meteorological or NWP models and atmospheric aerosol and chemical transport models gives a possibility to utilise all meteorological 3D fields in ACTM at each time step and to consider feedbacks of air pollution (e.g. urban aerosols) on meteorological processes and climate forcing, and further on the chemical composition (as a chain of dependent processes). This very promising way for future atmospheric simulation systems (as a part of and a step to Earth Modelling Systems) will lead to a new generation of models for meteorological, environmental and chemical weather forecasting.

The current COST728 Action "Enhancing meso-scale meteorological modelling capabilities for air pollution and dispersion applications" (http://www.cost728.org) addresses key issues concerning the development of meso-scale modelling capabilities for air pollution and dispersion applications and, in particular, it encourages the advancement of science in terms of integration methodologies and strategies in Europe. The final integration strategy will not be focused around any particular model, instead it will be possible to consider an open integrated system with a fixed architecture (module interface structure) and with a possibility of incorporating different MMMs/NWP and ACT models (ACTM). Such a strategy may only be realised through jointly agreed specifications of module structure for easy-to-use interfacing and integration.

The overall aim of the working group 2 (WG2), 'Integrated systems of MMM and ACTM: strategy, interfaces and module unification', is to identify the requirements for the unification of MMM and ACTM modules and to propose recommendations for a European strategy for integrated meso-scale modelling capabilities. The first report of WG2 (COST–WMO, 2007) compiles the existing state-of-the-art methodologies, approaches, models and practices for building integrated (off-line and on-line) meso-scale systems in different, mostly European, countries. The report also includes an overview and a summary of the existing integrated models and their characteristics as they are presently used. The model contributions were compiled using COST member contributions, each focusing on national model systems.

The methodology how to realise the suggested integrated CWF concept is demonstrated on examples of the European Enviro–HIRLAM [3,14] and American WRF–Chem [10] integrated systems. Importance of different feedback mechanisms for CWF is also discussed in the paper.

2 Methodology for model integration

The modern strategy for integrating MMMs and ACTMs is suggested to consider air quality modelling as a combination of (at least) the following factors: air pollution, regional/urban climate/meteorological conditions and population exposure. This combination is reasonable due to the following facts: meteorology is the main source of uncertainty in air pollution and emergency preparedness models, meteorological and pollution components have complex and combined effects on human health (e.g., hot spots in Paris, July 2003), pollutants, especially aerosols, influence climate forcing and meteorological events (precipitation, thunderstorms, etc.).

The integration/coupling of the NWP/MMM and ACT models could be realized by different ways using the on-line and off-line modelling approaches. In more details the definition and specifics of the approaches, as well as the advantages and disadvantages of the on-line and off-line modelling are described in [5] and [8]. It could be realized using the following possible variants (see Fig. 1):

One-way integration (off-line coupling):

1. MMM (or any other regional climate or NWP model) meteorological fields as a driver for ACTM (this way is traditionally used already by many air pollution modellers) (<—);
2. ACTM chemical composition fields as a driver for regional climate modelling or for NWP (e.g. for aerosol forcing on meteo-processes) (--->).

Two-way integration:

1. Driver and partly feedbacks, for ACTM or for NWP (data exchange via an interface with a limited time period: off-line or on-line access coupling, with or without second iteration with corrected fields) (<= =>);
2. ACTM is inside MMM or NWP model with full feedbacks included on each time step (on-line coupling) (<=>).

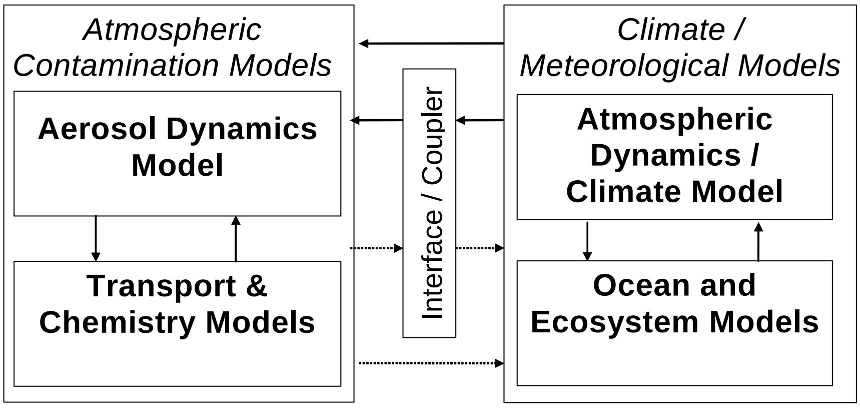

Fig. 1 – Integrated Atmospheric System Model Structure.

