Influence of meteorology and other input parameters on levels and loads of pollutants relevant to energy systems: a sensitivity study

S. Andreani-Aksoyoglu, J. Keller
Paul Scherrer Institute, CH-5232, Villigen PSI, Switzerland

Abstract

A comprehensive assessment of energy systems includes environmental impacts, health risks, and economic aspects. One important issue deals with air pollution caused by the anthropogenic emissions from these systems. In the frame of the Swiss project "Comprehensive Assessment of Energy Systems" (Ganzheitliche Betrachtung von Energiesystemen, GaBE), concentrations and deposition of pollutants in Switzerland are calculated using a 3-dimensional chemical dispersion model. In view of the future energy systems, influences of variations in input parameters such as emissions, wind and pollutant concentrations in Switzerland as well as beyond the Swiss borders are investigated. Results will be interpreted in terms of damage for the environment using critical levels and loads approach. In this sensitivity study, the effects of initial and boundary concentrations of species, surface temperature, wind fields, pressure, mixing layer height, and top of the model region on the levels and daily loads of the pollutants were investigated. It was shown that initial concentrations do not have any significant effect, whereas boundary concentrations may play a very important role. The results indicated that temperature, pressure, mixing layer height, wind fields and top of region affect the concentrations and depositions significantly.

1 Introduction

Air pollution is changing ecosystems especially in Europe and north America. Such changes result from acid deposition, photo-oxidants and nitrogen accumulation leading to serious deterioration of terrestrial and aquatic ecosystems[1]. The nature and severity of this deterioration vary from area to area depending on the ecosystem sensitivity, pollution, and

climate. Political decisions regarding air pollution control strategies require scientific studies of critical levels and loads above which pollutant concentrations and depositions may cause adverse effects on the environment[2].

In the frame of the Swiss project "Comprehensive Assessment of Energy Systems", we investigate the impacts of energy related air pollutants on the ecosystems[3]. In this context, we established the correlation between the emission rates of species released by various energy systems and the resulting concentration and load pattern due to transport, dispersion, chemical conversion and deposition. The consequences of the emission scenarios resulting from the energy systems today and in the future, will be simulated using a three-dimensional chemical dispersion model, and the concentrations and depositions of the pollutants under the prevailing conditions will be calculated. The results will be compared with the critical levels and loads for the relevant air pollutants and ecosystems in order to interpret them in terms of damage for the environment, using the exposure-response functions.

Some assumptions concerning the input parameters for such complex simulations are inevitable. It is therefore necessary to analyze the sensitivity of the model to the variations of the input parameters, before performing the scenario analyses. In this paper, sensitivity tests concerning the effects of the meteorological conditions and other input parameters on the levels and the loads of the pollutants relevant to energy systems are discussed.

2 Methodology

The model used for the simulations is the Urban Airshed Model (UAM) which is a three dimensional grid model developed by Systems Applications, USA[4]. The chemical reactions are described by the Carbon Bond Mechanism (CBM IV)[5]. The model domain is 350 km in the east-west and 220 km in the north-south direction with a 5km x 5km horizontal resolution. Boundary regions vary between 5 and 40 km outside the state borders. In the vertical direction, there are 5 layers, 2 below and 3 above the mixing layer height. The mixing layer heights were determined using the temperature data. Wind fields were first obtained from the routine weather forecast high-resolution subgrid model "HRM"[6]. We resampled them for the model domain with 5km x 5km grid of the UAM. Then, we prepared time and space dependent ground level emission fields for VOC (volatile organic compounds), NO_x ($NO+NO_2$) and CO using data from traffic and industry[7]. A biogenic VOC emission inventory (isoprene, alpha-pinene) was included in the emission inventory as well[8].

Simulations were run for July 28-29, 1993 by starting at 12:00 CEST (Central European Summer Time) on July 28 and ending at 24:00 on July 29. In that period, an air quality field experiment took place where the most important meteorological and chemical parameters were measured. The first 12 hours of the simulation served to initialize the parameters. The model results for July 29 were validated with the field measurements[9].

