AEROSOL CHARACTERISATION AT THE FEBUKO UPWIND STATION GOLDLAUTER (II): DETAILED ORGANIC CHEMICAL CHARACTERISATION

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ELECTRONIC SUPPLEMENTAL MATERIAL

Table 1: Concentrations of monocarboxylic acids at the upwind site during FEBUKO (all data in pptV)

start time (UTC)	sampling time (min)	formic acid	acetic acid	propionic acid	butyric acid
Event I					
26.10.2001 22:00	120	179	145	bdl	20
27.10.2001 00:06	114	139	95	bdl	bdl
27.10.2001 02:05	115	138	78	bdl	bdl
27.10.2001 04:09	111	197	168	bdl	20
27.10.2001 06:05	115	201	122	bdl	bdl
27.10.2001 08:05	115	180	257	bdl	bdl
27.10.2001 10:05	115	292	329	20	23
27.10.2001 12:04	116	408	391	26	29
Event II					
07.10.2001 20:00	120	249	224	20	22
07.10.2001 22:09	111	164	207	bdl	bdl
08.10.2001 00:07	113	133	200	bdl	bdl
08.10.2001 02:07	126	145	225	bdl	bdl
08.10.2001 04:20	100	151	178	bdl	bdl
08.10.2001 06:07	113	247	289	20	24
08.10.2001 08:05	115	312	417	23	41
08.10.2001 10:05	115	308	428	26	36
Event III					
16.10.2002 21:00	120	158	98	15	bdl
16.10.2002 23:00	120	122	83	bdl	bdl
17.10.2002 01:00	110	108	72	bdl	bdl
17.10.2002 03:00	79	139	91	bdl	bdl

bdl: concentration below analytical detection limit

Table 2: Concentrations of dicarboxylic acids at the upwind site during FEBUKO (all data in ng m^{-3})

start time (UTC)	sampling time (min)	oxalic acid	malonic acid	succinic acid	glutaric acid	suberic acid	azelaic acid
Event I							
26.10.2001 22:00	120	44.2	9.5	4.5	bdl	3.5	bdl
27.10.2001 00:06	114	63.2	10.2	4.4	bdl	bdl	bdl
27.10.2001 02:05	115	56.1	9.1	5.8	bdl	bdl	2.2
27.10.2001 04:09	111	55.8	8.4	5.6	bdl	bdl	bdl
27.10.2001 06:05	115	65.2	12.9	6.9	bdl	bdl	bdl
27.10.2001 08:05	115	80.1	21.2	12.2	2.2	2.8	3.3
27.10.2001 10:05	115	91.3	23.8	11.9	2.1	3.1	4.1
27.10.2001 12:04	116	104.4	23.1	15.5	2.8	3.2	8.3
Event II							
07.10.2001 20:00	120	22.5	5.1	bdl	bdl	bdl	bdl
07.10.2001 22:09	111	31.5	7.2	4.5	bdl	bdl	bdl
08.10.2001 00:07	113	28.3	5.3	4.0	bdl	bdl	bdl
08.10.2001 02:07	126	38.1	6.1	4.0	bdl	bdl	bdl
08.10.2001 04:20	100	27.5	6.2	bdl	bdl	bdl	bdl
08.10.2001 06:07	113	41.1	5.8	bdl	bdl	bdl	2.4
08.10.2001 08:05	115	68.9	11.2	6.5	bdl	bdl	4.1
08.10.2001 10:05	115	101.8	14.5	8.7	2.0	bdl	8.0
Event III							
16.10.2002 21:00	120	31.5	11.6	13.9	2.8	2.2	28.1
16.10.2002 23:00	120	39.0	7.3	6.8	2.4	1.9	18.6
17.10.2002 01:00	110	28.1	5.4	7.9	2.0	2.0	15.4
17.10.2002 03:00	79	28.4	4.4	4.9	2.0	1.8	10.0

bdl: concentration below analytical detection limit, NA: sample not available

Table 3: Size resolved concentrations of dicarboxylic acids at the upwind site during FEBUKO (all data in ng m^{-3})

