

Chapter 7

Source-receptor calculations

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7.1 Introduction

This chapter presents an updated set of source-receptor matrices calculated with the Lagrangian oxidant model. This update is presented for two main reasons:

1. The officially submitted emission estimates (Vestreng and Støren, 2000) for the Year 2010 have in a number of cases changed substantially from those used in the previous EMEP report (Simpson and Jonson, 1999).
2. The Tables presented in Simpson and Jonson (1999) contained an error. Although the numbers given are correct, Iceland should not have been in the list of receiver countries. All entries from Iceland and downwards therefore are shifted by one row. This error does not affect the plots presented in Report 2/99, or the numbers stored at the EMEP web site. However it seems prudent to publish here a set of tables with this mistake corrected.

Source-receptor (S-R) relationships give the change in ozone in each receptor country (or grid square) resulting from a change in emissions of either NO_x or VOC from each emitter country. They are generated for each country by reducing either NO_x or NMVOC emissions (anthropogenic) by a given percentage from that country, re-running the oxidant model, and comparing the resulting fields of ozone or AOTs with the base-case fields.

The first full set of such S-R matrices was presented in Simpson et al. (1997), where calculations were performed with the Lagrangian oxidant model for a 5 year period: 1989, 90, 92, 93, 94. A number of matrices with different assumptions (including 40% reductions) were calculated in order to supply results needed for the IIASA RAINS-ozone model (Schöpp et al., 1999). Extensive discussions of the behaviour of source-receptor matrices for ozone, and of the extent of linearity of these, have been presented elsewhere (Simpson, 1991, Simpson and Malik, 1996, Simpson et al., 1997).

The basic methodology used to calculate S-R matrices is identical to that of Simpson and Jonson (1999) with calculations performed for 40% emission reductions. The base-emission case is for the year 2010, using the EMEP emissions estimates as given in Vestreng and Støren (2000). The meteorology for the 5-year calculations is from April-September of 1992, 93, 94, 95 and 96.

The tables to be presented make use of two-letter country codes. These codes are:

AL	Albania	LT	Lithuania
AT	Austria	LU	Luxembourg
BY	Belarus	NL	Netherlands
BE	Belgium	NO	Norway
BA	Bosnia and Herzegovina	PL	Poland
BG	Bulgaria	PT	Portugal
HR	Croatia	MD	Republic of Moldova
CZ	Czech Republic	RO	Romania
DK	Denmark	RU	Russian Federation
EE	Estonia	SK	Slovakia
FI	Finland	SI	Slovenia
FR	France	ES	Spain
DE	Germany	SE	Sweden
GR	Greece	CH	Switzerland
HU	Hungary	MK	The FYR Macedonia
IS	Iceland	TR	Turkey
IE	Ireland	UA	Ukraine
IT	Italy	GB	United Kingdom
LV	Latvia	YU	Yugoslavia

Unfortunately the model domain of the Lagrangian has not yet been extended to cover the territories of all new Parties to the Convention, so we cannot present source-receptor calculations for these countries. This problem will be solved in future reports by performing such calculations with the 3-D Eulerian models with the extended domain.

The results of the updated S-R calculations are given in Tables 7.1-7.6 for 6-monthly mean of daily max. ozone, AOT40_c, and AOT60. These tables, also that for AOT40_f (not shown) and indeed the country-to-grid results from which they are constructed will be made available as ASCII files on the EMEP web-site, <http://www.emep.int>.

The matrices will not be discussed further here as the results are very similar to those previously reported in (Simpson et al., 1997) and Simpson and Jonson (1999). The latter reference also presents comparison with results from the Eulerian oxidant model of Jonson et al. (1998).