In this context, several levels of MMM and ACTM coupling/integration can be considered:

off-line:

- separate ACTMs driven by meteorological input data from meteo-preprocessors, measurements or diagnostic models,
- separate ACTMs driven by analysed or forecasted meteorological data from NWP archives or datasets,
- separate ACTMs reading output-files from operational NWP models or specific MMMs at limited time intervals (e.g. 1, 3, 6 hours).

on-line:

- on-line access models, when meteorological data are available at each time step (possibly via a model interface as well),
- on-line integration of ACTM into MMM, where two-way feedbacks may be considered. We will use this definition for on-line coupled/integrated modelling.

The main advantages of the on-line coupled modelling approach comprise:

- Only one grid, no interpolation in space,
- No time interpolation,
- Physical parameterizations and numerical schemes (e.g. for advection) are the same, no inconsistencies,
- All 3D meteorological variables are available at the right time (each time step),
- No restriction in variability of meteorological fields,
- Possibility to consider feedback mechanisms, e.g. aerosol forcing,
- Does not need meteorological pre- or post-processors.

However, not always the on-line approach is the best way of the model integration. For some specific tasks (e.g., for emergency preparedness, when low resolution NWP data are available) the off-line coupling is more efficient way. The main advantages of off-line models comprise:

- Possibility of independent parameterizations,
- More suitable for ensembles activities,
- Easier to use for the inverse modelling and adjoint problem,
- Independence of atmospheric pollution model runs on meteorological model computation,
- More flexible grid construction and generation for ACT models,
- Suitable for emission scenarios analysis and air quality management.

The on-line integration of meso-scale meteorological models and atmospheric aerosol and chemical transport models enables the utilisation of all meteorological 3D fields in ACTMs at each time step and the consideration of feedbacks between air pollution (e.g. urban aerosols), meteorological processes and climate forcing. These integration methodologies have been realised by several of the COST action partners such as the Danish Meteorological Institute, with the Enviro–HIRLAM model [3,14,16] and the COSMO consortium with the Lokal Modell [28,30].

These model developments will lead to a new generation of integrated models for: climate change modelling, weather forecasting (e.g., in urban areas, severe weather events, etc.), air quality, long-term assessments of chemical composition and chemical weather forecasting (an activity of increasing importance which is due to be supported by the new recently started COST action ES0602).

3 Overview of European on-line integrated models

Existing experience of the integrated modelling (mostly for research) in Europe as well as in other countries around the world should be analyzed first. On-line coupling was first employed at the Novosibirsk scientific school of Acad. G.I. Marchuk [1,23,24], for environmental modelling, in particular, of active artificial/anthropogenic impacts on atmospheric processes. Currently American, Canadian and Japanese institutions develop and use on-line coupled models operationally for air quality forecasting [10,13,20,21,25]. A nice overview of US integrated models was done in [31].

Such activities in Europe are widely dispersed and the COST Action 728 (see WG2: ‘Integrated systems of MMM and ACTM: strategy, interfaces and module unification’ on the web-site: http://cost728.org) seems to be the best approach to integrate, streamline and harmonize these national efforts towards a leap forward for new breakthroughs beneficial for a wide community of scientists and users [7,8].

Such a model integration should be realized following a joint elaborated specification of module structure for potential easy interfacing and integration. It might develop into a system, e.g. similar to the USA ESMF (Earth System Modelling Framework, see e.g. [9]) or European PRISM (Program for Integrating Earth System Modelling) specification for integrated Earth System Models: http://prism.enes.org/ [27].

