Results of the first planning meeting for the AIDA SOA08 campaign

Forschungszentrum Karlsruhe, September 29, 2008

Participants of the meeting:

Neil Donahue (Carnegie Mellon) Thomas Mentel (Research Centre Jülich) Ralf Tillmann (Research Centre Jülich) Kent Salo (Gothenburg University) Josef Dommen (PSI Villigen) Harald Saathoff (Research Centre Karlsruhe)

Participants of the SOA08 campaign and instrumentation provided by different groups:

Participant	Institute	Instruments	
Astrid Kiendler- Scharr, Thomas F. Mentel, Ralf Tillmann, Theo Brauers	Research Centre Jülich	W-TOF-AMS (Inlet line automated w/wo Thermodenuder), Isotope-MS (analysis of filter samples), CCNC(only if needed), PTR-MS (detection limit 0.1 ppb; higher sensitivity would be helpful to detect SVOC's)	
Mattias Hallquist, Kent Salo	University of Gothenburg	VTDMA	
Neil Donahue	Carnegie Mellon University	Support for dark OH source	
Yoshi Iinuma	IfT Leipzig	Chemical analysis (CE-MS) of filter samples	
Stefan Benz, Ottmar Möhler, Karl-Heinz Naumann, Harald Saathoff, Martin Schnaiter, Robert Wagner	Research Centre Karlsruhe	FTIR, Ozone, Water-TDL, Light- Scattering, Thermodenuder, SMPS, DMPS, CPC's, IC analysis of filter samples (e.g. sulphate), WELAS and SOA-Modelling	
Thorsten Hoffmann	University of Mainz	On-line APCI-MS or LC-ESI-MS of filter samples	

Selected goals sorted according to their priority:

- 1. Chemical ageing of SOA from α -pinene (limonene, β -pinene) (OH made in dark reaction, e.g. O3 + propene, trans-2-butene or TME?) This type of experiments will also be done in the simulation chambers of PSI-Villigen and FZ-Jülich.
 - The SOA oxidation may be dominated by reactions of the OH radicals with semivolatile species in the gas phase compared to heterogeneous reactions.
 - > α -pinene has the highest priority but experiments with limonene or β -pinene may follow in the second week.
 - OH will be generated in steps (stepwise addition of OH precursor) to allow to distinguish better between aerosol dynamics and oxidation.

- The evolution of volatility of higher-volatility products is monitored by VTDMA, O:C ratio (AMS), OOA1/OOA2 ratio. These values are indicators to stop the experiments.
- (NH₄)₂SO₄ may be added as inorganic seed aerosol to be able to measure the organics relative to sulphate (AMS).
- > OH levels are monitored with 2-butanol as tracer (PTR-MS).
- The time scale for one experiment may be 10-12 hours with the option to make a longer one over the weekend. This will be decided after the first experiment.
- Experiments will be done at 293 K (same in SAPHIR and PSI chambers), 273 K, and 253 K. The relative humidity will be 40% with the option to choose higher values at lower temperatures.
- Initial particle concentrations should be between 30-50 µg m⁻³ for all temperatures. One experiment with significantly lower concentrations may be useful to increase the OH to hydrocarbon ratio.
- > Dark OH source: TME may be to slow at 253 K? Neil and Karl-Heinz will check if trans-2-butene is the better source over the whole temperature range. (Include some ppb of SVOC's with $k_{OH} = 2*10^{-11}$ cm3/s into kinetic model calculation for OH source and 2-butanol tracer with same initial concentration as the terpene.)
- A meeting to discuss the results of SOA08 and to prepare the next experiments at PSI chamber and SAPHIR will be held in the first week of December 2008 in Karlsruhe.
- 2. SOA yields for isoprene (OH made in dark reaction, organic seed aerosol)
 - Experiments will be done at 303 K, 273 K, and 243 K. The relative humidity will be 40% with the option to choose higher values at lower temperatures
 - Rates of trans-2-butene with OH/O3 compared to Isoprene?
- 3. Formation and partitioning of semivolatile VOC's as indicators for temperature and humidity dependent reaction channels for SOA formation (beta-pinene, norpinone).
 - Norpinone partitioning coefficient
 - > Temperature dependence of 13 C partitioning (beta-pinene)
- OH yields from ozonolysis at low temperatures and different humidities
 ➤ Stability of Criegee radical for selected alkenes (TME, Butene,...?)
- 5. SOA yields for mixtures of terpenes (including Isoprene?, 303-273-243 K, with OH scavenger)
- 6. SOA yields for small concentrations (0.1-10 $\mu g/m3$) and for temperatures down to -30 to -60°C

The mechanistic aspects of the terpene degradation may be addressed in more detail in a separate campaign in 2009.

Time frame for the SOA08 campaign (November 3-28, 2008):

The first week will be used for technical preparations and to test the dark OH source. After successful tests of the dark OH source chemical ageing experiments will start with the α -

pinene/O₃/OH-system because this is best documented (option to use also limonene or β -pinene as SOA precursor after successful experiments with α -pinene).

In the second half of the experiment time SOA yields for Isoprene will be investigated at different temperatures. In the last week experiments regarding temperature dependence of partitioning and OH yield can be done.

Nov 2008		Experiment type or activity at AIDA	Tgas [K]	Comment
3		AIDA technical preparation		
4		Set up & connection of new instruments		
5	01	Test of dark OH source at AIDA	293	
6	02	Test of dark OH source at AIDA	293	
7	03	Test of dark OH source at AIDA	273	
10	1	Chemical ageing experiment (α-pinene/O ₃ /OH)	293	
11	2	Chemical ageing experiment (α-pinene/O ₃ /OH)	273	
12	3	Chemical ageing experiment (α-pinene/O ₃ /OH)	253	
13	4	Chemical ageing experiment (α-pinene/O ₃ /OH)	233	Buffer day
14	5*	Chemical ageing experiment (α-pinene/O ₃ /OH)	?	
17	6	Chemical ageing experiment (limonene, β -pinene)	293	
18	7	Chemical ageing experiment (limonene, β-pinene)	253	
19	8	Isoprene + OH (SOA yield, organic seed)	303	
20	9	Isoprene + OH (SOA yield, organic seed)	273	
21	10	Isoprene + OH (SOA yield, organic seed)	243	
24	11	Experiments without dark OH source	293	
25	12	partitioning, & OH yields	273	
26	13		253	
27	14		233	
28	15		?	Buffer day

*It will be decided during the campaign if a long time scale experiment (50 h) e.g. over the weekend should be done.

Experimental procedure:

- 1. AIDA will be filled with humidified synthetic air
- 2. Ozone will be added (300-600 ppb as required for OH precursor)
- 3. Terpene will be added (equivalent leading to formation of $40 \ \mu g \ m^{-3}$ SOA).
- 4. OH precursor will be added stepwise over a total time period of about 10 hours.