Table 1 shows the variations of the parameters during the sensitivity tests. The concentrations of the species to be used at the beginning of simulations on July 28, originate from the measurements where available, otherwise data from literature were used[10-11]. The initial concentrations were reduced individually by 20 % for the following UAM species : NO_x, O_3, CO, FORM, ALD2, PAR, OLE, ETH, PAN (see Table 2 for their definitions). In general, the concentrations of species in the boundary regions are governed by the emissions abroad and may affect the air quality in Switzerland. Therefore we checked the effect of transboundary pollution by reducing the boundary concentrations by 20%. During the simulation period chosen, there was a moderate, westerly wind blowing over the model domain. We investigated the sensitivity of the model to very low wind fields, which is usually the case for indifferent pressure distributions. We generated reduced wind fields by subtracting the daily averages of the wind vectors from the basic wind fields. The effects of other parameters such as temperature, pressure, top of region and mixing layer height were investigated too.

Table 1 Parameter variations in the sensitivity tests

parameter	variation	remarks
initial concentrations of the species	20 % reduced	one species reduced at each run
boundary concentrations of the species	20 % reduced	one species reduced at each run
atmospheric pressure	reduced from 1 atm to 0.87 atm	homogeneous over whole domain
surface temperature	reduced by 5 and 10°C	to investigate the cooler conditions
top of region	increased from 1400 to 2000 m	
mixing layer height	decreased by 20% during daytime	
wind fields	reduced by subtracting the daily averages of the wind fields	to investigate the low wind situation

Table 2. Some UAM species varied in the sensitivity studies

species	definition
NO	nitric oxide
NO2	nitrogen dioxide
O3	ozone
ETH	ethene
PAR	paraffinic carbon bond
OLE	olefinic carbon bond
FORM	formaldehyde
ALD2	high molecular weight aldehydes
CO	carbon monoxide
PAN	peroxyacetylnitrate

3 Results and discussion

3.1 Initial Concentrations

The concentrations of O_3, NO_2, PAN and VOC between 16:00-17:00 CEST on July 29 and the deposition of ozone and NO_2 during that day were compared with the results of the base case. The changes in the concentrations due to 20 % reduction in initial concentrations of species were less than 0.1 % for all the species. The results show that the effect of initial concentrations is significant only during the first few hours of simulations. The changes in O_3 and NO_2 deposition were less than 1%.

3.2 Boundary Concentrations

Boundary concentrations of the species are controlled by the emissions abroad and may have significant effects on the results depending on the meteorological conditions. After having reduced the boundary concentrations, we compared the levels of O_3, NO_2, PAN, and VOC between 16:00-17:00 CEST on July 29 and deposition of ozone and NO_2 with the results of the base case (Tables 3a,4). We found the highest changes for those species whose concentration was decreased. When NO_x, CO or PAR were reduced, the peak ozone concentrations decreased by about 1-2 %. Reducing NO_x boundary concentrations affected mainly NO_2 and PAN levels. The effect of decreasing PAR concentrations was observed especially on NO_2, PAN and VOC. Aldehydes affect mainly PAN levels, and the boundary PAN level is important for NO_2. NO_x reduction caused a substantial decrease (22%) in NO_2 deposition. Reducing boundary ozone concentrations by 20 %, caused a change between -25 % and +2% in peak ozone concentrations over the whole area. The decrease was observed especially on the western regions from where the wind was blowing. NO_2 and PAN concentrations were also affected significantly. Ozone deposition decreased by 1-20%. Deposition of NO_2 changed between -5 and +11 %.