	Compound	impactor stage 1 (0.05-0.14 µm)	impactor stage 2 (0.14-0.42 µm)	impactor stage 3 (0.42-1.2 µm)	impactor stage 4 (1.2-3.5 µm)	impactor stage 5 (3.5-10 µm)	sum (0.05-10 µm)
Event I	oxalate	1.6	8.0	20.8	5.0	bdl	35.3
	malonate	bdl	4.5	17.0	3.4	0.8	25.6
	succinate (incl. isomer)	0.4	3.4	14.7	1.6	0.5	20.6
	glutarate (incl. isomers)	bdl	5.9	17.2	bdl	bdl	23.1
	tartronate	bdl	1.0	2.9	bdl	bdl	3.8
	malate	0.5	2.0	6.5	1.2	0.7	10.9
	tartrate	bdl	1.2	3.3	bdl	bdl	4.5
	citramalate	bdl	bdl	1.7	bdl	bdl	1.7
	maleinate	bdl	1.1	5.3	0.4	bdl	6.8
Event II	oxalate	1.8	9.7	15.6	3.2	0.4	30.6
	malonate	bdl	3.4	8.7	1.7	0.5	14.3
	succinate (incl. isomer)	0.2	1.8	4.4	0.5	0.1	7.1
	glutarate (incl. isomers)	bdl	6.1	9.0	bdl	bdl	15.1
	tartronate	bdl	0.8	1.1	bdl	bdl	1.9
	malate	0.3	2.7	4.7	2.0	1.1	10.8
	tartrate	bdl	1.7	2.2	bdl	bdl	3.9
	citramalate	bdl	0.8	1.2	bdl	bdl	2.0
	maleinate	bdl	0.5	0.7	bdl	bdl	1.2
Event III	oxalate	bdl	6.2	10.8	6.6	bdl	23.6
	malonate	bdl	1.4	2.3	1.5	bdl	5.2
	succinate (incl. isomer)	bdl	1.0	1.3	0.6	bdl	2.9
	glutarate (incl. isomers)	bdl	bdl	bdl	bdl	bdl	bdl
	tartronate	bdl	bdl	0.3	bdl	bdl	0.3
	malate	bdl	1.4	2.2	1.6	0.7	5.9
	tartrate	bdl	0.4	0.4	bdl	bdl	0.8
	citramalate	bdl	bdl	bdl	bdl	bdl	bdl
	maleinate	bdl	bdl	bdl	bdl	bdl	bdl

bdl: concentration below analytical detection limit

Table 4: Carbonyl compounds at the upwind site during FEBUKO (all data in ppbv)

	UTC-mean time	FA	AA	AC	PA	MVK	CA	MEK	MACR	BU	BA	CHN	MPK	ISO
E I	26.10.01 23:00	0.858	0.482	0.389	0.060	0.008	0.009	0.114	0.016	0.042	0.030	0.035	0.014	0.033
	27.10.01 01:00	0.931	0.489	0.375	0.079	0.014	0.010	0.104	0.021	0.066	0.034	0.038	0.016	0.037
	27.10.01 03:00	0.750	0.445	0.440	0.082	0.010	0.012	0.130	0.026	0.055	0.034	0.045	0.014	0.038
	27.10.01 05:00	0.692	0.313	0.370	0.033	0.007	0.009	0.134	0.023	0.024	0.023	0.037	0.012	0.032
	27.10.01 07:00	0.738	0.348	0.376	0.061	0.007	0.009	0.139	0.018	0.026	0.025	0.034	0.010	0.036
	27.10.01 09:00	1.171	0.648	0.579	0.073	0.007	0.010	0.163	0.024	0.102	bdl	0.056	0.014	0.056
	27.10.01 11:00	1.474	0.835	0.507	0.137	0.011	0.009	0.156	0.018	0.206	0.081	0.064	0.018	0.077
	27.10.01 13:00	0.975	0.520	0.499	0.114	0.013	0.014	0.156	0.046	0.172	0.037	0.034	0.012	0.050
E II	07.10.01 19:00	0.382	0.368	0.241	0.014	bdl	0.027	0.094	0.015	0.043	0.025	bdl	bdl	0.013
	07.10.01 21:00	0.638	0.412	0.352	0.039	0.007	0.005	0.121	0.012	0.004	0.048	bdl	bdl	0.026
	07.10.01 23:00	1.207	0.719	0.303	0.086	0.011	0.006	0.112	0.018	0.008	0.176	0.025	0.029	0.036
	08.10.01 01:00	1.378	0.726	0.319	0.125	0.004	0.007	0.127	0.012	bdl	0.197	0.029	0.013	0.006
	08.10.01 03:00	0.456	0.301	0.259	0.021	bdl	0.006	0.082	0.012	0.009	0.002	bdl	bdl	bdl
	08.10.01 05:00	0.435	0.336	0.367	0.049	0.007	0.008	0.094	0.027	0.009	0.015	bdl	bdl	bdl
	08.10.01 07:00	0.535	0.461	0.407	0.054	0.008	0.006	0.101	0.016	bdl	0.013	bdl	bdl	0.029
	08.10.01 09:00	0.653	0.599	0.591	0.072	0.007	0.007	0.147	0.018	0.025	0.017	bdl	bdl	0.025
	08.10.01 11:00	0.909	0.674	0.651	0.078	0.023	0.020	0.155	0.025	0.045	0.025	bdl	bdl	0.024
E III	16.10.02 22:02	0.587	0.505	0.652	0.018	0.004	0.005	0.048	0.003	bdl	bdl	0.023	0.028	0.015
	17.10.02 00:02	0.360	0.277	0.292	bdl	0.004	0.004	0.056	0.004	0.006	bdl	0.021	0.035	0.009
	17.10.02 02:02	0.343	0.221	0.235	0.012	0.003	0.005	0.031	0.001	0.006	bdl	0.052	0.029	0.018
	17.10.02 04:02	0.174	0.122	0.304	bdl	0.008	0.005	0.103	bdl	0.013	bdl	0.021	0.019	0.008