Table 7.5: Source-receptor relationships for AOT60 - NOx
(Emission base-year 2010, meteorology: from 5 years - 1992-1996)

Country	emitters																		
	AL	AT	BY	BE	BA	BG	HR	CZ	DK	EE	FI	FR	DE	GR	HU	IS	IE	IT	LV
Albania	6	0	0	0	7	5	7	0	0	0	0	1	1	16	5	0.	0	9	0
Austria	0	27	0	1	2	0	11	13	0	0	0	15	42	0	19	0.	0	56	0
Belarus	0	0	5	0	0	0	0	1	0	0	0	0	1	0	4	0.	0	1	0
Belgium	0	5	0	93	0	0	0	11	0	0	0	284	234	0	3	0.02	0	7	0
Bosnia and Herzegovina	0	3	0	0	18	0	17	5	0	0	0	2	7	0	30	0.	0	28	0
Bulgaria	0	0	0	0	1	45	2	1	0	0	0	1	3	0	8	0.	0	3	0
Croatia	0	10	0	0	23	2	55	9	0	0	0	14	22	0	57	0.	0	119	0
Czech Republic	0	29	1	0	2	0	9	124	0	0	0	27	117	0	29	0.	0	24	0
Denmark	0	1	1	3	0	0	1	13	19	0	0	16	77	0	3	0.	0	3	0
Estonia	0	0	0	0	0	0	0	1	2	1	0	2	9	0	0	0.	0	0	0
Finland	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0.	0	0	0
France	0	2	0	14	0	0	1	4	0	0	0	265	74	0	1	0.	0	37	0
Germany	0	12	1	9	0	0	2	38	0	0	0	96	320	0	7	0.01	0	18	0
Greece	0	0	0	0	1	26	1	0	0	0	0	1	1	25	3	0.	0	9	0
Hungary	0	26	1	0	8	3	33	23	0	0	0	20	39	0	200	0.	0	50	0
Ireland	0	0	0	0	0	0	0	1	0	0	0	18	8	0	0	0.01	4	1	0
Italy	0	5	0	0	11	2	20	4	0	0	0	32	9	1	16	0.	0	255	0
Latvia	0	0	0	0	0	0	0	1	0	0	0	2	8	0	2	0.	0	1	2
Lithuania	0	0	0	0	0	0	1	3	0	0	0	2	8	0	5	0.	0	2	2
Luxembourg	0	4	0	69	0	0	0	8	0	0	0	372	453	0	0	0.01	0	20	0
Netherlands	0	5	1	30	0	0	0	17	0	0	0	132	175	0	7	0.02	0	3	0
Norway	0	0	0	0	0	0	0	0	1	0	0	2	4	0	0	0.	0	0	0
Poland	0	7	4	0	0	0	2	29	0	0	0	11	48	0	17	0.	0	7	0
Portugal	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0.	0	1	0
Republic of Moldova	0	2	0	0	1	9	2	3	0	0	0	3	5	-1	14	0.	0	6	0
Romania	0	2	0	0	2	10	4	3	0	0	0	3	6	0	24	0.	0	10	0
Russian Federation	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.	0	0	0
Slovakia	0	27	2	0	2	0	11	45	0	0	0	21	37	0	122	0.	0	23	0
Slovenia	0	17	0	0	8	1	37	8	0	0	0	14	25	0	29	0.	0	194	0
Spain	0	0	0	0	0	0	0	0	0	0	0	12	1	0	0	0.	0	3	0
Sweden	0	0	0	0	0	0	0	1	2	0	0	1	11	0	0	0.	0	0	0
Switzerland	0	2	0	0	0	0	2	0	0	0	0	26	44	0	1	-0.00	0	82	0
The FYR Macedonia	0	0	0	0	0	7	0	0	0	0	0	0	0	1	1	0.	0	1	0
Turkey	0	0	0	0	0	7	0	0	0	0	0	0	0	7	0	0.	0	3	0
Ukraine	0	1	1	0	0	2	1	2	0	0	0	1	3	0	7	0.	0	3	0
United Kingdom	0	1	0	0	0	0	0	3	0	0	0	52	32	0	1	0.	0	1	0
Yugoslavia	0	3	0	0	5	9	11	6	0	0	0	2	7	0	42	0.	0	17	0
Europe*	0	2	0	1	0	2	2	4	0	0	0	22	21	0	6	0.	0	14	0

