Separating the HROrg Species – one example

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Dec 1, 2009

V-mode Aerodyne ambient lab data

The default HR frag and batch table separates the pCO2 (particulate CO2) from the HROrg species. We can use this example as a guide to separate other aerosol ions.

In particular, suppose I want to group HROrg into these groups (my own particular made-up names are in bold – these are only for simplicity, I can call them anything):

All ions in organic aerosol that only have only C and H **HOA**
All ions in organic aerosol that come from water (including H2O isotopes) **pOrgH2O**
All ions in organic aerosol that are CO (including CO isotopes) **pCO**
All ions in organic aerosol that are CO2 (including CO2 isotopes) **pCO2**
All ions in organic aerosol that have one O but are not from CO, CO2, or H2O **O1OA**
All ions in organic aerosol that have two + Os but are not from CO, CO2, or H2O **O2OA**
All ions in organic aerosol that fit into none of the above categories **XOA**

For this example, I have deliberately grouped all of HROrg so that their sum will equal HROrg, but I can create these HR species any way I want.

I create HR frag waves and modified the HR batch table. (It is better to create the HRfrag waves first, so that when the HR frag table is popped they will appear)

i.e. duplicate root:HR_frag:HR_frag_organic root:HR_frag:HR_frag_pCO, etc

The batch table with these new HROrg-ish species is:

HRBatchTable

R8 | 1.4

Point	HR_specname_list	HR_spec_list	HR_specFrag_list	HR_sp	HR_s	HR_specFamilyBase	HR_specFam	HR_specC	HR_specCorr_list	HR_specColor_R	HR_specColor_G	HR_specColor_B
0	HRair	HRair	HR_frag_air	1	1	familyAir		1		47872	47872	47872
1	HRPwater	HRPwater	HR_frag_Pwater	1	1	familyHO		1		0	49152	49152
2	HRammonium	HRNH4	HR_frag_ammonium	4	1	familyNH		0.25		65535	43690	0
3	HRnitrate	HRNO3	HR_frag_nitrate	1.1	1	familyNO		0.909091		0	0	65535
4	HRsulphate	HRSO4	HR_frag_sulphate	1.2	1	familySO		0.833333		65535	0	0
5	HRorganic	HROrg	HR_frag_organic	1.4	1	familyCx;familyCH;familyCHO1;f		0.714286		0	52224	0
6	HRchloride	HRChl	HR_frag_chloride	1.3	1	familyCl		0.769231		65280	0	52224
7	HRpCO2	HRpCO2	HR_frag_pCO2	1.4	1			0.714286		12224	52224	0
8	HRHOA	HRHOA	HR_frag_HOA	1.4	1	familyCx;familyCH;		0.714286		0	52224	12224
9	HRO1OA	HRO1OA	HR_frag_O1OA	1.4	1	familyCHO1;familyCHO1N		0.714286		0	26224	0
10	HRO2OA	HRO2OA	HR_frag_O2OA	1.4	1	familyCHOgt1;familyCHOgt1N;		0.714286		0	13224	0
11	HRXOA	HRXOA	HR_frag_XOA	1.4	1	familyCHN;familyCS		0.714286		12224	52224	12224
12	HRpCO	HRPCO	HR_frag_pCO	1.4	1			0.714286		6224	52224	6224
13	HRpOrgH2O	HRpOrgH2O	HR_frag_pOrgH2O	1.4	1			0.714286		0	52224	6224
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I created some default color values for my new HR org species (in columns HR_SpecColor_R, etc). This is only for convenience.

The text values in the specname_list and spec_list are the same. They need not be the same but I kept them the same for simplicity. Also, normally everything we do is case INsensitive, but Pika does have some case sensitivity (to distinguish between CO and Co=cobalt, for example).

