Risk and impact assessment through air, water and soil quality modelling: an integrated approach

A. Ebel[1] & T. Davitashvili[2]
[1]Rhenish Institute for Environmental Research at the University of Cologne (RIU), Cologne, Germany
[2]State University Tbilisi, Vekua Institute for Applied Mathematics (VIAM), Tbilisi, Georgia

Abstract

The demand for integrated modelling of different environmental compartments is increasing. With steadily growing computational power it seems possible to overcome the obstacles still preventing the comprehensive numerical treatment of the environmental system including society and economy. This article deals with approaches to the combined treatment of air, water and soil pollution aiming at impact and risk assessment. The design of forward and inverse (adjoint) model systems is discussed and examples of applications focussing on air pollution impacts are given. It is evident that complex system applications to risk and impact assessment are still at their beginning and that there is still considerable potential to be exploited.
Keywords: pollution, forward modelling, inverse modelling, data assimilation, integrated modelling, air, water, soil, environmental impacts, risks.

1 Introduction

Though it is well known that changes of a specific component of the environmental system, e.g. in air, water, soil, usually also affects the other components it is still common to treat the different media without caring too much about their interactions and interdependence. There are severe obstacles to multi- or interdisciplinary research of the integral environmental system. These are, among others, fundamental differences of physical and chemical processes controlling the various compartments (or components) of the environment,

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significant deviations of dominant temporal and spatial scales and deviating characteristics of typical risks and impacts. Also socio-economic aspects may contribute to an isolated view of environmental compartments or sub-domains of it which seems to be reflected in many environmental research programmes of the past, particularly when the main weight is put on application of environmental science.

During the last years the efforts to establish integrating research for sustainability dealing with the complete earth system have considerably been intensified. The perspective of earth system analysis is first of all a global one [1, 2]. Yet it is evident that the main sources of global change, the Achilles' heels as they are coined in [2], are of regional nature. They may be made up by an accumulation of smaller scale anthropogenic impacts, e.g. emissions from fossil fuel plants, or larger scale natural processes, e.g. methane emission changes in the Arctic tundra. It may happen on all spatial scales that changes in air, water and soil interact. This interrelationship which is characterized by complex feed back mechanisms was the main topic of a NATO Advanced Research Workshop in September 2005 [3]. The results and ideas presented there form the background of this study. Inverse methods combining observations and numerical models through data assimilation are discussed in Section 2. Section 3 deals with problems of combined use of air, water and soil quality models. Some examples of model applications are given in Section 4. Section 5 addresses future needs of integrated modelling for environmental risk and impact assessment.

2 Numerical methods of risk assessment and control

The traditional approach to numerical treatment of environmental problems is forward modelling. Regarding the complexity of isolated environmental systems and even more of combined ones like that of air, (surface and ground) water and soil it is extremely difficult to arrive at a comprehensive and reliable assessment of possible adverse impacts in this way. Therefore advanced methods of risk assessment and system control based on backward modelling have been developed in recent years [4, 5, 6]. They combine computations and observations by assimilating measurement data into the employed model or model system. Theoretically it is possible to apply the combined method of forward and inverse modelling to larger integrated environmental complexes. Yet it seems that due to immense computational requirements most applications are still restricted to individual environmental compartments with a confined number of processes taken into account. For instance, 4-dimensional variational data assimilation in atmospheric modelling has long been restricted to meteorological measurements only, before it became theoretically and computationally possible to extend the method to the more complex chemistry and transport processes of the atmosphere [7, 8]. Though the principals of numerical risk assessment and control are well known, it is obvious that with regard to computer resources and algorithm development it is still a long way towards its application to an integrated treatment of interconnected environmental compartments.

First advances in this field may be found in the literature. An important one is the estimate of emissions into the lower atmosphere where the sources may be anthropogenic or natural. In the latter one has an example of interactive processes between atmosphere and soil if one includes deposition of trace substances on the earth's surface. An illuminating example how the methodology can be applied to the estimation of risks and vulnerability of territories, the assessment of observability and thus control in selected regions and source detection in case of atmospheric aerosols is given by Penenko and Tsvetova [9].

