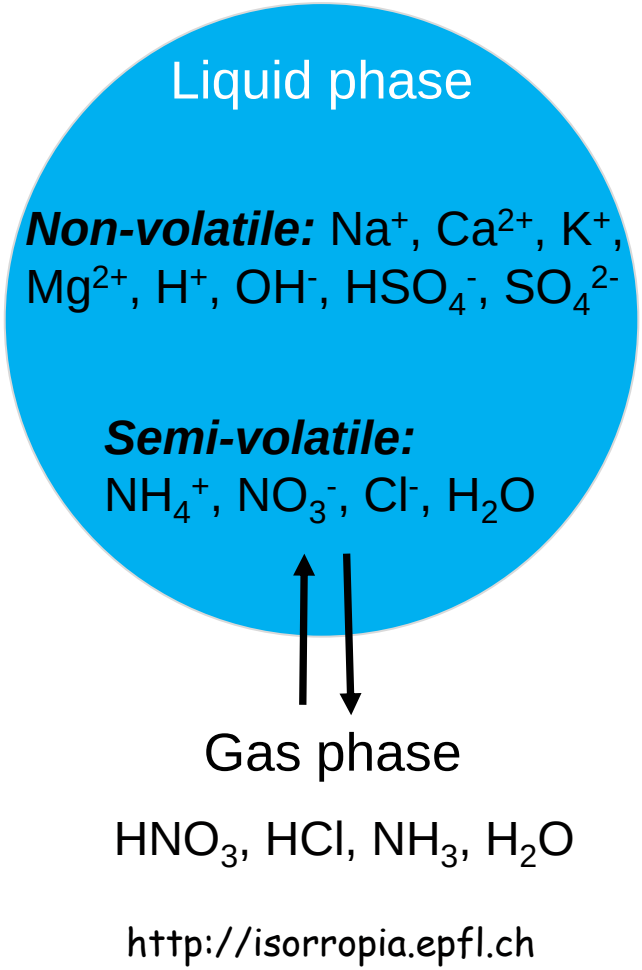
ISORROPIA-II

ISORROPIA-II calculates:

the composition and phase state of an NH_4^+-SO_4^{2-}-NO_3^--Cl^--Na^+-Ca^{2+}-K^+-Mg^{2+}-water inorganic aerosol in equilibrium with gases

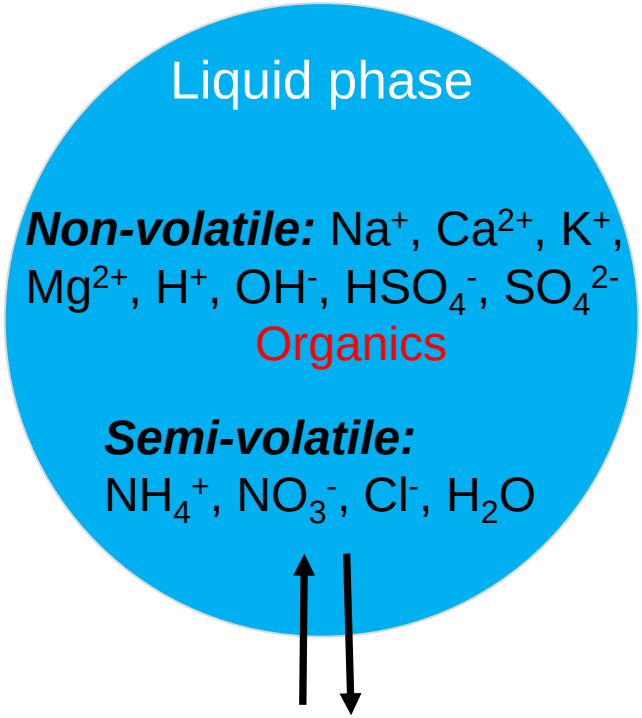


http://isorropia.epfl.ch

ISORROPIA-Lite (Kakavas et al., 2021)

ISORROPIA-lite calculates:

the composition and phase state of an NH_4^+-SO_4^{2-}-NO_3^--Cl^--Na^+-Ca^{2+}-K^+-Mg^{2+}-Org-water inorganic aerosol in equilibrium with gases



Assumptions:

