



Box Modeling

Less GAUs more FUN!

<http://boxmodeling.meteo.physik.uni-muenchen.de/index.html#>

(or just Google “BOXMOX”)

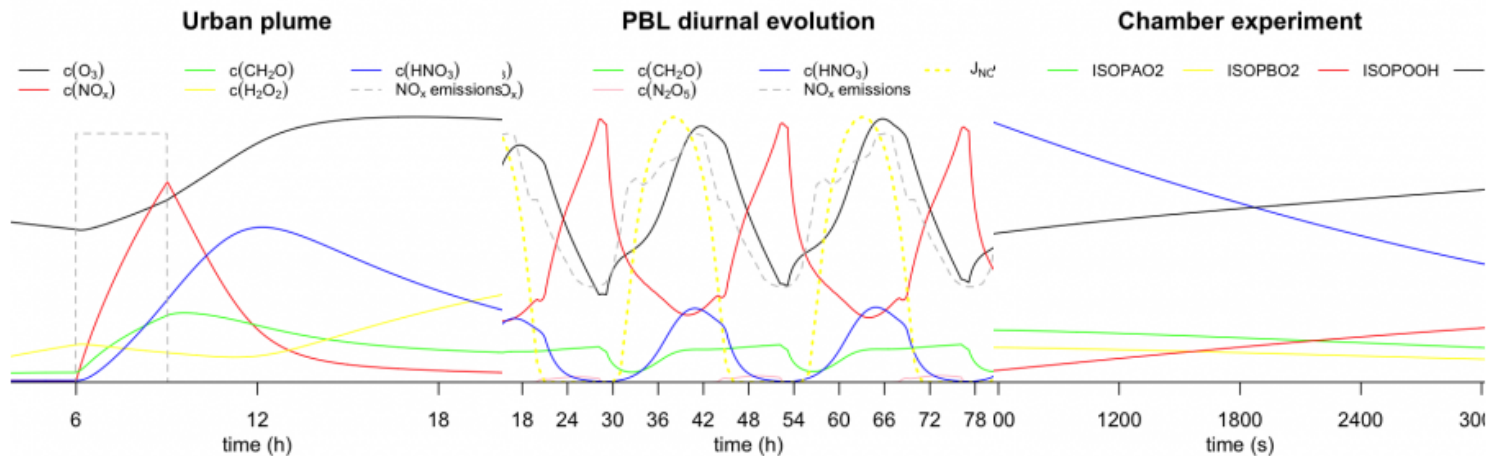
Modeling

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BOXMOX - BOX MODEL EXTENSIONS TO KPP

BOXMOX is an extension to the Kinetic PreProcessor (KPP, <http://people.cs.vt.edu/~asandu/Software/Kpp/>) that allows for an easy set up of box model simulations by providing input data (initial conditions, environmental parameters, mixing/ventilation) as simple text files.

The system can be used to simulate chamber experiments, Lagrange-type air parcel studies, as well as to describe chemistry in the atmospheric boundary layer. An example application has been published in Knote et al. (2015).



BOXMOX is a collaborative effort of the LMU Munich, Germany and NCAR, Boulder. You can find more information, online tools and downloads on the BOXMOX website:

<http://boxmodeling.meteo.physik.uni-muenchen.de>

BOXMOX (BOX MOdeling eXtensions to KPP)

Can be used to simulate:

- Chamber experiments
- Lagrange-type air parcel studies
- Boundary layer chemistry

Can be run online, or downloaded and compiled to run on your own system.

Uses the KPP (*Kinetic Preprocessor* [Sandu and Sander, 2006])

- User-selected input data, meteorological parameters, etc.
- Optional dilution, entrainment, mixing, deposition, etc.
- *Essentially puts the air parcel in a jar then follows the chemistry*

Currently available Mechanisms:

CB05TUCI_EPA	CBMZ
MCMv3_3	RACM
MOZART_4	RADM2
MOZART_T1	SAPRC99

Future:
GECKO_A



BOXMOX Inputs

environment.csv – space-delimited or fixed-width file (basically, temperature)

Constant

I15		
	A	B
1	1	
2	0	
3	TEMP	
4	295	
5		
6		
7		

Diurnal

(note = 25 hours, with 0h = 24h)

** Not specific to the mechanism being used*

line 1: the first row in each file states the number of species / parameters values are provided (not counting a "time" / "tau" variable).