3 Integrated modelling of air, water and soil

The basic principles of numerical quality model formulation are straightforward for all media under consideration. The central principle is the conservation of mass expressed by the continuity equation relating the local change of the concentration C of a species contaminating air, water or soil to mean, turbulent and diffusive transport (flux, including Darcy flux), its sources and sinks (including production (P) and loss (L) through chemical and physical transformation, internal sources (I_P) and sinks (I_L) of natural and anthropogenic substances:

$$\frac{\partial C}{\partial t} = -div(flux) + P - L + I_P - I_L \tag{1}$$

Boundary conditions describe gain or loss of a species from and to places outside a confined model domain. Differing chemical and physical characteristics of the media, specific conditions at the boundaries and peculiar morphological features lead to quite different complex model formulations for individual environmental regimes. Different typical time and spatial scales exist in different media. Till now such features have prevented the design of closely integrated systems of compatible environmental quality models, taken into account all significant feedback mechanisms between the media.

The most frequently applied concept is what may be called handover approach. Matter from one compartment is handed over to another one through the formulation of suitable boundary conditions. For instance, nitrate in the atmosphere is handed over to soil and water via dry and wet deposition. In the soil it may be transported through ground water flow. It may accumulate in lakes and cause eutrophication or act as a fertilizer. Feedback effects could be land type changes and/or modifications of natural emissions. These are important factors for environmental impact and thus risk assessment which motivates the development of integrated environmental quality models.

4 Interfaces of media: examples

Numerous studies exist about interactive processes and changes in environmental compartments (e.g. [12]). Deposition of toxic substances through air on water and soil surfaces being finally fed into the food chain or harmful substances leaving a landfill site and fertilizers penetrating from the earth's surface into the soil, heavily contaminating ground water resources are well known examples. The atmospheric boundary layer (ABL) is of outstanding importance for the interrelation of the three media. In this section we are therefore briefly discussing three cases of impacts occurring in the ABL and controlled by it to a high degree. These are the accumulation of ozone impacts at or near the surface over land, the role of land type and use changes for air quality and effects of dry and wet deposition.

A dosis value has been defined for ozone to measure the impact of this pollutant on plants and its damage to crops and other agricultural products. It is derived from measured or modelled hourly mixing rations exceeding a given threshold (40 ppb, chosen by the European Commission [10]) between 8 and 20 hours and accumulated from May to June. The respective dosis value AOT40 (accumulated ozone over a threshold of 40 ppb) is thus related to the ozone mixing ratio c_n (in ppb) through

$$AOT40 = \sum_{n=1}^{N} \max(0, c_n - 40) \tag{2}$$

with N the number of hours with $c_n > 40$ ppb. Though somewhat ambiguous in its relation to impacts on plants and crops, this is an important parameter for risk and impact assessment regarding air pollution through photo-oxidants and its precursors. It has been used to evaluate existing regional differences of harmful ozone effects as well as risks due to uncontrolled anthropogenic and biogenic emissions and countermeasures for avoiding them. Air pollution models have been used to demonstrate how climate change and anthropogenic emission reduction may change the ozone load. An example (Fig. 1) is taken from a study by Geernaert and Zlatev [11]. It shows where the most endangered areas can be found in Europe and what improvement of the situation can be expected from emission reductions as enforced by the EC. Till now little attention has been given to the fact that AOT measures contain valuable information about possible changes of land surfaces (and thus soil) due to air pollution effects. Land surface properties may be changed on short and long time scales and lead to unfavourable changes in the comportments air and soil and their interrelation (e.g. damage of plants changing the water balance in the air/soil system which in turn may affect the ABL properties in an unfavourable way).

Deposition of pollutants as the main process in the atmosphere affecting the soil is largely controlled by turbulence of the air and land type properties mainly related to the structure of the surface and its natural cover. Deposition velocities (V_D) of minor constituents which are deposited in a similar way like sulphur [14] exhibit a clear dependence on surface roughness (z_0), turbulent friction velocity of air (u^*) and its stratification which is characterised by the Obukhov length [13]. For a large range of meteorological conditions with unstable stratification V_D/u^* is approximately linearly decreasing with increasing $\sqrt{z_0}$.