Community Earth System Models (COSMOS) is a major international project (http://cosmos.enes.org) involving different institutes in Europe, in the US and in Japan, for the development of complex Earth System Models (ESM). Such models are needed to understand large climate variations of the past and to predict future climate changes. The main differences between the COST728 integrating strategy for meso-scale models and the COSMOS integration strategy regard the spatial and temporal scales. COSMOS is focusing on climate time-scale processes, general (global and regional) atmospheric circulation models and atmosphere, ocean, cryosphere and biosphere integration, while the meso-scale integration strategy is focusing on forecast time-scales of one to four days and omit the cryoshpere and the larger temporal and spatial scales in atmosphere, ocean and biosphere.

The WMO–COST728 overview [8] shows a surprisingly large (at least 10) number of on-line coupled MMM and ACTM model systems already being used in Europe (Table 1):

Table 1

Model name	On-line coupled chemistry	Time step for coupling	Feedback
BOLCHEM	Ozone as prognostic chemically active tracer		None
Enviro-HIRLAM	Gas phase, aerosol and heterogeneous chemistry	Each HIRLAM time step	Yes
WRF-Chem	RADM+Carbon Bond, Madronich+Fast-J photolysis, modal+sectional aerosol	Each model time step	Yes
COSMO LM-ART	Gas phase chem (58 variables), aerosol physics (102 variables), pollen grains	Each LM time step	Yes (*
COSMO LM-MUSCAT (**	Several gas phase mechanisms, aerosol physics	Each time step or time step multiple	None
MCCM	RADM and RACM, photolysis (Madronich), modal aerosol	Each model time step	(Yes) (***
MESSy: ECHAM5	Gases and aerosols		Yes
MC2-AQ	Gas phase: 47 species, 98 chemical and 16 photolysis reactions	Each model time step	None
GEM/LAM-AQ	Gas phase, aerosol and heterogeneous chemistry	Set up by user – in most cases every time step	None
ECMWF GEMS modelling	GEMS chemistry	Each model time step	Yes (*
GME	Progn. stratos passive O_3 tracer	Each model time step	
OPANA=MEMO+CBMIV		Each model time step	

*) Direct effects only; **) On-line access model; ***) Only via photolysis

However, it is necessary to mention, that many of the above on-line models were not built for the mesometeorological scale, and several of them (GME, ECMWF GEMS, MESSy) are global-scale modelling systems, originating from the climate modelling community. Besides, as it was shown in COST–WMO integrated models overview, at the current stage most of the on-line coupled models do not consider feedback mechanisms or include only simple 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.

4 Feedback mechanisms and aerosol Forcing in meso-scale models

In a general sense air quality and ACT modelling is a natural part of the climate change and MMM/NWP modelling. The role of greenhouse gases (such as water vapour, CO_2, O_3

and CH_4) and aerosols in climate change has been highlighted as a key area of future research [12]. In relation to aerosols, their diverse sources, complex physicochemical characteristics and large spatial gradients make their role in climate forcing particularly challenging to quantify. In addition to primary emissions, secondary particles, such as, nitrates, sulphates and organic compounds, also result from chemical reactions involving precursor gases such as SO_x, DMS, NO_x, volatile organic compounds and oxidising agents including ozone. One consequence of the diverse nature of aerosols is that they exhibit negative (e.g. sulphates) as well as positive (e.g. black carbon) radiative forcing characteristics [20]. Although much effort has been directed towards gaseous species, considerable uncertainties remain in size dependent aerosol compositional data, physical properties as well as processes controlling their transport and transformation, all of which affect the composition of the atmosphere [12]. Probably one of the most important sources of uncertainties relates to the indirect effect of aerosols as they also contribute to multiphase and microphysical cloud processes, which are of considerable importance to the global radiative balance [26].

In addition to better parameterisations of above mentioned key processes in climate models, on the meteorological time-scale and meso-spatial scale more improvements are required in resolving of two-way feedbacks with a suitable resolution. Averaging/integration and poor resolution of regional climate information from atmosphere-ocean general circulation models remains a limiting factor. Vertical profiles of turbulence, temperature and wind characteristics within PBL, for example, in CWF models need to be well resolved and better described for considering both directions chains of aerosol feedbacks on the meteorological and chemical composition. So, even for climate modelling, to understand the main mechanisms of aerosol feedback chains we have to start building on-line integrated models on the meteorological time-scale and resolving main meso-scale features and PBL structure.