Country	receivers																		
	LT	LU	NL	NO	PL	PT	MD	RO	RU	SK	SI	ES	SE	CH	MK	TR	UA	GB	YU
Albania	0	0	0	0	3	0	0	5	1	1	0	2	0	0	4	4	0	7	0
Austria	0	0	0	0	13	0	0	5	1	21	9	0	0	4	0	0	4	-2	2
Belarus	1	0	0	0	14	0	0	2	7	4	0	0	0	0	0	14	0	1	0
Belgium	0	13	-24	0	11	0	0	2	1	4	0	15	0	14	0	0	3	-46	0
Bosnia and Herzegovina	0	0	0	0	6	0	0	8	0	16	3	0	0	0	0	3	0	22	0
Bulgaria	0	0	0	0	3	0	2	79	5	5	0	0	0	0	7	14	0	9	0
Croatia	0	0	-1	0	15	0	0	21	1	26	12	2	0	2	0	5	0	25	0
Czech Republic	0	0	-1	0	55	0	0	7	3	50	5	0	0	4	0	9	-1	4	0
Denmark	1	0	7	0	32	0	0	1	3	3	0	0	1	1	0	4	-12	0	0
Estonia	0	0	0	0	6	0	0	0	3	0	0	0	2	0	0	0	0	0	0
Finland	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0
France	0	3	-1	0	3	1	0	0	0	1	0	40	0	10	0	0	0	-8	0
Germany	0	4	-1	0	28	0	0	2	1	11	1	2	0	14	0	5	-8	1	0
Greece	0	0	0	0	2	0	2	21	10	1	0	1	0	0	0	71	19	0	4
Hungary	0	0	-1	0	43	0	1	39	3	95	11	2	0	4	0	16	0	28	0
Ireland	0	0	1	0	2	0	0	0	0	0	0	0	1	0	0	0	6	0	0
Italy	0	0	0	0	5	0	0	7	0	9	6	6	0	2	0	2	0	9	0
Latvia	4	0	0	0	16	0	0	0	5	2	0	0	0	0	0	1	0	0	0
Lithuania	10	0	0	0	37	0	0	1	4	3	0	0	0	0	0	2	-10	1	0
Luxembourg	0	48	-11	0	7	0	0	0	0	2	0	10	0	23	0	1	-1	0	0
Netherlands	0	2	1	0	19	0	0	4	2	10	0	11	0	5	0	7	-26	0	0
Norway	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Poland	2	0	0	0	138	0	1	6	0	28	1	0	0	1	0	15	-1	2	0
Portugal	0	0	0	0	0	141	0	0	0	0	0	125	0	0	0	0	0	0	0
Republic of Moldova	0	0	0	0	9	0	23	62	3	12	1	0	0	0	6	21	0	5	0
Romania	0	0	0	0	7	0	3	108	2	18	1	0	0	0	1	13	0	13	0
Russian Federation	0	0	0	0	0	0	0	0	16	0	0	0	0	0	0	8	0	0	0
Slovakia	0	0	-2	0	76	0	1	18	3	153	5	1	0	2	0	23	-1	8	0
Slovenia	0	0	0	0	14	0	0	12	1	18	29	2	0	2	0	4	0	8	0
Spain	0	0	0	0	0	32	0	0	0	0	0	220	0	0	0	0	0	0	0
Sweden	0	0	0	0	7	0	0	0	1	0	0	0	2	0	0	0	-1	0	0
Switzerland	0	0	0	0	0	0	0	0	0	1	0	0	0	19	0	0	0	0	0
The FYR Macedonia	0	0	0	0	0	0	0	7	0	0	0	0	0	0	0	1	0	2	0
Turkey	0	0	0	0	0	0	1	7	13	0	0	0	0	0	369	14	0	0	0
Ukraine	0	0	0	0	9	0	5	18	27	7	0	0	0	0	3	97	0	1	0
United Kingdom	0	0	-1	0	7	0	0	1	1	1	0	1	0	1	0	2	-72	0	0
Yugoslavia	0	0	0	0	9	0	0	28	1	17	2	0	0	0	0	4	0	59	0
Europe*	0	0	0	0	8	3	0	7	10	5	0	15	0	1	0	21	12	-2	2