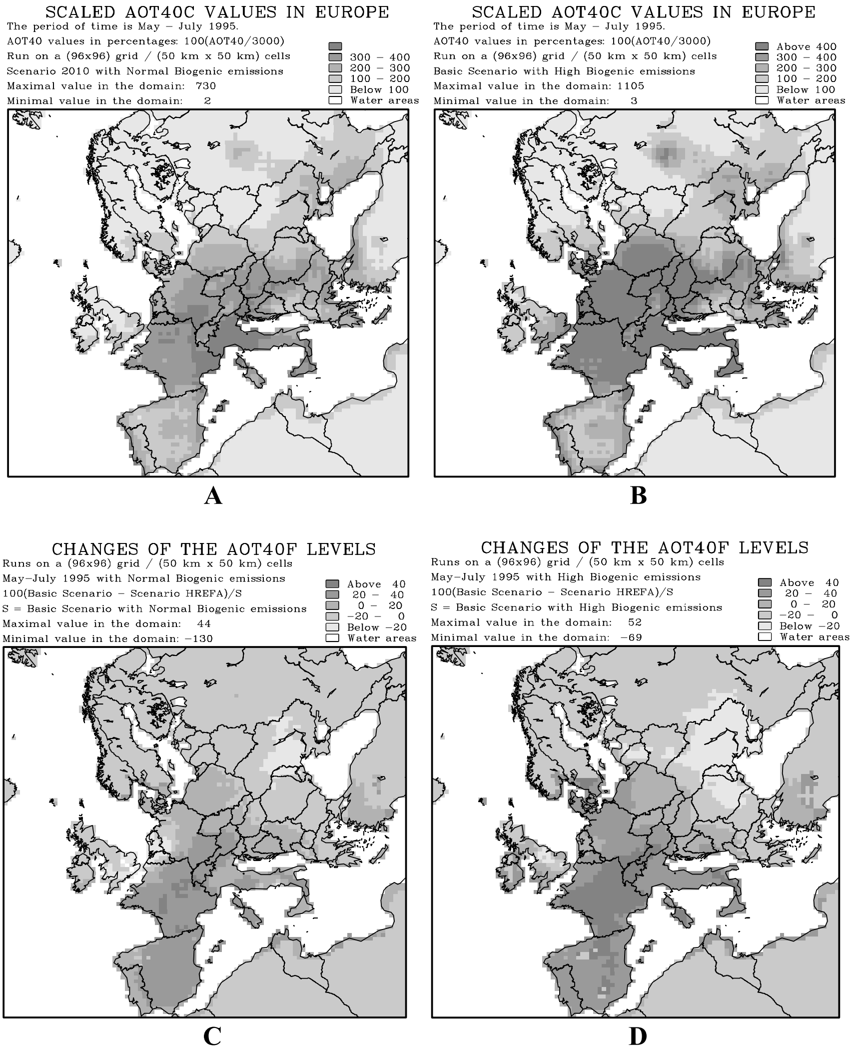

Figure 1: Upper panels: AOT40 - scaled values (100·AOT40/100) for EUROPE. A: Basic scenario 1995 with normal biogenic emissions. B: The same with high biogenic emissions. Lower panels: Relative changes of AOT40, C: (BN - RNO_x)/BN, D: (BH - RNO_x)/BN. BN - basic scenario 1995 with normal biogenic emissions; BH - basic scenario 1995 with high biogenic emissions; RNO_x - scenario with NO_x reduction as estimated for the year 2010. (Figures by courtesy of G. Geernaert and Z. Zlatev [11], reproduced with permission of Inderscience Publishers.)

Table 1: Normalized deposition flux of ozone and NO_x simulated with the EURAD system [21] for Berlin and its suburbs, episode July 21 – 27, 1994. Coarse grid: Value 1 corresponds to 378 tons and 1.6 tons for ozone and NO_x, respectively, deposited in the total domain during the episode.

horizontal resolution	*54 km*	*18 km*	*2 km*
deposition flux, ozone	1	1.9	1.7
deposition flux, NO_x	1	7.0	4.7

The roughness of surfaces and friction velocity are generally larger in cities than in parks or forests. And here they are larger than on grass or farmland. It depends on the relative change of V_D and u* if V_D is steadily increasing when going to places with smaller surface roughness. Real conditions with finer details may show a slight reduction of V_D compared to urban conditions. Such behaviour is well reproduced in atmospheric chemistry transport models. Table 1 is referring to a sensibility study for photo-oxidant formation in which the resolution of an urban domain (Berlin) has been increased from 54 km to 18 and 2 km thus allowing the land type to change from mainly urban to a mixture of suburban, forest and water with growing detail. The increase of deposition fluxes for O_3 and NO_x found in the first step from 54 km to 18 km with a larger fraction of land with smaller roughness and then (2 km) a slight decrease with higher resolution is evident. Such estimates may be used to assess additional stresses through air pollution impacts exerted on soil anyway due to urbanization of a region. In the same way risks resulting from conversion of forests into other land types (e.g. farm land) or effects of desertification in the course of climate change may be evaluated.

