SPACCIM: Simulations of the multiphase chemistry occurring in the FEBUKO hill cap cloud experiments

A. Tilgner, Z. Majdik, A.M. Sehili, M. Simmel, R. Wolke and H. Herrmann*

Leibniz-Institut für Troposphärenforschung, Permoserstr. 15, D-04303 Leipzig, Germany

ELECTRONIC SUPPLEMENTARY MATERIAL (ESM)

*corresponding author. tel.: +49-341-2352446; fax: +49 341 235-2325; e-mail: herrmann@tropos.de

A. Material to the chapter : “model initialisation”

The chemical composition of the gas and aerosol phase was measured in FEBUKO with a high analytical work (cp. Gnauk et al., 2005; Müller et al., 2005; Brüggemann et al., 2005; van Pinxteren et al., 2005) at all three sites. The most part of the gas phase initial concentrations are due to the upwind site measurements, implemented with 15-min average for time resolved measured species such as SO_2 according to a realistic transport times between upwind and summit (cp. Heinold et al., 2005) or with the nearest measurement for non-continuously measured species. In the case of the not measured as well as relatively constant species the initial concentration were taken from the urban scenario of the CAPRAM model (cp. Ervens et al., 2003) according to the typical concentration levels of other tracer gases observed during FEBUKO. The concentrations of included lumped RACM species such as ALD (acetaldehyde and higher aldehydes) were derived from a summation of all measured associated gas phase species. The derived gas phase compositions of the three pre-selected cloud events are given in the appendix (Table A I-III) including comments to data implementation and the associated list of references.

In contrast to, the implementation of the initial gas phase concentrations the chemical initialisation of the aerosol composition was much more complex. Because of the size-dependent chemical composition of aerosols particles and accordingly cloud droplets, the aerosol initialisation is based on the size resolved experimental data of the 5-stage Berner impactor. But additionally, also integral values of High-Volume Sierra Anderson filter sampler as well as steamjet measurements were used for a complete as possible model input. The explicit description of the chemical input aerosol generation is given in Table I.

Table I: Description to the initialisation of the upwind aerosol composition.

Aerosol compound	Comments
WSOC (water soluble organic mass)	Calculated from the impactor organic carbon mass measurements; the mass conversion from organic carbon mass to the total organic mass, due to the mass contributions of other constituents such as hydrogen and oxygen atoms, were calculated for an altered urban aerosol after Turpin et al. (2001); the separation between soluble and insoluble organic mass based on estimated mass ratios (Gnauk; 2004); due to the separate implementation of the dicarboxylic acids the mass of the WSOC was reduced accordingly [mass ratio (WSOC/WISOC)= 40%/60%; mass correction factor WSOC/WISOC=2.1/1.3]
WISOC (water insoluble organic mass)	
Elemental carbon	Measured impactor values
Nitrate	Based on steamjet measurements distributed over size according to impactor results (caused by the assumed impactor mass losses during sampling (Gnauk et al., 2005)); to correct the steamjet values for particles larger than 10 µm; the steamjet value was reduced by the percentage difference of sulphate mass between steamjet and impactor
Chloride	
Nitrite	Based on steamjet measurements; the value was distributed over size according to the total impactor stage mass ratios
Sulphate	Measured impactor values
Ammonium	
Sodium	
Potassium	

Magnesium	
Calcium	
Aluminium	
Zinc	
Iron	Water souluble part of the High-volume ANDERSON filter sampler (PM_{10}) values distributed over size according to the total impactor mass ratios
Manganese	
Copper	
Oxalate	Mean between the impactor and spray sampler measurements (the spray sampler value was distributed over size according to the impactor stage oxalate mass ratios)
Malonate	
Succinate	spray sampler value distributed over size according to the (Succinate+Isomers) impactor stage ratios
Succinate Isomers	Impactor values (Succinate+Isomers) reduced by the succinate value (above)
Glutarate	spray sampler value distributed over size according to the (Glutarate+Isomers) impactor stage ratios
Glutarate Isomers	Impactor values (Glutarate+Isomers) reduced by the glutarate value (above)
Tatronate	Measured impactor values
Malate	
Tatrate	
Citramalate	
Maleinate	
Suberate	spray sampler value distributed over size according to the total impactor mass ratios
Acelate	
Unknown residual mass	Calculated from the difference of the determined (uncorrected) and total dry impactor mass for each stage; the total dry mass was calculated using an aerosol density of 1.6 g cm^{-3} and growth factors for each impactor stage (Neusüß et al., 2000), an explicit description of the mass ratios is given in Gnauk et al. (2005) including the used calculation formulas

The finally derived chemical particle composition of the three pre-selected cloud events can be found in the appendix (Table A IV-VI). Figure I illustrates exemplarily for all three cloud events the resultant chemical aerosol particle composition of E I. The initial concentrations of the particle compounds are calculated in the model form the aerosol distribution (cp. next subchapter) and the associated impactor stage mass ratios. Additionally, the size resolved soluble particle fraction ε is an important initial parameter in the microphysical model (Simmel et al., 2005) in order to a correct nucleation description.

The physical model initialisation based mainly on the measurements of the upwind site Goldlauter. The used aerosol number concentrations for the three cloud event were derived from fits (three-parameter lognormal distributions) of the observed Twin Differential Mobility Particle Sizer (T-DMPS) measurements (Gnauk et al., 2005). The T-DMPS system detect particles in the size range of about 3-900 nm. However, Berner impactor samplings indicate also substantial mass contributions (up to about 30 % of the total mass) of aerosol particles at sizes larger than 900 nm. To compensate this deficit an additional coarse mode had to be generated which contains the mass contribution of the last two impactor stages. Exemplarily for all three treated cloud events, Figure I illustrates the resultant aerosol particle number concentration fit for the cloud event EI including the generated coarse mode. The associated parameters of the lognormal distributions are given in Table II.

Table II: Parameters of the used lognormal distributions for the three treated cloud events.

Event1	Particle mode	N	D	σ
E I	1	182.0	7.9	1.33
	2	5078.7	68.2	1.87
	3	535.3	335.5	1.39
	Coarse mode	1.3	1250.0	1.50
E II	1	1873.8	57.8	1.92
	2	481.7	228.0	1.52
	Coarse mode	0.30	1400.0	1.60
E III	1	430.7	15.2	1.30
	2	2696.4	34.0	1.63
	3	1186.3	162.5	1.52
	Coarse mode	0.7	1350.0	1.55

Particularly, with regard to aerosol constituents which can be found in larger particles, the cloud water concentrations would be underestimated without the added coarse mode mass contribution. Afterwards, performed comparisons between the total gravimetric determined impactor mass as well the integrated mass from T-DMPS spectra showed a good concurrence. The relative fulfilled mass closure was a strong quality criterion and the base for realistic comparisons between model results and observations especially in the cloud.

In addition to the aerosol initialisation also meteorological parameters had to be initialized for realistic as possible model conditions. Particularly, a reasonable implementation of the radiation conditions during the cloud passage was an essential aspect of the physical initialisation due to the control of the tropospheric radical chemistry and the resulting oxidation potential. At upwind site, a (4π sr) radiometer was used to measure the $j(NO_2)$ photolysis rate (Herrmann et al., 2005). The photolysis rates were calculated in the ordinary chemistry module in terms of clear sky conditions for the respective geographic position, date and time. For FEBUKO scenarios the photolysis rates had to be scaled according to the reduced radiation under capped cloud conditions. For this purpose, all calculated clear-sky photolysis rates were reduced by a scaling factor which were determined from the measured $j(NO_2)$ and the modelled $j(NO_2)$ for clear sky conditions so that the model conditions corresponds approximately the real value.

The dynamical flow conditions were initialised, like mentioned above, mainly with the measured data. The disadvantageous valley location for wind measurements at upwind site resulted in relatively inaccurate wind data so that other data had to be used. Therefore, the wind speed at upwind site was initialised using data from the meteorological observations of the German weather service (DWD) at the station Meiningen (30 km to the south-west of upwind site). In contrast to upwind site, at summit and downwind site measured flow conditions were used as input for the model. All other meteorological data needed by the adiabatic parcel model such as temperature and pressure are based on weather observations of the three measurement stations and were initialised for the selected modelling times by means of 15 min averages.

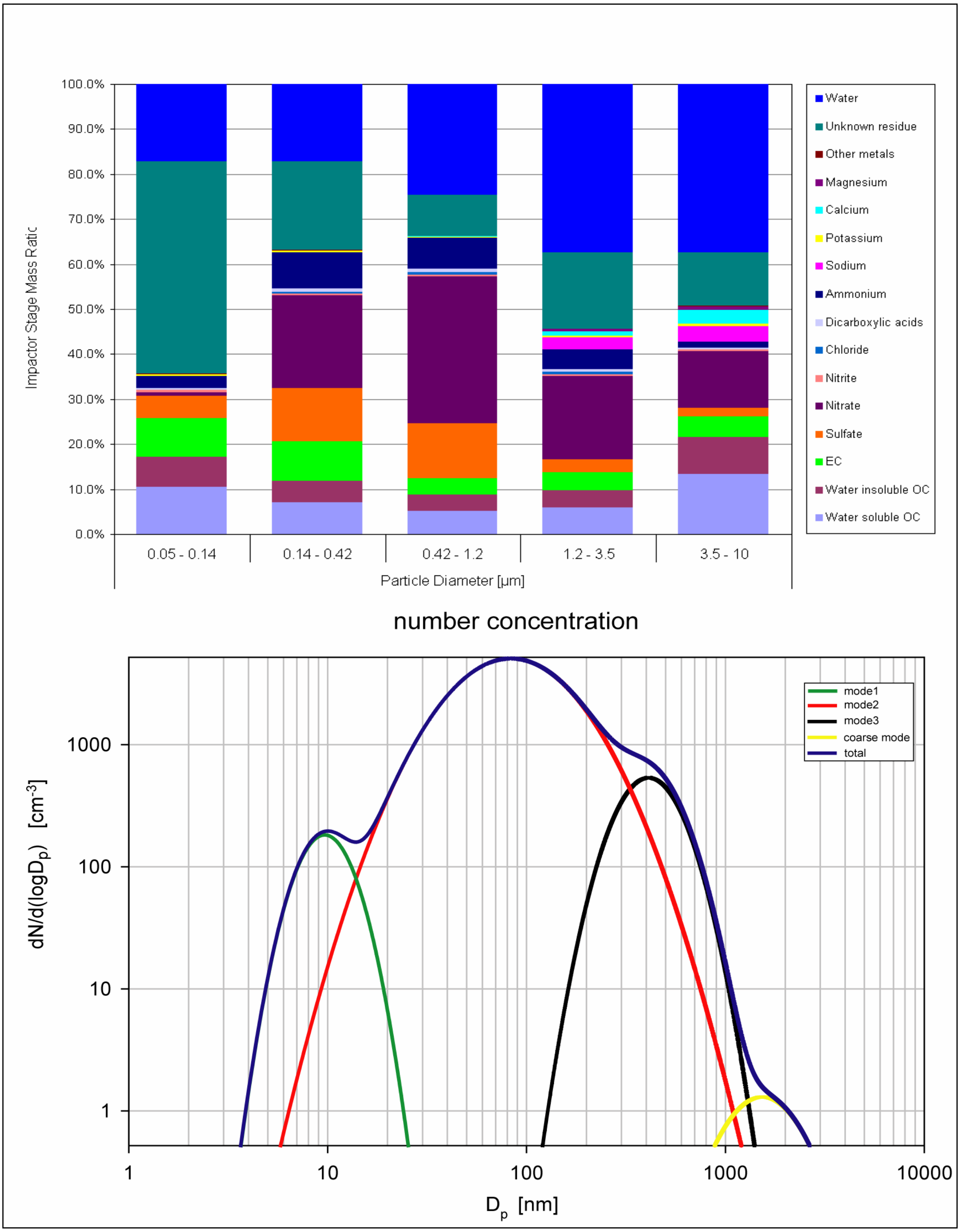


Fig. I: Chemical composition of the wet aerosol based on the Berner impactor distribution (left) and fit of the associated measured particle number concentration including the estimated coarse mode (right) for the cloud event EI.

B. Material to the chapter: "results and discussion"

1. Microphysical conditions and pH

The comparison between the model results and measured microphysical data for all treated cloud events shows that the adiabatically calculated liquid water content was overestimated in the most cases as discussed by Simmel et al. (2005). The fast transport including high vertical velocities produce a high peak in the supersaturation so that more and smaller droplets can be activated. Therefore, the microphysical model tends to result in a narrower modelled droplet spectrum than the measured one. The causes of the deviations between modelled and measured conditions are discussed extensively by Simmel et al. (2005). However, the microphysical model describes the conditions in an orographic cloud well enough to drive the multiphase chemistry in the coupled model SPACCIM.

Figure II shows the predicted temporal evolution of mean radius and LWC for all size bins of the particle/droplet spectra during the cloud passage for the three treated cloud events. As can be seen from Figure II the transport of the air parcel takes about 23 minutes from upwind to downwind site at E I as well as 21 and 16 minutes for E II and E III, respectively. The difference is caused by the different flow conditions at each cloud event. The droplet activation occurs at about 325 s (E I), 330 s (E II) and 325 s (E III). Consequently, droplets larger than the activation diameter of about 180 nm (E I), 120 nm (E II) and 90 nm (E III) are activated to cloud droplets with a huge increase of the mean diameter especially within the first 100 s due to the peak of the supersaturation. Therefore, an interstitial aerosol spectrum as well as a cloud droplet spectrum arises from the relatively uniform deliquescent aerosol spectra. The LWC predicted by the model follows the mean diameter as well the corresponding number concentration and reach the total maximum value of about 0.52 g m^{-3} at the summit (E II: 0.45 g m^{-3}, E III: 0.21 g m^{-3}). Characteristic for microphysical model, the observed value is about 20 % below the predicted value of the model at summit site (E II: 40 %, E III: 0 % g m^{-3}). After the summit passage, the total LWC decreases in relation to the descent in the lee of the mountain and the following cloud evaporation. The small droplets evaporate earlier due to the higher required supersaturation in the cloud. The in-cloud residence time of the air parcel which is decisive for the duration of effective multiphase cloud processes, differs between E I with about 980 s as well as 550 s and 280 s for E II and E III, respectively. As a result of the longer travelling and in-cloud times as well as the bigger droplets, it can be assumed that also depositions might be more efficient for the cloud event E I than for E II and especially for E III. This fact is important for the subsequent comparison between model results and measurements.

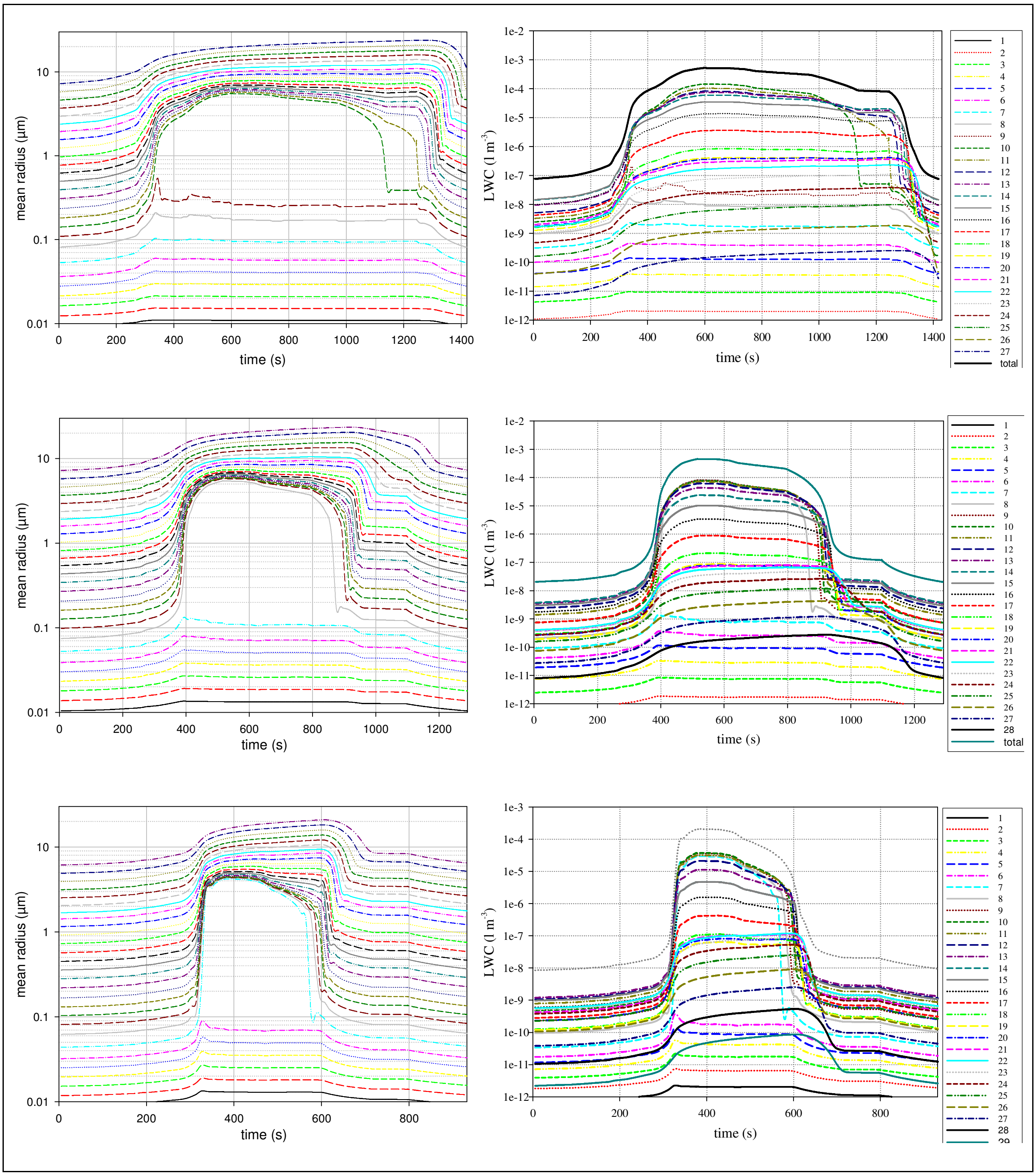


Fig. II: Mean radius and LWC of each size bin for the cloud event E I as a function of transfer time from the upwind site to downwind site.

The pH-value is the one of the most important aqueous phase process control parameter which is mainly affected by the microphysical processes as well as the initial aerosol composition and uptake processes of gaseous acids or bases. Within the SPACCIM model the H^+ concentration is initialised by a charge balance and calculated dynamically over the whole simulation time. Figure III illustrates the pH-value in each size bin as a function of the transport time for the cloud event E I. As can be seen from the plot, within the first 100 s the pH-value is characterised by transient effects. These effects are caused particularly by the adjustment of the equilibriums of soluble species between the gas phase and the aqueous phase depending on the current pH. For this reason, the first 100 s of the simulation time will not be considered in much detail in the analysis of the model results. Additionally, it can be seen from Figure III that the pH-value shows huge variations over the size bin spectra. This fact is caused like mentioned above mainly by the size depended aerosol composition. The pH is generally higher before the droplet activation than after the cloud evaporation. This increase in the acidity of the particles is a direct consequence of multiphase cloud processing which will be discussed in the following subchapters. The comparison between the modelled and the measured pH-value at the summit implicate that the model reproduce the observed values relatively well (cp. Table III).

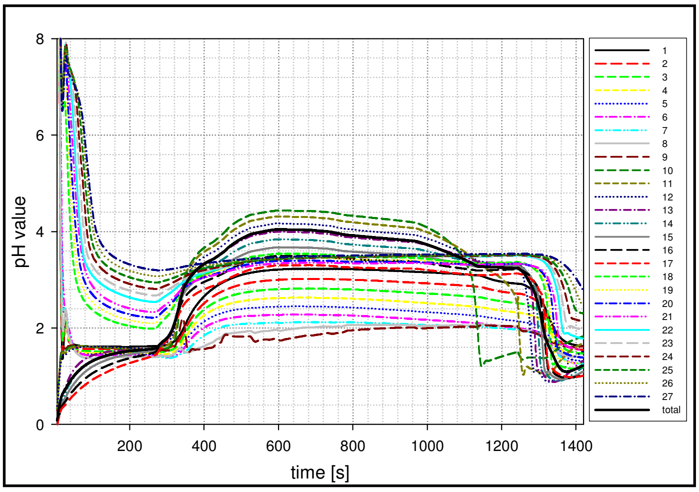


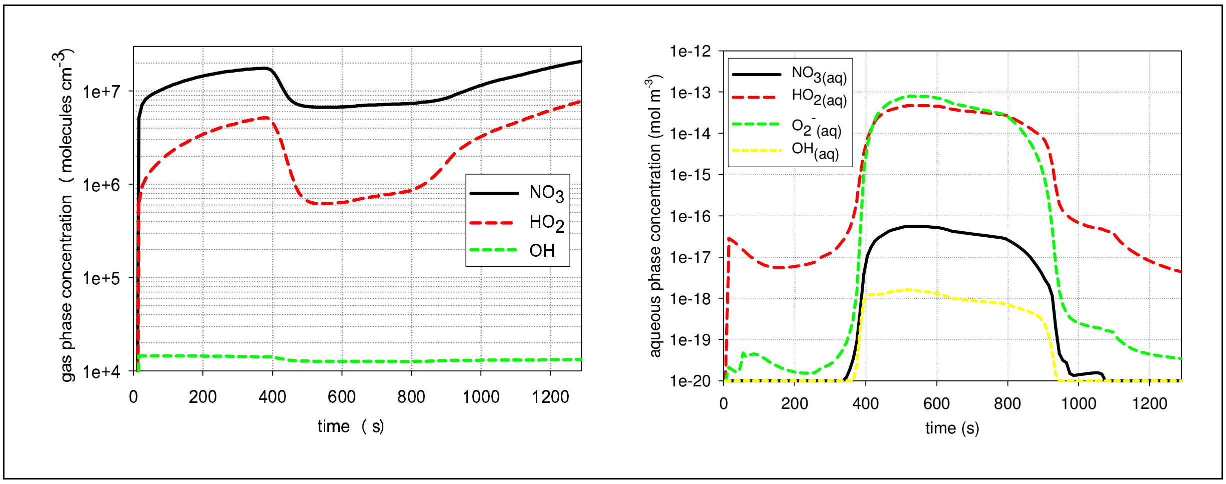
Fig. III: pH-value of each size bin for the cloud event E I as a function of transfer time from the upwind site to downwind site.