I modified the new HR frag waves as follows:

HRFragTable

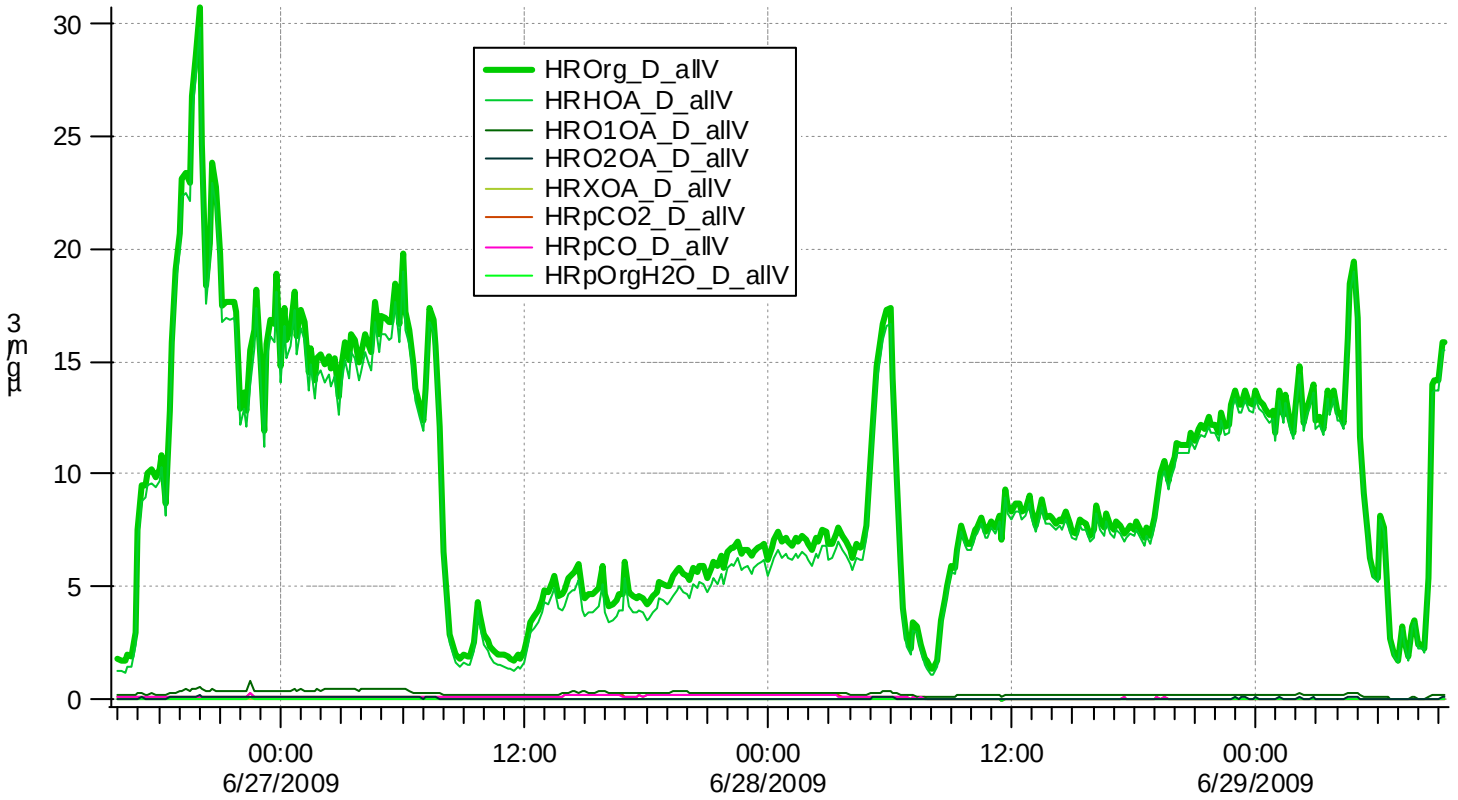
R17

Point	HR_specMassA	HR_frag_organic	HR_frag_pCO2	HR_frag_pCO	HR_frag_pOrgH2O	HR_frag_HOA	HR_frag_XOA	HR_frag_O1OA	HR_frag_O2OA
0	N								
1	j15N								
2	O	0.04*HR_frag_organic[{H2O}]			0.04*HR_frag_orgai				
3	HO	0.25*HR_frag_organic[{H2O}]			0.25*HR_frag_orgai				
4	j18O	0.00205000*HR_frag_organic[{O}]			0.00205000*HR_fra				
5	H2O	0.225*HR_frag_organic[{CO2}]			0.225*HR_frag_org:				
6	Hj18O	0.00205000*HR_frag_organic[{HO}]			0.00205000*HR_fra				
7	H2j18O	0.00205000*HR_frag_organic[{H2O}]			0.00205000*HR_fra				
8	CO2plus2	{CO2plus2}	{CO2plus2}						
9	CO	HR_frag_organic[{CO2}]		HR_frag_organic[					
10	Cj18O	0.00205000*HR_frag_organic[{CO}]		0.00205000*HR_					