Units: ppb.h per 40% emission reduction; * Average over all land-areas of Europe

Table 7.6: Source-receptor relationships for AOT60 - VOC
(Emission base-year 2010, meteorology: from 5 years - 1992-1996)

Country	emitters																		
	AL	AT	BY	BE	BA	BG	HR	CZ	DK	EE	FI	FR	DE	GR	HU	IS	IE	IT	LV
Albania	3	1	0	0	3	0	3	1	0	0	0	3	4	3	1	0	0	76	0
Austria	0	4	0	1	0	0	2	4	0	0	0	9	23	0	3	0	0	53	0
Belarus	0	0	0	0	0	0	0	1	0	0	0	0	3	0	1	0	0	3	0
Belgium	0	6	1	64	0	0	0	17	0	0	0	89	254	0	2	0,01	0	13	0
Bosnia and Herzegovina	0	1	0	0	2	0	2	2	0	0	0	4	8	0	4	0	0	52	0
Bulgaria	0	0	0	0	0	4	1	1	0	0	0	1	7	2	3	0	0	5	0
Croatia	0	4	0	1	3	0	7	5	0	0	0	17	26	0	8	0	0	158	0
Czech Republic	0	8	1	2	1	0	3	26	0	0	0	15	51	0	7	0	0	33	0
Denmark	0	2	1	5	0	0	0	11	2	0	0	16	55	0	1	0	0	8	0
Estonia	0	0	0	0	0	0	0	1	0	0	0	4	7	0	0	0	0	1	0
Finland	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
France	0	2	0	10	0	0	1	4	0	0	0	54	61	0	1	0	0	34	0
Germany	0	6	1	12	0	0	1	17	0	0	0	38	135	0	3	0	0	29	0
Greece	1	0	0	0	1	5	1	1	0	0	0	2	3	54	1	0	0	45	0
Hungary	0	7	1	2	2	1	6	13	0	0	0	16	40	0	23	0	0	72	0
Ireland	0	0	0	3	0	0	0	1	0	0	0	13	18	0	0	0	0	2	0
Italy	0	5	0	1	5	1	9	5	0	0	0	32	19	1	6	0	0	415	0
Latvia	0	0	0	0	0	0	0	3	0	0	0	3	7	0	0	0	0	4	0
Lithuania	0	1	0	0	0	0	0	3	0	0	0	3	8	0	1	0	0	5	1
Luxembourg	0	5	0	34	0	0	0	10	0	0	0	76	226	0	0	0	0	24	0
Netherlands	0	5	2	47	0	0	0	22	0	0	0	73	250	0	3	0,01	0	16	0
Norway	0	0	0	0	0	0	0	0	0	0	0	2	4	0	0	0	0	1	0
Poland	0	5	2	1	0	0	1	15	0	0	0	10	26	0	6	0	0	16	0
Portugal	0	0	0	0	0	0	0	0	0	0	0	7	1	0	0	0	0	1	0
Republic of Moldova	0	1	0	0	0	2	1	3	0	0	0	5	8	2	3	0	0	6	0
Romania	0	1	0	0	1	2	1	3	0	0	0	3	10	0	4	0	0	14	0
Russian Federation	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Slovakia	0	7	1	2	1	0	3	19	0	0	0	14	33	0	19	0	0	36	0
Slovenia	0	5	0	0	1	0	5	4	0	0	0	16	21	1	4	0	0	237	0
Spain	0	0	0	0	0	0	0	0	0	0	0	7	3	0	0	0	0	4	0
Sweden	0	0	0	0	0	0	0	1	0	0	0	2	10	0	0	0	0	1	0
Switzerland	0	1	0	0	0	0	1	0	0	0	0	7	14	0	1	0	0	73	0
The FYR Macedonia	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
Turkey	0	0	0	0	0	1	0	0	0	0	0	0	1	10	0	0	0	4	0
Ukraine	0	0	1	0	0	0	0	1	0	0	0	2	5	1	1	0	0	5	0
United Kingdom	0	1	0	12	0	0	0	5	0	0	0	39	63	0	1	0	0	3	0
Yugoslavia	0	1	0	0	1	1	2	4	0	0	0	3	11	0	6	0	0	22	0
Europe*	0	1	0	1	0	0	0	2	0	0	0	8	15	1	1	0	0	22	0