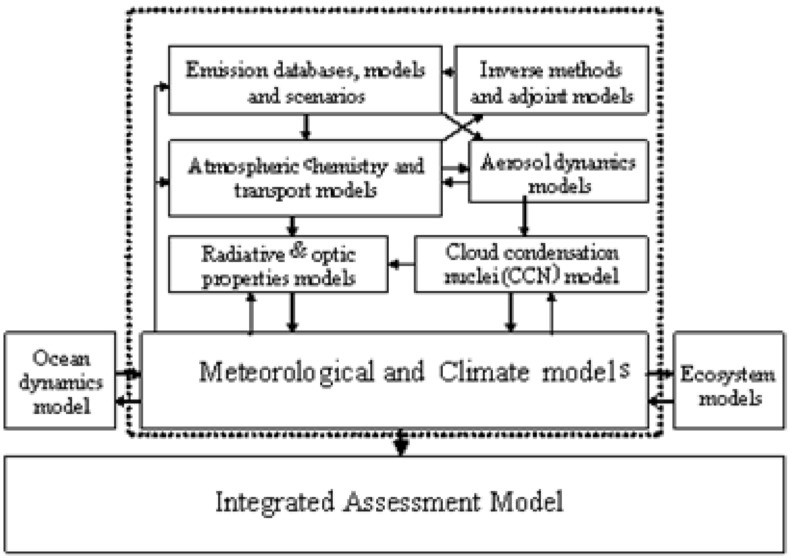

Fig. 2 – Two-way on-line integrated system structure for studies of the meso-scale meteorology and air pollution, and their interaction.

In this concern one of the important tasks is to develop a modelling instrument of two-way coupled 'Atmospheric chemistry/Aerosol' and 'Atmospheric Dynamics/Climate' models for integrated studies, which is able to consider the feedback mechanisms, e.g. aerosol forcing (direct and indirect) on the meteorological processes and climate change (see Fig. 2).

Chemical species influencing weather and atmospheric processes include greenhouse gases which warm near-surface air and aerosols such as sea salt, dust, primary and secondary particles of anthropogenic and natural origin. Some aerosol particle components (black carbon (BC), iron, aluminium, polycyclic and nitrated aromatic compounds) warm the air by absorbing solar and thermal-infrared (IR) radiation, while others (water, sulphate, nitrate, most of organic compounds (OC)) cool the air by backscattering incident short-wave radiation to space.

It is necessary to highlight, that effects of aerosols and other chemical species on meteorological parameters have many different pathways (direct, indirect, semi-direct effects, etc.) and they have to be prioritised and considered in on-line coupled modelling systems. Proceedings from [19] the following effects of aerosol particles on meteorology and climate can be distinguished:

- Self-Feedback Effect,
- Photochemistry Effect,
- Smudge-Pot Effect,
- Daytime Stability Effect,
- Particle Effect through Surface Albedo,
- Particle Effect through Large-Scale Meteorology,
- Indirect Effect,
- Semi-direct Effect,
- BC-Low-Cloud-Positive Feedback Loop.

It is important to stress, that many of the above-mentioned mechanisms to be described need the on-line integration and resolving the mesometeorological phenomena and detailed PBL structure.

The aerosol feedback mechanisms to be considered in the models are the following (see also in [7]):

1. <u>Direct effect</u> – Decrease solar/thermal-infrared radiation and visibility:
   a. Processes involved: radiation (scattering, absorption, refraction, etc.);
   b. Key variables: refractive indices, extinction coefficient, single-scattering albedo, asymmetry factor, aerosol optical depth, visual range;
   c. Key species: - cooling: water, sulphate, nitrate, most OC;
      - warming: BC, OC, Fe, Al, polycyclic/nitrated aromatic compounds;
2. <u>Semi-direct effect</u> – Affect PBL meteorology and photochemistry:
   a. Processes involved: PBL, surface layer, photolysis, meteorology-dependent processes;
   b. 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;
3. <u>First indirect effect</u> (so called the Twomey effect) – Affect clouds drop size, number, reflectivity, and optical depth via CCN or ice nuclei:
   a. Processes involved: aerodynamic activation/resuspension, clouds microphysics, hydrometeor dynamics;
   b. Key variables: int./act. fractions, CCN size/compound, clouds drop size/number/liquid water content, cloud optical depth, updraft velocity;
4. <u>Second indirect effect</u> (also called as the lifetime or suppression effect) – Affect cloud liquid water content, lifetime and precipitation:
   a. Processes involved: clouds microphysics, washout, rainout, droplet sedimentation;
   b. Key variables: scavenging efficiency, precipitation rate, sedimentation rate.