11	S								
12	j33S								
13	j34S								
14	CO2	HR_frag_pco2[{CO2}]	{CO2},-HR_frag_air[{CO2}]						
15	j13CO2	HR_frag_pco2[{j13CO2}]	0.01112*HR_frag_pco2[{CO2}]						
16	Cj18OO	HR_frag_pco2[{Cj18OO}]	0.004*HR_frag_pco2[{CO2}]						
17									

Recall that an HR species uses 2 pieces of information:
(1) Possible list of any families (from the batch table entries)
(2) Possible fragments of individual HR ions (from the frag table entries)

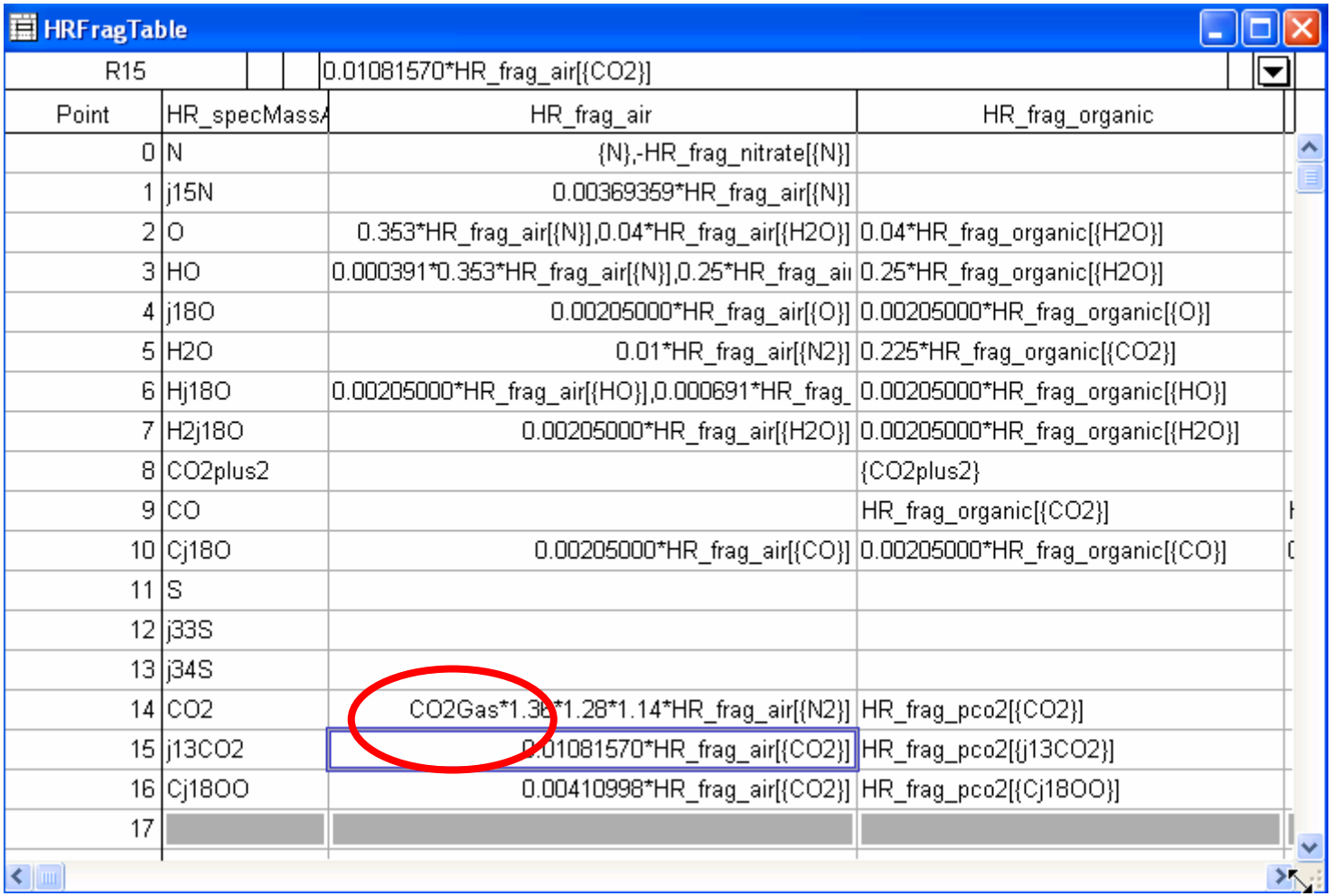
The individual HR ion entries in the HR frag table take precedence over any family inclusion/exclusion designation. Thus while the HR ion CO2 is a member of the CHOgt1 family it will not be ‘counted twice’ (by it’s inclusion in the frag table and as a member of the CHOgt1 family).