- One phase where organics are mixed with inorganics – in metastable state.
- Effect of organics is to increase the aerosol liquid water content affecting inorganic partitioning
- Water uptake is parameterized in terms of organic mass, and hygroscopicity parameter

http://isorropia.epfl.ch

Lite version: metastable aerosol only

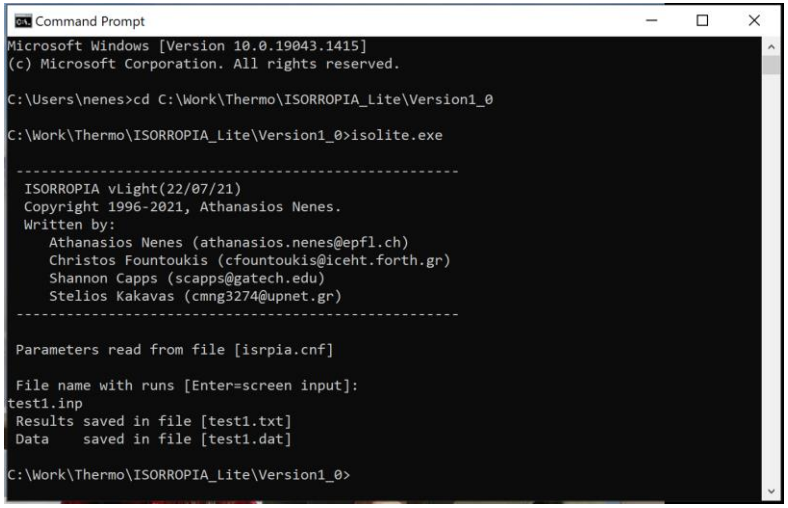
Full version: stable/metastable option also (this will be released later as ISORROPIA – III, but we don't care about this for all our applications.

ISORROPIA-Lite (standalone code)

Changes – from the user side - compared to ISORROPIA 2.3:

1. Input file has 3 more columns to describe the amount and properties of the organics internally mixed with the inorganic aerosol.
2. Two more output files are generated, in addition to the .txt, .dat files with the output from the simulations. These extra files have the activitity coefficients (.act) and the water content associated with each aerosol species (.wat).
3. The .txt file has a little more information compared to ISORROPIA 2.3 because the effect of the organics is also summarized.

Execution: similar to older versions, see example with the demo input file test1.inp:



Output files (with new in italics):

test1	ACT File	*Activity coefficients (new)*
test1.dat	DAT File	.dat file (*with more info on organics*)
test1.inp	INP File	Input file (*with more info on organics*)
test1	Text Document	.txt file (*with more info on organics*)
test1.wat	WAT File	*Liquid water content file (new)*

ISORROPIA-Lite (standalone code)

Input file:

Very similar format to .inp file of ISORROPIA 2.3, only that you need to have 3 extra columns (shaded in blue) to describe the organic mass and their properties.

DEMO - Notepad

File Edit Format View Help

```
Input units (0=umol/m3, 1=ug/m3) ; sample input file
       1

Problem type (0=forward, 1=reverse); Phase state (0=solid+liquid, 1=metastable)
0, 1

NH4-SO4-NO3 system case
Na      SO4     NH3     NO3     Cl      Ca      K       Mg      Org     k_org   rho_org RH      TEMP
0.0     10.0    0.01    0.01    0.0     0.0     0.0     0.0     10      0.15    1.0     0.80    298.15
0.0     10.0    0.01    0.01    0.0     0.0     0.0     0.0     10      0.15    1.0     0.85    298.15
0.0     10.0    0.01    0.01    0.0     0.0     0.0     0.0     10      0.15    1.0     0.90    298.15
0.0     10.0    0.01    0.01    0.0     0.0     0.0     0.0     10      0.15    1.0     0.95    298.15
0.0     10.0    0.01    0.01    0.0     0.0     0.0     0.0     10      0.15    1.0     1.00    298.15
```

Mass of organics in aerosol (always in μg m^{-3})

Density of hygroscopic organics (g cm^{-3})

Hygroscopicity of organics (*κ* parameter of Petters and Kreidenweis, 2007)

Notes:

1. Phase state parameter should still be included (for compatibility with ISORROPIA-III, when it is released), but ISORROPIA-Lite ignores it and always assignes to 1.
2. k_org = 0.15 and rho_org = 1.4 are good values. Organic mass *always* in μg m^{-3}.
3. Specifying k_org=0 or Org (mass) = 0 means organics do not take up water and affect the solution. This is identical to running ISORROPIA 2.3 in metastable mode.

ISORROPIA-Lite (standalone code)

Activity coefficient (.act) output file:

test1 - Notepad

File Edit Format View Help

"NaCl"	"Na2SO4"	"NaNO3"	"(NH4)2SO4"	"NH4NO3"	"NH4Cl"	"2H-SO4"	"H-HSO4"	"NH4HSO4"
0.10000	0.10000	0.10000	0.17475	0.37675	0.10000			0.19323
0.10000	0.10000	0.10000	0.16842	0.37203	0.10000			0.19918
0.10000	0.10000	0.10000	0.16464	0.35975	0.10000			0.20016
0.10000	0.10000	0.10000	0.14894	0.33708	0.10000			0.16653
0.10000	0.10000	0.10000	0.14377	0.32670	0.10000			0.17278
0.10000	0.10000	0.10000	0.13899	0.31625	0.10000			0.17444
0.10000	0.10000	0.10000	0.11485	0.27651	0.10000			0.13104
0.10000	0.10000	0.10000	0.11245	0.27809	0.10000			0.14027
0.10000	0.10000	0.10000	0.11133	0.26782	0.10000			0.14421

Text file, each row contains the results from the corresponding row in the input (.inp) file

Each column has the value of the mean activity coefficient of the salt (e.g., γ_{NaCl}, γ_{NaNO3}, etc.).