Sensitivity studies are needed to understand the relative importance of different feedback mechanisms. Implementation of the feedbacks into integrated models could be realized in different ways with varying complexity. The following variants serve as examples:
One-way integration (off-line):
- The chemical composition fields from ACTMs may be used as a driver for Regional/Global Climate Models, including aerosol forcing on meteorological processes. This strategy could also be realized for NWP or MMMs.

Two-way integration:
- Driver and partly aerosol feedbacks, for ACTMs or for NWP (data exchange with a limited time period); off-line or on-line access coupling, with or without the following iterations with corrected fields).
- Two-way/chain full feedbacks included on each time step (on-line coupling/integration).

For the realisation of all aerosol forcing mechanisms in integrated systems it is necessary to improve not only ACTMs, but also NWP/MMMs. The boundary layer structure and processes, including radiation transfer, cloud microphysics and precipitation formation must be improved. Convection and condensation schemes need to be adjusted to take the aerosol-microphysical interactions into account, and the radiation scheme needs to be modified to include accurately the aerosol effects.

5 Example of integrated CWF realization: Enviro–HIRLAM system

The realisation of the on-line integration for such CWF system could be demonstrated using the Enviro–HIRLAM integrated system, recently developed by DMI and other collaborators[1] [2,3,6,14,16]. Enviro–HIRLAM is an on-line coupled model for research and forecasting of both meteorological and chemical weather. It includes two-way feedbacks between air pollutants and meteorological processes. Atmospheric chemical transport equations are implemented inside the meteorological corner on each time step [6]. To make the model suitable for CWF in urban areas, where most of population is concentrated, the meteorological part is improved by implementation of urban sublayer modules and parameterisations [4]. The aerosol module in Enviro–HIRLAM comprises two parts: (i) a thermodynamic equilibrium model (NWP–Chem–Liquid) and (ii) the aerosol dynamics model CAC [11] based on the modal approach. Parameterisations of the aerosol feedback mechanisms in the Enviro–HIRLAM model are described in [14] and [16]. Several chemical mechanisms could be chosen depending on the specific tasks: well-known RADM2 and RACM or new-developed economical NWP–Chem [14].

Validation and sensitivity tests of the on-line versus off-line integrated versions of Enviro–HIRLAM [17] showed that the on-line coupling improved the results. Different parts of Enviro–HIRLAM were evaluated versus the ETEX–1 experiment, Chernobyl accident and Paris study datasets and showed that the model performs satisfactorily [16].

In [14,15] it was shown that aerosol feedbacks through the first indirect effect could lead to modifications up to 7% in dry and wet deposition patterns over major polluted areas in Europe. The effects of urban aerosols on the urban boundary layer height, could be of the same order of magnitude as the effects of the urban heat island (Δh is up to 100–200 m for stable boundary layer). A consistent explanation is suggested: the first indirect effect affects

[1] At the current stage the Enviro-HIRLAM model is used as the baseline system for the HIRLAM chemical brunch, and additionally to the HIRLAM community the following groups join the development team: University of Copenhagen, Tartu University (Estonia), Russian State Hydro-Meteorological University and Tomsk State University, Odessa State Environmental University (Ukraine), etc.

the dispersion of pollutants through regulation of atmospheric stability, thereby leading to a redistribution of the pollutant.

Other specific case study for the Paris metropolitan region by Korsholm et al. (2009b) shows that feedbacks through the second indirect effect lead to even stronger effects than the first indirect effect:

- Indirect aerosol effects induce considerable changes in meteorological fields and large changes in chemical composition, in particular NO_2, in a case of convective cloud caver and little precipitation.
- The changes mediated mostly through changes in dynamics, however the indirect aerosol effects are considerable for changes in chemistry as well.
- The residual circulation induced by temperature changes acts to redistribute the species both vertically and horizontally.
- The second indirect effect dominates in most of cases; its effect on 2m temperature was stronger than the direct effect.
- Non-linearity component of the aerosol-meteorology interactions is very important and acts to decrease the effects of the feedbacks on NO_2.