Country	receivers																		
	LT	LU	NL	NO	PL	PT	MD	RO	RU	SK	SI	ES	SE	CH	MK	TR	UA	GB	YU
Albania	0	0	0	0	2	0	0	3	1	1	0	2	0	0	3	5	0	2	0
Austria	0	0	1	0	9	0	0	2	1	4	1	1	0	3	0	0	3	4	1
Belarus	0	0	0	0	5	0	0	0	6	1	0	0	0	0	0	0	6	0	0
Belgium	0	2	45	1	23	0	0	3	2	4	0	14	0	10	0	0	4	63	0
Bosnia and Herzegovina	0	0	0	0	4	0	0	5	0	3	0	1	0	1	0	0	2	1	7
Bulgaria	0	0	0	0	4	0	1	30	4	2	0	0	0	0	7	9	0	3	0
Croatia	0	0	2	0	12	0	0	12	2	7	3	4	0	4	0	0	4	6	9
Czech Republic	0	0	3	0	27	0	0	4	3	12	2	1	0	4	0	0	7	8	3
Denmark	0	0	8	0	18	0	0	2	3	2	0	0	0	3	0	0	3	16	0
Estonia	0	0	0	0	3	0	0	0	1	0	0	0	0	0	0	0	0	1	0
Finland	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
France	0	0	7	0	6	2	0	1	0	1	0	34	0	4	0	0	0	14	0
Germany	0	0	13	0	24	0	0	2	2	6	1	5	0	9	0	0	4	24	0
Greece	0	0	0	0	2	0	1	13	9	1	0	2	0	0	0	58	16	1	3
Hungary	0	0	2	0	28	0	0	17	3	17	2	4	0	4	0	0	10	7	12
Ireland	0	0	5	0	3	0	0	0	0	0	1	0	1	0	0	1	34	0	0
Italy	0	0	1	0	9	0	0	8	1	5	4	9	0	5	0	1	3	4	7
Latvia	0	0	0	0	8	0	0	0	2	1	0	0	0	0	0	1	1	0	0
Lithuania	0	0	0	0	15	0	0	1	1	2	0	0	0	0	0	0	1	0	0
Luxembourg	0	4	17	0	14	0	0	1	0	2	0	8	0	13	0	0	1	14	0
Netherlands	0	2	54	0	31	0	1	4	3	6	0	12	0	5	0	0	9	68	0
Norway	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	3	0
Poland	0	0	2	0	48	0	0	4	4	11	0	1	0	2	0	0	7	3	2
Portugal	0	0	0	0	0	241	0	0	0	0	0	256	0	0	0	0	0	3	0
Republic of Moldova	0	0	0	0	6	0	3	21	2	3	0	0	0	0	0	9	6	3	2
Romania	0	0	1	0	7	0	1	35	1	4	0	0	0	1	0	3	7	1	5
Russian Federation	0	0	0	0	0	0	0	0	8	0	0	0	0	0	0	0	5	0	0
Slovakia	0	0	3	0	37	0	0	8	3	23	1	3	0	3	0	0	11	9	5
Slovenia	0	0	1	0	12	0	0	6	1	5	5	5	0	5	0	1	4	3	2
Spain	0	0	0	0	0	33	0	0	0	0	0	182	0	0	0	0	0	2	0
Sweden	0	0	1	0	3	0	0	0	1	0	0	0	0	0	0	0	0	1	0
Switzerland	0	0	0	0	1	0	0	0	0	0	1	0	0	4	0	0	0	0	0
The FYR Macedonia	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	3	0	0
Turkey	0	0	0	0	1	0	0	5	10	0	0	0	0	0	0	250	12	0	0
Ukraine	0	0	0	0	4	0	1	7	15	1	0	0	0	0	0	6	41	1	1
United Kingdom	0	0	16	0	9	0	0	2	1	1	0	2	0	2	0	0	3	90	0
Yugoslavia	0	0	0	0	7	0	0	13	0	4	0	0	0	0	0	0	3	1	12
Europe*	0	0	1	0	5	4	0	3	6	1	0	14	0	1	0	15	6	5	1