Table III: Comparison between measured and modelled pH-values at the summit.

pH-value / Cloud event	measured	modelled
E I	4.2	4.05
E II	4.8	4.82
E III	4.4	4.42

2. Oxidants

Radical oxidants



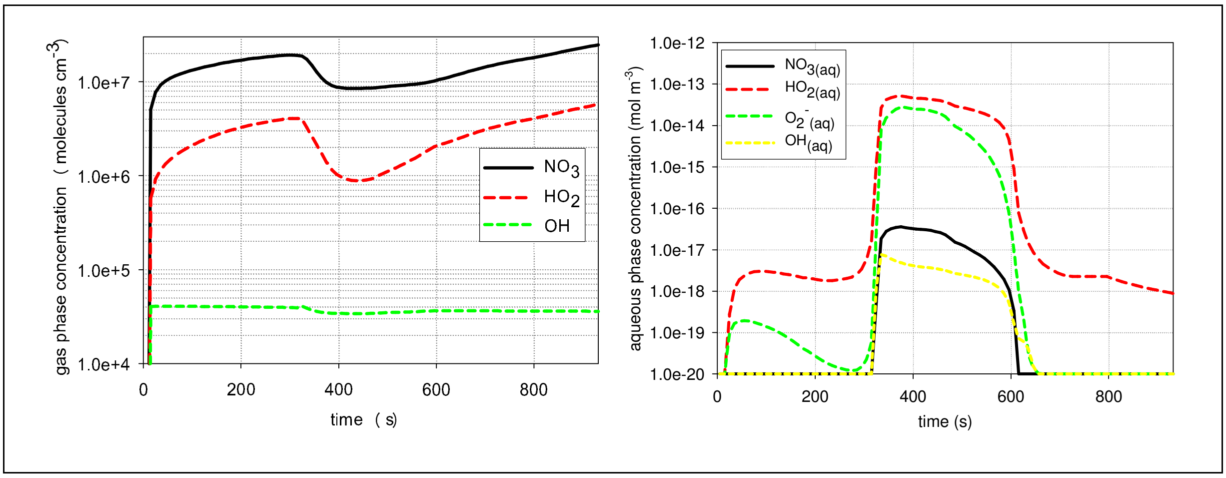
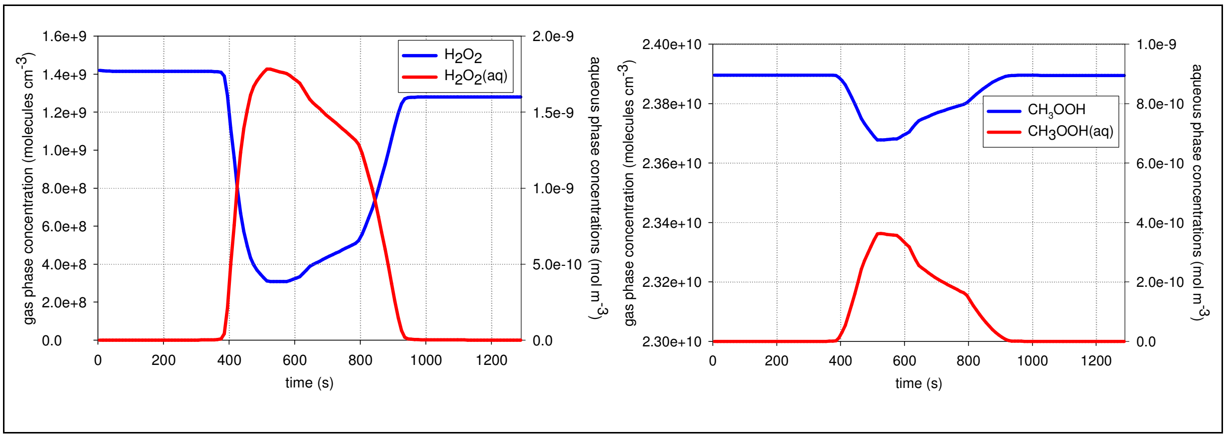


Fig. IV: Gas and aqueous phase concentration of the radicals OH, $HO_2(/O_2^-)$ and NO_3 as function of the travelling time for the cloud event E II(above) and E III(below).

Table IV: Percentage difference of oxidant gas phase concentrations between cloud-free and in-cloud conditions, and phase partitioning coefficient ε ($\varepsilon = \dfrac{c_{aq}}{c_{aq} + c_g}$; cp. Herrmann et al., 2000) at the summit for the three treated cloud events.

Oxidant	E I		E II		E III	
	Percentage decrease	Partitioning coefficient ε at the summit	Percentage decrease	Partitioning coefficient ε at the summit	Percentage decrease	Partitioning coefficient ε at the summit
OH	-44 %	$1.7 \cdot 10^{-5}$	-11 %	$7.7 \cdot 10^{-5}$	-12 %	$8.4 \cdot 10^{-5}$
HO_2	-73 %	$2.2 \cdot 10^{-1}$	-88 %	$1.1 \cdot 10^{-1}$	-67 %	$3.4 \cdot 10^{-2}$
NO_3	-28 %	$6.0 \cdot 10^{-6}$	-61 %	$5.0 \cdot 10^{-6}$	-49 %	$2.2 \cdot 10^{-6}$
H_2O_2	-87 %	$8.4 \cdot 10^{-1}$	-78 %	$7.7 \cdot 10^{-1}$	-65 %	$6.4 \cdot 10^{-1}$
O_3	< -1 %	$2.3 \cdot 10^{-7}$	< -1 %	$1.8 \cdot 10^{-7}$	< -1 %	$8.7 \cdot 10^{-8}$
CH_3OOH	-1 %	$1.3 \cdot 10^{-2}$	-1 %	$9.1 \cdot 10^{-3}$	-1 %	$4.7 \cdot 10^{-3}$

Non-radical oxidants



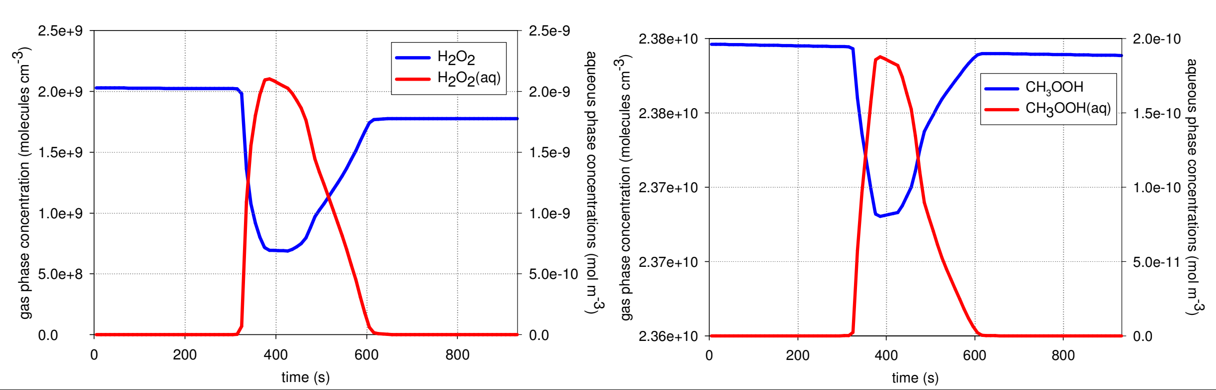


Fig. V: Gas and aqueous phase concentration of the peroxides H_2O_2 (left) and CH_3OOH (right) as function of the travelling time for the cloud event E II(above) and E III (below).

3. Sulphur chemistry

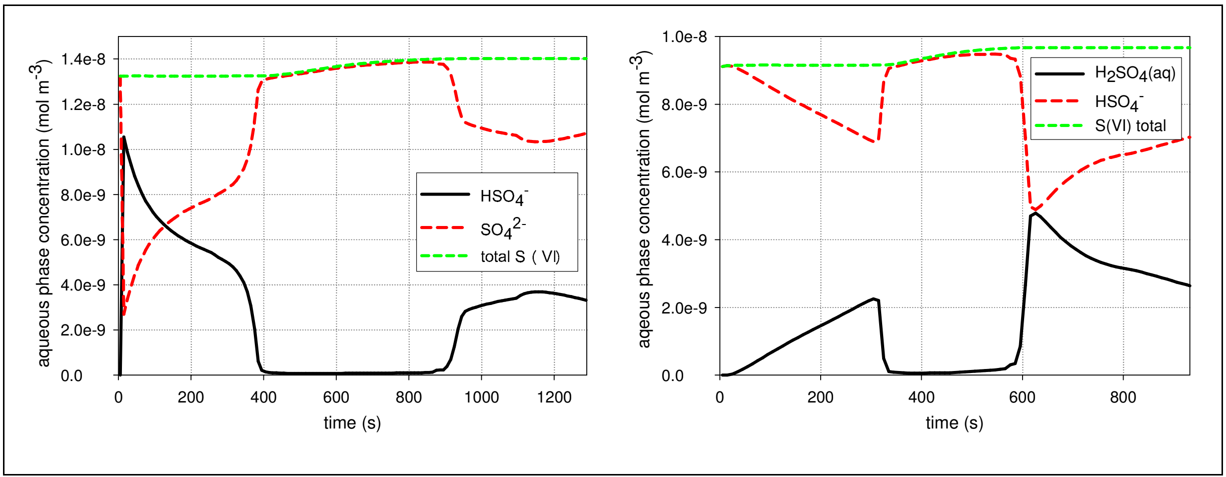


Fig. VI: S(VI) species and total S(VI) as function of the travelling time for the cloud event E II (left) and E III (right).

4. Mass production by aerosol cloud processing

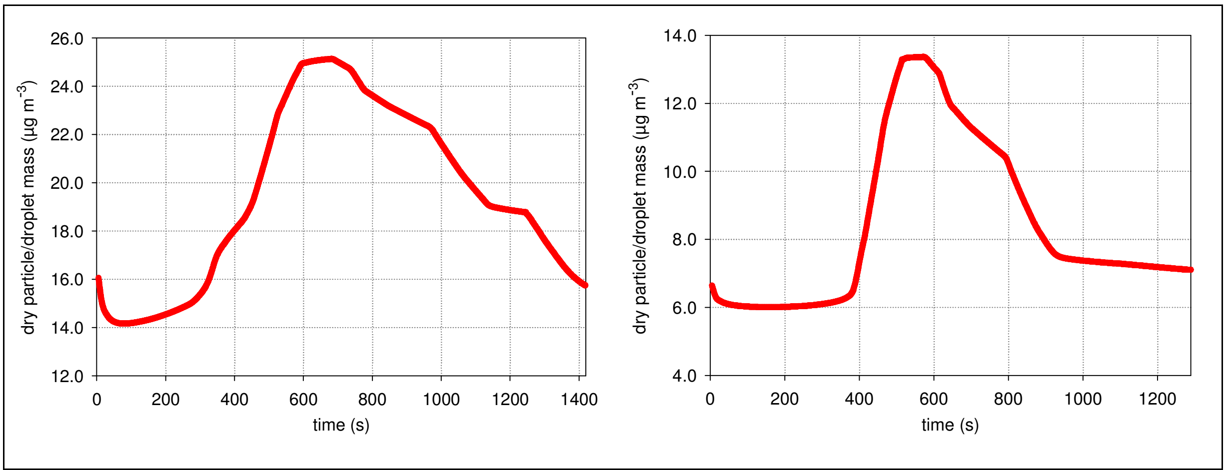


Fig. VII: Total dry condensed non-water mass as function of the travelling time for E I (left) and E II (right).

C. Material to the chapter: “Comparison between measurements and model results”

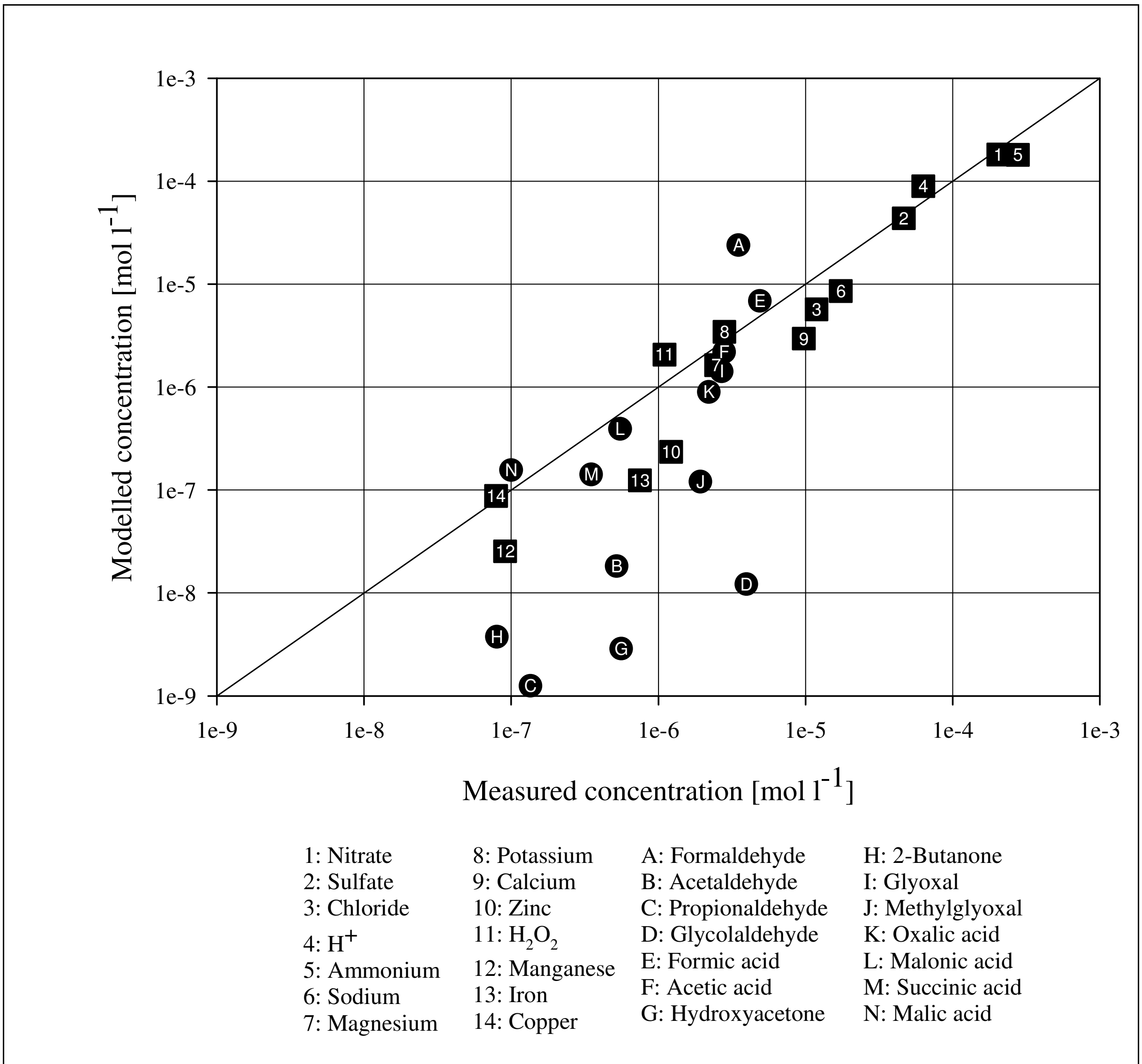


Fig. VIII: Comparison between the measured and modelled cloud water concentrations (mol l^{-1}) at the summit for the cloud event E I.

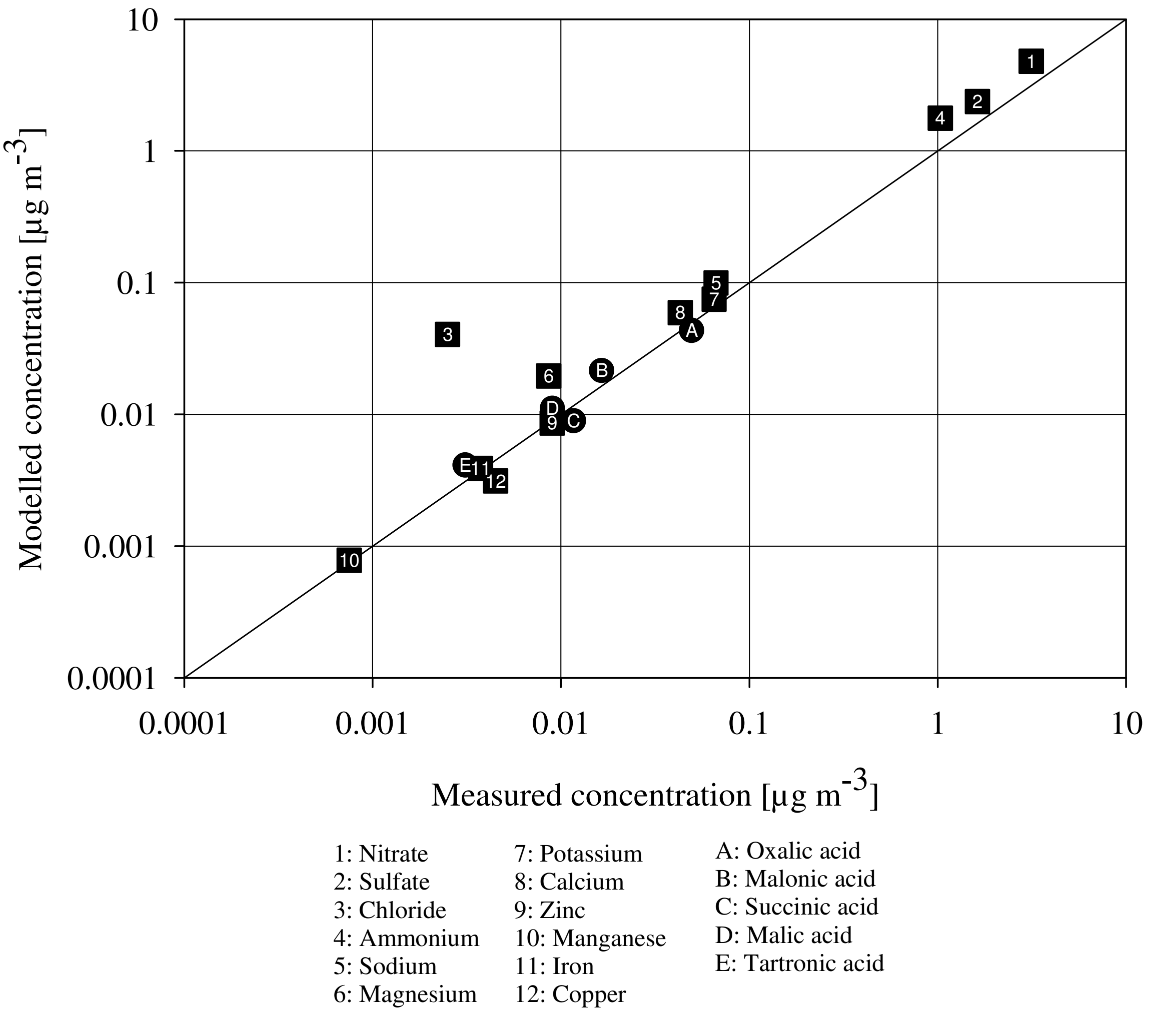


Fig. IX: Comparison between the measured and modelled aerosol particle concentrations (µg m^{-3}) at the downwind site for the cloud event E I.

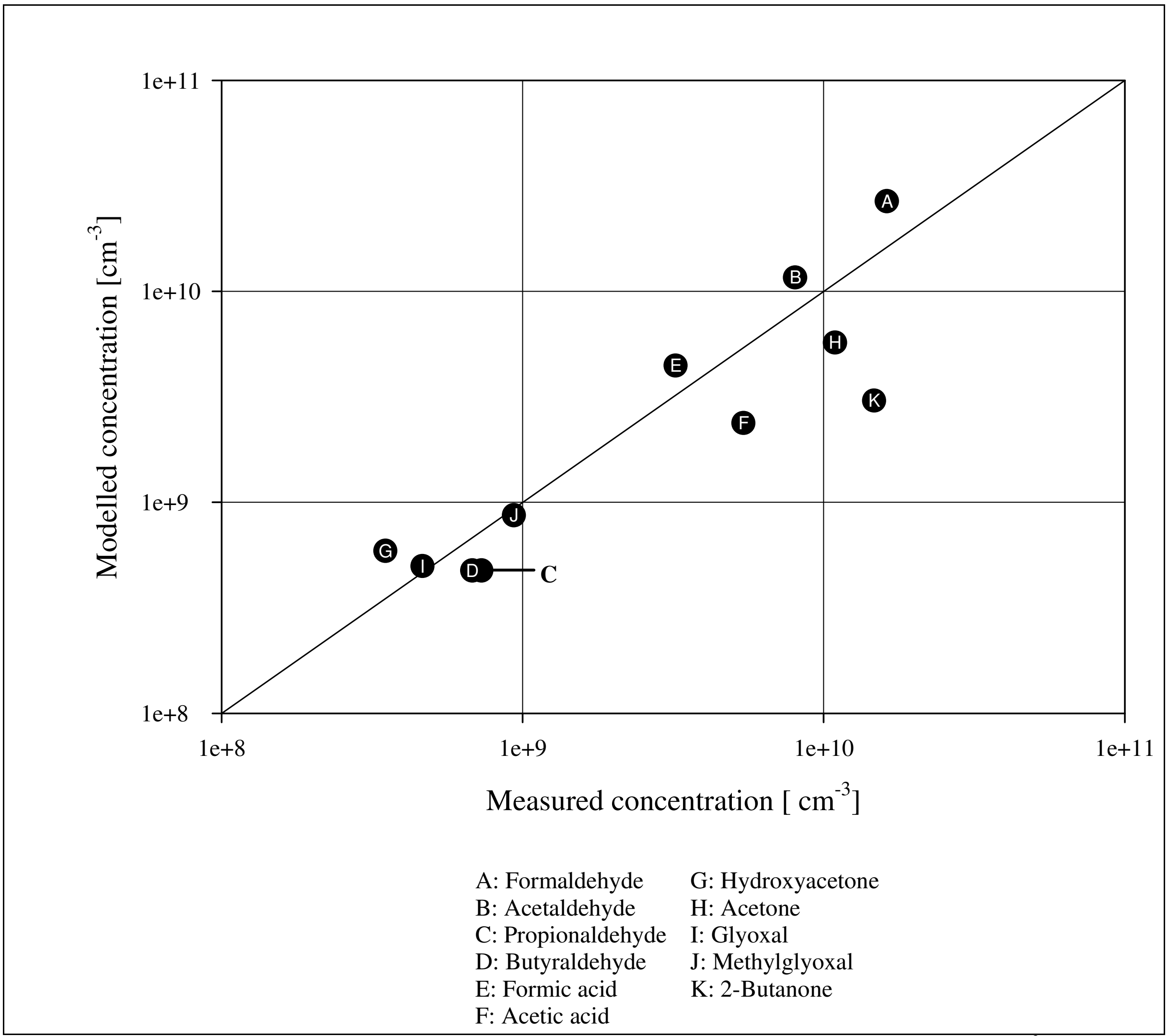


Fig. X: Comparison between the measured and modelled gas phase concentrations (molecules cm^{-3}) of organic compounds at the downwind site for the cloud event E I.