The absolute supply of pollutants by the atmosphere to its adjacent compartments water and soil not only depends on surface characteristics but also on emissions and meteorological and chemical processes controlling transport and transformation in the atmosphere. Reliable estimates therefore need to be based on budget calculations taking into account all relevant sources and sinks of a component. Fig. 2 contains results of an estimate of NO_x and SO_2 dry deposition for Central Europe and the Iberian Peninsula during an episode of high photo-oxidant formation. The percentage of emissions of the pollutants which are absorbed by the surface is shown. For comparison the fraction of ozone generated in and transported into the domains under consideration in layers up to 3600 m are shown. The percentage of sulphur deposition is always larger than that of NO_x because the latter species is partly used up through chemical transformations. Similar estimates can easily be derived for smaller spatial (i.e. local) and longer temporal (i.e. climatological) scales.

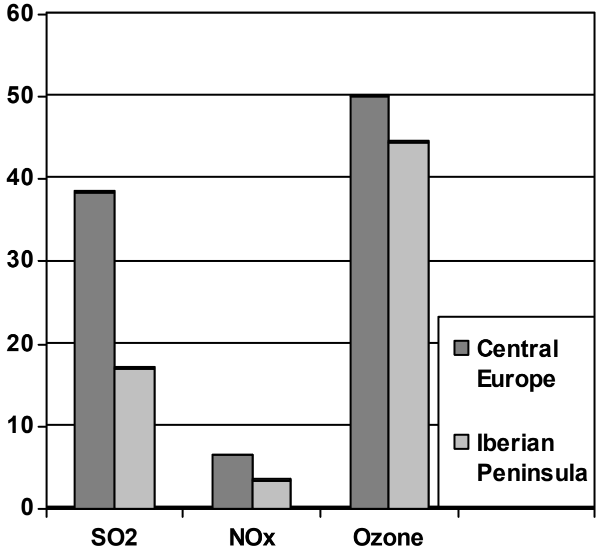

Figure 2: Fraction (in percent, vertical axis) of emitted SO_2 and NO_x deposited to the earth's surface during from July 31 to August 4, 1990 in Central Europe and the Iberian Peninsula. The deposition of ozone (fraction of gain through chemical production and transport) is shown for comparison. Results obtained with the EURAD model system [21].

5 Extension of the system: challenges to future integrated modelling

From the discussion in the previous section it is evident that modelling for environmental risk and impact assessment needs to integrate the biosphere. Also the compartment "water" should not be restricted to land surface and ground water as it has been done here for practical reasons since we have been focusing on limited area modelling. It should also include the ocean explicitly which is actually done in global models when emission and deposition are treated.

The complete system of environmental cause-effect relationships will also have to deal with its social and economic components not only to find an optimum of sustainability but also for assessing risks for and impacts on human health, economy and the importance of possible feedbacks between all compartments [15, 20]. A helpful scheme, DPSIR, for treatment of such effects has been suggested by OECD [16] for social studies. It also proves useful for integrated environmental studies. It interrelates **D**riving forces of environmental change, **P**ressures on the environment, **S**tate of the environmental compartments, **I**mpacts on these compartments and **R**esponse of the society (Fig. 3). Approaches of this kind are the RAINS model [17], the ExterneE methodology [18] and the UNECE Task Force on Integrated Assessment Modelling [19].

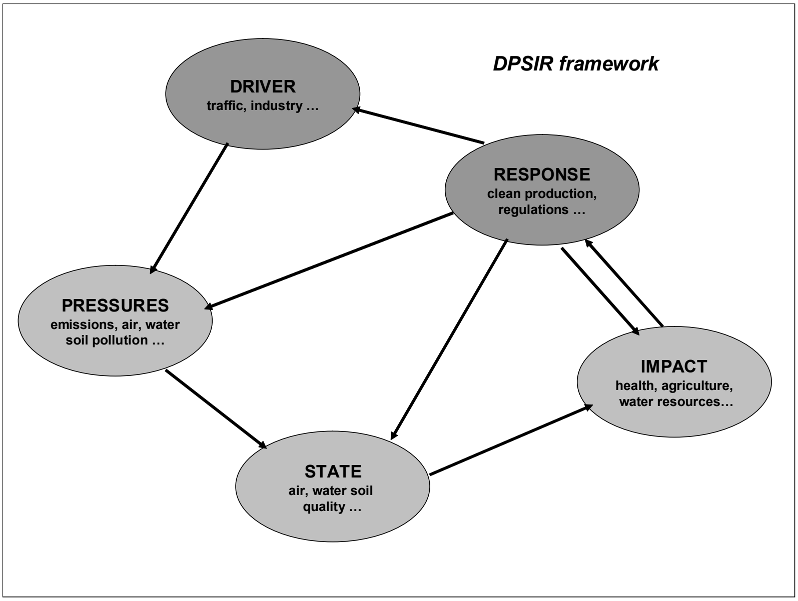

Figure 3: DPSIR scheme after [16, 20].