Units: ppb.h per 40% emission reduction; * Average over all land-areas of Europe

7.2 References

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Chapter 8

Towards a modular CTM system for EMEP

David Simpson and Steffen Unger

8.1 Introduction:

The modelling tools available at EMEP MSC-W consist of two main Eulerian models, the acidification model (MADE) of Berge and Jakobsen (1998), Olendrzyński (1997) and the oxidant model (MACHO) of Jonson et al. (1997,1998). The acidification model now uses the 3-hourly resolution meteorological data of Tsyro and Støren (1999), whereas the oxidant model uses 6-hourly data.

The acidification model has recently been extended to include primary aerosol emissions and transport (Tsyro and Erdman, 2000), and a new aerosol module which includes secondary formation and dynamics is under development. Schemes for including secondary organic aerosol formation have been developed and applied for the Lagrangian oxidant model (Andersson-Sköld and Simpson, 2000). And finally, an offline deposition module for ozone (see chapter 2) is under development, which although intended for ozone bears many resemblances to the deposition scheme used in the acidification models. Merging these two deposition approaches into one scheme suitable for all models is therefore practical in the near future.

With all these different models and future possibilities, there is a clear need for a more modular approach within the EMEP modelling system. Ideally there would be one core model, which can optionally run different chemical schemes and/or aerosol modules. Such a system would greatly ease the maintenance of the current models and would significantly ease any future changes to such models.

Such a modular system is now under construction. Although this new model system still requires a substantial effort to complete, this work is well under-way and preliminary model versions should be available by the end of year 2000. We here outline the approach taken and discuss the type of system envisaged for the new EMEP models.

8.2 Approach

The program codes of the two Eulerian models were carefully examined to identify similar and different features. A preliminary "common" model was built where both models were available from the same directory, with as many already-common subroutines as possible, but with a large number of other subroutines specific to either MADE or MACHO. Either MADE or MACHO can be built ("made") from within this directory through the use of a common Makefile. At this stage the code for the common modelling system is substantially more complex than that of the individual models (Stage B, fig. 8.1), but at least all of the code is located in one place and similarities and differences clearly identified.

Starting from this stage B mixture, work has proceeded to identify which differences are fundamental to the different models, and which can be overcome with re-coding for a more flexible structure. For example, many subroutines to handle the meteorology were already

Stage A	<u>MADE</u>		<u>MACHO</u>	
	sub1		sub1	
	sub2		sub2	
	sub3		sub3	
	... subN		... subN	
Stage B	<u>Common directory</u>			
	sub1_MADE		sub1_MACHO	
	sub3_MADE		sub3_MACHO	
	subN_MADE		subN_MACHO	
	sub2 sub4 ...			
Stage C	<u>Modular structure</u>			
	User-supplied		<u>CORE routines</u>	
	model_def		Advection+meteorology	
	aerosol_def		Chemical solver	
	chemistry_def		Emissions	

Table 8.1: Illustration of the 3 stages of model development. Starting from separate models in Stage A, a common directory has been established in Stage B. The subroutines are then re-written in Stage C to those modules (CORE routines) common to all model versions, and some smaller user-supplied routines to specify details

very similar in the two codes, and only minor changes were needed to unify these routines. Similarly, the MADE model has advection for just the main chemical species, whereas MACHO also advected air density as a check on the numerical advection schemes. Such differences are easily removed by defining the start and end indices of species/components to advect. The advection routines themselves need know nothing of the species to be used.