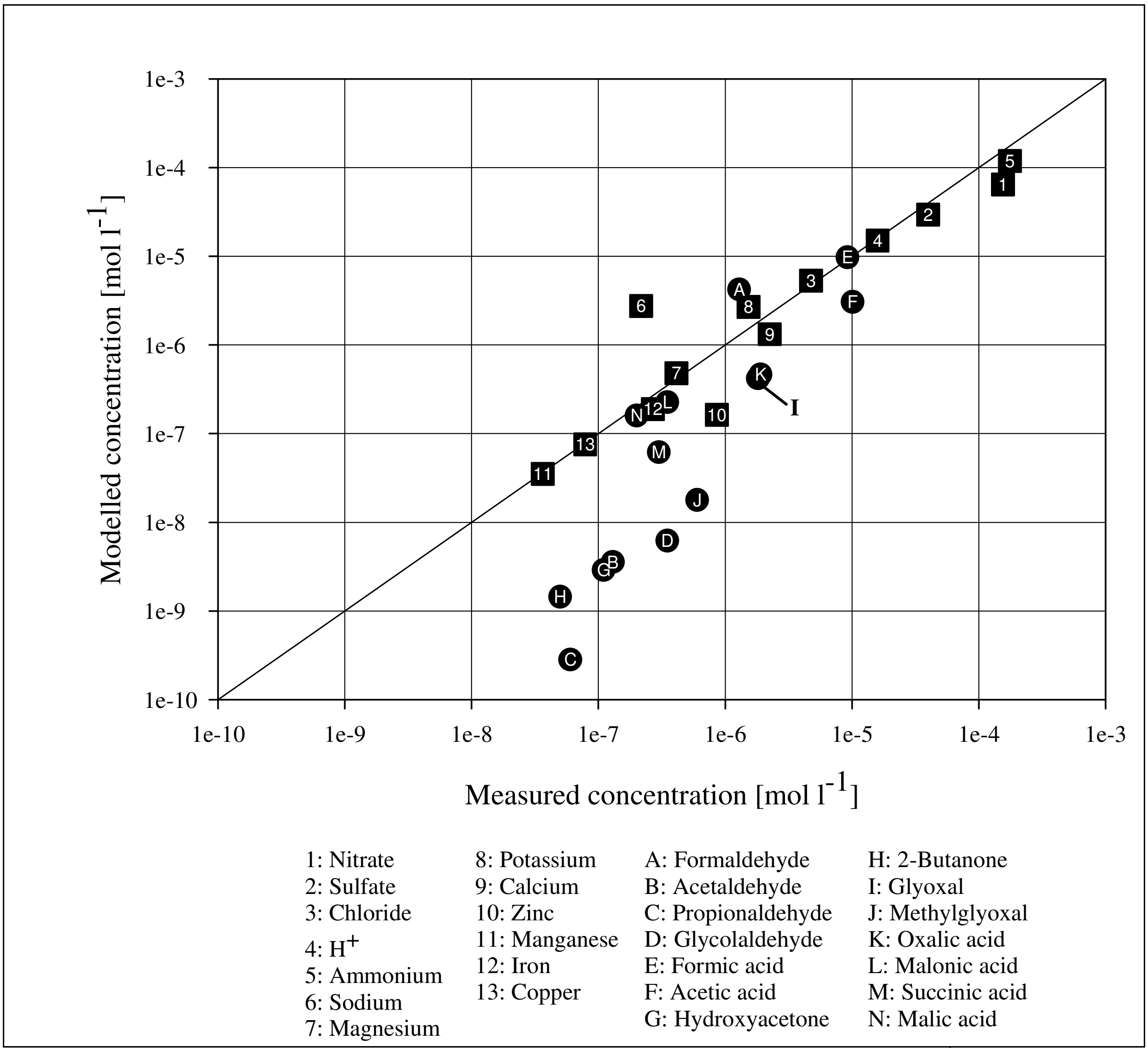


Fig. XI: Comparison between the measured and modelled cloud water concentrations (mol l^{-1}) at the summit for the cloud event E II.

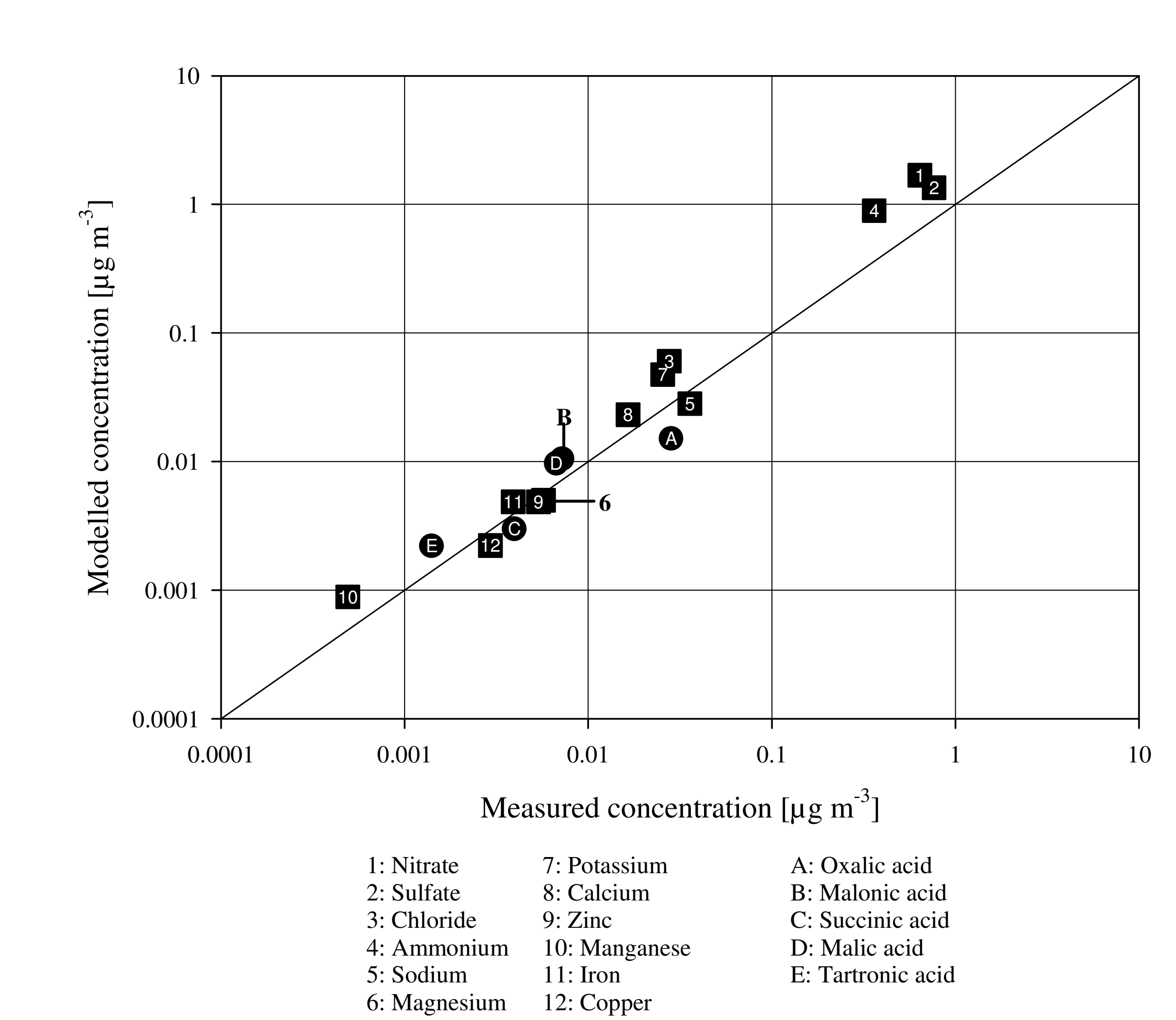


Fig. XII: Comparison between the measured and modelled aerosol particle concentrations (µg m^{-3}) at the downwind site for the cloud event E II.

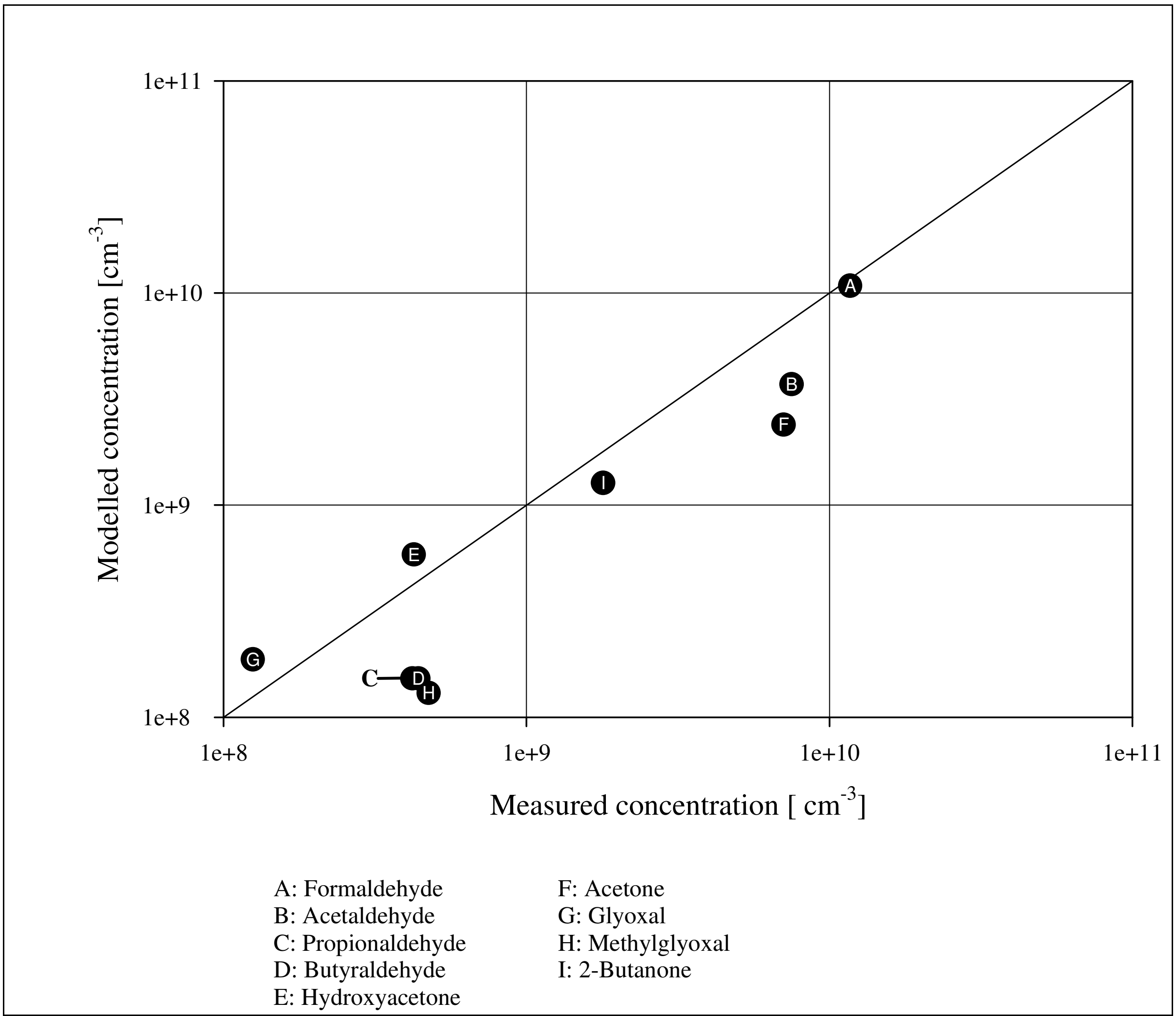


Fig. XIII: Comparison between the measured and modelled gas phase concentrations (molecules cm^{-3}) of organic compounds at the downwind site for the cloud event E II.

Table V: Measured and modelled cloud water concentrations at summit for the cloud event EI.

Species	Species name CAPRAM 3.0 / RACM	Measured concentration Place: Schmücke Date/Time: 27-10-2001/ 09:00 UTC Unit: $mol \cdot l^{-1}$ LWC_{summit}[g/m³]=0.3958[9^{00} - 9^{30}][2]	Calculated concentration CAPRAM 3.0 Unit: $mol \cdot l^{-1}$ LWC_{summit} [g/m³]=0.52
NO_3^-	NO3m	$2.04 \cdot 10^{-4}$ [1]	$1.82 \cdot 10^{-4}$
HNO_3	aHNO3		$9.91 \cdot 10^{-10}$
SO_4^{2-}	SO4mm	$4.65 \cdot 10^{-5}$ [1]	$4.32 \cdot 10^{-5}$
HSO_4^-	HSO4m		$4.32 \cdot 10^{-7}$
H_2SO_4	aSULF		$1.17 \cdot 10^{-13}$
HMSm	HMSm	---	$3.18 \cdot 10^{-8}$
Cl^-	CLm	$1.19 \cdot 10^{-5}$ [1]	$5.70 \cdot 10^{-6}$
HCl	aHCL		$1.16 \cdot 10^{-16}$
H^+	Hp	$6.31 \cdot 10^{-5}$ (pH=4.20) [2]	$8.93 \cdot 10^{-5}$
NH_4^+	NH4p	$2.77 \cdot 10^{-4}$ [1]	$1.79 \cdot 10^{-4}$
NH_3	aNH3		$2.17 \cdot 10^{-10}$
Na^+	NAp	$1.74 \cdot 10^{-5}$ [1]	$8.55 \cdot 10^{-6}$
Mg^{2+}	MGpp	$2.47 \cdot 10^{-6}$ [1]	$1.63 \cdot 10^{-6}$
K^+	Kp	$2.81 \cdot 10^{-6}$ [1]	$3.46 \cdot 10^{-6}$
Ca^{2+}	CApp	$9.73 \cdot 10^{-6}$ [1]	$2.95 \cdot 10^{-6}$
Al^{3+}	ALppp	$4.19 \cdot 10^{-6}$ [1]	0
Zn^{2+}	ZNpp	$1.22 \cdot 10^{-6}$ [1]	$2.36 \cdot 10^{-7}$
H_2O_2	aH2O2	$1.1 \cdot 10^{-6}$ [1]	$2.06 \cdot 10^{-6}$
Mn^{3+}	MNppp	$9.1 \cdot 10^{-8}$ [1]	$7.15 \cdot 10^{-16}$
Mn^{2+}	MNpp		$2.17 \cdot 10^{-8}$
Mn^{4+}	MNpppp		0
$MnBr_2^+$	MNBR2p		0
$MnCl_2^+$	MNCL2p		0
$MnHSO_3^+$	MNHSO3p		$1.78 \cdot 10^{-10}$
$Mn(OH)_2^+$	MNOH2p		$3.12 \cdot 10^{-9}$
$MnOH^{2+}$	MNOHpp		$3.72 \cdot 10^{-10}$
MnO^{2+}	MNOpp		$1.20 \cdot 10^{-12}$
MnO_2^+	MNO2p		$1.23 \cdot 10^{-14}$
Fe^{3+}	FEppp	$7.5 \cdot 10^{-7}$ [1]	$3.55 \cdot 10^{-10}$
Fe^{2+}	FEpp		$2.77 \cdot 10^{-8}$
$Fe(OH)_2^+$	FEOH2p		$2.44 \cdot 10^{-10}$
$FeOH^{2+}$	FEOHpp		$7.06 \cdot 10^{-9}$
$FeSO_4^+$	FESO4p		$2.01 \cdot 10^{-11}$
$Fe(C_2O_4)_2^-$	FEC2O42m		$6.28 \cdot 10^{-8}$
$Fe(C_2O_4)_3^{3-}$	FEC2O43mmm		$7.16 \cdot 10^{-9}$

Species	Species name CAPRAM 3.0 / RACM	Measured concentration Place: Schmücke Date/Time: 27-10-2001/ 09:00 UTC Unit: mol·l^{-1} LWC$_{summit}$[g/m³]=0.3958[9^{00} - 9^{30}][2]	Calculated concentration CAPRAM 3.0 Unit: mol·l^{-1} LWC$_{summit}$ [g/m³]=0.52
$Fe(C_2O_4)^+$	FEC2O4p		$1.93\cdot10^{-8}$
$FeCl^{2+}$	FECLpp		$1.98\cdot10^{-14}$
FeO^{2+}	FEOpp		$3.93\cdot10^{-12}$
$[FeCH_3OO]^{2+}$	FEMO2pp		$6.18\cdot10^{-15}$
$[Fe(OH)_2Fe]^{4+}$	FEOH2FEpppp		$1.72\cdot10^{-13}$
Cu^{2+}	CUpp	$7.9\cdot10^{-8}$ [1]	$8.74\cdot10^{-8}$
Cu^+	CUp		$1.61\cdot10^{-10}$
Formaldehyde	aHCHO	$3.5\cdot10^{-6}$ [3]	$1.05\cdot10^{-8}$
Formaldehyde (hydrated)	aCH2OH2		$2.39\cdot10^{-5}$
Acetaldehyde	aCH3CHO	$5.2\cdot10^{-7}$ [3]	$8.85\cdot10^{-9}$
Acetaldehyde	aCH3CHOH2		$9.33\cdot10^{-9}$
Propionaldehyde	aC2H5CHO	$0.135\cdot10^{-6}$ [3]	$8.62\cdot10^{-10}$
Propionaldehyde (hydrated)	aCH3CH2CHOH2		$3.88\cdot10^{-10}$
Butyraldehyde	aCH3CH2CH2CHO	n.d. [3]	$7.14\cdot10^{-10}$
Butyraldehyde (hydrated)	aCH3CH2CH2CHOH2		$1.57\cdot10^{-10}$
Glycolaldehyde	aOHCCH2OH	$3.97\cdot10^{-6}$ [3]	$1.72\cdot10^{-9}$
Glycolaldehyde (hydrated)	aOH2CHCH2OH		$1.04\cdot10^{-8}$
Formic acid	aORA1	$4.90\cdot10^{-6}$ [3]	$1.73\cdot10^{-6}$
Formate	HCOOm		$5.11\cdot10^{-6}$
Acetic acid	aORA2	$2.80\cdot10^{-6}$ [3]	$1.69\cdot10^{-6}$
Acetate	MCOOm		$4.98\cdot10^{-7}$
Propanoic acid	aCH2CH3COOH	n.d. [3]	$1.53\cdot10^{-14}$
Propionate	C2H5COO$^-$		$3.47\cdot10^{-15}$
Butyric acid	aCH3CH2CH2COOH	n.d. [3]	$1.30\cdot10^{-14}$
Butyrate	CH3CH2CH2COOm		$2.96\cdot10^{-15}$
Acetone	aCH3C(O)CH3		$2.60\cdot10^{-8}$
Biacetyl / 2,3-butanedione	aCH3COCOCH3	$0.24\cdot10^{-6}$ [3]	$1.27\cdot10^{-14}$
Hydroxyaceton	aCH3COCH2OH	$5.60\cdot10^{-7}$ [3]	$2.88\cdot10^{-9}$
Methylethylketone	aCH3COCH2CH3	$0.08\cdot10^{-6}$ [3]	$3.74\cdot10^{-9}$
Glyoxal	aGLY	$2.69\cdot10^{-6}$ [3]	$9.26\cdot10^{-12}$
Glyoxal (hydrated)	aCHOH2CHOH2		$1.41\cdot10^{-6}$
Methylglyoxal	aMGLY	$1.93\cdot10^{-6}$ [3]	$4.48\cdot10^{-11}$

Species	Species name CAPRAM 3.0 / RACM	Measured concentration Place: Schmücke Date/Time: 27-10-2001/ 09:00 UTC Unit: $mol \cdot l^{-1}$ LWC_{summit}[g/m³]=0.3958[9^{00} - 9^{30}][2]		Calculated concentration CAPRAM 3.0 Unit: $mol \cdot l^{-1}$ LWC_{summit} [g/m³]=0.52
Methylglyoxal (hydrated)	aCH3COCHOH2			$1.20 \cdot 10^{-7}$
Oxalic acid	C2O4mm	$2.1 \cdot 10^{-6}$ [3]	$2.3 \cdot 10^{-6}$ [3]	$2.65 \cdot 10^{-7}$
Oxalat MA	HC2O4m			$6.27 \cdot 10^{-7}$
Oxalat DA	aH2C2O4			$2.24 \cdot 10^{-9}$
Malonic acid	aHOOCCH2COOH	$0.6\ 10^{-6}$ [3]	$0.5\ 10^{-6}$ [3]	$5.08 \cdot 10^{-8}$
Malonate MA	HOOCCH2COOm			$3.36 \cdot 10^{-7}$
Malonate DA	OOCCH2COOmm			$4.93 \cdot 10^{-9}$
Succinic acid	aC2H4COOH2	$0.3\ 10^{-6}$ [3]	$0.4\ 10^{-6}$ [3]	$1.00 \cdot 10^{-7}$
Succinate MA	HOOCC2H4COOm			$4.02 \cdot 10^{-8}$
Succinate DA	OOCCH2CH2COOmm			$8.57 \cdot 10^{-10}$
Malic acid	aHOOCCHOHCH2COOH	$0.1\ 10^{-6}$ [3]		$1.91 \cdot 10^{-8}$
Malate MA	HOOCCHOHCH2COOm			$1.29 \cdot 10^{-7}$
Malate DA	OOCCHOHCH2COOmm			$7.48 \cdot 10^{-9}$
Tartronic acid	aHOOCCHOHCOOH	n.d. [3]		$9.43 \cdot 10^{-10}$
Tartronate MA	HOOCCHOHCOOm			$4.43 \cdot 10^{-8}$
Tartronate DA	OOCCHOHCOOmm			$1.86 \cdot 10^{-8}$
OH^{*}	aHO	---		$1.54 \cdot 10^{-15}$
HO_2^{*}	aHO_2	---		$2.98 \cdot 10^{-10}$
NO_3^{*}	aNO3	---		$5.59 \cdot 10^{-14}$
Cl^{*}	aCL	---		$1.42 \cdot 10^{-16}$
Cl_2^{-*}	CL2m	---		$1.98 \cdot 10^{-16}$
Br^{*}	aBR	---		n. i. c.
Br_2^{-*}	aBR2m	---		n. i. c.

Table VI: Measured and modelled cloud water concentrations at summit for the cloud event E II.