Input file can also be easily read in Excel, Igor, etc. (following the same procedure as done for the .dat file).

test1 - Excel

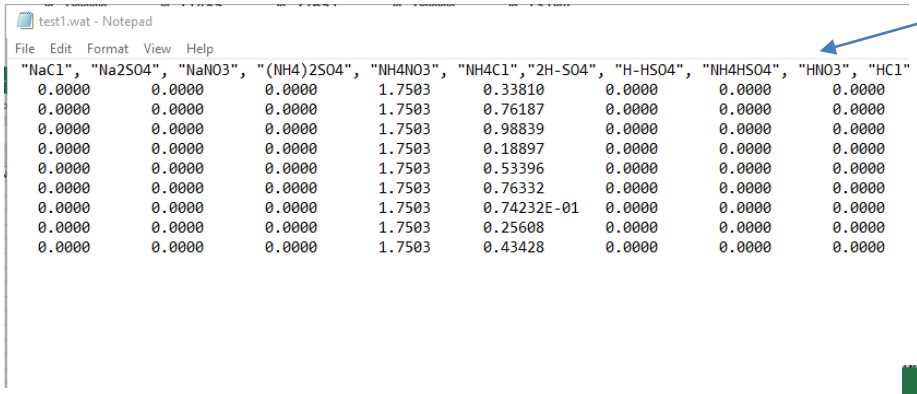
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	NaCl	Na2SO4	NaNO3	(NH4)2SO4	NH4NO3	NH4Cl	2H-SO4	H-HSO4	NH4HSO4	HNO3	HCl	NaHSO4	LC	CaSO4	Ca(NO3)2	CaCl2
2	0.1	0.1	0.1	0.17475	0.37675	0.1	0.19323	0.54599	0.50635	0.40625	0.1	0.1	0.26745	0.1	0.1	0.1
3	0.1	0.1	0.1	0.16842	0.37203	0.1	0.19918	0.58052	0.5119	0.4219	0.1	0.1	0.26273	0.1	0.1	0.1
4	0.1	0.1	0.1	0.16464	0.35975	0.1	0.20016	0.58654	0.50662	0.41651	0.1	0.1	0.25811	0.1	0.1	0.1
5	0.1	0.1	0.1	0.14894	0.33708	0.1	0.16653	0.5787	0.53222	0.36652	0.1	0.1	0.24788	0.1	0.1	0.1
6	0.1	0.1	0.1	0.14377	0.3267	0.1	0.17278	0.61972	0.53991	0.37499	0.1	0.1	0.24407	0.1	0.1	0.1
7	0.1	0.1	0.1	0.13899	0.31625	0.1	0.17444	0.66032	0.55689	0.37498	0.1	0.1	0.24216	0.1	0.1	0.1
8	0.1	0.1	0.1	0.11485	0.27651	0.1	0.13104	0.70308	0.63689	0.30526	0.1	0.1	0.22788	0.1	0.1	0.1
9	0.1	0.1	0.1	0.11245	0.27809	0.1	0.14027	0.77718	0.65844	0.32825	0.1	0.1	0.22802	0.1	0.1	0.1
10	0.1	0.1	0.1	0.11133	0.26782	0.1	0.14421	0.7868	0.648	0.32518	0.1	0.1	0.22522	0.1	0.1	0.1

Notes:

1. The activity coefficients are used to plot maps, partitioning curves, etc. See relevant papers on how they can be used.
2. If a binary pair was not present in solution (see above, e.g., NaCl), then the program defaults the γ to 0.1. Don't use them if they weren't in the aerosol though!

ISORROPIA-Lite (standalone code)

Liquid water content (.wat) output file:


test1.wat - Notepad

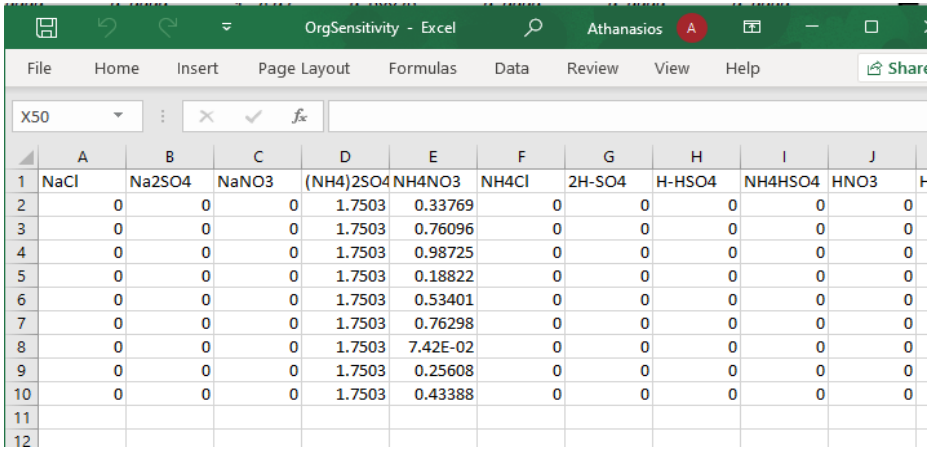
File Edit Format View Help

```
"NaCl", "Na2SO4", "NaNO3", "(NH4)2SO4", "NH4NO3", "NH4Cl","2H-SO4", "H-HSO4", "NH4HSO4", "HNO3", "HCl"
  0.0000       0.0000       0.0000       1.7503       0.33810       0.0000       0.0000       0.0000
  0.0000       0.0000       0.0000       1.7503       0.76187       0.0000       0.0000       0.0000
  0.0000       0.0000       0.0000       1.7503       0.98839       0.0000       0.0000       0.0000
  0.0000       0.0000       0.0000       1.7503       0.18897       0.0000       0.0000       0.0000
  0.0000       0.0000       0.0000       1.7503       0.53396       0.0000       0.0000       0.0000
  0.0000       0.0000       0.0000       1.7503       0.76332       0.0000       0.0000       0.0000
  0.0000       0.0000       0.0000       1.7503       0.74232E-01   0.0000       0.0000       0.0000
  0.0000       0.0000       0.0000       1.7503       0.25608       0.0000       0.0000       0.0000
  0.0000       0.0000       0.0000       1.7503       0.43428       0.0000       0.0000       0.0000
```

Text file, each row contains the results from the corresponding row in the input (.inp) file

Each column has the value of the liquid water content (always in μg m^{-3}) associated with the salt specified in the header. Organics and total water is also provided.

Input file can also be easily read in Excel, Igor, etc. (following the same procedure as done for the .dat file).


OrgSensitivity - Excel — Athanasios

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X50

	A	B	C	D	E	F	G	H	I	J
1	NaCl	Na2SO4	NaNO3	(NH4)2SO4	NH4NO3	NH4Cl	2H-SO4	H-HSO4	NH4HSO4	HNO3
2	0	0	0	1.7503	0.33769	0	0	0	0	0
3	0	0	0	1.7503	0.76096	0	0	0	0	0
4	0	0	0	1.7503	0.98725	0	0	0	0	0
5	0	0	0	1.7503	0.18822	0	0	0	0	0
6	0	0	0	1.7503	0.53401	0	0	0	0	0
7	0	0	0	1.7503	0.76298	0	0	0	0	0
8	0	0	0	1.7503	7.42E-02	0	0	0	0	0
9	0	0	0	1.7503	0.25608	0	0	0	0	0
10	0	0	0	1.7503	0.43388	0	0	0	0	0
11										
12										

Notes:

1. The sum of the water from each of the salts and the organics should give you the total LWC.
2. The contribution of each salt is now directly known for each input. This provides all the information required to understand if the aerosol is in a “sulfate-dominated”, “nitrate-dominated”, “chloride-dominated”, or “organics-dominated” regime in terms of liquid water.

ISORROPIA-Lite (standalone code)

Changes to (.txt) output files – compared to those from ISORROPIA 2.3:

test1 - Notepad

File Edit Format View Help

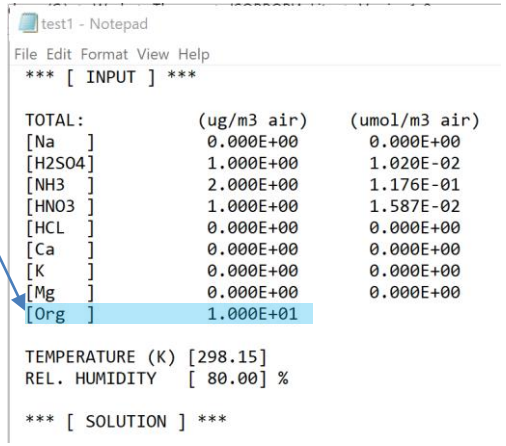
```
 [TOTAL ]          9.713E+00
 [LIQUID]          9.713E+00       100.000

 NO SOLID AEROSOL PHASE

 LIQUID AEROSOL:  (ug/m3 air)    (umol/m3 air)   (% mass)    (% mole)
 [WATER ]          8.088E+00       4.494E-01      83.277      92.294
 [H+    ]          2.170E-05       2.170E-05       0.000       0.004
 [Na+   ]          0.000E+00       0.000E+00       0.000       0.000
 [NH4+  ]          4.285E-01       2.381E-02       4.412       4.890
 [Cl-   ]          0.000E+00       0.000E+00       0.000       0.000
 [NO3-  ]          2.160E-01       3.485E-03       2.224       0.716
 [SO4-- ]          9.734E-01       1.014E-02      10.022       2.083
 [HSO4- ]          6.293E-03       6.487E-05       0.065       0.013
 [Ca    ]          0.000E+00       0.000E+00       0.000       0.000
 [K     ]          0.000E+00       0.000E+00       0.000       0.000
 [Mg    ]          0.000E+00       0.000E+00       0.000       0.000
 [NH3aq ]          0.000E+00       0.000E+00       0.000       0.000
 [HClaq ]          0.000E+00       0.000E+00       0.000       0.000
 [HNO3aq]          0.000E+00       0.000E+00       0.000       0.000
 [WatNaCl]         0.000E+00       0.000E+00       0.000       0.000
 [WatNa2SO4]       0.000E+00       0.000E+00       0.000       0.000
 [WatNaNO3]        0.000E+00       0.000E+00       0.000       0.000
 [Wat(NH4)2SO4]    1.750E+00       9.724E-02      18.021      19.972
 [WatNH4NO3]       3.381E-01       1.878E-02       3.481       3.858
 [WatNH4Cl]        0.000E+00       0.000E+00       0.000       0.000
 [Wat2H-SO4]       0.000E+00       0.000E+00       0.000       0.000
 [WatH-HSO4]       0.000E+00       0.000E+00       0.000       0.000
 [WatNH4HSO4]      0.000E+00       0.000E+00       0.000       0.000
 [WatHNO3]         0.000E+00       0.000E+00       0.000       0.000
 [WatHCl]          0.000E+00       0.000E+00       0.000       0.000
 [WatNaHSO4]       0.000E+00       0.000E+00       0.000       0.000
 [WatLC]           0.000E+00       0.000E+00       0.000       0.000
 [WatCaSO4]        0.000E+00       0.000E+00       0.000       0.000
 [WatCa(NO3)2]     0.000E+00       0.000E+00       0.000       0.000
 [WatCaCl2]        0.000E+00       0.000E+00       0.000       0.000
 [WatK2SO4]        0.000E+00       0.000E+00       0.000       0.000
 [WatKHSO4]        0.000E+00       0.000E+00       0.000       0.000
 [WatKNO3]         0.000E+00       0.000E+00       0.000       0.000
 [WatKCl]          0.000E+00       0.000E+00       0.000       0.000
 [WatMgSO4]        0.000E+00       0.000E+00       0.000       0.000
 [WatMgNO3]        0.000E+00       0.000E+00       0.000       0.000
 [WatMgCl2]        0.000E+00       0.000E+00       0.000       0.000
 [WatOrg]          6.000E+00       3.333E-01      61.775      68.464
 [pH    ]          2.571E+00
 [IONIC STRENGTH]  4.295E+00
```

Output section for each input now contains the water contributions from each salt.

Input section also notes the amount of organics in the simulation.



ISORROPIA-Lite (standalone code)

Changes to (.dat) output files – compared to those from ISORROPIA 2.3:

test1 - Notepad

File Edit Format View Help

```
 [TOTAL ]          9.713E+00
 [LIQUID]          9.713E+00       100.000

 NO SOLID AEROSOL PHASE

 LIQUID AEROSOL:  (ug/m3 air)    (umol/m3 air)   (% mass)    (% mole)
 [WATER ]          8.088E+00       4.494E-01      83.277      92.294
 [H+    ]          2.170E-05       2.170E-05       0.000       0.004
 [Na+   ]          0.000E+00       0.000E+00       0.000       0.000
 [NH4+  ]          4.285E-01       2.381E-02       4.412       4.890
 [Cl-   ]          0.000E+00       0.000E+00       0.000       0.000
 [NO3-  ]          2.160E-01       3.485E-03       2.224       0.716
 [SO4-- ]          9.734E-01       1.014E-02      10.022       2.083
 [HSO4- ]          6.293E-03       6.487E-05       0.065       0.013
 [Ca    ]          0.000E+00       0.000E+00       0.000       0.000
 [K     ]          0.000E+00       0.000E+00       0.000       0.000
 [Mg    ]          0.000E+00       0.000E+00       0.000       0.000
 [NH3aq ]          0.000E+00       0.000E+00       0.000       0.000
 [HClaq ]          0.000E+00       0.000E+00       0.000       0.000
 [HNO3aq]          0.000E+00       0.000E+00       0.000       0.000
 [WatNaCl]         0.000E+00       0.000E+00       0.000       0.000
 [WatNa2SO4]       0.000E+00       0.000E+00       0.000       0.000
 [WatNaNO3]        0.000E+00       0.000E+00       0.000       0.000
 [Wat(NH4)2SO4]    1.750E+00       9.724E-02      18.021      19.972
 [WatNH4NO3]       3.381E-01       1.878E-02       3.481       3.858
 [WatNH4Cl]        0.000E+00       0.000E+00       0.000       0.000
 [Wat2H-SO4]       0.000E+00       0.000E+00       0.000       0.000
 [WatH-HSO4]       0.000E+00       0.000E+00       0.000       0.000
 [WatNH4HSO4]      0.000E+00       0.000E+00       0.000       0.000
 [WatHNO3]         0.000E+00       0.000E+00       0.000       0.000
 [WatHCl]          0.000E+00       0.000E+00       0.000       0.000
 [WatNaHSO4]       0.000E+00       0.000E+00       0.000       0.000
 [WatLC]           0.000E+00       0.000E+00       0.000       0.000
 [WatCaSO4]        0.000E+00       0.000E+00       0.000       0.000
 [WatCa(NO3)2]     0.000E+00       0.000E+00       0.000       0.000
 [WatCaCl2]        0.000E+00       0.000E+00       0.000       0.000
 [WatK2SO4]        0.000E+00       0.000E+00       0.000       0.000
 [WatKHSO4]        0.000E+00       0.000E+00       0.000       0.000
 [WatKNO3]         0.000E+00       0.000E+00       0.000       0.000
 [WatKCl]          0.000E+00       0.000E+00       0.000       0.000
 [WatMgSO4]        0.000E+00       0.000E+00       0.000       0.000
 [WatMgNO3]        0.000E+00       0.000E+00       0.000       0.000
 [WatMgCl2]        0.000E+00       0.000E+00       0.000       0.000
 [WatOrg]          6.000E+00       3.333E-01      61.775      68.464
 [pH    ]          2.571E+00
 [IONIC STRENGTH]  4.295E+00
```