6 Conclusion and discussion

The new concept and methodology considering the chemical weather as two-way interacted meteorological weather and chemical composition of the atmosphere is suggested for future chemical weather forecasting systems.

The on-line integration of meso-scale meteorological models and atmospheric aerosol and chemical transport models enables the utilisation of all meteorological 3D fields in ACTMs at each time step and the consideration of the feedbacks of air pollution (e.g. urban aerosols) on meteorological processes and climate forcing.

These on-line coupled model developments will lead to a new generation of integrated models not only for the chemical weather forecasting, but also for climate change modelling, weather forecasting (e.g., in urban areas, severe weather events, etc.), air quality analysis and mitigations, long-term assessment chemical composition, etc.

Main advantages of the on-line modelling approach include: (i) Only one grid for MMM and ACTM, no interpolation in space and time, (ii) Physical parameterizations are the same, no inconsistencies; (iii) All 3D meteorological variables are available at the right time at each time step; (iv) No restriction in variability of meteorological fields; (v) Possibility to consider two-way feedback mechanisms; (vi) Does not need meteo- pre/post-processors.

While for specific tasks the off-line approach could also be useful and includes the following advantages in specific cases, e.g. for risk assessments: (i) Possibility of independent parameterizations; (ii) More suitable for ensemble activities; (iii) Easier to use for the inverse modelling and adjoint problem; (iv) Independence of atmospheric pollution model runs on meteorological model computations; (v) More flexible grid construction and generation for ACTMs, (vi) Suitable for emission scenarios analysis and air quality management.

The WMO–COST728 overview shows a quite surprising number of on-line coupled MMM and ACTM model systems already being used in Europe. However, many of the on-line coupled models were not built for the mesometeorological scale, and they (e.g. GME, ECMWF GEMS, MESSy) are global-scale modelling systems and first of all designed for climate change modelling. Besides, at the current stage most of the on-line 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.

To conclude this paper we can answer that the scientific hypothesis (formulated on COST–NetFAM workshop in Copenhagen, May 2007, see [7]), that feedback mechanisms are important in accurate CWF modelling and quantifying direct and indirect effects of aerosols, is really correct and supported by simulation results.

However the following key scientific questions are (at least particularly) still waiting for further research and justified 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 are the two-way/chain feedbacks among meteorology, climate, and air quality in the estimated effects?
- What is the relative importance of aerosol direct and indirect effects in the estimates on different space and time scales?
- What are the key uncertainties associated with model predictions of those effects?
- How can simulated feedbacks be verified with available datasets?

Acknowledgements. This study was supported by the COST Actions 728 and ES0602, NetFAM, EC FP7 Project MEGAPOLI and the Copenhagen Global Change Initiative (COGCI). The author is grateful to a number of COST728, FUMAPEX, MEGAPOLI and DMI colleagues, who participated in the above-mentioned projects, for productive collaboration and discussions. Especial thanks are to my PhD student Ulrik Korsholm (DMI) who realised most of the Enviro–HIRLAM model coding, simulation runs and studies of the aerosol indirect effects.