Even apparently fundamental differences can hopefully be resolved. For example, the oxidant model has arrays which store the speciation of VOC emissions, such that an input total VOC amount is split into say six different hydrocarbon species, with this split depending on the emission sector and time of year. The acidification model has no such complex speciations, with only simple splits of SO_x emissions into SO₂ and SO₄, and of NO_x into NO and NO₂. However, this apparent difference is easily resolved by the introduction of an array NEMIS_SPLIT, which gives the number of speciations for each emission input. Thus NEMIS_SPLIT(SO_x) = 1, whereas NEMIS_SPLIT(NMVOC) = 6 for example. By introducing this new array the acidification version becomes slightly more complicated, but is now identical to the ozone version. The introduction of particulates is at the same time a trivial exercise. If we wish to split our input PM_{2.5} emissions into, say, EC (elemental carbon), ORG (organics) and INORG (inorganics), we simply set NEMIS_SPLIT(PM_{2.5}) = 3.

Other differences have arisen for historical reasons, as different workers have modified different codes. Thus, the deposition routines are very different in the current models, with the oxidant model using a drag-coefficient approach for the whole grid-square (Berge and Jakobsen, 1998) whereas the acidification model uses a sub-grid treatment as discussed in Jakobsen et al. (1996) and Olendrzyński (1997). In future it is hoped that a modular approach will allow either level

of complexity, although the sub-grid treatments for ozone and acidifying compounds can be made almost identical by combining the different sub-grid approaches.

Whilst converting the above codes, we are also taking to opportunity to introduce much more FORTRAN'90, replacing the FORTRAN'77 in which most of the model is written. FORTRAN'90 has superior array-handling abilities, and is specifically designed to enable modular program design. This change will result in a virtual elimination of error-prone 'common blocks' and lead to more compact and more structured code.

The chemical scheme will hopefully be written as chemical equations (rather than as differential equations or Jacobian), and pre-processed to FORTRAN code with scripts written in *Perl* which are currently under development (indeed, one version of the Lagrangian oxidant model is already chemically-blind as far as the ozone/SOA chemistry is concerned. Changing the chemistry can often be done with just some minutes work).

The final model is expected to look something like the stage C in Figure 8.1. Details required to define the model (number of advected and non-advected species, emission to be used, inclusion of aerosols etc., will be specified in a "model definition" module. The rest of the code should not need to know whether it is to run acidification chemistry, ozone, aerosol, or indeed any combination of the above, as long as the equations can be written for the chemical pre-processor and the appropriate modules (e.g. for aerosols) are linked in as desired at compile-time. This final system should greatly ease future maintenance and improvements to the EMEP model system.

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Chapter 9

Conclusions and outlook

This summary report for photochemical oxidants has covered a number of topics related to the Lagrangian and Eulerian photo-oxidant models, measurements of ozone and VOC, and evaluation. In general, work in 1999-2000 has concentrated on new developments with the two models, and these are still in progress. Thus the forthcoming version of the EMEP models will contain new deposition and particle modules, new chemistry, and in general will have a much more modular and flexible structure to ease future usage.

Some of the main conclusions to be drawn from this report are:

- The requirements of the critical-levels community for oxidant models which can predict stomatal fluxes as well as concentrations are well on the way to being met. Despite conceptual and practical difficulties in implementing such a scheme, the resulting model predictions should be much more useful for so-called level II mapping and for vegetation-damage assessments in future.
- A number of modern isoprene chemical schemes have been found to give results for ozone which are similar, but show some scatter in high-NO_x conditions. It should be possible to construct a scheme for both oxidant models which is mid-way in complexity between the current Eulerian and Lagrangian schemes, but still consistent with modern state-of-the-art mechanisms. These schemes need to be checked for their consistency with respect to compounds such as HCHO though, see below.
- The problems found in last year's model predictions of the Eulerian model with respect to carbonyls, as compared to observations, have been largely solved. Addition of dry and wet deposition for HCHO has greatly improved the performance of the model. The Lagrangian and Eulerian models are now much more similar in their predictions of HCHO, although the Lagrangian model still shows a better correlation with the measurements than the Eulerian model. One possible reason for this may be the different isoprene schemes, as work elsewhere (Solberg et al., 2000) has shown that HCHO concentrations are very sensitive to this species.
- Comparison of the model's performance against formaldehyde measurements has been done on a transport-sector basis. This comparison showed that the models perform reasonably well in most situations, although for some sectors the Eulerian model was superior whereas for others it was the Lagrangian model. This type of analysis needs to be extended to draw further conclusions, but is a promising way of testing the models and their emission inputs.
- The long-term variations in surface ozone was studied by kriged maps of 99-percentiles of hourly ozone monitoring values for 1989-1998. The maps show large inter-annual variations, and it is not possible to identify any clear trends based on these maps alone. The kriged maps clearly shows the importance of increasing the number of ozone monitoring sites, both to get a better regional cover and also to reduce the uncertainty in the interpolated fields. It is quite clear that an evaluation of model results and monitoring data in close combination is needed to make a fruitful trend study of ozone.