3.3 Surface Temperature

The UAM reads the surface temperatures and temperature gradients from the input files and calculates the vertical temperature profile. Temperature may be important for the chemical reactions with temperature dependent rate constants (see Tables 3b, 4). When the temperatures were reduced by 5°C, peak ozone concentrations changed between -13 and +0.5% over the whole area, main decrease occurring over the Swiss Plateau. Changes especially in PAN concentrations were very large due to the strong temperature dependence of its stability. Ozone deposition changed between -6 (over the Swiss Plateau) and +2% (in the Alpine regions). The change in NO_2 deposition was about ± 11%. When temperatures were reduced by 10°C, peak ozone concentrations varied between -21 and +1 %. Changes in depositions were between -10 and +4 % for O_3, and between -18 (over the Swiss Plateau) and +14 % for NO_2. NO_2 levels decreased and PAN increased especially over the Swiss Plateau.

3.4 Atmospheric Pressure

The original version of the computer code assumes one homogeneous surface pressure field for the whole model domain. However, Switzerland has a complex topography, the altitudes varying between 200 and 4000 m a.s.l. To check for the effect of using a homogeneous pressure, we reduced it from 1 atm to about 0.87 atm which corresponds to an altitude of about 1100 m. Peak ozone concentrations changed by ± 4 % over the Swiss Plateau which is relatively flat (see Table 3b). On the other hand, deposition of ozone was decreased by about 12-17 %. Changes in NO_2, PAN and VOC concentrations and NO_2 deposition were significant especially over the Swiss Plateau (see Tables 3b,4). These results lead to the following modifications: The topography was included in the input data to calculate the altitude dependent surface pressure for each grid cell individually.

3.5 Top of Region

Ozone concentrations varied by ± 4%, when top of the model region was increased from 1400 m to 2000 m whereas the changes in NO_2, PAN, and VOC concentrations were more significant (see Table 3b). NO_2 concentrations decreased especially in the Alpine regions. Ozone deposition changed between -1.4 and 5% at a few locations (Table 4). On the other hand deposition of NO_2 changed between -19 and +6%, decrease being mainly in the Alpine regions.

3.6 Mixing Layer Height

The effect of mixing layer height seems to be quite important for all species (Tables 3b, 4). When the height was reduced by 20% during daytime, NO_2 and VOC concentrations increased mainly in the urban

areas where the emissions are high. Deposition of ozone decreased in these areas. NO_2 deposition changed between -4 and +28%, increasing especially in the urban areas.

3.7 Wind Fields

There was a westerly wind with speeds between 0.2 and 15 $m \cdot s^{-1}$ during the simulation period. In high pressure weather situations, the winds are usually very weak. This test was carried out to investigate the low wind situation. We derived reduced windfields by subtracting the daily averages of the wind fields from the original data. The resulting wind speeds vary between 0.03 and 7.6 $m \cdot s^{-1}$. Ozone and PAN concentrations increased in the sub-urban areas by ~50% and ~90% respectively. On the other hand, in the urban areas, NO_2 and VOC levels were much larger than before (about 40 and 7 times, respectively) and NO_2 deposition was 4 times higher (see Tables 3b,4). This effect is due to the high emissions which cannot be transported away by weak winds. Ozone levels, however, decreased in the urban areas. Deposition of ozone decreased mainly over the Alpine regions.

4 Summary and Conclusion

In the frame of the project GaBE, concentrations and deposition of air pollutants in Switzerland are calculated using a 3-dimensional chemical dispersion model. The results will be interpreted as damage to the environment using critical levels and loads approach and exposure-response functions. In view of the future energy systems, influences of variations in input parameters such as emissions, wind and pollutant concentrations in Switzerland as well as beyond the Swiss borders are investigated. In this sensitivity study, effects of meteorological and other input parameters on the concentrations and depositions of species are evaluated. Initial concentrations of the species do not have any significant effect. On the other hand, boundary concentrations play an important role on the concentrations and the depositions of the pollutants. As the boundary levels are controlled by the emissions abroad, they reflect the importance of transboundary pollution in Switzerland. Lower wind fields caused an increase in the NO_x and VOC concentrations leading to lower O_3 and PAN levels in the urban areas where the emissions are high. Surface temperature also plays an important role due to temperature dependence of some reactions. Other parameters such as pressure, mixing layer height and top of region have significant effects as well on the levels and loads of the pollutants. In the next step, effects of emissions in Switzerland as well as outside the borders will be investigated.