Output section for each input now contains the water contributions from each salt.

Input section also notes the amount of organics in the simulation.

test1 - Notepad

File Edit Format View Help

```
 *** [ INPUT ] ***

 TOTAL:            (ug/m3 air)     (umol/m3 air)
 [Na    ]           0.000E+00        0.000E+00
 [H2SO4]           1.000E+00        1.020E-02
 [NH3   ]           2.000E+00        1.176E-01
 [HNO3  ]           1.000E+00        1.587E-02
 [HCL   ]           0.000E+00        0.000E+00
 [Ca    ]           0.000E+00        0.000E+00
 [K     ]           0.000E+00        0.000E+00
 [Mg    ]           0.000E+00        0.000E+00
 [Org   ]           1.000E+01

 TEMPERATURE (K) [298.15]
 REL. HUMIDITY   [ 80.00] %

 *** [ SOLUTION ] ***
```

ISORROPIA-lite (some example results)

Input file

DEMO - Notepad

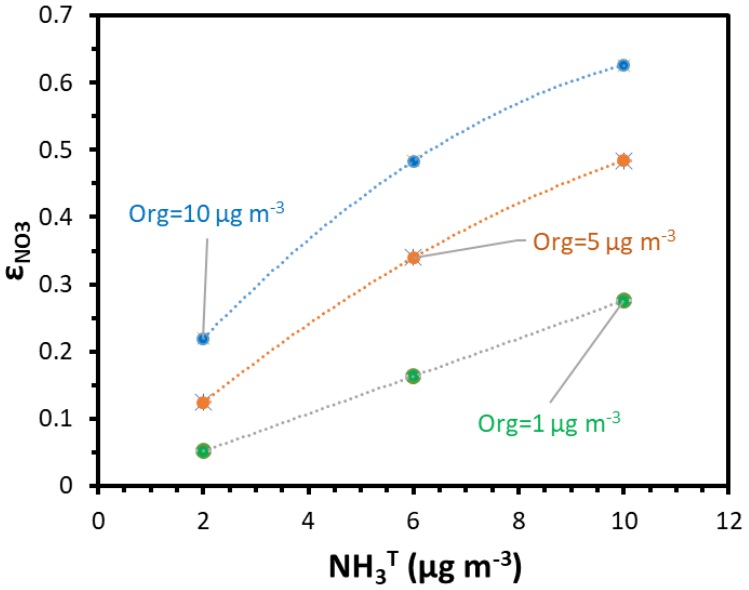
File Edit Format View Help

```
Input units (0=umol/m3, 1=ug/m3) ; sample input file
        1

Problem type (0=forward, 1=reverse); Phase state (0=solid+liquid, 1=metastable)
0, 1

NH4-SO4-NO3 system case
Na       SO4      NH3      NO3      Cl       Ca       K        Mg       Org    k_org    rho_org    RH       TEMP
0.0      10.0     0.01     0.01     0.0      0.0      0.0      0.0      10     0.15     1.0        0.80     298.15
0.0      10.0     0.01     0.01     0.0      0.0      0.0      0.0      10     0.15     1.0        0.85     298.15
0.0      10.0     0.01     0.01     0.0      0.0      0.0      0.0      10     0.15     1.0        0.90     298.15
0.0      10.0     0.01     0.01     0.0      0.0      0.0      0.0      10     0.15     1.0        0.95     298.15
0.0      10.0     0.01     0.01     0.0      0.0      0.0      0.0      10     0.15     1.0        1.00     298.15
```