- The importance of sea salt and sodium nitrate particles has been tested within the Eulerian oxidant model. The results show that inclusion of NaNO_3 leads to an increase in calculated total nitrate at all locations, but this still does not solve a problem with under-prediction of nitrate at remote sites. Other explanations for the deficit of total nitrate at remote locations should be sought.
- An updated set of source-receptor relationships was presented, calculated with the Lagrangian model for year 2010 emissions and five years of meteorology.
- A major re-write of the Eulerian model codes is underway. The aim is to build a modular system with a set of core subroutines for all Eulerian models, and as few chemistry- and model- specific routines as possible.

As noted last year, the measurements of carbonyls and hydrocarbons available within EMEP have proven extremely valuable in evaluating both the models and the emission inventories. It is recommended that such measurements continue and if possible be enhanced with other key-species for evaluating photochemical models, for example NO_y constituents and radical concentrations.

The 3-D model has much greater potential for evaluating measurements than the Lagrangian model, because of its much greater vertical and horizontal resolution. The model is particularly useful for dealing with pollutants which are known to have large vertical gradients much of the time (e.g. NO_2). Serious gaps in the measured species do exist, however, and efforts should be made to make use of data available from other activities, for example EUROTRAC or national programmes. By actively pursuing such comparisons both the model and its inputs (emissions, land-use) can be continuously evaluated and improved.

With the new flexible model system under development, it is anticipated that the addition of inorganic and inorganic aerosol modules will be possible in the near future.

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Appendices

Appendix A

Overview by Country

This Appendix presents brief country-by-country information on emission submissions, measurements of ozone and VOC, and on source-receptor calculations associated with each country. Two pages of information are presented for each country, consisting of:

Histogram plot - emissions - illustrates the data officially submitted for NO_x , NMVOC and CO. See Vestreng and Støren (2000) for more details. *Contact: egil.storen@dnmi.no*

Table - measurement overview - gives the number of ozone, hydrocarbon and aldehyde/carbonyl stations for that country. An assessment of the quality of the ozone data has been introduced. For more details of sites, sampling and quality terms see chapter 5. *Contact: Sverre.Solberg@nilu.no*

Pie chart - AOT40 Contributions to/from countries - see below. *Contact: david.simpson@ivl.se*

The pie charts probably require most explanation. These are derived from the country-to-country calculations (see chapter 7, The "Contrib. from" pie chart shows the countries and emissions most responsible for AOT40c changes in that country. The "Contrib. to" pie chart shows the effect of that country's emissions on other countries. The 5 biggest contributions in both cases are shown explicitly, with the remaining contributions to or from all other countries summed as REM:NO_x, REM:VOC (import) or NO_x:REM; VOC:REM (export). Note that in producing these pie charts only emission contributions which lead to ozone decreases were counted. Thus the 'negative' effects associated with NO_x emissions from some countries were excluded. The two-letter country-codes used in these charts have been given in chapter 7. Note that these pie charts show only relative contributions as modelled with the procedures discussed in chapter 7. Ozone over each country has also large contributions from background tropospheric ozone, not reflected here.

Taking Austria as an example, the biggest single country contribution to imports is from IT-VOC; i.e. VOC emissions from Italy. The number given (in this case 272) is the average change in AOT40_c (in ppb.h) over Austria caused by a 40% reduction in the Italy's VOC emissions. These numbers are identical to those presented in the source-receptor tables of chapter 7.

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