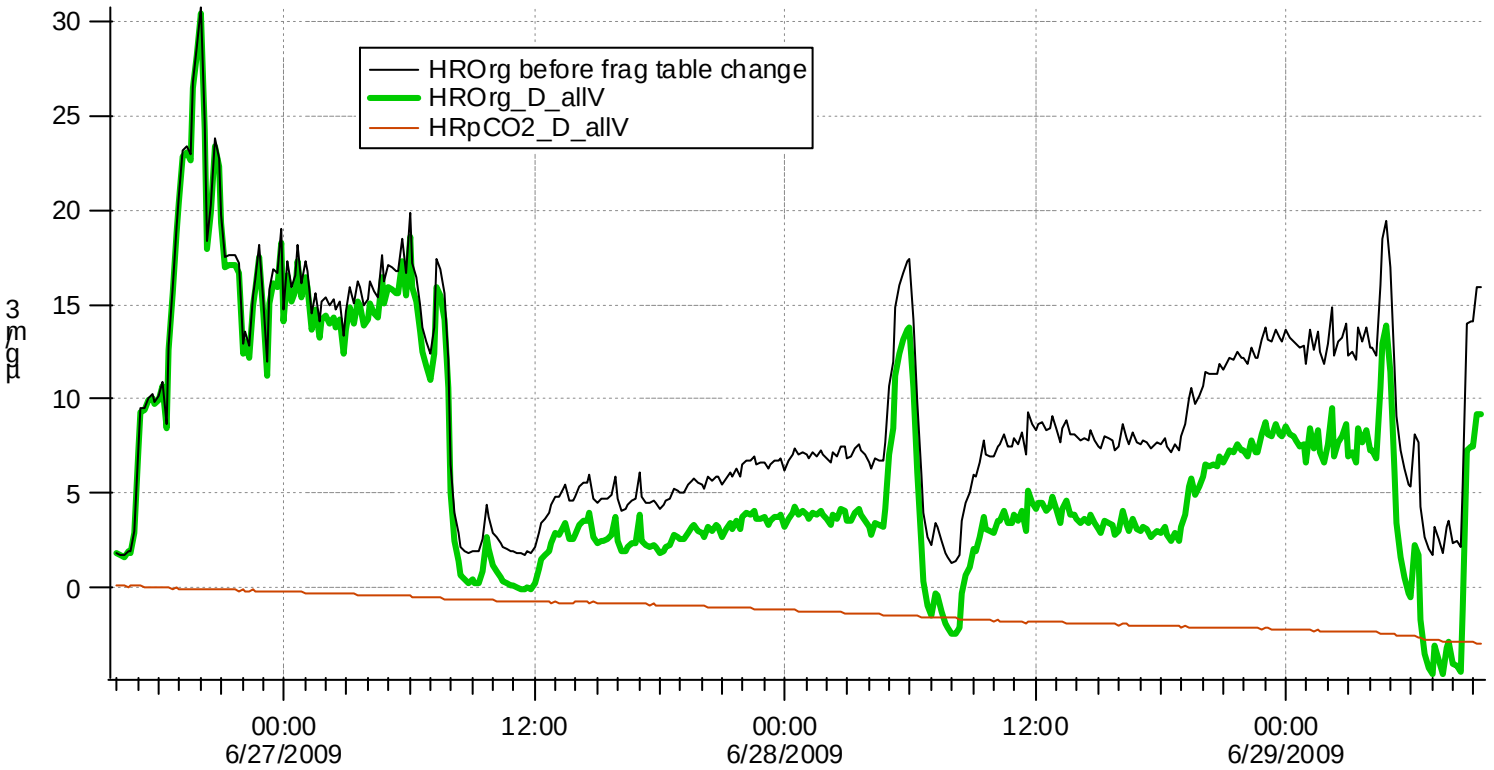
Now I can view my separate HROrg subgroups O1OA, etc.