Organic water impacts on ε_{NO3}

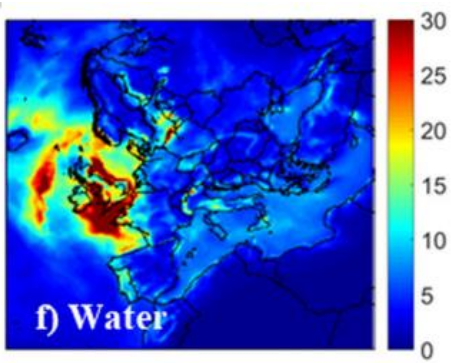


Sulfate, nitrate, organic contributions to water

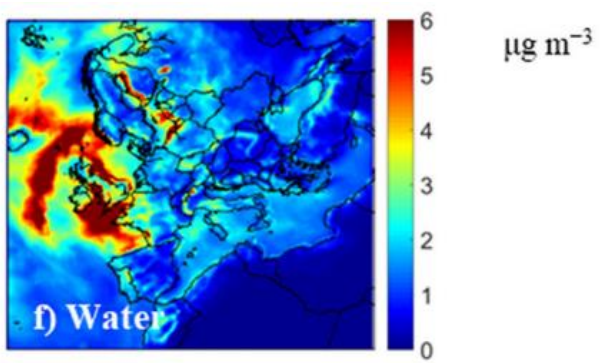
NH3T	Sulfate Water	Nitrate Water	Organic Water
2	22%	4%	74%
6	21%	9%	70%
10	20%	11%	69%
2	35%	4%	61%
6	33%	10%	57%
10	32%	14%	54%
2	72%	3%	25%
6	67%	10%	23%
10	63%	16%	22%

ISORROPIA-lite (results by Kakavas et al., Tellus B)

Aerosol water, no organic effects
(i.e., like ISORROPIA 2.3)



Aerosol water change from
including organic effects



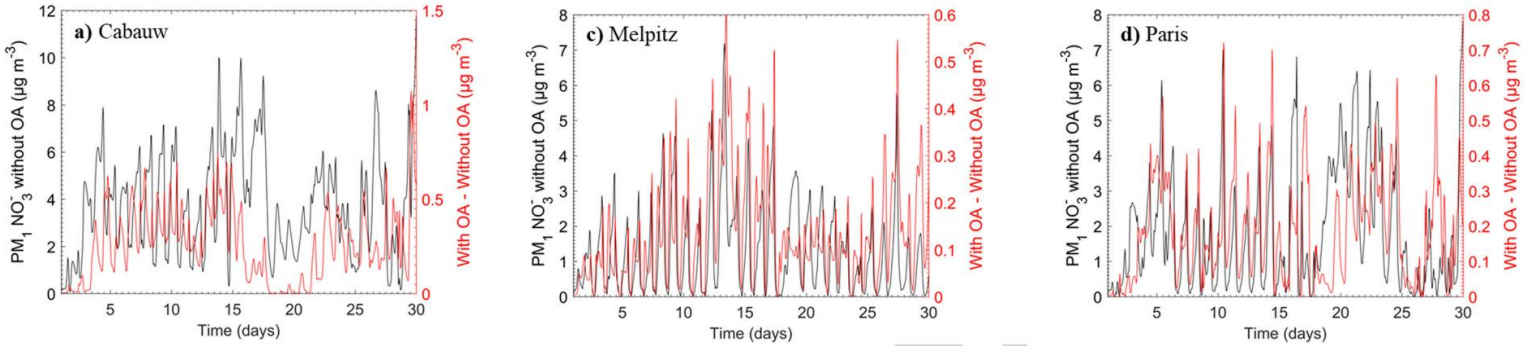


Fig. 11. PM_1 nitrate concentration (in µg m^{-3}) when the organic aerosol water is absent (black) and the corresponding concentration difference when is present (red) in the simulation for **a)** Cabauw, Netherlands; **b)** Finokalia, Greece; **c)** Melpitz, Germany; and **d)** Paris, France during May 2008.

Takehome message: the feedback of organic water can be important.