Species	Species name CAPRAM 3.0 / RACM	Measured concentration Place: Schmücke Date/Time: 08-10-2001/ 02:00 UTC Unit: mol·l^{-1} LWC [g/m³]=0.268 [02$^{\underline{00}}$ - 02$^{\underline{30}}$] [3]	Calculated concentration CAPRAM 3.0 Unit: mol·l^{-1} LWC [g/m³]=0.45
NO_3^-	NO3m	$1.55 \cdot 10^{-4}$ [1]	$6.44 \cdot 10^{-5}$
HNO_3	aHNO3		$1.29 \cdot 10^{-10}$
SO_4^{2-}	SO4mm	$3.99 \cdot 10^{-5}$ [1]	$2.93 \cdot 10^{-5}$
HSO_4^-	HSO4m		$9.46 \cdot 10^{-8}$
H_2SO_4	aSULF		$5.59 \cdot 10^{-14}$
Cl^-	CLm	$4.75 \cdot 10^{-6}$ [1]	$5.28 \cdot 10^{-6}$
HCl	aHCL		$2.93 \cdot 10^{-16}$
H^+	Hp	$1.59 \cdot 10^{-5}$ [pH=4.8] [2]	$1.50 \cdot 10^{-5}$
NH_4^+	NH4p	$1.76 \cdot 10^{-4}$ [1]	$1.19 \cdot 10^{-4}$
NH_3	aNH3		$1.24 \cdot 10^{-9}$
Na^+	NAp	$2.17 \cdot 10^{-7}$ [1]	$2.75 \cdot 10^{-6}$
Mg^{2+}	MGpp	$4.12 \cdot 10^{-7}$ [1]	$4.79 \cdot 10^{-7}$
K^+	Kp	$1.53 \cdot 10^{-6}$ [1]	$2.68 \cdot 10^{-6}$
Ca^{2+}	CApp	$2.25 \cdot 10^{-6}$ [1]	$1.32 \cdot 10^{-6}$
Al^{3+}	ALppp	$4.00 \cdot 10^{-6}$ [1]	0
Zn^{2+}	ZNpp	$8.57 \cdot 10^{-7}$ [1]	$1.62 \cdot 10^{-7}$
H_2O_2	aH2O2	$2.93 \cdot 10^{-6}$ [1]	$3.94 \cdot 10^{-6}$
Mn^{3+}	MNppp	$3.64 \cdot 10^{-8}$ [1]	$7.94 \cdot 10^{-16}$
Mn^{2+}	MNpp		$2.64 \cdot 10^{-8}$
Mn^{4+}	MNpppp		0
$MnBr_2^+$	MNBR2p		0
$MnCl_2^+$	MNCL2p		$1.47 \cdot 10^{-19}$
$MnHSO_3^+$	MNHSO3p		$2.20 \cdot 10^{-10}$
$Mn(OH)_2^+$	MNOH2p		$8.20 \cdot 10^{-9}$
$MnOH^{2+}$	MNOHpp		$2.20 \cdot 10^{-10}$
MnO^{2+}	MNOpp		$1.09 \cdot 10^{-12}$
MnO_2^+	MNO2p		$2.20 \cdot 10^{-14}$
Fe^{3+}	FEppp	$2.69 \cdot 10^{-7}$ [1]	$8.86 \cdot 10^{-10}$
Fe^{2+}	FEpp		$4.65 \cdot 10^{-9}$
$Fe(OH)_2^+$	FEOH2p		$4.92 \cdot 10^{-10}$
$FeOH^{2+}$	FEOHpp		$6.94 \cdot 10^{-9}$
$FeSO_4^+$	FESO4p		$8.89 \cdot 10^{-11}$
$Fe(C_2O_4)_2^-$	FEC2O42m		$9.96 \cdot 10^{-8}$
$Fe(C_2O_4)_3^{3-}$	FEC2O43mmm		$4.92 \cdot 10^{-8}$
$Fe(C_2O_4)^+$	FEC2O4p		$2.62 \cdot 10^{-8}$

Species	Species name CAPRAM 3.0 / RACM	Measured concentration Place: Schmücke Date/Time: 08-10-2001/ 02:00 UTC Unit: mol·l^{-1} LWC [g/m³]=0.268 [02$\underline{00}$ - 02$\underline{30}$] [3]	Calculated concentration CAPRAM 3.0 Unit: mol·l^{-1} LWC [g/m³]=0.45
$FeCl^{2+}$	FECLpp		$1.46 \cdot 10^{-11}$
FeO^{2+}	FEOpp		$8.69 \cdot 10^{-13}$
$[FeCH_3OO]^{2+}$	FEMO2pp		$6.43 \cdot 10^{-15}$
$[Fe(OH)_2Fe]^{4+}$	FEOH2FEpppp		$5.72 \cdot 10^{-14}$
Cu^{2+}	CUpp	$7.86 \cdot 10^{-8}$ [1]	$7.53 \cdot 10^{-8}$
Cu^{+}	CUp		$2.48 \cdot 10^{-10}$
Formaldehyde	aHCHO	$1.29\ 10^{-6}$ [3]	$3.58 \cdot 10^{-9}$
Formaldehyde (hydrated)	aCH2OH2		$4.20 \cdot 10^{-6}$
Acetaldehyde	aCH3CHO	$0.13\ 10^{-6}$ [3]	$2.18 \cdot 10^{-9}$
Acetaldehyde	aCH3CHOH2		$1.38 \cdot 10^{-9}$
Propionaldehyde	aC2H5CHO	$0.06\ 10^{-6}$ [3]	$2.17 \cdot 10^{-10}$
Propionaldehyde (hydrated)	aCH3CH2CHOH2		$6.51 \cdot 10^{-11}$
Butyraldehyde	aCH3CH2CH2CHO	n.d.	$1.76 \cdot 10^{-10}$
Butyraldehyde (hydrated)	aCH3CH2CH2CHOH2		$2.58 \cdot 10^{-11}$
Glycolaldehyde	aOHCCH2OH	$0.35\ 10^{-6}$ [3]	$1.4 \cdot 10^{-9}$
Glycolaldehyde (hydrated)	aOH2CHCH2OH		$4.77 \cdot 10^{-9}$
Formic acid	aORA1	$9.2\ 10^{-6}$ [3]	$4.98 \cdot 10^{-7}$
Formate	HCOOm		$9.18 \cdot 10^{-6}$
Acetic acid	aORA2	$10.1\ 10^{-6}$ [3]	$1.07 \cdot 10^{-6}$
Acetate	MCOOm		$1.97 \cdot 10^{-6}$
Propanoic acid	aCH2CH3COOH	$0.3\ 10^{-6}$ [3]	$2.39 \cdot 10^{-15}$
Propionate	$C2H5COO^{-}$		$3.36 \cdot 10^{-15}$
Butyric acid	aCH3CH2CH2COOH	$0.3\ 10^{-6}$ [3]	$2.10 \cdot 10^{-15}$
Butyrate	CH3CH2CH2COOm		$3.04 \cdot 10^{-15}$
Acetone	aCH3C(O)CH3	n.d.	$8.56 \cdot 10^{-9}$
Biacetyl / 2,3-butanedione	aCH3COCOCH3	$0.13\ 10^{-6}$ [3]	$1.52 \cdot 10^{-15}$
Hydroxyaceton	aCH3COCH2OH	$0.11\ 10^{-6}$ [3]	$2.89 \cdot 10^{-9}$
Methylethylketone	aCH3COCH2CH3	$0.05 \cdot 10^{-6}$ [3]	$1.44 \cdot 10^{-9}$
Glyoxal	aGLY	$1.81\ 10^{-6}$ [3]	$4.62 \cdot 10^{-12}$
Glyoxal (hydrated)	aCHOH2CHOH2		$4.18 \cdot 10^{-7}$
Methylglyoxal	aMGLY	$0.6\ 10^{-6}$ [3]	$6.65 \cdot 10^{-12}$
Methylglyoxal (hydrated)	aCH3COCHOH2		$1.78 \cdot 10^{-8}$

Species	Species name CAPRAM 3.0 / RACM	Measured concentration Place: Schmücke Date/Time: 08-10-2001/ 02:00 UTC Unit: mol·l^{-1} LWC [g/m³]=0.268 [02^{00} - 02^{30}] [3]		Calculated concentration CAPRAM 3.0 Unit: mol·l^{-1} LWC [g/m³]=0.45
Oxalic acid	C2O4mm	$2.2\ 10^{-6}$ [3]	$1.6\ 10^{-6}$ [3]	$2.86\cdot10^{-7}$
Oxalat MA	HC2O4m			$1.78\cdot10^{-7}$
Oxalat DA	aH2C2O4			$1.97\cdot10^{-10}$
Malonic acid	aHOOCCH2COOH	$0.5\ 10^{-6}$ [3]	$0.2\ 10^{-6}$ [3]	$1.06\cdot10^{-8}$
Malonate MA	HOOCCH2COOm			$2.02\cdot10^{-7}$
Malonate DA	OOCCH2COOmm			$1.29\cdot10^{-8}$
Succinic acid	aC2H4COOH2	$0.3\ 10^{-6}$ [3]		$2.37\cdot10^{-8}$
Succinate MA	HOOCC2H4COOm			$3.46\cdot10^{-8}$
Succinate DA	OOCCH2CH2COOmm			$3.24\cdot10^{-9}$
Malic acid	aHOOCCHOHCH2COOH	$0.2\ 10^{-6}$ [3]		$1.10\cdot10^{-8}$
Malate MA	HOOCCHOHCH2COOm			$1.21\cdot10^{-7}$
Malate DA	OOCCHOHCH2COOmm			$2.74\cdot10^{-8}$
Tartronic acid	aHOOCCHOHCOOH	n.d.		$8.00\cdot10^{-11}$
Tartronate MA	HOOCCHOHCOOm			$1.24\cdot10^{-8}$
Tartronate DA	OOCCHOHCOOmm			$2.07\cdot10^{-8}$
OH^{*}	aHO	---		$3.55\cdot10^{-15}$
HO_2^{*}	aHO_2	---		$1.02\cdot10^{-10}$
NO_3^{*}	aNO3	---		$1.23\cdot10^{-13}$
Cl^{*}	aCL	---		$3.18\cdot10^{-16}$
Cl_2^{-*}	CL2m	---		$6.10\cdot10^{-16}$
Br^{*}	aBR	---		n. i. c.
Br_2^{-*}	aBR2m	---		n. i. c.

Table VII: Measured and modelled cloud water concentrations at summit for the cloud event E III.

Species	Species name CAPRAM 3.0 / RACM	Measured concentration Place: Schmücke Date/Time: 17-10-2002/ 01:00 UTC Unit: $mol \cdot l^{-1}$ LWC [g/m³]=0.210 [1⁰⁰ - 1³⁰] [2]	Calculated concentration CAPRAM 3.0 Unit: $mol \cdot l^{-1}$ LWC [g/m³]=0.21
NO_3^-	NO3m	$1.04 \cdot 10^{-4}$ [1]	$9.91 \cdot 10^{-5}$
HNO_3	aHNO3		$2.79 \cdot 10^{-10}$
SO_4^{2-}	SO4mm	$4.90 \cdot 10^{-5}$ [1]	$4.47 \cdot 10^{-5}$
HSO_4^-	HSO4m		$2.42 \cdot 10^{-7}$
H_2SO_4	aSULF		$3.45 \cdot 10^{-14}$
Cl^-	CLm	$4.76 \cdot 10^{-5}$ [1]	$2.45 \cdot 10^{-5}$
HCl	aHCL		$2.78 \cdot 10^{-16}$
H^+	Hp	$4.07 \cdot 10^{-5}$ (pH=4.39) [2]	$3.79 \cdot 10^{-5}$
NH_4^+	NH4p	$1.69 \cdot 10^{-4}$ [1]	$1.60 \cdot 10^{-4}$
NH_3	aNH3		$5.09 \cdot 10^{-10}$
Na^+	NAp	$5.94 \cdot 10^{-5}$ [1]	$2.51 \cdot 10^{-5}$
Mg^{2+}	MGpp	$8.93 \cdot 10^{-6}$ [1]	$1.13 \cdot 10^{-5}$
K^+	Kp	$8.49 \cdot 10^{-6}$ [1]	$4.09 \cdot 10^{-6}$
Ca^{2+}	CApp	$7.11 \cdot 10^{-6}$ [1]	$5.59 \cdot 10^{-7}$
Al^{3+}	ALppp	$1.26 \cdot 10^{-6}$ [1]	$1.46 \cdot 10^{-6}$
Zn^{2+}	ZNpp	$1.93 \cdot 10^{-6}$ [1]	$1.06 \cdot 10^{-6}$
H_2O_2	aH2O2	$4.01 \cdot 10^{-6}$ [1]	$1.02 \cdot 10^{-5}$
Mn^{3+}	MNppp	$1.27 \cdot 10^{-7}$ [1]	$1.29 \cdot 10^{-15}$
Mn^{2+}	MNpp		$8.40 \cdot 10^{-8}$
Mn^{4+}	MNpppp		0
$MnBr_2^+$	MNBR2p		0
$MnCl_2^+$	MNCL2p		$9.58 \cdot 10^{-19}$
$MnHSO_3^+$	MNHSO3p		$1.08 \cdot 10^{-9}$
$Mn(OH)_2^+$	MNOH2p		$9.69 \cdot 10^{-9}$
$MnOH^{2+}$	MNOHpp		$8.50 \cdot 10^{-10}$
MnO^{2+}	MNOpp		$1.53 \cdot 10^{-12}$
MnO_2^+	MNO2p		$6.07 \cdot 10^{-14}$
Fe^{3+}	FEppp	$7.16 \cdot 10^{-7}$ [1]	$5.62 \cdot 10^{-10}$
Fe^{2+}	FEpp		$1.94 \cdot 10^{-8}$
$Fe(OH)_2^+$	FEOH2p		$1.93 \cdot 10^{-9}$
$FeOH^{2+}$	FEOHpp		$2.79 \cdot 10^{-8}$
$FeSO_4^+$	FESO4p		$9.16 \cdot 10^{-11}$
$Fe(C_2O_4)_2^-$	FEC2O42m		$5.21 \cdot 10^{-8}$
$Fe(C_2O_4)_3^{3-}$	FEC2O43mmm		$1.15 \cdot 10^{-7}$
$Fe(C_2O_4)^+$	FEC2O4p		$4.96 \cdot 10^{-9}$

Species	Species name CAPRAM 3.0 / RACM	Measured concentration Place: Schmücke Date/Time: 17-10-2002/ 01:00 UTC Unit: mol·l^{-1} LWC [g/m³]=0.210 [1$^{\underline{00}}$ - 1$^{\underline{30}}$] [2]	Calculated concentration CAPRAM 3.0 Unit: mol·l^{-1} LWC [g/m³]=0.21
$FeCl^{2+}$	FECLpp		$7.48 \cdot 10^{-12}$
FeO^{2+}	FEOpp		$9.40 \cdot 10^{-13}$
$[FeCH_3OO]^{2+}$	FEMO2pp		8.32·10-15
$[Fe(OH)_2Fe]^{4+}$	FEOH2Fepppp		$1.80 \cdot 10^{-12}$
Cu^{2+}	CUpp	$4.09 \cdot 10^{-8}$ [1]	$2.57 \cdot 10^{-7}$
Cu^{+}	CUp		$5.42 \cdot 10^{-10}$
Formaldehyde	aHCHO	$1.095 \cdot 10^{-6}$ [3]	$4.52 \cdot 10^{-9}$
Formaldehyde (hydrated)	aCH2OH2		$2.91 \cdot 10^{-6}$
Acetaldehyd	aCH3CHO	$0.226 \cdot 10^{-6}$ [3]	$2.39 \cdot 10^{-9}$
Acetaldehyd (hydrated)	aCH3CHOH2		$8.31 \cdot 10^{-10}$
Propionaldehyde	aC2H5CHO	$0.071 \cdot 10^{-6}$ [3]	$2.35 \cdot 10^{-10}$
Propionaldehyde (hydrated)	aCH3CH2CHOH2		$3.65 \cdot 10^{-11}$
Butyraldehyde	aCH3CH2CH2CHO	n.d.	$1.93 \cdot 10^{-10}$
Butyraldehyde (hydrated)	aCH3CH2CH2CHOH2		$1.46 \cdot 10^{-11}$
Glycolaldehyde	aOHCCH2OH	$0.28 \cdot 10^{-6}$ [3]	$7.00 \cdot 10^{-10}$
Glycolaldehyde (hydrated)	aOH2CHCH2OH		$1.18 \cdot 10^{-9}$
Formic acid	aORA1	$6.8\ 10^{-6}$ [3]	$1.09 \cdot 10^{-6}$
Formate	HCOOm		$6.24 \cdot 10^{-6}$
Acetic acid	aORA2	$2.0\ 10^{-6}$ [3]	$4.34 \cdot 10^{-7}$
Acetate	MCOOm		$2.48 \cdot 10^{-7}$
Propanoic acid	aCH2CH3COOH	n.d. [3]	$1.98 \cdot 10^{-15}$
Propionate	$C2H5COO^{-}$		$8.50 \cdot 10^{-16}$
Butyric acid	aCH3CH2CH2COOH	$0.2\ 10^{-6}$ [3]	$1.21 \cdot 10^{-15}$
Butyrate	CH3CH2CH2COOm		$5.30 \cdot 10^{-16}$
Acetone	aCH3C(O)CH3	$0.403 \cdot 10^{-6}$ [3]	$8.09 \cdot 10^{-9}$
Biacetyl / 2,3-butanedione	aCH3COCOCH3	$0.076 \cdot 10^{-6}$ [3]	$6.31 \cdot 10^{-15}$
Hydroxyaceton	aCH3COCH2OH	$0.163 \cdot 10^{-6}$ [3]	$5.77 \cdot 10^{-10}$
Methylethylketone	aCH3COCH2CH3	$0.062 \cdot 10^{-6}$ [3]	$1.25 \cdot 10^{-9}$
Glyoxal	aGLY	$1.005 \cdot 10^{-6}$ [3]	$3.93 \cdot 10^{-12}$
Glyoxal (hydrated)	aCHOH2CHOH2		$1.40 \cdot 10^{-7}$
Methylglyoxal	aMGLY	$0.578 \cdot 10^{-6}$ [3]	$1.96 \cdot 10^{-11}$
Methylglyoxal	aCH3COCHOH2		$5.16 \cdot 10^{-8}$

Species	Species name CAPRAM 3.0 / RACM	Measured concentration Place: Schmücke Date/Time: 17-10-2002/ 01:00 UTC Unit: $mol \cdot l^{-1}$ LWC [g/m³]=0.210 [1^{00} - 1^{30}] [2]		Calculated concentration CAPRAM 3.0 Unit: $mol \cdot l^{-1}$ LWC [g/m³]=0.21
(hydrated)				
Oxalic acid	C2O4mm	$2.2\ 10^{-6}$ [3]	$1.5\ 10^{-6}$ [3]	$2.71 \cdot 10^{-7}$
Oxalat MA	HC2O4m			$4.90 \cdot 10^{-7}$
Oxalat DA	aH2C2O4			$1.20 \cdot 10^{-9}$
Malonic acid	aHOOCCH2COOH	$0.4\ 10^{-6}$ [3]	$0.2\ 10^{-6}$ [3]	$1.91 \cdot 10^{-8}$
Malonate MA	HOOCCH2COOm			$2.05 \cdot 10^{-7}$
Malonate DA	OOCCH2COOmm			$4.92 \cdot 10^{-9}$
Succinic acid	aC2H4COOH2	$0.2\ 10^{-6}$ [3]	$0.2\ 10^{-6}$ [3]	$1.60 \cdot 10^{-7}$
Succinate MA	HOOCC2H4COOm			$1.11 \cdot 10^{-7}$
Succinate DA	OOCCH2CH2COOmm			$4.17 \cdot 10^{-9}$
Malic acid	aHOOCCHOHCH2COOH	$0.2\ 10^{-6}$ [3]]		$1.38 \cdot 10^{-8}$
Malate MA	HOOCCHOHCH2COOm			$1.53 \cdot 10^{-7}$
Malate DA	OOCCHOHCH2COOmm			$1.32 \cdot 10^{-8}$
Tartronic acid	aHOOCCHOHCOOH	n.d.		$1.16 \cdot 10^{-10}$
Tartronate MA	HOOCCHOHCOOm			$8.12 \cdot 10^{-9}$
Tartronate DA	OOCCHOHCOOmm			$4.00 \cdot 10^{-9}$
OH^*	aHO	---		$2.34 \cdot 10^{-14}$
HO_2^*	aHO_2	---		$2.48 \cdot 10^{-10}$
NO_3^*	aNO3	---		$1.75 \cdot 10^{-13}$
Cl^*	aCL	---		$1.83 \cdot 10^{-15}$
Cl_2^{-*}	CL2m	---		$7.03 \cdot 10^{-15}$
Br^*	aBR	---		n. i. c.
Br_2^{-*}	aBR2m	---		n. i. c.

Remarks to Table V-VII:

[1] **Brüggemann**, E., Gnauk, T., Mertes, S., Acker, K., Auel, R., Wieprecht, W., Möller, D., Collett, J.L., Jr., Chemnitzer, R., Rüd, C., Junek, R., Herrmann, H., 2005. Schmücke hill cap cloud and valley stations aerosol characterisation during FEBUKO (I): Particle size distribution and main components. Atmospheric Environment (this issue).

[2] **Wieprecht**, W., Acker, K., Mertes, S., Collett, J.L., Jr., Jaeschke, W., Brüggemann, E., Möller, D., Herrmann, H., 2005. Cloud physics and cloud water sampler comparison during FEBUKO. Atmospheric Environment (this issue).

[3] **van Pinxteren**, D., Plewka, A., Hofmann, D., Müller, K., Kramberger, H., Svrcina, B., Bächmann, K., Jaeschke, W., Mertes, S., Collett, J.L., Jr., Herrmann, H., 2005. Schmücke hill cap cloud and valley stations aerosol chemical composition during FEBUKO (II): Organic compounds. Atmospheric Environment (this issue).

Table VIII: Measured and modelled gas phase and particle phase concentrations at downwind site for the cloud event E I.