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Table 3a. Effect of 20% reduced boundary levels on the species concentrations (29.7.1993, 16:00-17:00 CEST, ranges over the model domain). Upper line as ppb, lower line as %. The significant effects are shadowed.

reduced species	change in O_3 (ppb) (%)	change in NO_2 (ppb) (%)	change in PAN (ppb) (%)	change in VOC (ppb) (%)
NO_x	(-1.1) - (+0.3) (-2.0) - (+0.7)	(-0.2) - (<+0.1) (-22) - (+3.4)	(<-0.1) - (<+0.1) (-9.0) - (+5.7)	(-0.1) - (+0.2) (-0.4) - (+1.0)
O_3	(-13) - (+1.0) (-25) - (+2.1)	(-0.3) - (+0.4) (-6.0) - (+13)	(-0.3) - (<+0.1) (-19) - (+1.7)	(<-0.1) - (+0.9) (-0.2) - (+2.6)
CO	(-0.9) - (+0.1) (-1.2) - (+0.1)	(-0.1) - (<+0.1) (-6.2) - (+0.4)	(<-0.1) - (<+0.1) (-0.5) - (+3.3)	(-0.3) - (<+0.1) (-1.5) - (+0.1)
PAR	(-1.1) - (+0.1) (-1.5) - (+0.2)	(<-0.1) - (+0.1) (-1.0) - (+6.3)	(-0.1) - (<+0.1) (-9.0) - (+1.4)	(-3.6) - (+0.3) (-23) - (+1.8)
FORM	(-0.3) - (<+0.1) (-0.4) - (+0.1)	(<-0.1) - (<+0.1) (-0.3) - (+2.8)	(<-0.1) - (<+0.1) (-2.0) - (+0.2)	(-0.2) - (+0.1) (-1.0) - (+0.2)
ALD2	(-0.3) - (+0.1) (-0.4) - (+0.2)	(<-0.1) - (<+0.1) (-2.9) - (+2.1)	(<-0.1) - (<+0.1) (-6.4) - (+0.5)	(-0.1) - (<+0.1) (-0.8) - (+0.1)
OLE	(-0.3) - (<+0.1) (-0.4) - (<+0.1)	(<-0.1) - (<+0.1) (-0.3) - (2.8)	(<-0.1) - (<+0.1) (-2.4) - (+0.5)	(-0.1) - (+0.1) (-0.4) - (+0.2)
ETH	(-0.3) - (<+0.1) (-0.5) - (<+0.1)	(<-0.1) - (<+0.1) (-0.4) - (+2.7)	(<-0.1) - (<+0.1) (-1.0) - (+0.3)	(-0.1) - (<+0.1) (-0.9) - (+0.1)
PAN	(-0.3) - (<+0.1) (-0.5) - (<+0.1)	(<-0.1) - (<+0.1) (-4.5) - (+0.8)	(-0.1) - (<+0.1) (-19) - (+0.6)	(<-0.1) - (+0.1) (-0.1) - (+0.2)

Table 3b. Effect of selected input parameter variations on the species concentrations (29.7.1993, 16:00-17:00 CEST, ranges over the model domain). Upper line as ppb, lower line as %. The significant effects are shadowed.