I put a cursor somewhere and note that HROrg_D_allV[pcsr(a)] –
(HRHOA_D_allV[pcsr(a)] + HRO2OA_D_allV[pcsr(a)] + HRO1OA_D_allV[pcsr(a)] + HRXOA_D_allV[pcsr(a)] + HRpCO2_D_allV[pcsr(a)] + HRpCO_D_allV[pcsr(a)] + HRpOrgH2O_D_allV[pcsr(a)])
= 2.85916e-07 ~ 0
So I think I successfully separated HROrg to chemically related subgroups.

The HR frag table can deal with dependencies, as in squirrel. For example the default entry for gas phase CO2 is 0.00037*1.36*1.28*1.14*HR_frag_air[{N2}]. In this example I create a fake gas-phase CO2 measurement that constantly increases and convert to mixing ratio and change the frag entry.
duplicate/o Org CO2gas; CO2Gas = 0.00037 +0.000015*p





Time series of HROrg using the original and time-dependent frag correction. The negative amount of particulate CO2 is not intended to reflect real conditions, only to demonstrate the functionality of a HR time-dependent frag correction.

Note that one could also generate an ‘gas’ CO2 similar to ‘pCO2’ or particulate CO2, just by copying the CO2 entry in HR_frag_air.

The ability to add new HR species in the batch table by directly referencing an HR ion is NOT yet available. If one were to attempt this, the resulting waves should be 0s.

HRBatchTable

1R X 12C

Point	HR_specname_list	HR_spec_list	HR_specFrag_list	HR_sp	HR_s	HR_specFamilyBase	HR_specFami	HR_spe
0	HRair	HRair	HR_frag_air	1	1	familyAir		
1	HRPwater	HRPwater	HR_frag_Pwater	1	1	familyHO		
2	HRammonium	HRNH4	HR_frag_ammonium	4	1	familyNH		0.
3	HRnitrate	HRNO3	HR_frag_nitrate	1.1	1	familyNO		0.9090
4	HRsulphate	HRSO4	HR_frag_sulphate	1.2	1	familySO		0.8333
5	HRorganic	HROrg	HR_frag_organic	1.4	1	familyCx;familyCH;familyCHO1;f		0.7142
6	HRchloride	HRChl	HR_frag_chloride	1.3	1	familyCl		0.7692
7	HRpCO2	HRpCO2	HR_frag_pCO2	1.4	1			0.7142
8	HRHOA	HRHOA	HR_frag_HOA	1.4	1	familyCx;familyCH;		0.7142
9	HRO1OA	HRO1OA	HR_frag_O1OA	1.4	1	familyCHO1;familyCHO1N		0.7142
10	HRO2OA	HRO2OA	HR_frag_O2OA	1.4	1	familyCHOgt1;familyCHOgt1N;		0.7142
11	HRXOA	HRXOA	HR_frag_XOA	1.4	1	familyCHN;familyCS		0.7142
12	HRpCO	HRPCO	HR_frag_pCO	1.4	1			0.7142
13	HRpOrgH2O	HRpOrgH2O	HR_frag_pOrgH2O	1.4	1			0.7142
14	HRpC3H7	HRpC3H7	HR_frag_organic[{C3H7}]	1.4	1			0.7142
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Will NOT work (yet)!