Febuko Event 27/10/2001_09^{00}UTC (**E I**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result GB
			µg·m^{-3}	molec·cm^{-3}	molec·cm^{-3}/ µg·m^{-3}	molec·cm^{-3}/ µg·m^{-3}
NO_3^-	NO3m	Impactor stage 1	0.006	-	0.0034	0.01140
NO_3^-	NO3m	Impactor stage 2	0.663	-	0.285	0.43400
NO_3^-	NO3m	Impactor stage3	2.186	-	2.517	2.19000
NO_3^-	NO3m	Impactor stage 4	0.238	-	2.511	1.74000
NO_3^-	NO3m	Impactor stage5	0.043	-	0.366	0.39800
NO_3^-	NO3m	Impactor total	3.136	-	5.704	4.77000
HNO_3	aHNO3	total	-	-	-	0.00871
HNO_3	HNO3	-	-	-	2.75E+09	1.41E+10
NO	NO	Mean [9:15-9:30]	-	-	1.89E+10	8.84E+9
NO2	NO2	Mean [9:15-9:30]	-	-	2.16E+11	2.23E+11
SO_4^{2-} & HSO_4^-	SO4mm & HSO4m	Impactor stage 1	0.05594	-	0.021	0.02180
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor stage 2	0.45852	-	0.183	0.23000
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor stage3	1.04995	-	1.046	1.14000
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor stage 4	0.05748	-	0.902	0.92300
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor stage5	0.0033	-	0.058	0.06000
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor total	1.62519	-	2.218	2.37000
H_2SO_4	aSULF	total	-	-	-	0.00012
SO_2	SO2	Mean [9:15-9:30]	-	0.85E+10	1.81E+10	1.71E+10
Cl^-	CLm	Impactor stage 1	0.0025	-	0	0.00015
Cl^-	CLm	Impactor stage 2	0	-	0.0047	0.00386
Cl^-	CLm	Impactor stage3	0	-	0.043	0.01300
Cl^-	CLm	Impactor stage 4	0	-	0.045	0.01660
Cl^-	CLm	Impactor stage5	0	-	0.0057	0.00691
Cl^-	CLm	Impactor total	0.0025	-	0.098	0.04050
HCl	aHCL	total	-	-	0.0	0.00000
HCl	HCL	-	-	-	1.2E+08	1.10E+9
NH_4^+	NH4p	Impactor stage 1	0.03029	-	0.012	0.00974
NH_4^+	NH4p	Impactor stage 2	0.3196	-	0.121	0.18900
NH_4^+	NH4p	Impactor stage3	0.62067	-	0.608	0.87200
NH_4^+	NH4p	Impactor stage 4	0.05896	-	0.524	0.63300
NH_4^+	NH4p	Impactor stage5	0.00471	-	0.072	0.06680
NH_4^+	NH4p	Impactor total	1.03423	-	1.332	1.77000
NH_3	aNH3	total	-	-	0.0	0.00000
NH_3	NH3	-	-	-	2.45E+10	2.82E+8

Febuko Event 27/10/2001_09[00]UTC (**E I**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result GB
			µg·m⁻³	molec·cm⁻³	molec·cm⁻³/ µg·m⁻³	molec·cm⁻³/ µg·m⁻³
H_2O_2	H2O2	-	-	-	9.26E+08	4.45E+8
O_3	O3	Mean [9:15-9:30]	-	4.25 E+11	4.13E+11	4.02E+11
Na^+	NAp	Impactor stage 1	0.00036	-	0.00000	0.00000
Na^+	NAp	Impactor stage 2	0.00155	-	0.00040	0.00040
Na^+	NAp	Impactor stage3	0.00695	-	0.00315	0.00315
Na^+	NAp	Impactor stage 4	0.04721	-	0.02590	0.02590
Na^+	NAp	Impactor stage5	0.01049	-	0.06990	0.06990
Na^+	NAp	Impactor total	0.06656	-	0.09935	0.09935
Mg^{2+}	MGpp	Impactor stage 1	0	-	0.00000	0.00000
Mg^{2+}	MGpp	Impactor stage 2	0	-	0.00000	0.00000
Mg^{2+}	MGpp	Impactor stage3	0.00109	-	0.00063	0.00063
Mg^{2+}	MGpp	Impactor stage 4	0.00576	-	0.00440	0.00440
Mg^{2+}	MGpp	Impactor stage5	0.00175	-	0.01460	0.01460
Mg^{2+}	MGpp	Impactor total	0.0086	-	0.01960	0.01960
K^+	Kp	Impactor stage 1	0.0053	-	0.00140	0.00140
K^+	Kp	Impactor stage 2	0.01702	-	0.00784	0.00784
K^+	Kp	Impactor stage3	0.03282	-	0.03020	0.03020
K^+	Kp	Impactor stage 4	0.00751	-	0.02530	0.02530
K^+	Kp	Impactor stage5	0.00228	-	0.01000	0.01000
K^+	Kp	Impactor total	0.06493	-	0.07490	0.07490
Ca^{2+}	CApp	Impactor stage 1	0.00537	-	0.00022	0.00022
Ca^{2+}	CApp	Impactor stage 2	0.00497	-	0.00021	0.00021
Ca^{2+}	CApp	Impactor stage3	0.00757	-	0.00093	0.00093
Ca^{2+}	CApp	Impactor stage 4	0.01547	-	0.01040	0.01040
Ca^{2+}	CApp	Impactor stage5	0.00969	-	0.04750	0.04750
Ca^{2+}	CApp	Impactor total	0.04307	-	0.05930	0.05930
Al^{3+}	ALppp	total	n.d.	-	0.00000	0.00000
Zn^{2+}	ZNpp	total	0.00897	-	0.00859	0.00859
Mn^{3+}	MNppp	total	7.5E-4	-	7.82E-4	1.55E-8
Mn^{2+}	MNpp	total		-		7.67E-4
Mn^{4+}	MNpppp	total		-		0
$MnBr_2^+$	MNBR2p	total		-		0
$MnCl_2^+$	MNCL2p	total		-		0
$MnHSO_3^+$	MNHSO3p	total		-		2.35E-8

Febuko Event 27/10/2001_09^{00}UTC (**E I**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result GB
			µg·m^{-3}	molec·cm^{-3}	molec·cm^{-3}/ µg·m^{-3}	molec·cm^{-3}/ µg·m^{-3}
$Mn(OH)_2^{\ +}$	MNOH2p	total		-		4.08E-7
$MnOH^{2+}$	MNOHpp	total		-		1.43E-5
MnO_2^+	MNO2p	total		-		3.33E-12
Fe^{3+}	FEppp	total		-		3.79E-5
Fe^{2+}	FEpp	total		-		1.22E-3
$Fe(OH)_2^{\ +}$	FEOH2p	total		-		1.73E-8
$FeOH^{2+}$	FEOHpp	total		-		2.01E-5
$FeSO_4^+$	FESO4p	total		-		9.09E-5
$Fe(C_2O_4)_2^{\ -}$	FEC2O42m	total	3.74E-3	-	3.89E-3	2.16E-3
$Fe(C_2O_4)_3^{\ 3-}$	FEC2O43mmm	total		-		1.57E-4
$Fe(C_2O_4)^+$	FEC2O4p	total		-		2.11E-4
$FeCl^{2+}$	FECLpp	total		-		2.63E-7
$[FeCH_3OO]^{2+}$	FEMO2pp	total		-		6.02E-12
$[Fe(OH)_2Fe]^{4+}$	FEOH2FEpppp	total		-		1.26E-7
Cu^{2+}	CUpp	total	4.49E-3	-	3.12E-3	3.12E-3
Cu^+	CUp	total		-		9.51E-7
HCHO	HCHO	-	-	1.62E+10	2.86E+10	2.67E+10
HCHO	aHCHO	-	-	-	-	5.37E-8
HCHO (hydrated)	aCH2OH2	-	-	-	-	1.77E-1
CH3CHO	CH3CHO	-	-	8.04E+9	1.15E+10	1.16E+10
aCH3CHO	aCH3CHO	-	-	-	-	2.50E-8
CH3CHO (hydrated)	aCH3CHOH2	-	-	-	-	8.43E-5
CH3CH2CHO	C2H5CHO	-	-	0.073E+10	4.69E+08	4.74E+8
CH3CH2CHO	aC2H5CHO	-	-	-	-	3.26E-9
CH3CH2CHO (hydrated)	aC2H5CHOH2	-	-	-	-	4.37E-6
CH3CH2CH2CHO	CH3CH2CH2CHO	-	-	0.068E+10	4.82E+8	4.74E+8
CH3CH2CH2CHO	aCH3CH2CH2CHO	-	-	-	-	3.30E-9
CH3CH2CH2CHO (hydrated)	aCH3CH2CH2CHOH2	-	-	-	-	2.07E-6
HCOOH	ORA1	-	-	3.22E+09	4.40E+09	4.44E+9
HCOOH	aORA1	-	-	-	-	1.02E-5
$HCOO^-$	HCOOm	-	-	-	-	4.22E-8
CH3COOH	CH3COOH	-	-	5.41E+09	3.94E+09	2.37E+9
CH3COOH	aCH3COOH	-	-	-	-	7.40E-6

Febuko Event 27/10/2001_09⁰⁰UTC (**E I**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result GB
			$\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$
$CH3COO^-$	MCOOm	-	-	-	-	3.08E-9
Hydroxyaceton	HKET	-	-	3.50E+08	5.87E+08	5.88E+8
Hydroxyaceton	aCH3COCH2OH	-	-	-	-	1.64E-8
Acetone	CH3COCH3	-	-	1.09E+10	5.68E+09	5.71E+9
Acetone	aCH3COCH3	-	-	-	-	9.80E-8
Biacetyl / 2,3-butanedione	---	-	-	1.48E+08	-	-
Biacetyl / 2,3-butanedione	aCH3COCOCH3	-	-	-	-	1.37E-8
Glyoxal	GLY	-	-	4.65E+08	6.36E+08	4.98E+8
Glyoxal	aGLY	-	-	-	-	2.64E-10
Glyoxal (hydrated)	aCHOH2CHOH2	-	-	-	-	1.88E-2
Methylglyoxal	MGLY	-	-	9.35E+08	8.81E+08	8.67E+8
Methylglyoxal	aMGLY	-	-	-	-	2.55E-10
Methylglyoxal (hydrated)	aCH3COCHOH2	-	-	-	-	8.73E-7
Methylethylketone	CH3COCH2CH3	-	-	1.47E+10	3.01E+09	3.03E+9
Methylethylketone	aCH3COCH2CH3	-	-	-	-	1.95E-8
Oxalic acid	aH2C2O4	Impactor stage 1	1.9E-3	-	1.12E-3	3.58E-4
Oxalate MA	HC2O4m					4.27E-4
Oxalate DA	C2O4mm					5.00E-7
Oxalic acid	aH2C2O4	Impactor stage 2	7.8E-3	-	5.11E-3	9.85E-4
Oxalate MA	HC2O4m					2.80E-3
Oxalate DA	C2O4mm					8.78E-6
Oxalic acid	aH2C2O4	Impactor stage3	1.35 E-2	-	2.34E-2	7.80E-3
Oxalate MA	HC2O4m					1.06E-2
Oxalate DA	C2O4mm					1.66E-5
Oxalic acid	aH2C2O4	Impactor stage 4	4.9E-3	-	2.16E-2	9.89E-3
Oxalate MA	HC2O4m					7.52E-3
Oxalate DA	C2O4mm					5.72E-6
Oxalic acid	aH2C2O4	Impactor stage5	n.d.	-	3.6E-3	9.93E-4
Oxalate MA	HC2O4m					1.84E-3
Oxalate DA	C2O4mm					3.41E-6
Oxalic acid	aH2C2O4	total	2.80E-2	-	5.47E-2	4.33E-2
Oxalate MA	HC2O4m		-			
Oxalate DA	C2O4mm		7.07E-2			
Malonic acid	aHOOCCH2COOH	Impactor stage 1	n.d.	-	~ 0.0	5.47E-10

Febuko Event 27/10/2001_09^{00}UTC (**E I**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result GB
			µg·m^{-3}	molec·cm^{-3}	molec·cm^{-3}/ µg·m^{-3}	molec·cm^{-3}/ µg·m^{-3}
Malonate MA	HOOCCH2COOm					1.44E-11
Malonate DA	OOCCH2COOmm					0
Malonic acid	aHOOCCH2COOH	Impactor stage 2	3.8E-3	-	1.17E-3	1.10E-3
Malonate MA	HOOCCH2COOm					8.43E-5
Malonate DA	OOCCH2COOmm					9.67E-9
Malonic acid	aHOOCCH2COOH	Impactor stage3	1.2 E-2	-	8.93E-3	8.74E-3
Malonate MA	HOOCCH2COOm					2.70E-4
Malonate DA	OOCCH2COOmm					1.42E-8
Malonic acid	aHOOCCH2COOH	Impactor stage 4	2.4E-3	-	8.86E-3	8.84E-3
Malonate MA	HOOCCH2COOm					1.48E-4
Malonate DA	OOCCH2COOmm					3.60E-9
Malonic acid	aHOOCCH2COOH	Impactor stage5	4.0E-4	-	2.58E-3	2.19E-3
Malonate MA	HOOCCH2COOm					1.60E-4
Malonate DA	OOCCH2COOmm					2.26E-8
Malonic acid	aHOOCCH2COOH	total	1.86E-2	-	2.14E-02	2.15E-2
Malonate MA	HOOCCH2COOm					
Malonate DA	OOCCH2COOmm		1.43E-2			
Succinic acid	aC2H4COOH2	Impactor stage 1	4.0E-4	-	7.00E-05	7.02E-5
Succinate MA	HOOCC2H4COOm					8.51E-8
Succinate DA	OOCCH2CH2COOmm					3.68E-12
Succinic acid	aC2H4COOH2	Impactor stage 2	3.5E-3	-	5.30E-04	5.31E-4
Succinate MA	HOOCC2H4COOm					1.76E-6
Succinate DA	OOCCH2CH2COOmm					2.26E-10
Succinic acid	aC2H4COOH2	Impactor stage3	9.5E-3	-	3.88E-03	3.91E-3
Succinate MA	HOOCC2H4COOm					5.49E-6
Succinate DA	OOCCH2CH2COOmm					3.26E-10
Succinic acid	aC2H4COOH2	Impactor stage 4	8.0E-4	-	3.79E-03	3.82E-3
Succinate MA	HOOCC2H4COOm					2.89E-6
Succinate DA	OOCCH2CH2COOmm					7.87E-11
Succinic acid	aC2H4COOH2	Impactor stage5	2.0E-4	-	5.90E-04	6.14E-4
Succinate MA	HOOCC2H4COOm					2.21E-6
Succinate DA	OOCCH2CH2COOmm					3.78E-10
Succinic acid	aC2H4COOH2	total	1.44E-2	-	8.91E-03	8.95E-3
Succinate MA	HOOCC2H4COOm					

Febuko Event 27/10/2001_09^{00}UTC (**E I**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result GB
			µg·m^{-3}	molec·cm^{-3}	molec·cm^{-3}/ µg·m^{-3}	molec·cm^{-3}/ µg·m^{-3}
Succinate DA	OOCCH2CH2COOmm		8.9E-3			
Malic acid	aHOOCCHOHCH2COOH					2.25E-4
Malate MA	HOOCCHOHCH2COOm	Impactor stage 1	5.00E-04	-	2.40E-04	6.25E-6
Malate DA	OOCCHOHCH2COOmm					9.46E-10
Malic acid	aHOOCCHOHCH2COOH					8.00E-4
Malate MA	HOOCCHOHCH2COOm	Impactor stage 2	2.30E-03	-	8.80E-04	5.58E-5
Malate DA	OOCCHOHCH2COOmm					2.36E-8
Malic acid	aHOOCCHOHCH2COOH					4.15E-3
Malate MA	HOOCCHOHCH2COOm	Impactor stage3	5.10E-03	-	4.50E-03	1.39E-4
Malate DA	OOCCHOHCH2COOmm					3.02E-8
Malic acid	aHOOCCHOHCH2COOH					4.06E-3
Malate MA	HOOCCHOHCH2COOm	Impactor stage 4	9.00E-04	-	4.30E-03	7.15E-5
Malate DA	OOCCHOHCH2COOmm					6.97E-9
Malic acid	aHOOCCHOHCH2COOH					1.48E-3
Malate MA	HOOCCHOHCH2COOm	Impactor stage5	2.00E-04	-	1.64E-03	1.37E-4
Malate DA	OOCCHOHCH2COOmm					8.74E-8
Malic acid	aHOOCCHOHCH2COOH					
Malate MA	HOOCCHOHCH2COOm	total	9.0E-3	-	1.16E-02	1.11E-2
Malate DA	OOCCHOHCH2COOmm					
Tartronic acid	aHOOCCHOHCOOH					0
Tatronate MA	HOOCCHOHCOOm	Impactor stage 1	n.d.	-	~ 0.0	0
Tatronate DA	OOCCHOHCOOmm					0
Tartronic acid	aHOOCCHOHCOOH					2.15E-4
Tatronate MA	HOOCCHOHCOOm	Impactor stage 2	8.00E-04	-	3.20E-04	1.11E-4
Tatronate DA	OOCCHOHCOOmm					3.64E-7
Tartronic acid	aHOOCCHOHCOOH	Impactor stage 3	2.30E-03	-	2.04E-03	1.69E-3

Febuko Event 27/10/2001_09^{00}UTC (**E I**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result GB
			µg·m^{-3}	molec·cm^{-3}	molec·cm^{-3}/ µg·m^{-3}	molec·cm^{-3}/ µg·m^{-3}
Tatronate MA	HOOCCHOHCOOm					3.63E-4
Tatronate DA	OOCCHOHCOOmm					5.61E-7
Tartronic acid	aHOOCCHOHCOOH	Impactor stage 4	n.d.	-	1.72E-03	1.55E-3
Tatronate MA	HOOCCHOHCOOm					1.69E-4
Tatronate DA	OOCCHOHCOOmm					1.11E-7
Tartronic acid	aHOOCCHOHCOOH	Impactor stage 5	n.d.	-	~ 0.0	1.12E-6
Tatronate MA	HOOCCHOHCOOm					6.65E-7
Tatronate DA	OOCCHOHCOOmm					3.04E-9
Tartronic acid	aHOOCCHOHCOOH	total	3.10E-03	-	4.08E-03	4.11E-3
Tatronate MA	HOOCCHOHCOOm					
Tatronate DA	OOCCHOHCOOmm					

Table IX: Measured and modelled gas phase and particle phase concentrations at downwind site for the cloud event E II.

Febuko Event 08/10/2001_02^{00}UTC (**E II**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			$\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$
NO_3^-	NO3m	Impactor stage 1	0.0020	-	0.00049	0.00382
NO_3^-	NO3m	Impactor stage 2	0.1828	-	0.15200	0.48400
NO_3^-	NO3m	Impactor stage3	0.3102	-	1.11000	0.93400
NO_3^-	NO3m	Impactor stage 4	0.0826	-	0.28100	0.19600
NO_3^-	NO3m	Impactor stage5	0.0462	-	0.06450	0.06300
NO_3^-	NO3m	Impactor total	0.6241	-	1.60000	1.68000
HNO_3	aHNO3	total	-	-	-	0.00027
HNO_3	HNO3	-	-	-	1.53E+9	1.78E+9
NO	NO	Mean [2:15-2:30]	-	-	2.39E+6	4.90E+4
NO2	NO2	Mean [2:15-2:30]	-	-	5.95E+10	5.79E+10
SO_4^{2-} & HSO_4^-	SO4mm & HSO4m	Impactor stage 1	0.0386	-	0.01240	0.01240
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor stage 2	0.2936	-	0.20000	0.26100
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor stage3	0.3828	-	0.85100	0.86700
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor stage 4	0.0367	-	0.18600	0.18700
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor stage5	0.0142	-	0.02200	0.02200
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor total	0.7659	-	1.27000	1.35000
H_2SO_4	aSULF	total	-	-	-	0.00000
SO_2	SO2	Mean [2:15-2:30]	-	5.41E+9	6.27E+9	5.78E+9
Cl^-	CLm	Impactor stage 1	0	-	0.00255	0.00011
Cl^-	CLm	Impactor stage 2	0	-	0.00208	0.01040
Cl^-	CLm	Impactor stage3	0	-	0.00032	0.02170
Cl^-	CLm	Impactor stage 4	0	-	0.00374	0.00640
Cl^-	CLm	Impactor stage5	0.0276	-	0.03860	0.02180
Cl^-	CLm	Impactor total	0.0276	-	0.04730	0.06040
HCl	aHCL	total	-	-		0.00000
HCl	HCL	-	-	-	5.82E+8	3.78E+8
NH_4^+	NH4p	Impactor stage 1	0.0175	-	0.00564	0.00466
NH_4^+	NH4p	Impactor stage 2	0.1430	-	0.08990	0.23400
NH_4^+	NH4p	Impactor stage3	0.1858	-	0.37100	0.54400
NH_4^+	NH4p	Impactor stage 4	0.0096	-	0.08000	0.10100
NH_4^+	NH4p	Impactor stage5	0.0048	-	0.00934	0.01060
NH_4^+	NH4p	Impactor total	0.3607	-	0.55600	0.89400

Febuko Event 08/10/2001_02^{00}UTC (**E II**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			µg·m^{-3}	molec·cm^{-3}	molec·cm^{-3}/ µg·m^{-3}	molec·cm^{-3}/ µg·m^{-3}
NH_3	aNH3	total	-	-	-	0.00000
NH_3	NH3	-	-	-	1.43E+10	3.01E+9
H_2O_2	H2O2	-	-	-	1.42E+9	1.28E+9
O_3	O3	Mean [2:15-2:30]	-	6.47E+11	6.17E+11	6.15E+11
Na^+	NAp	Impactor stage 1	0	-	0.00006	0.00006
Na^+	NAp	Impactor stage 2	0.0009	-	0.00119	0.00119
Na^+	NAp	Impactor stage3	0.0040	-	0.00615	0.00615
Na^+	NAp	Impactor stage 4	0.0221	-	0.01010	0.01010
Na^+	NAp	Impactor stage5	0.0088	-	0.01070	0.01070
Na^+	NAp	Impactor total	0.0358	-	0.02820	0.02820
Mg^{2+}	MGpp	Impactor stage 1	0	-	0.00000	0.00000
Mg^{2+}	MGpp	Impactor stage 2	0	-	0.00000	0.00000
Mg^{2+}	MGpp	Impactor stage3	0.002	-	0.00053	0.00053
Mg^{2+}	MGpp	Impactor stage 4	0.0033	-	0.00165	0.00165
Mg^{2+}	MGpp	Impactor stage5	0.0022	-	0.00283	0.00283
Mg^{2+}	MGpp	Impactor total	0.0057	-	0.00501	0.00501
K^+	Kp	Impactor stage 1	0.0013	-	0.00065	0.00065
K^+	Kp	Impactor stage 2	0.0079	-	0.00700	0.00700
K^+	Kp	Impactor stage3	0.0099	-	0.02560	0.02560
K^+	Kp	Impactor stage 4	0.0039	-	0.00827	0.00827
K^+	Kp	Impactor stage5	0.0025	-	0.00603	0.00603
K^+	Kp	Impactor total	0.0254	-	0.04750	0.04750
Ca^{2+}	CApp	Impactor stage 1	0.0018	-	0.00015	0.00015
Ca^{2+}	CApp	Impactor stage 2	0	-	0.00160	0.00160
Ca^{2+}	CApp	Impactor stage3	0.0004	-	0.00458	0.00458
Ca^{2+}	CApp	Impactor stage 4	0.0066	-	0.00568	0.00568
Ca^{2+}	CApp	Impactor stage5	0.0077	-	0.01120	0.01120
Ca^{2+}	CApp	Impactor total	0.0165	-	0.02320	0.02320
Al^{3+}	ALppp	total	0	-	0.00000	0.00000
Zn^{2+}	ZNpp	total	0.00536	-	0.00486	0.00486
Mn^{3+}	MNppp	total	4.90E-04	-	8.88E-4	1.38E-8
Mn^{2+}	MNpp	total		-		8.53E-4
Mn^{4+}	MNpppp	total		-		0
$MnBr_2^+$	MNBR2p	total		-		0