ISORROPIA-lite (more information)

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ISORROPIA-lite: a comprehensive atmospheric aerosol thermodynamics module for earth system models

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ABSTRACT

Aerosol simulations especially for Earth System Models require a thermodynamics module with a good compromise between rigor and computational efficiency. We present and evaluate ISORROPIA-lite, an accelerated and simplified version of the widely used ISORROPIA-II v.2.3 aerosol thermodynamics model, expanded to include the effects of water uptake from organics and an updated interface communicating simulation diagnostics and information. ISORROPIA-lite assumes the aerosol is in metastable equilibrium (i.e., salts do not precipitate from supersaturated solutions) and treats the thermodynamics of $Na^+ - NH_4^+ - SO_4^{2-} - NO_3^- - Cl^- - Ca^{2+} - K^+ - Mg^{2+} - Organics - H_2O$ aerosol using binary activity coefficients from precalculated look-up tables. Off-line comparison between ISORROPIA-II and ISORROPIA-lite (without organic water effects) for more than 330,000 atmospherically-relevant states demonstrated that *i)* ISORROPIA-lite provides virtually identical results with ISORROPIA-II in metastable mode and *ii)* differences between stable mode ISORROPIA-II and ISORROPIA-lite are less than 25% for the concentrations of the various semivolatile aerosol components and similar to the differences between stable and metastable modes of ISORROPIA-II. Using ISORROPIA-lite reduced computational cost by 35% compared to ISORROPIA-II simulations in stable mode with online calculation of binary activity coefficients. Application of ISORROPIA-lite in the PMCAMx chemical transport model accelerated the 3D simulations by about 10% compared to using ISORROPIA-II in stable mode with changes in the concentrations of the major aerosol components of less than 10%. Simulations considering the effects of the organic aerosol water did not slow down ISORROPIA-lite but increased the concentrations of the inorganic semivolatile components especially at nighttime. The temporal evolution shown that organic water could highly contribute to the total PM_1 water mass and increase the concentrations of fine nitrate and ammonium within 1 $\mu g\ m^{-3}$ in places where the organic aerosol and RH levels are high.

Keywords: aerosol thermodynamics, metastable state, nitrate, ammonium, organic water

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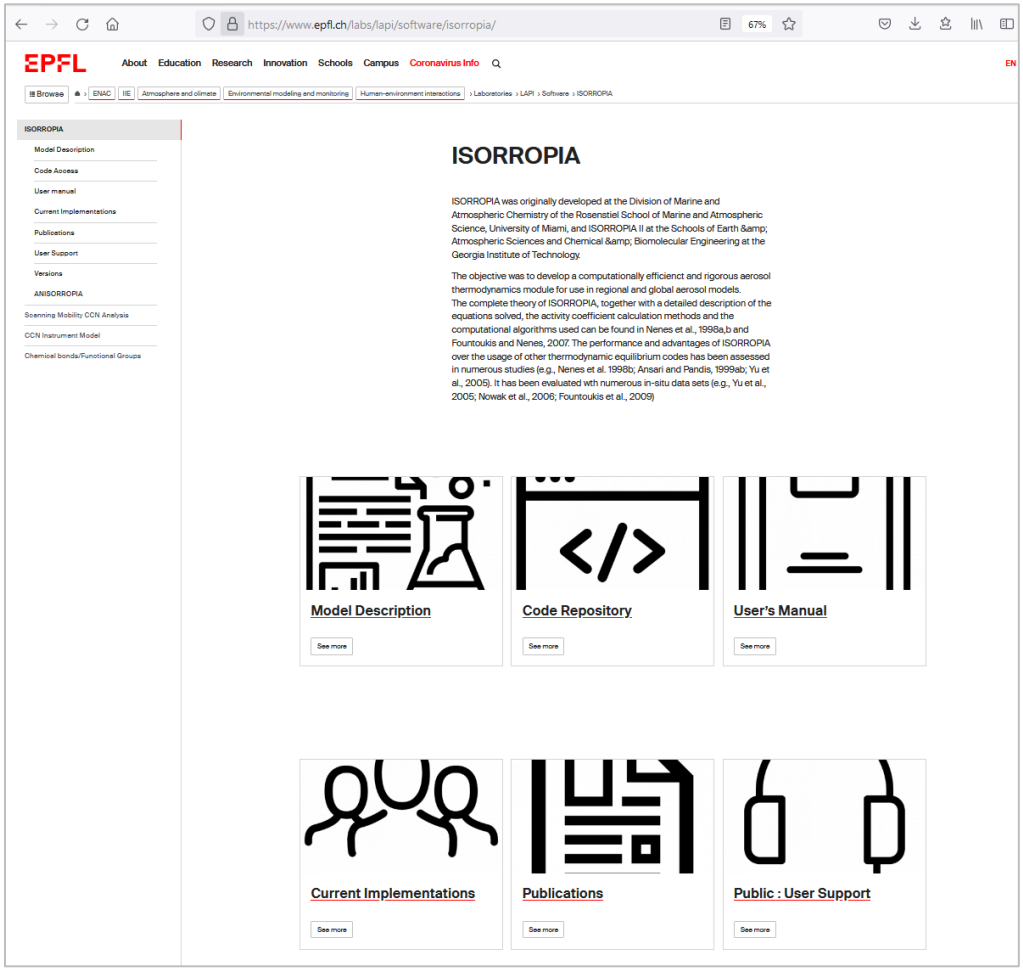

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