variations of parameters	change in O_3 (ppb) (%)	change in NO_2 (ppb) (%)	change in PAN (ppb) (%)	change in VOC (ppb) (%)
decrease in surface temperature (5°C)	(-9.6) - (+0.2) (-13) - (+0.5)	(-0.8) - (+0.3) (-56) - (+12)	(<+0.1) - (+0.7) (+2.0) - (+126)	(-0.8) - (+1.7) (-1.2) - (+5.3)
(10°C)	(-17) - (+0.4) (-21) - (+0.8)	(-1.6) - (+0.4) (-82) - (+18)	(<+0.1) - (+1.2) (+3.2) - (+242)	(-1.6) - (+3.2) (-2.3) - (+10)
decrease in pressure	(-2.7) - (+2.8) (-4.3) - (+3.8)	(<-0.1) - (+2.8) (-5.6) - (+45)	(-0.1) - (+0.2) (-7.6) - (+14)	(-0.3) - (+12) (-3.4) - (+16)
increase in top of region	(-2.7) - (+2.5) (-4.2) - (+4.4)	(-0.5) - (+0.5) (-30) - (+17)	(-0.1) - (+0.1) (-15) - (+36)	(-4.5) - (+3.9) (-14) - (+11)
decreased mixing layer	(-7.1) - (+3.7) (-9.8) - (+6.0)	(<-0.1) - (+4.2) (-13) - (+70)	(-0.3) - (+0.1) (-19) - (+26)	(-0.9) - (+20) (-7.1) - (+29)
reduced wind fields	(-26) - (+39) (-41) - (+75)	(-4.5) - (+25) (-98) - (+4744)	(-1.0) - (+2.0) (-81) - (+659)	(-19) - (+126) (-60) - (+723)

Table 4 Effect of selected input parameter variations on the deposition of O_3 and NO_2 (29.7.1993, ranges over the model domain). Upper line as ppb, lower line as %. The significant effects are shadowed.

variations of parameters		change in O_3 ($mg \cdot m^{-2} \cdot d^{-1}$) (%)	change in NO_2 ($mg \cdot m^{-2} \cdot d^{-1}$) (%)
20% reduction in boundary levels	NO_x	(-0.3) - (+0.1) (-0.8) - (+0.2)	(-0.2) - (<+0.1) (-22) - (<+0.1)
	O_3	(-9.1) - (<-0.1) (-20) - (-0.9)	(-0.3) - (+0.1) (-4.5) - (+11)
	CO	(-0.2) - (<+0.1) (-0.7) - (<+0.1)	(<-0.1) - (<-0.1) (-2.0) - (<-0.1)
	PAR	(-0.2) - (<+0.1) (-0.8) - (<+0.1)	(<-0.1) - (<+0.1) (-0.2) - (+ 0.9)
	FORM	(-0.1) - (<+0.1) (-0.4) - (<+0.1)	(<-0.1) - (<+0.1) (-0.1) - (+0.6)
	ALD2	(-0.1) - (<+0.1) (-0.3) - (+0.1)	(<-0.1) - (<+0.1) (-0.1) - (+0.9)
	OLE	(-0.1) - (<+0.1) (-0.3) - (<+0.1)	(<-0.1) - (<+0.1) (-0.2) - (+0.3)
	ETH	(-0.1) - (<+0.1) (-0.3) - (<+0.1)	(<-0.1) - (<+0.1) (-0.1) - (+0.2)
	PAN	(-0.1) - (<+0.1) (-0.4) - (<+0.1)	(<-0.1) - (<+0.1) (-1.4) - (+0.2)
decrease in surface temperature	5°C	(-2.0) - (+0.8) (-6.4) - (+1.9)	(-0.2) - (+0.1) (-12) - (+11)
	10°C	(-3.3) - (+1.5) (-10) - (+3.8)	(-0.4) - (+0.2) (-18) - (+14)
decrease in pressure		(-8.6) - (<-0.1) (-17) - (-12)	(-0.1) - (+0.2) (-15) - (+8.6)
increase in top of region		(-0.5) - (+3.0) (-1.4) - (+5.0)	(-0.2) - (+0.1) (-19) - (+5.9)
decreased mixing layer		(-2.0) - (+2.5) (-6.0) - (+6.0)	(<-0.1) - (+1.7) (-3.7) - (+28)
reduced wind fields		(-32) - (+12) (-69) - (+57)	(-2.3) - (+5.5) (-90) - (+400)