Febuko Event 08/10/2001_02[00]UTC (**E II**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			$\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$
$MnCl_2^+$	MNCL2p	total		-		0
$MnHSO_3^+$	MNHSO3p	total		-		6.50E-8
$Mn(OH)_2^+$	MNOH2p	total		-		1.41E-5
$MnOH^{2+}$	MNOHpp	total		-		2.07E-5
MnO_2^+	MNO2p	total		-		7.33E-11
Fe^{3+}	FEppp	total	3.90E-03	-	4.85E-3	3.09E-5
Fe^{2+}	FEpp	total		-		6.20E-5
$Fe(OH)_2^+$	FEOH2p	total		-		1.01E-7
$FeOH^{2+}$	FEOHpp	total		-		3.95E-5
$FeSO_4^+$	FESO4p	total		-		1.02E-4
$Fe(C_2O_4)_2^-$	FEC2O42m	total		-		1.38E-3
$Fe(C_2O_4)_3^{3-}$	FEC2O43mmm	total		-		2.91E-3
$Fe(C_2O_4)^+$	FEC2O4p	total		-		3.13E-4
$FeCl^{2+}$	FECLpp	total		-		2.01E-5
$[FeCH_3OO]^{2+}$	FEMO2pp	total		-		2.50E-11
$[Fe(OH)_2Fe]^{4+}$	FEOH2FEpppp	total		-		4.98E-9
Cu^{2+}	CUpp	total	2.93E-03	-	2.22E-3	2.22E-3
Cu^+	CUp	total		-		5.65E-7
HCHO	HCHO	-	-	1.17E+10	1.09E+10	1.08E+10
HCHO	aHCHO	-	-	-	-	2.25E-9
HCHO (hydrated)	aCH2OH2	-	-	-	-	1.68E-2
CH3CHO	CH3CHO	-	-	0.75E+10	3.50E+9	3.71E+9
aCH3CHO	aCH3CHO	-	-	-	-	1.64E-9
CH3CHO (hydrated)	aCH3CHOH2	-	-	-	-	5.79E-6
CH3CH2CHO	C2H5CHO	-	-	0.042E+10	1.54E+8	1.52E+8
CH3CH2CHO	aC2H5CHO	-	-	-	-	2.20E-10
CH3CH2CHO (hydrated)	aC2H5CHOH2	-	-	-	-	3.37E-7
CH3CH2CH2CHO	CH3CH2CH2CHO	-	-	0.044E+10	1.54E+8	1.52E+8
CH3CH2CH2CHO	aCH3CH2CHO	-	-	-	-	2.18E-10
CH3CH2CH2CHO (hydrated)	aCH3CH2CHOH2	-	-	-	-	1.52E-7
HCOOH	ORA1	-	-	x	3.47E+9	3.50E+9
HCOOH	aORA1	-	-	-	-	1.69E-6
$HCOO^-$	HCOOm	-	-	x	-	7.45E-8
CH3COOH	CH3COOH	-	-	-	2.02E+9	2.04E+9

Febuko Event 08/10/2001_02^{00}UTC (**E II**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			µg·m^{-3}	molec·cm^{-3}	molec·cm^{-3}/ µg·m^{-3}	molec·cm^{-3}/ µg·m^{-3}
CH3COOH	aCH3COOH	-	-	-	-	1.33E-6
CH3COO^{-}	MCOOm	-	-	-	-	5.85E-9
Hydroxyaceton	HKET	-	-	0.043E+10	5.84E+8	5.84E+8
Hydroxyaceton	aCH3COCH2OH	-	-	-	-	4.42E-9
Acetone	CH3C(O)CH3	-	-	0.706E+10	2.25E+9	2.39E+9
Acetone	aCH3C(O)CH3	-	-	-	-	8.61E-9
Biacetyl / 2,3-butanedione	aCH3COCOCH3	-		n.d.	-	6.10E-9
Glyoxal	GLY	-	-	0.013E+10	2.04E+8	1.87E+8
Glyoxal	aGLY	-	-	-	-	1.91E-11
Glyoxal (hydrated)	aCHOH2CHOH2	-	-	-	-	1.79E-3
Methylglyoxal	MGLY	-	-	0.048E+10	1.28E+8	1.30E+8
Methylglyoxal	aMGLY	-	-	-	-	1.04E-11
Methylglyoxal (hydrated)	aCH3COCHOH2	-	-	-	-	3.52E-8
Methylethylketone	CH3COCH2CHCH3	-	-	0.18E+10	1.30E+9	1.27E+9
Methylethylketone	aCH3COCH2CHCH3	-	-	-	-	2.01E-9
Oxalic acid	H2C2O4	Impactor stage 1	1.10E-03	-	6.00E-4	1.75E-5
Oxalate MA	HC2O4m					1.81E-4
Oxalate DA	C2O4mm					1.86E-6
Oxalic acid	H2C2O4	Impactor stage 2	6.40E-03	-	5.13E-3	4.54E-5
Oxalate MA	HC2O4m					1.43E-3
Oxalate DA	C2O4mm					5.44E-5
Oxalic acid	H2C2O4	Impactor stage3	9.20E-03	-	2.10E-2	8.28E-4
Oxalate MA	HC2O4m					9.18E-3
Oxalate DA	C2O4mm					1.02E-4
Oxalic acid	H2C2O4	Impactor stage 4	2.60E-03	-	5.89E-3	2.46E-4
Oxalate MA	HC2O4m					2.55E-3
Oxalate DA	C2O4mm					2.87E-5
Oxalic acid	H2C2O4	Impactor stage5	n.d.	-	1.47E-3	1.76E-5
Oxalate MA	HC2O4m					3.79E-4
Oxalate DA	C2O4mm					7.95E-6
Oxalic acid	H2C2O4	total	1.94E-02	-	3.41E-2	1.51E-2
Oxalate MA	HC2O4m					
Oxalate DA	C2O4mm		3.70E-02			
Malonic acid	aHOOCCH2COOH	Impactor stage 1	n.d.	-	0	7.34E-11

Febuko Event 08/10/2001_02^{00}UTC (**E II**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			$\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$
Malonate MA	HOOCCH2COOm					1.66E-11
Malonate DA	OOCCH2COOmm					0
Malonic acid	aHOOCCH2COOH	Impactor stage 2	2.30E-03	-	1.01E-3	5.76E-4
Malonate MA	HOOCCH2COOm					4.40E-4
Malonate DA	OOCCH2COOmm					5.91E-7
Malonic acid	aHOOCCH2COOH	Impactor stage3	4.00E-03	-	6.80E-3	5.49E-3
Malonate MA	HOOCCH2COOm					1.35E-3
Malonate DA	OOCCH2COOmm					4.88E-7
Malonic acid	aHOOCCH2COOH	Impactor stage 4	1.50E-03	-	2.03E-3	1.59E-3
Malonate MA	HOOCCH2COOm					3.92E-4
Malonate DA	OOCCH2COOmm					1.58E-7
Malonic acid	aHOOCCH2COOH	Impactor stage5	5.00E-04	-	7.11E-4	5.05E-4
Malonate MA	HOOCCH2COOm					2.08E-4
Malonate DA	OOCCH2COOmm					1.40E-7
Malonic acid	aHOOCCH2COOH	total	8.30E-03	-	1.06E-2	1.05E-2
Malonate MA	HOOCCH2COOm					
Malonate DA	OOCCH2COOmm		6.10E-03			
Succinic acid	aC2H4COOH2	Impactor stage 1	2.00E-04	-	2.89E-5	2.88E-5
Succinate MA	HOOCC2H4COOm					3.05E-7
Succinate DA	OOCCH2CH2COOmm					1.17E-10
Succinic acid	aC2H4COOH2	Impactor stage 2	1.20E-03	-	3.60E-4	3.46E-4
Succinate MA	HOOCC2H4COOm					1.44E-5
Succinate DA	OOCCH2CH2COOmm					2.71E-8
Succinic acid	aC2H4COOH2	Impactor stage3	2.00E-03	-	2.20E-3	2.18E-3
Succinate MA	HOOCC2H4COOm					2.49E-5
Succinate DA	OOCCH2CH2COOmm					1.04E-8
Succinic acid	aC2H4COOH2	Impactor stage 4	2.00E-04	-	5.82E-4	5.63E-4

Febuko Event 08/10/2001_02^{00}UTC (**E II**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			μg·m^{-3}	molec·cm^{-3}	molec·cm^{-3}/ μg·m^{-3}	molec·cm^{-3}/ μg·m^{-3}
Succinate MA	HOOCC2H4COOm					6.10E-6
Succinate DA	OOCCH2CH2COOmm					2.64E-9
Succinic acid	aC2H4COOH2	Impactor stage5	2.00E-04	-	1.32E-4	1.30E-4
Succinate MA	HOOCC2H4COOm					2.59E-6
Succinate DA	OOCCH2CH2COOmm					2.02E-9
Succinic acid	aC2H4COOH2	total	3.90E-3	-	3.30E-3	3.0E-3
Succinate MA	HOOCC2H4COOm					
Succinate DA	OOCCH2CH2COOmm		4.0E-03			
Malic acid	aHOOCCHOHCH2COOH	Impactor stage 1	2.00E-04	-	8.10E-5	6.22E-5
Malate MA	HOOCCHOHCH2COOm					1.51E-5
Malate DA	OOCCHOHCH2COOmm					2.01E-8
Malic acid	aHOOCCHOHCH2COOH	Impactor stage 2	1.70E-03	-	1.12E-3	5.19E-4
Malate MA	HOOCCHOHCH2COOm					4.31E-4
Malate DA	OOCCHOHCH2COOmm					2.44E-6
Malic acid	aHOOCCHOHCH2COOH	Impactor stage3	2.60E-03	-	5.09E-3	3.66E-3
Malate MA	HOOCCHOHCH2COOm					9.70E-4
Malate DA	OOCCHOHCH2COOmm					1.44E-6
Malic acid	aHOOCCHOHCH2COOH	Impactor stage 4	1.20E-03	-	1.90E-3	1.35E-3
Malate MA	HOOCCHOHCH2COOm					4.08E-4
Malate DA	OOCCHOHCH2COOmm					7.63E-7
Malic acid	aHOOCCHOHCH2COOH	Impactor stage5	1.00E-03	-	1.68E-3	1.17E-3
Malate MA	HOOCCHOHCH2COOm					4.87E-4
Malate DA	OOCCHOHCH2COOmm					1.31E-6
Malic acid	aHOOCCHOHCH2COOH	total	6.70E-03	-	9.87E-3	9.70E-3
Malate MA	HOOCCHOHCH2COOm					
Malate DA	OOCCHOHCH2COOmm					
Tartronic acid	aHOOCCHOHCOOH	Impactor stage 1	n.d.	-	0	0

Febuko Event 08/10/2001_02^{00}UTC (**E II**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			µg·m^{-3}	molec·cm^{-3}	molec·cm^{-3}/ µg·m^{-3}	molec·cm^{-3}/ µg·m^{-3}
Tatronate MA	HOOCCHOHCOOm					0
Tatronate DA	OOCCHOHCOOmm					0
Tartronic acid	aHOOCCHOHCOOH	Impactor stage 2	7.00E-04	-	3.59E-4	5.94E-5
Tatronate MA	HOOCCHOHCOOm					2.89E-4
Tatronate DA	OOCCHOHCOOmm					1.02E-5
Tartronic acid	aHOOCCHOHCOOH	Impactor stage3	7.00E-04	-	1.54E-3	5.67E-4
Tatronate MA	HOOCCHOHCOOm					9.67E-4
Tatronate DA	OOCCHOHCOOmm					1.03E-5
Tartronic acid	aHOOCCHOHCOOH	Impactor stage 4	n.d.	-	2.99E-4	1.30E-4
Tatronate MA	HOOCCHOHCOOm					1.79E-4
Tatronate DA	OOCCHOHCOOmm					1.53E-6
Tartronic acid	aHOOCCHOHCOOH	Impactor stage5	n.d.	-	0	1.45E-7
Tatronate MA	HOOCCHOHCOOm					4.05E-7
Tatronate DA	OOCCHOHCOOmm					7.98E-9
Tartronic acid	aHOOCCHOHCOOH	total	1.40E-03	-	2.20E-3	2.21E-3
Tatronate MA	HOOCCHOHCOOm					
Tatronate DA	OOCCHOHCOOmm					

Table X: Measured and modelled gas phase and particle phase concentrations at downwind site for the cloud event E III.

Febuko Event 17/10/2002_01^{00}UTC (**E III**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			$\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$
NO_3^-	NO3m	Impactor stage 1	0.0072	-	0.00049	0.07770
NO_3^-	NO3m	Impactor stage 2	0.0760	-	0.15800	0.39600
NO_3^-	NO3m	Impactor stage3	0.0512	-	0.17700	0.32600
NO_3^-	NO3m	Impactor stage 4	0.1962	-	0.19600	0.11700
NO_3^-	NO3m	Impactor stage5	0.0392	-	0.07240	0.15500
NO_3^-	NO3m	Impactor total	0.3700	-	0.60400	1.07000
HNO_3	aHNO3	total	-	-		0.00015
HNO_3	HNO3	-	-	-	6.06E+9	2.07E+9
NO	NO	Mean [1:15-1:30]	-	2.46e+09	0.0	3.54E+4
NO2	NO2	Mean [1:15-1:30]	-	2.46e+10	4.21E+10	4.10E+10
SO_4^{2-} & HSO_4^-	SO4mm & HSO4m	Impactor stage 1	0.0385	-	0.00405	0.01150
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor stage 2	0.348	-	0.35200	0.24800
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor stage3	0.3173	-	0.44700	0.59800
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor stage 4	0.0321	-	0.04880	0.03590
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor stage5	0.0149	-	0.02250	0.03650
SO_4^{2-}& HSO_4^-	SO4mm & HSO4m	Impactor total	0.7508	-	0.87400	0.93000
H_2SO_4	aSULF	total	-	-		0.00000
SO_2	SO2	Mean [1:15-1:30]	-	2.46e+09	1.51E+10	1.48E+10
Cl^-	CLm	Impactor stage 1	0.0068	-	0.00008	0.00685
Cl^-	CLm	Impactor stage 2	0.0000	-	0.00174	0.02540
Cl^-	CLm	Impactor stage3	0.0077	-	0.00000	0.01640
Cl^-	CLm	Impactor stage 4	0.0261	-	0.01980	0.01190
Cl^-	CLm	Impactor stage5	0.0286	-	0.02760	0.03600
Cl^-	CLm	Impactor total	0.0693	-	0.04920	0.09650
HCl	aHCL	total	-	-		0.00000
HCl	HCL	-	-	-	2.19E+9	1.37E+9
NH_4^+	NH4p	Impactor stage 1	0.0239	-	0.00173	0.03020
NH_4^+	NH4p	Impactor stage 2	0.1967	-	0.19500	0.22300
NH_4^+	NH4p	Impactor stage3	0.1584	-	0.23400	0.30100
NH_4^+	NH4p	Impactor stage 4	0.005	-	0.02240	0.01450
NH_4^+	NH4p	Impactor stage5	0	-	0.00252	0.00626
NH_4^+	NH4p	Impactor total	0.3841	-	0.45600	0.57500

Febuko Event 17/10/2002_01^{00}UTC (**E III**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			$\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$
NH_3	aNH3	total	-	-		0.00000
NH_3	NH3		-	-	4.76E+9	7.98E+8
H_2O_2	H2O2		-	1.23E+09	2.03E+9	1.78E+9
O_3	O3	Mean [1:15-1:30]	-	8.73E+11	7.77E+11	7.76E+11
Na^+	NAp	Impactor stage 1	0.0005	-	0.00000	0.00000
Na^+	NAp	Impactor stage 2	0.0001	-	0.00011	0.00007
Na^+	NAp	Impactor stage3	0.0166	-	0.01500	0.01510
Na^+	NAp	Impactor stage 4	0.0812	-	0.06450	0.03670
Na^+	NAp	Impactor stage5	0.0296	-	0.03860	0.06510
Na^+	NAp	Impactor total	0.128	-	0.11800	0.11700
Mg^{2+}	MGpp	Impactor stage 1	0.0003	-	0.00130	0.00148
Mg^{2+}	MGpp	Impactor stage 2	0	-	0.00827	0.00548
Mg^{2+}	MGpp	Impactor stage3	0.0032	-	0.01180	0.01460
Mg^{2+}	MGpp	Impactor stage 4	0.0108	-	0.01730	0.01000
Mg^{2+}	MGpp	Impactor stage5	0.0049	-	0.01750	0.02420
Mg^{2+}	MGpp	Impactor total	0.0193	-	0.05620	0.05580
K^+	Kp	Impactor stage 1	0.0003	-	0.00000	0.00000
K^+	Kp	Impactor stage 2	0.0097	-	0.00843	0.00510
K^+	Kp	Impactor stage3	0.0127	-	0.01070	0.01410
K^+	Kp	Impactor stage 4	0.0066	-	0.00633	0.00376
K^+	Kp	Impactor stage5	0.0056	-	0.00723	0.00956
K^+	Kp	Impactor total	0.0349	-	0.03270	0.03250
Ca^{2+}	CApp	Impactor stage 1	0.0029	-	0.00000	0.00000
Ca^{2+}	CApp	Impactor stage 2	0.0004	-	0.00000	0.00000
Ca^{2+}	CApp	Impactor stage3	0.002	-	0.00000	0.00000
Ca^{2+}	CApp	Impactor stage 4	0.0045	-	0.00459	0.00260
Ca^{2+}	CApp	Impactor stage5	0.0071	-	0.00000	0.00200
Ca^{2+}	CApp	Impactor total	0.017	-	0.00459	0.00459
Al^{3+}	ALppp	total	n.d.	-	0.00817	0.00817
Zn^{2+}	ZNpp	total	0.0239	-	0.01430	0.01430
Mn^{3+}	MNppp	total	5.60E-04	-	1.09E-3	1.47E-7
Mn^{2+}	MNpp	total		-		1.09E-3
Mn^{4+}	MNpppp	total		-		0
$MnBr_2^+$	MNBR2p	total		-		0

Febuko Event 17/10/2002_01^{00}UTC (**E III**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			µg·m⁻³	molec·cm⁻³	molec·cm⁻³/ µg·m⁻³	molec·cm⁻³/ µg·m⁻³
$MnCl_2^+$	MNCL2p	total		-		0
$MnHSO_3^+$	MNHSO3p	total		-		4.77E-7
$Mn(OH)_2^+$	MNOH2p	total		-		6.34E-7
$MnOH^{2+}$	MNOHpp	total		-		1.47E-6
MnO_2^+	MNO2p	total		-		1.14E-11
Fe^{3+}	FEppp	total		-		2.80E-5
Fe^{2+}	FEpp	total		-		1.70E-4
$Fe(OH)_2^+$	FEOH2p	total		-		1.11E-6
$FeOH^{2+}$	FEOHpp	total		-		1.26E-4
$FeSO_4^+$	FESO4p	total		-		2.60E-4
$Fe(C_2O_4)_2^-$	FEC2O42m	total	n.d.	-	2.58E-3	4.54E-4
$Fe(C_2O_4)_3^{3-}$	FEC2O43mmm	total		-		1.52E-3
$Fe(C_2O_4)^+$	FEC2O4p	total		-		8.63E-7
$FeCl^{2+}$	FECLpp	total		-		2.05E-5
$[FeCH_3OO]^{2+}$	FEMO2pp	total		-		2.63E-11
$[Fe(OH)_2Fe]^{4+}$	FEOH2FEpppp	total		-		3.51E-8
Cu^{2+}	CUpp	total	5.77E-03	-	3.40E-3	3.40E-3
Cu^+	CUp	total		-		3.05E-7
HCHO	HCHO	-	-	0.53E+10	1.09E+10	1.08E+10
HCHO	aHCHO	-	-	-	-	1.20E-9
HCHO (hydrated)	aCH2OH2	-	-	-	-	1.22E-2
CH3CHO	CH3CHO	-	-	0.59E+10	3.35E+9	3.54E+9
aCH3CHO	aCH3CHO	-	-	-	-	8.15E-10
CH3CHO (hydrated)	aCH3CHOH2	-	-	-	-	3.62E-6
CH3CH2CHO	C2H5CHO	-	-	0.05E+10	1.47E+8	1.44E+8
CH3CH2CHO	aC2H5CHO	-	-	-	-	1.08E-10
CH3CH2CHO (hydrated)	aC2H5CHOH2	-	-	-	-	1.94E-7
CH3CH2CH2CHO	CH3CH2CH2CHO	-	-	0.015E+10	1.47E+8	1.44E+8
CH3CH2CH2CHO	aCH3CH2CH2CHO	-	-	-	-	1.08E-10
CH3CH2CH2CHO (hydrated)	aCH3CH2CH2CHOH2	-	-	-	-	9.08E-8
HCOOH	ORA1	-	-	x	2.57E+9	2.58E+9
HCOOH	aORA1	-	-	-	-	6.42E-7
$HCOO^-$	HCOOm	-	-	x	-	4.53E-8
CH3COOH	CH3COOH	-	-	-	6.40E+8	6.49E+8

Febuko Event 17/10/2002_01^{00}UTC (**E III**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			µg·m^{-3}	molec·cm^{-3}	molec·cm^{-3}/ µg·m^{-3}	molec·cm^{-3}/ µg·m^{-3}
CH3COOH	aCH3COOH	-	-	-	-	2.19E-7
CH3COO^{-}	MCOOm	-	-	-	-	1.54E-9
Hydroxyaceton	HKET	-	-	0.013E+10	1.17E+8	1.17E+8
Hydroxyaceton	aCH3COCH2OH	-	-	-	-	4.12E-10
Acetone	CH3C(O)CH3	-	-	0.62E+10	1.87E+9	1.99E+9
Acetone	aCH3C(O)CH3	-	-	-	-	3.69E-9
Biacetyl / 2,3-butanedione	aCH3COCOCH3	-		0.008E+10	-	8.67E-9
Glyoxal	GLY	-	-	0.013E+10	3.39E+7	8.83E+7
Glyoxal	aGLY	-	-	-	-	4.62E-12
Glyoxal (hydrated)	aCHOH2CHOH2	-	-	-	-	7.55E-4
Methylglyoxal	MGLY	-	-	0.038E+10	3.73E+8	3.73E+8
Methylglyoxal	aMGLY	-	-	-	-	1.38E-11
Methylglyoxal (hydrated)	aCH3COCHOH2	-	-	-	-	4.70E-8
Methylethylketone	CH3COCH2CH3	-	-	0.47E+10	1.08E+9	1.05E+9
Methylethylketone	aCH3COCH2CH3	-	-	-	-	8.07E-10
Oxalic acid	H2C2O4	Impactor stage 1	n.d.	-	0	0
Oxalate MA	HC2O4m					5.95E-12
Oxalate DA	C2O4mm					4.12E-12
Oxalic acid	H2C2O4	Impactor stage 2	4.60E-03	-	5.16E-3	3.65E-5
Oxalate MA	HC2O4m					9.09E-4
Oxalate DA	C2O4mm					3.00E-5
Oxalic acid	H2C2O4	Impactor stage3	5.80E-03	-	1.20E-2	1.18E-3
Oxalate MA	HC2O4m					7.87E-3
Oxalate DA	C2O4mm					5.24E-5
Oxalic acid	H2C2O4	Impactor stage 4	2.50E-03	-	5.42E-3	1.33E-4
Oxalate MA	HC2O4m					1.86E-3
Oxalate DA	C2O4mm					2.84E-5
Oxalic acid	H2C2O4	Impactor stage5	8.00E-04	-	0	6.93E-5
Oxalate MA	HC2O4m					1.25E-3
Oxalate DA	C2O4mm					2.19E-5
Oxalic acid	H2C2O4	total	1.37E-02	-	2.26E-2	1.34E-2
Oxalate MA	HC2O4m					
Oxalate DA	C2O4mm		2.68E-02			
Malonic acid	aHOOCCH2COOH	Impactor stage 1	n.d.	-	0	0

Febuko Event 17/10/2002_01^{00}UTC (**E III**)

Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			$\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$
Malonate MA	HOOCCH2COOm					0
Malonate DA	OOCCH2COOmm					0
Malonic acid	aHOOCCH2COOH					4.14E-4
Malonate MA	HOOCCH2COOm	Impactor stage 2	7.00E-04	-	1.17E-3	2.82E-4
Malonate DA	OOCCH2COOmm					4.04E-7
Malonic acid	aHOOCCH2COOH					2.60E-3
Malonate MA	HOOCCH2COOm	Impactor stage3	9.00E-04	-	2.58E-3	4.00E-4
Malonate DA	OOCCH2COOmm					9.16E-8
Malonic acid	aHOOCCH2COOH					5.16E-4
Malonate MA	HOOCCH2COOm	Impactor stage 4	1.10E-03	-	1.23E-3	1.74E-4
Malonate DA	OOCCH2COOmm					8.89E-8
Malonic acid	aHOOCCH2COOH					3.49E-4
Malonate MA	HOOCCH2COOm	Impactor stage5	n.d.	-	0	1.38E-4
Malonate DA	OOCCH2COOmm					7.75E-8
Malonic acid	aHOOCCH2COOH		2.70E-03			
Malonate MA	HOOCCH2COOm	total		-	4.97E-3	4.88E-3
Malonate DA	OOCCH2COOmm		5.30E-03			
Succinic acid	aC2H4COOH2					0
Succinate MA	HOOCC2H4COOm	Impactor stage 1	n.d.	-	0	0
Succinate DA	OOCCH2CH2COOmm					0
Succinic acid	aC2H4COOH2					1.17E-3
Succinate MA	HOOCC2H4COOm	Impactor stage 2	4.00E-04		2.01E-3	4.32E-5
Succinate DA	OOCCH2CH2COOmm					8.40E-8
Succinic acid	aC2H4COOH2					4.26E-3
Succinate MA	HOOCC2H4COOm	Impactor stage3	6.00E-04	-	3.49E-3	3.10E-5
Succinate DA	OOCCH2CH2COOmm					8.38E-9
Succinic acid	aC2H4COOH2	Impactor stage 4	n.d.	-	1.22E-3	6.89E-4

Febuko Event 17/10/2002_01^{00}UTC (**E III**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			µg·m^{-3}	molec·cm^{-3}	molec·cm^{-3}/ µg·m^{-3}	molec·cm^{-3}/ µg·m^{-3}
Succinate MA	HOOCC2H4COOm					1.05E-5
Succinate DA	OOCCH2CH2COOmm					6.09E-9
Succinic acid	aC2H4COOH2	Impactor stage5	n.d.	-	0	4.65E-4
Succinate MA	HOOCC2H4COOm					8.47E-6
Succinate DA	OOCCH2CH2COOmm					5.47E-9
Succinic acid	aC2H4COOH2	total	1.00E-03	-	6.72E-3	6.68E-3
Succinate MA	HOOCC2H4COOm		-			
Succinate DA	OOCCH2CH2COOmm		6.20E-03			
Malic acid	aHOOCCHOHCH2COOH	Impactor stage 1	n.d.	-	0	0
Malate MA	HOOCCHOHCH2COOm					0
Malate DA	OOCCHOHCH2COOmm					0
Malic acid	aHOOCCHOHCH2COOH	Impactor stage 2	8.00E-04	-	9.73E-4	3.16E-4
Malate MA	HOOCCHOHCH2COOm					2.27E-4
Malate DA	OOCCHOHCH2COOmm					1.30E-6
Malic acid	aHOOCCHOHCH2COOH	Impactor stage3	1.40E-03	-	2.05E-3	1.97E-3
Malate MA	HOOCCHOHCH2COOm					3.21E-4
Malate DA	OOCCHOHCH2COOmm					2.95E-7
Malic acid	aHOOCCHOHCH2COOH	Impactor stage 4	1.20E-03	-	1.08E-3	4.54E-4
Malate MA	HOOCCHOHCH2COOm					1.65E-4
Malate DA	OOCCHOHCH2COOmm					3.41E-7
Malic acid	aHOOCCHOHCH2COOH	Impactor stage5	4.00E-04	-	9.46E-4	7.06E-4
Malate MA	HOOCCHOHCH2COOm					5.45E-4
Malate DA	OOCCHOHCH2COOmm					2.80E-6
Malic acid	aHOOCCHOHCH2COOH	total	3.80E-03	-	5.05E-3	4.71E-3
Malate MA	HOOCCHOHCH2COOm					
Malate DA	OOCCHOHCH2COOmm					
Tartronic acid	aHOOCCHOHCOOH	Impactor stage 1	n.d	-	0	0

Febuko Event 17/10/2002_01^{00}UTC (**E III**)						
Species	CAPRAM 3.0 / RACM	remarks	Aerosol particle concentration GB	Gas phase concentration GB	Initial concentration GL	SPACCIM result
			$\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$	$molec \cdot cm^{-3}$/ $\mu g \cdot m^{-3}$
Tatronate MA	HOOCCHOHCOOm					0
Tatronate DA	OOCCHOHCOOmm					0
Tartronic acid	aHOOCCHOHCOOH	Impactor stage 2	n.d.	-	0	2.12E-7
Tatronate MA	HOOCCHOHCOOm					8.31E-7
Tatronate DA	OOCCHOHCOOmm					2.47E-8
Tartronic acid	aHOOCCHOHCOOH	Impactor stage3	n.d.	-	2.79E-4	1.43E-4
Tatronate MA	HOOCCHOHCOOm					1.38E-4
Tatronate DA	OOCCHOHCOOmm					8.06E-7
Tartronic acid	aHOOCCHOHCOOH	Impactor stage 4	n.d.	-	1.08E-5	7.27E-6
Tatronate MA	HOOCCHOHCOOm					1.08E-5
Tatronate DA	OOCCHOHCOOmm					1.21E-7
Tartronic acid	aHOOCCHOHCOOH	Impactor stage5	n.d.	-	0	1.38E-7
Tatronate MA	HOOCCHOHCOOm					3.72E-7
Tatronate DA	OOCCHOHCOOmm					6.03E-9
Tartronic acid	aHOOCCHOHCOOH	total	n.d.	-	2.90E-4	3.01E-4
Tatronate MA	HOOCCHOHCOOm					
Tatronate DA	OOCCHOHCOOmm					

D. Appendix

(1) Gas and particle phase initialisation

Table A I: Derived initial gas phase composition at the upwind site for the cloud event E I (27-10-2001 09:00 UTC).

Chemical gas phase composition 27-10-01 09:00 UTC (E I)				
Gas phase species	RACM species	Concentration [ppb]	Concentration [molec.cm^{-3}] (p=950.2 hPa, T=281.35 K)	Remarks
Sulphur dioxide	SO2	**0.739**	**1.81E+10**	Measured by BTU [1]
Carbon monoxide	CO	**300.000**	**7.34E+12**	urban case
Nitrogen monoxide	NO	**0.772**	**1.89E+10**	Measured by BTU [1]
Nitrogen dioxide	NO2	**8.840**	**2.16E+11**	Measured by BTU [1]
Ozone	O3	**16.903**	**4.13E+11**	Measured by BTU [1]
Nitrous acid	HONO	**0.117**	**2.86E+09**	Measured by BTU [1]
Nitric acid	HNO3	**0.113**	**2.75E+09**	Measured by BTU [1]
Formic acid	ORA1	**0.180**	**4.40E+09**	Measured by TUD [2]
Acetic acid	ORA2	0.257	6.29E+09	Measured by TUD [2]
Propionic acid	ORA2	0.000	0.00E+00	Measured by TUD [2]
Butyric acid	ORA2	0.000	0.00E+00	Measured by TUD [2]
Σ ORA2	ORA2	**0.257**	**6.29E+09**	---
Glyoxal	GLY	**0.026**	**6.36E+08**	Measured by TUD [2]
Methyl glyoxal	MGLY	**0.036**	**8.81E+08**	Measured by TUD [2]
Acetaldehyde	ALD	0.648	1.59E+10	Measured by IfT [2]
Propanal	ALD	0.073	1.79E+09	Measured by IfT [2]
Butanal	ALD	0.102	2.50E+09	Measured by IfT [2]
Pentanal	ALD	0.037	9.05E+08	Measured by IfT [2]
Hexanal	ALD	0.080	1.96E+09	Measured by IfT [2]
Heptanal	ALD	0.069	1.69E+09	Measured by IfT [2]
Octanal	ALD	0.025	6.12E+08	Measured by IfT [2]
Nonanal	ALD	0.074	1.81E+09	Measured by IfT [2]
Decanal	ALD	0.015	3.67E+08	Measured by IfT [2]
Benzaldehyde	ALD	0.015	3.67E+08	Measured by TUD [2]
m-Toluylaldehyde	ALD	0.008	1.96E+08	Measured by TUD [2]
p-Toluylaldehyde	ALD	0.008	1.96E+08	Measured by TUD [2]
Acrolein	MACR	0.043	1.05E+09	Measured by TUD [2]
Methacrolein	MACR	0.024	5.87E+08	Measured by TUD [2]
Crotonaldehyde	MACR	0.010	2.45E+08	Measured by TUD [2]
Σ MACR	MACR	**0.077**	**1.88E+09**	---
Glycolaldehyde	ALD	0.071	1.74E+09	Measured by TUD [2]
Isobutanal	ALD	0.012	2.94E+08	Measured by TUD [2]
Isovaleraldehyde	ALD	0.056	1.37E+09	Measured by IfT [2]
Undecanal	ALD	0.005	1.22E+08	Measured by IfT [2]
Dodecanal	ALD	0.005	1.22E+08	Measured by IfT [2]
Pinonaldehyde	ALD	0.090	2.20E+09	Measured by IfT [2]
Dimethylbenzaldehyde	ALD	0.000	0.00E+00	Measured by IfT [2]
Σ ALD	ALD	**1.393**	**3.60E+10**	---
Acetone	KET	0.579	1.42E+10	Measured by IfT [2]
Cyclohexanone	KET	0.056	1.37E+09	Measured by IfT [2]
Diacetyl	KET	0.008	1.96E+08	Measured by TUD [2]
Methylvinylketone	KET	0.007	1.71E+08	Measured by TUD [2]
2-Pentanone	KET	0.014	3.42E+08	Measured by TUD [2]
3-Pentanone	KET	0.009	2.20E+08	Measured by TUD [2]
3-Hexanone	KET	0.007	1.71E+08	Measured by TUD [2]
Methyl ethyl ketone	KET	0.163	3.99E+09	Measured by IfT [2]
Σ KET	KET	**0.843**	**2.06E+10**	---
Hydroxy acetone	HKET	**0.024**	**5.87E+08**	Measured by TUD [2]
Methane	CH4	**1700.000**	**4.16E+13**	urban case
Hydrogen peroxide	H2O2	**0.038**	**9.26E+08**	Estimated (respectively to ZUF measurements 2002 [1])
Hydrogen	H2	**500.000**	**1.22E+13**	urban case
Hydrogen chloride	HCL	**0.005**	**1.23E+08**	Measured by BTU [1]
Ammonia	NH3	**0.600**	**1.47E+10**	Estimated
Propane	HC3	2.900	7.09E+10	Mean value of UBA measurements oct. 2001 [2]
n-Butane	HC3	10.340	2.53E+11	Mean value of UBA measurements oct. 2001 [2]
Isobutane	HC3	4.690	1.15E+11	Mean value of UBA measurements oct. 2001 [2]
Σ Aliphatic k_{OH}<3.4E-12	HC3	**17.930**	**4.39E+11**	---
Isopentane	HC5	6.130	1.50 E+11	Mean value of UBA measurements oct. 2001 [2]
n-Hexane	HC5	0.810	1.98 E+10	Mean value of UBA measurements oct. 2001 [2]
n-Pentane	HC5	2.400	5.87E+10	Mean value of UBA measurements oct. 2001 [2]
2-Methylpentane	HC5	1.930	4.72E+10	Mean value of UBA measurements oct. 2001 [2]
3- Methylpentane	HC5	1.130	2.76E+10	Mean value of UBA measurements oct. 2001 [2]
Σ Aliphatic 3.4E-12<k_{OH}<6.8E-12	HC5	**12.400**	**3.03E+11**	---
n-Heptane	HC8	0.380	9.30E+09	Mean value of UBA measurements oct. 2001 [2]
Σ Aliphatic k_{OH}>3.4E-12	HC8	**0.380**	**9.30E+09**	---
Ethene	ETE	**1.010**	**2.47E+10**	Mean value of UBA measurements oct. 2001 [2]
Propene	OLT	0.350	8.56E+09	Mean value of UBA measurements oct. 2001 [2]

Chemical gas phase composition 27-10-01 09:00 UTC (E I)				
Gas phase species	RACM species	Concentration [ppb]	Concentration [molec.cm^{-3}] (p=950.2 hPa, T=281.35 K)	Remarks
1-Butene	OLT	0.860	2.10E+10	Mean value of UBA measurements oct. 2001 [2]
Σ OLT	OLT	**1.210**	**2.96E+10**	---
Cresol …	CSL	**0.001**	**2.45E+07**	urban case
Methyl hydrogen peroxide	OP1	**1.000**	**2.45E+10**	urban case
higher organic peroxides	OP2	**0.100**	**2.45E+09**	urban case
Peroxy acetyl acid	PAA	**0.001**	**2.45E+07**	urban case
Methanol	CH3OH	**5.000**	**1.22E+11**	urban case
Ethanol	ETOH	**1.000**	**2.45E+10**	urban case
α-Pinene …	API	**0.040**	**9.78E+08**	urban case
d-Limonen …	LIM	**0.020**	**4.89E+08**	urban case
Toluene	TOL	2.830	6.92E+10	Mean value of UBA measurements oct. 2001 [2]
Benzene	TOL	0.610	1.49E+10	Mean value of UBA measurements oct. 2001 [2]
Ethyl benzene	TOL	0.590	1.44E+10	Mean value of UBA measurements oct. 2001 [2]
Σ TOL	TOL	**4.030**	**9.85E+10**	---
Xylene	XYL	**2.400**	**5.87E+10**	Mean value of UBA measurements oct. 2001 [2]
Ethane	ETH	**1.390**	**3.40E+10**	Mean value of UBA measurements oct. 2001 [2]
Formaldehyde	HCHO	**1.171**	**2.86E+10**	Measured by IfT [2]
Isoprene	ISO	**0.530**	**1.30E+10**	Mean value of UBA measurements oct. 2001 [2]
Peroxy acetyl nitrate …	PAN	**0.500**	**1.23E+10**	urban case
Water vapour	[H2O]	**20000000**	**4.89E+17**	urban case
Oxygen	[O2]	**200000000**	**4.89E+18**	urban case
Nitrogen	[N2]	**780000000**	**1.91E+19**	urban case

Table A II: Derived initial gas phase composition of the upwind site for the cloud event E II (08-10-2001 02:00 UTC).

Chemical gas phase composition 08-10-01 02:00 UTC (E II)				
Gas phase species	RACM species	Concentration [ppb]	Concentration [molec.cm^{-3}] (p=940.4 hPa, T=284.8 K)	Remarks
Sulphur dioxide	SO2	**0.262**	**6.27E+09**	Measured by BTU [1]
Carbon monoxide	CO	**300.000**	**7.18E+12**	urban case
Nitrogen monoxide	NO	**0.000**	**2.39E+06**	Measured by BTU [1]
Nitrogen dioxide	NO2	**2.488**	**5.95E+10**	Measured by BTU [1]
Ozone	O3	**25.806**	**6.17E+11**	Measured by BTU [1]
Nitrous acid	HONO	**0.038**	**9.09E+08**	Measured by BTU [1]
Nitric acid	HNO3	**0.064**	**1.53E+09**	Measured by BTU [1]
Formic acid	ORA1	**0.145**	**3.47E+09**	Measured by TUD [2]
Acetic acid	ORA2	0.225	5.39E+09	Measured by TUD [2]
Propionic acid	ORA2	0.000	0.00E+00	Measured by TUD [2]
Butyric acid	ORA2	0.000	0.00E+00	Measured by TUD [2]
Σ ORA2	ORA2	**0.225**	**5.39E+09**	---
Glyoxal	GLY	**0.009**	**2.04E+08**	Measured by TUD [2]
Methyl glyoxal	MGLY	**0.053**	**1.28E+09**	Measured by TUD [2]
Acetaldehyde	ALD	0.301	7.20E+09	Measured by IfT [2]
Propanal	ALD	0.021	5.09E+08	Measured by IfT [2]
Butanal	ALD	0.037	8.76E+08	Measured by IfT [2]
Pentanal	ALD	0.000	0.00E+00	Measured by IfT [2]
Hexanal	ALD	0.027	6.35E+08	Measured by IfT [2]
Heptanal	ALD	0.000	0.00E+00	Measured by IfT [2]
Octanal	ALD	0.009	2.05E+08	Measured by IfT [2]
Nonanal	ALD	0.014	3.26E+08	Measured by IfT [2]
Decanal	ALD	0.000	0.00E+00	Measured by IfT [2]
Benzaldehyde	ALD	0.010	2.47E+08	Measured by TUD [2]
m-Toluylaldehyde	ALD	0.006	1.49E+08	Measured by TUD [2]
p-Toluylaldehyde	ALD	0.000	0.00E+00	Measured by TUD [2]
Acrolein	MACR	0.018	4.42E+08	Measured by TUD [2]
Methacrolein	MACR	0.012	2.81E+08	Measured by TUD [2]
Crotonaldehyde	MACR	0.006	1.53E+08	Measured by TUD [2]
Σ MACR	MACR	**0.037**	**8.77E+08**	---
Glycolaldehyde	ALD	0.055	1.31E+09	Measured by TUD [2]
Isobutanal	ALD	0.002	3.64E+07	Measured by TUD [2]
Isovaleraldehyde	ALD	0.000	0.00E+00	Measured by IfT [2]
Undecanal	ALD	0.000	0.00E+00	Measured by IfT [2]
Dodecanal	ALD	0.000	0.00E+00	Measured by IfT [2]
Pinonaldehyde	ALD	0.000	0.00E+00	Measured by IfT [2]
Dimethylbenzaldehyde	ALD	0.000	0.00E+00	Measured by IfT [2]
Σ ALD	ALD	**0.480**	**1.15E+10**	---
Acetone	KET	0.259	6.19E+09	Measured by IfT [2]
Cyclohexanone	KET	0.000	0.00E+00	Measured by IfT [2]
Diacetyl	KET	0.000	0.00E+00	Measured by TUD [2]
Methylvinylketone	KET	0.000	0.00E+00	Measured by TUD [2]
2-Pentanone	KET	0.005	1.28E+08	Measured by TUD [2]
3-Pentanone	KET	0.007	1.77E+08	Measured by TUD [2]
3-Hexanone	KET	0.007	1.74E+08	Measured by TUD [2]
Methyl ethyl ketone	KET	0.082	1.96E+09	Measured by IfT [2]
Σ KET	KET	**0.361**	**8.63E+09**	---
Hydroxy acetone	HKET	**0.024**	**5.84E+08**	Measured by TUD [2]

Chemical gas phase composition 08-10-01 02:00 UTC (E II)				
Gas phase species	RACM species	Concentration [ppb]	Concentration [molec.cm^{-3}] (p=940.4 hPa, T=284.8 K)	Remarks
Methane	CH4	**1700.000**	**4.07E+13**	urban case
Hydrogen peroxide	H2O2	**0.060**	**1.42E+09**	Estimated (respectively to ZUF measurements 2002 [1])
Hydrogen	H2	**500.000**	**1.20E+13**	urban case
Hydrogen chloride	HCL	**0.012**	**5.82E+08**	Measured by BTU [1]
Ammonia	NH3	**0.600**	**1.43E+10**	Estimated
Propane	HC3	9.108	2.18E+11	Measured by UBA [2]
n-Butane	HC3	18.720	4.47E+11	Measured by UBA [2]
Isobutane	HC3	8.484	2.03E+11	Measured by UBA [2]
Σ Aliphatic k_{OH}<3.4E-12	HC3	**3.631**	**8.67E+11**	---
Isopentane	HC5	2.232	5.33E+10	Measured by UBA [2]
n-Hexane	HC5	0.402	9.61E+09	Measured by UBA [2]
n-Pentane	HC5	0.921	2.20E+10	Measured by UBA [2]
2-Methylpentane	HC5	0.897	2.14E+10	Measured by UBA [2]
3- Methylpentane	HC5	0.531	1.27E+10	Measured by UBA [2]
Σ Aliphatic 3.4E-12<k_{OH}<6.8E-12	HC5	**4.980**	**1.19E+11**	---
n-Heptane	HC8	0.272	6.50E+09	Measured by UBA [2]
Σ Aliphatic k_{OH}>3.4E-12	HC8	**0.272**	**6.50E+09**	---
Ethene	ETE	**0.867**	**2.07E+10**	Measured by UBA [2]
Propene	OLT	0.193	4.61E+09	Measured by UBA [2]
1-Butene	OLT	0.317	7.58E+09	Measured by UBA [2]
Σ OLT	OLT	**0.510**	**1.22E+10**	---
Cresol …	CSL	**0.001**	**2.39E+07**	urban case
Methyl hydrogen peroxide	OP1	**1.000**	**2.39E+10**	urban case
higher organic peroxides	OP2	**0.100**	**2.39E+09**	urban case
Peroxy acetyl acid …	PAA	**0.001**	**2.39E+07**	urban case
Methanol	CH3OH	**5.000**	**1.20E+11**	urban case
Ethanol	ETOH	**1.000**	**2.39E+10**	urban case
α-Pinene …	API	**0.040**	**9.57E+08**	urban case
d-Limonen …	LIM	**0.020**	**4.78E+08**	urban case
Toluene	TOL	1.809	4.32E+10	Measured by UBA [2]
Benzene	TOL	0.336	8.03E+09	Measured by UBA [2]
Ethyl benzene	TOL	0.366	8.75E+09	Measured by UBA [2]
Σ TOL	TOL	**2.511**	**6.00E+10**	---
Xylene	XYL	**2.400**	**5.74E+10**	Measured by UBA [2]
Ethane	ETH	**1.198**	**2.86E+10**	Measured by UBA [2]
Formaldehyde	HCHO	**0.456**	**1.09E+10**	Measured by IfT [2]
Isoprene	ISO	**0.530**	**1.27E+10**	Measured by UBA [2]
Peroxy acetyl nitrate …	PAN	**0.500**	**1.20E+10**	urban case
Water vapour	[H2O]	**20000000.000**	**4.78E+17**	urban case
Oxygen	[O2]	**200000000.000**	**4.78E+18**	urban case
Nitrogen	[N2]	**780000000.000**	**1.87E+19**	urban case

Table A III: Derived initial gas phase composition of the upwind site for the cloud event E III (17-10-2002 01:00 UTC).