References

1. *Baklanov, A.* (1988) Numerical modelling in mine aerology, Apatity: USSR Academy of Science, 200 pp. (in Russian).
2. *Baklanov, A., A. Gross, J.H. Sørensen* (2004) Modelling and forecasting of regional and urban air quality and microclimate. J. Computational Technologies, 9, pp. 82–97.
3. *Baklanov, A., U. Korsholm, A. Mahura, C. Petersen, A. Gross* (2008a) Enviro–HIRLAM: on-line coupled modelling of urban meteorology and air pollution. Advances in Science and Research, 2, pp. 41–46.
4. *Baklanov, A., P. Mestayer, A. Clappier, S. Zilitinkevich, S. Joffre, A. Mahura, N.W. Nielsen*, (2008b) Towards improving the simulation of meteorological fields in urban areas through updated/advanced surface fluxes description. Atmospheric Chemistry and Physics, 8, pp. 523–543.
5. *Baklanov, A. and U. Korsholm* (2007) On-line integrated meteorological and chemical transport modelling: advantages and prospective. In: ITM 2007: 29th NATO/SPS International Technical Meeting on Air Pollution. Modelling and its Application, 24-28.09.2007, University of Aveiro, Portugal, pp. 21–34.
6. *Chenevez, J., A. Baklanov, J.H. Sørensen* (2004) Pollutant transport schemes integrated in a numerical weather prediction model: Model description and verification results. Meteorological Applications, 11(3), pp. 265–275.
7. *COST–NetFAM* (2008) Integrated systems of meso-meteorological and chemical transport models/ Baklanov, A., A. Mahura, R. Sokhi (eds), Materials of the COST–728/NetFAM workshop, DMI, Copenhagen, 21–23 May 2007, 183 pp. Springer (in press). Available on: http://www.cost728.org.

8. *COST–WMO* (2007) Overview of existing integrated (off-line and on-line) meso-scale systems in Europe/Baklanov, A., B. Fay, J. Kaminski, R. Sokhi. Joint Report of COST728 and GURME, May 2007. WMO–COST publication. GAW Report No. 177, WMO TD No. 1427. Available also from: http://www.cost728.org.
9. *Dickenson, R.E., S.E. Zebiak, J.L. Anderson, M.L. Blackmon, C. DeLuca, T.F. Hogan, M. Iredell, M. Ji, R. Rood, M.J. Suarez, K.E. Taylor* (2002) How can we advance our weather and climate models as a community? Bull. Am. Met. Soc., 83, pp. 431–434.
10. *Grell, G.A., S.E. Peckham, R. Schmitz, S.A. McKeen, G. Frost, W.C. Skamarock, B. Eder* (2005) Fully coupled "on-line" chemistry within the WRF model, Atmos. Environ., 39(37), pp. 6957-6975.
11. *Gross, A. and A. Baklanov* (2004) Modelling the influence of dimethyl sulphid on the aerosol production in the marine boundary layer. International Journal of Environment and Pollution, 22, pp. 51–71.
12. *IPCC* (2005) IPCC Expert Meeting on Emission Estimation of Aerosols Relevant to Climate Change held on 2–4 May 2005, Geneva, Switzerland
13. *Kaminski, J., L. Neary, J. Struzewska and J.C. McConnell* (2008) Multiscale Atmospheric Chemistry Modelling with GEM–AQ. In: Integrated systems of mesometeorological and chemical transport models, Materials of the COST–728/NetFAM workshop, DMI, Copenhagen, 21–23 May 2007, pp. 42–47. Springer (in press). Available on http://www.cost728.org.
14. *Korsholm U.S., A. Baklanov, A. Gross, A. Mahura, B.H. Sass, E. Kaas* (2008a) On-line coupled chemical weather forecasting based on HIRLAM – overview and prospective of Enviro–HIRLAM. HIRLAM Newsletter, 54, pp. 1–17.
15. *Korsholm, U., A. Baklanov and J.H. Sørensen* (2008b) Status and Evaluation of Enviro–HIRLAM: Differences between on-line and off-line Models. In: Integrated systems of meso-meteorological and chemical transport models, Materials of the COST–728/NetFAM workshop, DMI, Copenhagen, 21–23 May 2007, pp. 47–61. Springer (in press). Available: http://www.cost728.org.
16. *Korsholm, U.* (2009) Integrated modeling of aerosol indirect effects – develoment and application of a chemical weather model. PhD thesis University of Copenhagen, Niels Bohr Institute and DMI, Research department.
17. *Korsholm, U.S., A. Baklanov, A. Gross, J.H. Sørensen* (2009a) On the importance of the meteorological coupling interval in dispersion modeling during ETEX–1, Atmospheric Environment, DOI:10.1016/j.atmosenv.2008.11.017 (available at ScienceDirect).
18. *Korsholm U, A. Mahura, A. Baklanov, A. Gross, C. Petersen, M. Bechmann* (2009b) Aerosol–meteorology feedbacks on short time-scale in a convective case. Atmospheric Environment (submitted).
19. *Jacobson, M.Z.* (2002) Atmospheric Pollution: History, Science and Regulation. Cambridge University Press.
20. *Jacobson, M.Z.* (2005) Fundamentals of Atmospheric Modeling, Second Edition, Cambridge University Press, New York, 813 pp.
21. *Jacobson, M.Z.* (2006) Comment on "Fully coupled 'on-line' chemistry within the WRF model," by Grell et al., Atmos. Environ., 39, pp. 6957–697.
22. *Lawrence, M.G., Ø. Hov, M. Backmann, J. Brandt, H. Elbern, H. Eskes, H. Feichter, M. Takigawa* (2005) The Chemical Weather. Envir. Chem., 2, pp. 6–8.
23. *Marchuk, G.I.* (1982) Mathematical modeling in the environmental problems. Moscow, Nauka.
24. *Penenko, V.V., A.E. Aloyan* (1985) Models and methods for environment protection problems. Nauka, Novosibirsk (in Russian).