FA- formaldehyde; AA- acetaldehyde; AC- acetone; PA- propionaldehyde; MVK- methyl vinyl ketone; CA- crotonaldehyde; MACR- methacroleine; BU- butyraldehyde; BA- benzaldehyde; CHN- cyclohexanone; ISO- iso-valeraldehyde (iso-pentanal)

Table 4: continued

	UTC-mean time	VA	m-TO	p-TO	HEX	MGX	HEP	Pinon	OCT	NON	DEC	UND	DOD
	26.10.01 23:00	0.020	0.008	0.008	0.041	0.020	0.040	0.011	0.017	0.057	0.020	0.007	bdl
	27.10.01 01:00	0.033	0.008	0.008	0.063	0.020	0.070	0.009	0.030	0.080	0.032	0.010	0.009
	27.10.01 03:00	0.028	0.007	0.007	0.048	0.021	0.047	0.014	0.028	0.071	0.039	0.006	0.006
E I	27.10.01 05:00	0.036	0.007	0.006	0.030	0.015	0.029	bdl	0.009	0.008	bdl	0.005	bdl
	27.10.01 07:00	0.018	0.008	0.008	0.028	0.022	0.034	0.020	0.057	0.024	bdl	bdl	bdl
	27.10.01 09:00	0.037	0.008	0.008	0.080	0.036	0.069	0.009	0.025	0.074	0.015	0.005	0.005
	27.10.01 11:00	0.048	0.009	bdl	0.113	0.060	0.095	0.009	0.043	0.137	0.039	0.014	0.010
	27.10.01 13:00	0.027	0.007	0.009	0.056	0.060	0.037	0.007	0.022	0.055	0.024	0.007	bdl
	07.10.01 19:00	bdl	bdl	bdl	0.037	bdl	0.019	bdl	0.010	0.024	bdl	bdl	bdl
	07.10.01 21:00	0.022	0.006	bdl	0.040	0.036	0.029	bdl	0.012	0.039	0.004	bdl	bdl
	07.10.01 23:00	0.043	0.013	bdl	0.133	0.055	0.045	bdl	0.057	0.172	0.061	bdl	bdl
	08.10.01 01:00	0.067	0.005	bdl	0.146	0.043	0.027	0.014	0.068	0.213	0.073	0.010	0.008
E II	08.10.01 03:00	bdl	0.006	bdl	0.027	0.053	0.017	bdl	0.009	0.014	bdl	bdl	bdl
	08.10.01 05:00	bdl	0.018	bdl	0.036	0.064	0.038	bdl	0.013	0.038	0.005	bdl	bdl
	08.10.01 07:00	bdl	0.006	bdl	0.030	0.077	0.028	bdl	0.015	0.035	0.006	bdl	bdl
	08.10.01 09:00	0.037	0.006	bdl	0.039	0.121	0.034	bdl	0.015	0.039	0.015	bdl	bdl
	08.10.01 11:00	0.026	0.005	bdl	0.059	0.147	0.039	bdl	0.032	0.087	0.025	bdl	bdl
	16.10.02 22:02	0.015	bdl	bdl	0.064	0.018	0.018	bdl	0.119	0.192	0.140	0.003	0.001
E III	17.10.02 00:02	0.001	bdl	bdl	0.009	0.015	0.015	bdl	0.009	0.041	0.032	0.003	bdl
	17.10.02 02:02	0.014	bdl	bdl	0.027	0.016	0.015	bdl	0.022	0.048	0.056	0.003	0.001
	17.10.02 04:02	0.008	0.002	bdl	0.018	0.019	0.014	bdl	0.009	0.036	0.038	0.001	bdl