Chemical gas phase composition 17-10-02 01:00 UTC (E III)				
Gas phase species	RACM species	Concentration [ppb]	Concentration [molec.cm^{-3}] (p=931.7 hPa, T=283.3 K)	Remarks
Sulphur dioxide	SO2	**0.634**	**1.51E+10**	Measured by BTU [1]
Carbon monoxide	CO	**185.929**	**4.43E+12**	Measured by IfT [1]
Nitrogen monoxide	NO	**0.000**	**0.00E+00**	Measured by BTU [1]
Nitrogen dioxide	NO2	**1.769**	**4.21E+10**	Measured by BTU [1]
Ozone	O3	**32.631**	**7.77E+11**	Measured by BTU [1]
Nitrous acid	HONO	**0.055**	**1.31E+09**	Measured by BTU [1]
Nitric acid	HNO3	**0.255**	**6.06E+09**	Measured by BTU [1]
Formic acid	ORA1	**0.108**	**2.57E+09**	Measured by TUD [2]
Acetic acid	ORA2	0.072	1.71E+09	Measured by TUD [2]
Propionic acid	ORA2	0.000	0.00E+00	Measured by TUD [2]
Butyric acid	ORA2	0.000	0.00E+00	Measured by TUD [2]
Σ ORA2	ORA2	**0.072**	**1.71E+09**	---
Glyoxal	GLY	**0.004**	**9.39E+07**	Measured by TUD [2]
Methyl glyoxal	MGLY	**0.016**	**3.73E+08**	Measured by TUD [2]
Acetaldehyde	ALD	0.221	5.25E+09	Measured by IfT [2]
Propanal	ALD	0.012	2.85E+08	Measured by IfT [2]
Butanal	ALD	0.000	0.00E+00	Measured by IfT [2]
Pentanal	ALD	0.014	3.23E+08	Measured by IfT [2]
Hexanal	ALD	0.027	6.41E+08	Measured by IfT [2]
Heptanal	ALD	0.030	7.08E+08	Measured by IfT [2]
Octanal	ALD	0.022	5.13E+08	Measured by IfT [2]
Nonanal	ALD	0.048	1.14E+09	Measured by IfT [2]
Decanal	ALD	0.056	1.34E+09	Measured by IfT [2]
Benzaldehyde	ALD	0.002	3.59E+07	Measured by TUD [2]
m-Toluylaldehyde	ALD	0.002	4.98E+07	Measured by TUD [2]
p-Toluylaldehyde	ALD	0.000	0.00E+00	Measured by TUD [2]
Acrolein	MACR	0.008	1.99E+08	Measured by TUD [2]

Chemical gas phase composition 17-10-02 01:00 UTC (E III)				
Gas phase species	RACM species	Concentration [ppb]	Concentration [molec.cm^{-3}] (p=931.7 hPa, T=283.3 K)	Remarks
Methacrolein	MACR	0.001	3.30E+07	Measured by TUD [2]
Crotonaldehyde	MACR	0.005	1.19E+08	Measured by TUD [2]
Σ MACR	MACR	**0.015**	**3.51E+08**	---
Glycolaldehyde	ALD	0.007	1.75E+08	Measured by TUD [2]
Isobutanal	ALD	0.000	0.00E+00	Measured by TUD [2]
Isovaleraldehyde	ALD	0.018	4.39E+08	Measured by IfT [2]
Undecanal	ALD	0.003	6.01E+07	Measured by IfT [2]
Dodecanal	ALD	0.001	1.62E+07	Measured by IfT [2]
Pinonaldehyde	ALD	0.000	0.00E+00	Measured by IfT [2]
Dimethylbenzaldehyde	ALD	0.000	0.00E+00	Measured by IfT [2]
Σ ALD	ALD	**0.461**	**1.10E+10**	---
Acetone	KET	0.235	5.59E+09	Measured by IfT [2]
Cyclohexanone	KET	0.052	1.23E+09	Measured by IfT [2]
Diacetyl	KET	0.004	9.03E+07	Measured by TUD [2]
Methylvinylketone	KET	0.003	8.28E+07	Measured by TUD [2]
2-Pentanone	KET	0.005	1.15E+08	Measured by TUD [2]
3-Pentanone	KET	0.003	7.78E+07	Measured by TUD [2]
3-Hexanone	KET	0.000	0.00E+00	Measured by TUD [2]
Methylethylketone	KET	0.000	0.00E+00	Measured by IfT [2]
Σ KET	KET	**0.302**	**7.18E+09**	---
Hydroxyacetone	HKET	**0.005**	**1.17E+08**	Measured by TUD [2]
Methane	CH4	**1700.000**	**4.05E+13**	urban case
Hydrogen peroxide	H2O2	**0.085**	**2.03E+09**	Measured by ZUF [1]
Hydrogen	H2	**500.000**	**1.19E+13**	urban case
Hydrogen chloride	HCL	**0.092**	**2.19E+09**	Measured by BTU [1]
Ammonia	NH3	**0.200**	**4.76E+09**	Estimated
Propane	HC3	0.748	1.78E+10	Mean value of UBA measurements oct. 2002
n-Butane	HC3	0.310	7.38E+09	Mean value of UBA measurements oct. 2002
Isobutane	HC3	0.207	4.93E+09	Mean value of UBA measurements oct. 2002
Σ Aliphatic k_{OH}<3.4E-12	HC3	**1.265**	**3.01E+10**	---
Isopentane	HC5	0.251	5.97 E+09	Mean value of UBA measurements oct. 2002
n-Hexane	HC5	0.048	1.14 E+09	Mean value of UBA measurements oct. 2002
n-Pentane	HC5	0.199	4.74E+09	Mean value of UBA measurements oct. 2002
2-Methylpentane	HC5	0.082	1.95E+09	Mean value of UBA measurements oct. 2002
3- Methylpentane	HC5	0.047	1.14 E+09	Mean value of UBA measurements oct. 2002
Σ Aliphatic 3.4E-12<k_{OH}<6.8E-12	HC5	**0.627**	**1.49E+10**	---
n-Heptane	HC8	0.025	5.95E+08	Mean value of UBA measurements oct. 2002
Σ Aliphatic k_{OH}>3.4E-12	HC8	**0.025**	**5.95E+08**	---
Ethene	ETE	**0.798**	**1.90E+10**	Mean value of UBA measurements oct. 2002
Propene	OLT	0.150	3.57E+09	Mean value of UBA measurements oct. 2002
1-Butene	OLT	0.033	7.85E+08	Mean value of UBA measurements oct. 2002
Σ OLT	OLT	**0.183**	**4.36E+09**	---
Cresol	CSL	**0.001**	**2.38E+07**	urban case
Methyl hydrogen peroxide	OP1	**1.000**	**2.38E+10**	urban case
higher organic peroxides	OP2	**0.100**	**2.38E+09**	urban case
Peroxy acetyl acid ...	PAA	**0.001**	**2.38E+07**	urban case
Methanol	CH3OH	**5.000**	**1.19E+11**	urban case
Ethanol	ETOH	**1.000**	**2.38E+10**	urban case
α-Pinene …	API	**0.040**	**9.53E+08**	urban case
d-Limonen …	LIM	**0.020**	**4.76E+08**	urban case
Toluene	TOL	0.238	5.66E+09	Mean value of UBA measurements oct. 2002
Benzene	TOL	0.220	5.24E+09	Mean value of UBA measurements oct. 2002
Ethylbenzene	TOL	0.041	9.76E+08	Mean value of UBA measurements oct. 2002
Σ TOL	TOL	**0.499**	**1.19E+10**	---
Xylene	XYL	**0.130**	**3.09E+09**	Mean value of UBA measurements oct. 2002
Ethane	ETH	**1.524**	**3.63E+10**	Mean value of UBA measurements oct. 2002
Formaldehyde	HCHO	**0.343**	**1.09E+10**	Measured by IfT [2]
Isoprene	ISO	**0.021**	**5.00E+08**	Mean value of UBA measurements oct. 2002
Peroxy acetyl nitrate …	PAN	**0.500**	**1.19E+10**	urban case
Water vapour	[H2O]	**20000000.000**	**4.78E+17**	urban case
Oxygen	[O2]	**200000000.000**	**4.78E+18**	urban case
Nitrogen	[N2]	**780000000.000**	**1.87E+19**	urban case

Remarks to Table A I-III:

IfT Leibniz-Institut für Troposphärenforschung, Permoserstr. 15, 04318 Leipzig, Germany.

BTU Brandenburgische Technische Universität Cottbus, Lehrstuhl für Luftchemie und Luftreinhaltung, Volmer Str.13, 12489 Berlin, Germany.

ZUF Johann-Wolfgang-Goethe Universität Frankfurt, Zentrum für Umweltforschung, Georg-Voigt-Str. 14, 60325 Frankfurt a.M., Germany.

TUD Technische Universität Darmstadt. Institut für Anorganische Chemie, Petersenstrasse 18, 64287 Darmstadt, Germany.

UBA Umweltbundesamt Messstelle Schmücke 98559 Gehlberg, Germany.

[1] **Gnauk**, T., Brüggemann, E., Müller, K., Chemnitzer, R., Rüd, C., Galgon, D., Wiedensohler, A., Acker, K., Auel, R., Wieprecht, W., Möller, D., Jaeschke, W., Herrmann, H., 2005. Aerosol characterisation at the FEBUKO upwind station Goldlauter (I): Particle mass, main ionic components, OC/EC, and mass closure. Atmospheric Environment (this issue).

[2] **Müller**, K., van Pinxteren, D., Plewka, A., Svrcina, B., Kramberger, H., Hofmann, D., Bächmann, K., Herrmann, H., 2005. Aerosol characterisation at the FEBUKO upwind station Goldlauter (II): Detailed organic chemical characterisation. Atmospheric Environment (this issue).

Table A IV: Derived size resolved initial aerosol particle composition at the upwind site for the cloud event E I (27-10-2001 09:00 UTC).

Chemical composition of the aerosol particles [µg m^{-3}]						
Chemical Components	**FEBUKO 26./27-10-2001 (E I)**					
	total	Berner impactor stages (aerodynamic diameter)				
		1	2	3	4	5
		0.05 - 0.14 µm	0.14 - 0.42 µm	0.42 - 1.2 µm	1.2 - 3.5 µm	3.5 - 10 µm
Water soluble organic carbon [WSOC] (without dicarboxylic acids)	1.247222	0.098906	0.289209	0.618686	0.152697	0.087723
Water insoluble organic carbon [WISOC]	0.850200	0.062400	0.195000	0.436800	0.101400	0.054600
Elemental cabon [EC]	1.000000	0.080000	0.360000	0.430000	0.100000	0.030000
Sulfate [$SO4^{2-}$]	2.100190	0.046650	0.489350	1.475690	0.075150	0.013350
Nitrate [NO_3^-]	5.355280	0.007552	0.841889	3.941419	0.481956	0.082464
Nitrite [NO_2^-]	0.091000	0.005014	0.019431	0.051425	0.011915	0.003215
Chloride [Cl^-]	0.094196	0.000000	0.013898	0.068607	0.011692	0.000000
Oxalate dianion [$(C_2O_4)^{2-}$]	0.052670	0.002390	0.011916	0.030969	0.007395	0.000000
Malonate monoanion [$(C_3H_3O_4)^-$]	0.020201	0.000000	0.003510	0.013388	0.002663	0.000640
Succinate monoanion [$(C_4H_5O_4)^-$]	0.008350	0.000153	0.001390	0.005982	0.000642	0.000183
Succinate Isomers monoanion [$(C_4H_5O_4)^-$]	0.012226	0.000224	0.002035	0.008759	0.000941	0.000268
Glutarate monoanion [$(C_5H_7O_4)^-$]	0.000890	0.000000	0.000228	0.000662	0.000000	0.000000
Glutarate Isomers monoanion [$(C_5H_7O_4)^-$]	0.022167	0.000000	0.005670	0.016497	0.000000	0.000000
Tartronate monoanion [$(C_3H_3O_5)^-$]	0.003845	0.000000	0.000974	0.002870	0.000000	0.000000
Malate monoanion [$(C_4H_5O_5)^-$]	0.010864	0.000516	0.001991	0.006549	0.001158	0.000650
Tartrate monoanion [$(C_4H_5O_6)^-$]	0.004515	0.000000	0.001182	0.003333	0.000000	0.000000
Citramalate monoanion [$(C_5H_7O_5)^-$]	0.001672	0.000000	0.000000	0.001672	0.000000	0.000000
Maleinate monoanion [$(C_4H_3O_4)^-$]	0.006759	0.000000	0.001080	0.005275	0.000404	0.000000
Suberate monoanion [$(C_8H_{13}O_4)^-$]	0.001580	0.000087	0.000337	0.000893	0.000207	0.000056
Acetate monoanion [$(C_9H_{15}O_4)^-$]	0.002240	0.000123	0.000478	0.001266	0.000293	0.000079
Ammonium [$NH4^+$]	1.290530	0.025910	0.326420	0.810960	0.117760	0.009480
Manganese [Mn^{3+}]	0.000750	0.000041	0.000160	0.000424	0.000098	0.000026
Iron [Fe^{3+}]	0.003740	0.000206	0.000799	0.002114	0.000490	0.000132
Cupper [Cu^{2+}]	0.002990	0.000165	0.000638	0.001690	0.000391	0.000106
Sodium [Na^+]	0.095320	0.000000	0.001190	0.004770	0.066630	0.022730
Potassium [K^+]	0.072480	0.003060	0.019590	0.036540	0.010210	0.003080
Calcium [Ca^{2+}]	0.049830	0.000490	0.000000	0.001810	0.027030	0.020500
Magnesium [Mg^{2+}]	0.017480	0.000000	0.000000	0.001220	0.010600	0.005660
Aluminium [Al^{3+}]	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Zinc [Zn^{2+}]	0.008230	0.000453	0.001757	0.004651	0.001078	0.000291
Unknown residual mass	2.886634	0.443779	0.808556	1.112762	0.442748	0.078790
Dry mass (total)	**15.314049**	**0.778120**	**3.398678**	**9.097681**	**1.625547**	**0.414023**
Soluble dry mass (total)	**10.577216**	**0.191941**	**2.035123**	**7.118119**	**0.981399**	**0.250633**
Insoluble dry mass (total)	**4.736834**	**0.586179**	**1.365558**	**1.979562**	**0.644148**	**0.163390**
Water mass	**5.040775**	**0.160974**	**0.703102**	**2.961722**	**0.968344**	**0.246635**
Total mass	**20.354824**	**0.939094**	**4.101780**	**12.059402**	**2.593891**	**0.660657**

Table A V: Derived size resolved initial aerosol particle composition of the upwind site for the cloud event E II (07/08-10-2001 02:00 UTC).

Chemical composition of the aerosol particles [µg m^{-3}]						
Chemical Components	**FEBUKO (06-08)-10-2001 (E II)**					
	total	Berner impactor stages (aerodynamic diameter)				
		1	2	3	4	5
		0.05 - 0.14 µm	0.14 - 0.42 µm	0.42 - 1.2 µm	1.2 - 3.5 µm	3.5 - 10 µm
Water soluble organic carbon [WSOC] (without dicarboxylic acids)	1.270384	0.077463	0.466309	0.428352	0.137906	0.160354
Water insoluble organic carbon [WISOC]	0.830542	0.048935	0.302152	0.291526	0.088877	0.099051
Elemental cabon [EC]	0.446885	0.076681	0.136778	0.173010	0.025764	0.034652
Sulfate [$SO4^{2-}$]	1.366650	0.045640	0.490530	0.777150	0.042840	0.010490
Nitrate [NO_3^-]	1.634862	0.001792	0.391502	1.105402	0.098982	0.037185
Nitrite [NO_2^-]	0.058000	0.003621	0.018625	0.025108	0.005626	0.005020
Chloride [Cl^-]	0.052008	0.009406	0.000000	0.000000	0.008299	0.034303
Oxalate dianion [$(C_2O_4)^{2-}$]	0.037799	0.002212	0.011982	0.019209	0.003953	0.000444
Malonate monoanion [$(C_3H_3O_4)^-$]	0.010990	0.000000	0.002613	0.006713	0.001305	0.000359
Succinate monoanion [$(C_4H_5O_4)^-$]	0.003463	0.000107	0.000868	0.002163	0.000264	0.000061
Succinate Isomers monoanion [$(C_4H_5O_4)^-$]	0.003623	0.000111	0.000909	0.002263	0.000276	0.000064
Glutarate monoanion [$(C_5H_7O_4)^-$]	0.000250	0.000000	0.000101	0.000149	0.000000	0.000000
Glutarate Isomers monoanion [$(C_5H_7O_4)^-$]	0.014849	0.000000	0.005974	0.008876	0.000000	0.000000
Tartronate monoanion [$(C_3H_3O_5)^-$]	0.001882	0.000000	0.000751	0.001131	0.000000	0.000000
Malate monoanion [$(C_4H_5O_5)^-$]	0.010828	0.000298	0.002725	0.004728	0.001970	0.001106
Tartrate monoanion [$(C_4H_5O_6)^-$]	0.003863	0.000000	0.001666	0.002197	0.000000	0.000000
Citramalate monoanion [$(C_5H_7O_5)^-$]	0.001990	0.000000	0.000833	0.001157	0.000000	0.000000
Maleinate monoanion [$(C_4H_3O_4)^-$]	0.001207	0.000000	0.000528	0.000679	0.000000	0.000000
Suberate monoanion [$(C_8H_{13}O_4)^-$]	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Acetate monoanion [$(C_9H_{15}O_4)^-$]	0.001813	0.000113	0.000582	0.000785	0.000176	0.000157
Ammonium [$NH4^+$]	0.598790	0.020740	0.219820	0.336020	0.017630	0.004580
Manganese [Mn^{3+}]	0.000980	0.000061	0.000315	0.000424	0.000095	0.000085
Iron [Fe^{3+}]	0.005360	0.000335	0.001721	0.002320	0.000520	0.000464
Cupper [Cu^{2+}]	0.002440	0.000152	0.000784	0.001056	0.000237	0.000211
Sodium [Na^+]	0.033980	0.000210	0.002960	0.005840	0.019560	0.005410
Potassium [K^+]	0.053180	0.002380	0.016730	0.022610	0.007600	0.003860
Calcium [Ca^{2+}]	0.026880	0.000560	0.003820	0.003740	0.010800	0.007960
Magnesium [Mg^{2+}]	0.005830	0.000000	0.000000	0.000600	0.003370	0.001860
Aluminium [Al^{3+}]	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Zinc [Zn^{2+}]	0.005360	0.000335	0.001721	0.002320	0.000520	0.000464
Unknown residual mass	0.787370	0.139152	0.328524	0.138593	0.090075	0.091026
Dry mass (total)	**7.272058**	**0.430303**	**2.411823**	**3.364122**	**0.566643**	**0.499167**
Soluble dry mass (total)	**5.207261**	**0.165535**	**1.644368**	**2.760993**	**0.361928**	**0.274437**
Insoluble dry mass (total)	**2.064797**	**0.264768**	**0.767454**	**0.603129**	**0.204715**	**0.224730**
Water mass	**2.318051**	**0.089019**	**0.498946**	**1.095180**	**0.337551**	**0.297355**
Total mass	**9.590109**	**0.519322**	**2.910769**	**4.459302**	**0.904194**	**0.796522**

Table A VI: Derived size resolved initial aerosol particle composition of the upwind site for the cloud event E III (16/17-10-2002 01:00 UTC).

Chemical composition of the aerosol particles [µg m^{-3}]						
Chemical Components	**FEBUKO (16/17)-10-2002 (E III)**					
	total	Berner impactor stages (aerodynamic diameter)				
		1	2	3	4	5
		0.05 - 0.14 µm	0.14 - 0.42 µm	0.42 - 1.2 µm	1.2 - 3.5 µm	3.5 - 10 µm
Water soluble organic carbon [WSOC] (without dicarboxylic acids)	1.290674	0.166362	0.320869	0.307269	0.259616	0.236558
Water insoluble organic carbon [WISOC]	0.830090	0.102260	0.208594	0.204349	0.168692	0.146194
Elemental cabon [EC]	0.405714	0.046422	0.191456	0.105469	0.027918	0.034449
Sulfate [$SO4^{2-}$]	1.069914	0.022526	0.500565	0.479921	0.050261	0.016641
Nitrate [NO_3^-]	0.776242	0.002727	0.226114	0.190845	0.302970	0.053586
Nitrite [NO_2^-]	0.029500	0.001918	0.010345	0.007964	0.005765	0.003508
Chloride [Cl^-]	0.054681	0.000000	0.002512	0.000001	0.031755	0.020414
Oxalate dianion [$(C_2O_4)^{2-}$]	0.027675	0.000000	0.007271	0.012665	0.007740	0.000000
Malonate monoanion [$(C_3H_3O_4)^-$]	0.006188	0.000000	0.001666	0.002737	0.001785	0.000000
Succinate monoanion [$(C_4H_5O_4)^-$]	0.008375	0.000000	0.002888	0.003754	0.001733	0.000000
Succinate Isomers monoanion [$(C_4H_5O_4)^-$]	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Glutarate monoanion [$(C_5H_7O_4)^-$]	0.002288	0.000149	0.000802	0.000618	0.000447	0.000272
Glutarate Isomers monoanion [$(C_5H_7O_4)^-$]	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Tartronate monoanion [$(C_3H_3O_5)^-$]	0.000300	0.000000	0.000000	0.000300	0.000000	0.000000
Malate monoanion [$(C_4H_5O_5)^-$]	0.005900	0.000000	0.001400	0.002200	0.001600	0.000700
Tartrate monoanion [$(C_4H_5O_6)^-$]	0.000800	0.000000	0.000400	0.000400	0.000000	0.000000
Citramalate monoanion [$(C_5H_7O_5)^-$]	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Maleinate monoanion [$(C_4H_3O_4)^-$]	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Suberate monoanion [$(C_8H_{13}O_4)^-$]	0.001975	0.000128	0.000693	0.000533	0.000386	0.000235
Acetate monoanion [$(C_9H_{15}O_4)^-$]	0.018025	0.001172	0.006321	0.004866	0.003522	0.002144
Ammonium [$NH4^+$]	0.561809	0.009612	0.277571	0.251525	0.021240	0.001860
Manganese [Mn^{3+}]	0.001340	0.000087	0.000470	0.000362	0.000262	0.000159
Iron [Fe^{3+}]	0.003170	0.000206	0.001112	0.000856	0.000619	0.000377
Cupper [Cu^{2+}]	0.004170	0.000271	0.001462	0.001126	0.000815	0.000496
Sodium [Na^+]	0.146956	0.000000	0.000155	0.016176	0.102067	0.028558
Potassium [K^+]	0.038475	0.000000	0.012145	0.011525	0.009457	0.005349
Calcium [Ca^{2+}]	0.007339	0.000000	0.000000	0.000000	0.007339	0.000000
Magnesium [Mg^{2+}]	0.069984	0.007235	0.010129	0.012713	0.026977	0.012930
Aluminium [Al^{3+}]	0.010020	0.000651	0.003514	0.002705	0.001958	0.001192
Zinc [Zn^{2+}]	0.017530	0.001140	0.006147	0.004733	0.003426	0.002085
Unknown residual mass	0.882325	0.076496	0.627750	0.080743	0.040429	0.056905
Dry mass (total)	**6.271458**	**0.439362**	**2.422349**	**1.706355**	**1.078779**	**0.624613**
Soluble dry mass (total)	**4.153329**	**0.214184**	**1.394549**	**1.315793**	**0.841739**	**0.387064**
Insoluble dry mass (total)	**2.118129**	**0.225178**	**1.027800**	**0.390562**	**0.237040**	**0.237549**
Water mass	**2.162231**	**0.090893**	**0.501123**	**0.555499**	**0.642632**	**0.372084**
Total mass	**8.433688**	**0.530255**	**2.923473**	**2.261853**	**1.721410**	**0.996697**

E. Literature

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