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References

[1] Schellnhuber, H.-J. & Wenzel, V., (eds). Earth System Analysis, Integrating Science for Sustainability, Springer-Verlag: Berlin, Heidelberg, 1998.

[2] Schellnhuber, H.-J., Crutzen, P. J., Clark, W. C. & Hunt, J., Earth System Analysis for Sustainability. *Environment*, 47, pp. 10 - 25, 2005.

[3] NATO Programme Security Through Science, Advanced Research Workshop; Air, Water and Soil Quality Modelling for Risk and Impact Assessment, Tabakhmela/Tbilisi, Georgia, Sept. 2005, www.eurad.uni-koeln.de/NATO-ARW-Georgia/index.html.

[4] Marchuk, G.I., *Adjoint Equations and Analysis of Complex Systems*, Kluwer Academic Publishers, Dordrecht, 1995.

[5] Penenko, V.V., Numerical models and methods for the solution of problems of ecological forecasting and design. *Rev. appl. indust. math.*, **1(6),** pp. 917 - 941, 1994.

[6] Penenko, V.V. & Tsvetova, E. A., Mathematical models for studying risks of environment pollution. *Appl. Mech. Tech. Phys.,* **45 (2),** pp. 136 - 146, 2004.

[7] Elbern, H., Schmidt, H. & Ebel, A., Variational data assimilation for tropospheric chemistry modelling. *J. Geophys. Res*., **104**, pp. 18583 - 18598, 1997.

[8] Elbern, H. & Schmidt, H., Chemical 4D variational data assimilation and its numerical implications for case study analyses. *IMA Vol, in Mathem. and its Appl., Atmospheric Modeling*, eds. D. P. Chock & G. R. Carmichael, **130,** pp. 165 - 184, 2001.

[9] Penenko, V. V. & Tsvetova, E., Variational technique for environmental risk/vulnerability assessment and control. *Air, Water and Soil Modelling for Risk and Impact Assessment*, eds. A. Ebel and T. Davitashvili, Springer Verlag: Berlin and New York, in preparation, 2006.

[10] Directive 2002/3/EC of the European Parliament and the Council of 12 February 2002 relating to ozone in ambient air. *Official Journal of the European Communities,* **L67**, 9.3.2002, pp. 14 - 30, 2002.

[11] Geernaert, G. & Zlatev, Z., Studying the influence of biogenic emissions on AOT40 levels. *Int. J. Environm. and Pollution*, **22**, pp. 29 - 42, 2004.

[12] Ebel, A. & Davitashvili, T., (eds). *Air, Water and Soil Modelling for Risk and Impact Assessment*, Springer Verlag: Berlin and New York, in preparation, 2006.

[13] Stull, R. B., *An Introduction to Boundary Layer Meteorology*. Kluwer Academic Publ.: Dordrecht, 1988.

[14] Chang, J. S., Brost, R. A., Isaksen, I. S. A., Madronich, S., Middleton, P., Stockwell, W. R. & Walcek, C. J., A three-dimensional acid deposition model: Physical concepts and formulation. *J. Geophys. Res.,* **92**, pp. 14681 – 14700, 1987.

[15] Mensink, C., Integrated modelling and applications. *Air, Water and Soil Modelling for Risk and Impact Assessment*, eds. A. Ebel and T. Davitashvili, Springer Verlag: Berlin and New York, in preparation, 2006.

[16] OECD, *OECD Core Set of Indicators for Environmental Performance Views*. OECD Environment Monographs No. 83, OECD/GD(93)179, 39.p, 1993.

[17] IIASA, www.iiasa.ac.at/~rains/ 2005.

[18] Friedrich,R. & Bickel, P. (eds). Environmental Costs of Transport. Springer Verlag: Berlin and New York, 2001.

[19] UNECE, www.unece.org/env/tfiam/welcome.html.

[20] Mensink, C., De Nocker, L. & and De Ridder, K., Integrated assessment modelling: applications of the impact pathway methodology. *Air, Water and Soil Modelling for Risk and Impact Assessment*, eds. A. Ebel and T. Davitashvili, Springer Verlag: Berlin and New York, in preparation, 2006.

[21] Memmesheimer, M., Friese, E., Ebel, A., Jakobs, H. J., Feldmann, H., Kessler, C. & Piekorz, G., Long-term simulations of particulate matter in Europe on different scales using sequential nesting of a regional model. *Int. J. Environm. and Pollution*, **22**, pp. 108 - 132, 2004.