25. *Uno, I. et al.,* (2003) Regional chemical weather forecasting system CFORS: Model descriptions and analysis of surface observations at Japanese island stations during the ACE–Asia experiment, J. Geophys. Res., 108 (D23), 8668, DOI: 10.1029/2002JD002845.
26. *Semazzi, F.* (2003) Air quality research: perspective from climate change modelling research. Environment International, 29, pp. 253–261.
27. *Valcke, S., E. Guilyardi, C. Larsson* (2006) PRISM and ENES: A European approach to Earth system modelling. Concurrency Computat.: Pract. Exper., 18, pp. 231–245.
28. *Vogel, B., C. Hoose, H. Vogel, Ch. Kottmeier* (2006) A model of dust transport applied to the Dead Sea area. Meteorologische Zeitschrift, 14, pp. 611–624.
29. *Watson, R.T. et al.* (1997) The regional impacts of climate change: an assessment of vulnerability. Special Report for the Intergovernmental Panel on Climate Change.
30. *Wolke, R., O. Hellmuth, O. Knoth, W. Schröder, B. Heinrich, E. Renner* (2003) The chemistry-transport modeling system LM–MUSCAT: Description and CITYDELTA applications. Proceedings of the 26-th International Technical Meeting on Air Pollution and Its Application. Istanbul, May 2003, pp. 369–379.
31. *Zhang, Y.* (2008) Online-coupled meteorology and chemistry models: history, current status, and outlook. Atmos. Chem. Phys., 8, pp. 2895–2932.

Прогноз химической погоды: новая концепция и методология двусторонне-интегрированного мезомасштабного моделирования

Аннотация. *В течение последнего десятилетия быстро развивается новая область атмосферного моделирования – прогноз химической погоды. Однако в настоящий момент в большинстве исследований и публикаций эта область рассматривается упрощенно: запуск модели переноса химических веществ осуществляется в режиме "оффлайн", использующей данные из оперативного численного прогноза погоды только, как входные поля. Предлагается и анализируется новая концепция, рассматривающая химическую погоду как двусторонне-взаимодействующие процессы метеорологии и химического состава атмосферы. Интегрирование мезометеорологических моделей и моделей переноса атмосферных аэрозолей и химических веществ в режиме "онлайн" дает возможность использовать все трехмерные метеорологические поля в моделях переноса химических веществ на каждом временном шаге и учитывать обратные связи, то есть учитывать влияние загрязняющих веществ (например, городских аэрозолей) на метеорологические процессы/ климатические изменения и в дальнейшем на химический состав. Этот перспективный путь для будущих атмосферных моделирующих систем (как часть и шаг к моделированию системы “Земля”) ведет к новому поколению моделей для метеорологического и химического прогнозов и оценки воздействий на окружающую среду. Методология реализации предложенной интегрированной концепции для прогноза химической погоды рассматривается на примере европейской системы Enviro–HIRLAM. Значимость различных механизмов обратных связей для прогноза химической погоды также обсуждается в данной статье.*

Ключевые слова: *прогноз химической погоды, моделирование переноса химических веществ в режимах "оффлайн" и "онлайн", механизмы обратных связей, двустороннее совместное мезомасштабное моделирование.*