VA- valeraldehyde (pentanal); m-TO- m-tolyaldehyde; p-TO- p-tolyaldehyde; BIAC- biacetyl; HEX- hexanal; MGX- methyl glyoxal; HEP- heptanal; Pinon- pinonaldehyde; OCT- octanal; NON- nonanal; DEC- decanal; UND- undecanal; DOD- dodecanal;

Table 4: continued

	UTC-mean time	IBu	BIAC	MEK	MPK	DEK	EPK	GLX	GLYALD	HYAC	ACR
E I	26.10.01 23:00	0.011	0.005	0.114	0.014	0.010	0.007	0.026	0.044	0.018	0.040
	27.10.01 01:03	0.018	0.006	0.104	0.016	0.011	bdl	0.021	0.050	0.011	0.049
	27.10.01 03:03	0.015	0.007	0.130	0.014	0.010	0.007	0.021	0.047	0.014	0.037
	27.10.01 05:06	0.013	0.005	0.134	0.012	0.009	0.009	0.017	0.039	0.008	0.032
	27.10.01 07:03	0.012	0.006	0.139	0.010	0.004	0.005	0.016	0.046	0.015	0.040
	27.10.01 09:03	0.012	0.008	0.163	0.014	0.009	0.007	0.026	0.071	0.024	0.043
	27.10.01 11:03	0.014	0.012	0.156	0.018	0.009	bdl	0.031	0.085	0.035	0.045
	27.10.01 13:03	0.014	0.013	0.156	0.012	bdl	0.006	0.028	0.091	0.052	0.066
E II	07.10.01 19:00	nm	bdl	bdl	bdl	bdl	0.037	nm	nm	nm	bdl
	07.10.01 21:00	0.011	bdl	0.094	0.009	bdl	0.009	0.007	0.037	0.022	0.022
	07.10.01 23:05	0.013	0.005	0.121	0.009	0.005	0.012	0.010	0.044	0.024	0.028
	08.10.01 01:01	0.009	bdl	0.112	0.005	0.008	bdl	0.006	0.028	0.020	0.020
	08.10.01 03:10	0.002	bdl	0.127	0.005	bdl	0.007	0.009	0.055	0.024	0.018
	08.10.01 05:10	0.014	0.006	0.082	0.017	0.007	0.015	0.008	0.040	0.027	0.023
	08.10.01 07:03	0.009	0.006	0.094	0.006	0.007	0.011	0.009	0.042	0.024	0.026
	08.10.01 09:03	bdl	0.008	0.101	0.008	bdl	0.003	0.019	0.057	0.031	0.027
	08.10.01 11:03	0.015	0.015	0.147	0.022	bdl	0.007	0.021	0.083	0.032	0.027
E III											
	16.10.02 22:02	0.006	0.003	0.048	0.002	0.036	0.002	0.006	0.011	0.006	0.010
	17.10.02 00:02	0.004	0.003	0.056	0.005	0.025	0.002	0.005	0.009	0.005	0.008
	17.10.02 02:02	0.005	0.004	0.031	0.003	0.042	bdl	0.004	0.007	0.005	0.008
	17.10.02 04:02	0.005	0.003	0.103	0.010	0.020	0.003	0.008	0.011	0.006	0.015

IBu- i-butanal; MEK- methyl ethyl ketone; MPK- methyl propyl ketone (pentanone-2); DEK- diethyl ketone (pentanone-3); EPK- ethyl propyl ketone (hexanone-3); GLX- glyoxal; GLYALD- glycolaldehyde; HYAC- hydroxyacetone; ACR- acroleine

nm – not measured bdl – concentration below analytical detection limit