- line 2: the second line defines whether the units of time are
- "0": without time dependency, one line of values expected (see below).
- "1": seconds since simulation start.
- "2": hour of day for an idealized diurnal cycle.

E3		
	A	B
1	1	
2	2	
3	time TEMP	
4	0.000000	284.779492
5	1.000000	284.779492
6	2.000000	284.779492
7	3.000000	284.779492
8	4.000000	284.779492
9	5.000000	284.779492
10	6.000000	285.342824
11	7.000000	288.208903
12	8.000000	291.094748
13	9.000000	293.802698
14	10.000000	296.144976
15	11.000000	297.973336
16	12.000000	299.149416
17	13.000000	299.604036
18	14.000000	299.297662
19	15.000000	298.259944
20	16.000000	296.550180
21	17.000000	294.286966
22	18.000000	291.638314
23	19.000000	288.762353
24	20.000000	285.876508
25	21.000000	284.779492
26	22.000000	284.779492
27	23.000000	284.779492
28	24.000000	284.779492

BOXMOX Inputs

PhotolysisRates.csv

** Not specific to the mechanism being used*

Constant

	A	B	C	D	E	F	G	H	I	J	K	L	M	N			
1	57																
2	0																
3	mek 1_c4h9ono2 ch2or n2o o31d c2cho ch2cch3cho_hco hocl ch2om pooh no2 ch3coo2h mvk_mcm_co h2o2 hno4_2 hno2 no3o2 o33p hno3 c5hpalld hc																
4	0.000010	0.000003	0.000041	0.000000	0.000047	0.000026	0.000001	0.000350	0.000061	0.000006	0.010009	0.000001	0.000003	0.000009	0.000009	0.001637	0.0
5																	

Diurnal

(again, 25 hours, with 0h = 24h)

*you can initialize the model to a specific time of day in the compiled version.

	A	B	C	D	E	F	G	H	I
1	57								
2	2								
3	time mek 1_c4h9ono2 ch2or n2o o31d c2cho ch2cch3cho_hco hocl ch2om pooh no2 ch3coo2h r								
4	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
5	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
6	2.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
7	3.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
8	4.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
9	5.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
10	6.000000	0.000001	0.000000	0.000006	0.000000	0.000005	0.000001	0.000000	0.000037
11	7.000000	0.000003	0.000000	0.000016	0.000000	0.000014	0.000004	0.000000	0.000125
12	8.000000	0.000005	0.000001	0.000023	0.000000	0.000020	0.000009	0.000001	0.000199
13	9.000000	0.000006	0.000001	0.000027	0.000000	0.000023	0.000014	0.000001	0.000251
14	10.000000	0.000006	0.000002	0.000029	0.000000	0.000025	0.000018	0.000001	0.000286
15	11.000000	0.000006	0.000002	0.000031	0.000000	0.000027	0.000020	0.000001	0.000306
16	12.000000	0.000007	0.000002	0.000031	0.000000	0.000027	0.000021	0.000001	0.000312
17	13.000000	0.000006	0.000002	0.000031	0.000000	0.000027	0.000021	0.000001	0.000307
18	14.000000	0.000006	0.000002	0.000030	0.000000	0.000026	0.000018	0.000001	0.000289
19	15.000000	0.000006	0.000002	0.000027	0.000000	0.000024	0.000015	0.000001	0.000256
20	16.000000	0.000005	0.000001	0.000023	0.000000	0.000020	0.000010	0.000001	0.000206
21	17.000000	0.000004	0.000001	0.000017	0.000000	0.000015	0.000005	0.000000	0.000135
22	18.000000	0.000001	0.000000	0.000007	0.000000	0.000006	0.000001	0.000000	0.000047
23	19.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000001
24	20.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25	21.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
26	22.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
27	23.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
28	24.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
29									

BOXMOX Inputs

InitialConditions.csv – space delimited file

** Specific to the mechanism being used*

BOXMOX Online Examples

http://boxmodeling.meteo.physik.uni-muenchen.de/online_tools/inbox.html

Select pull-down “Run BOXMOX online”.

Mechanism: MOZART_4

Check “use example”

Select “chamber_experiment”

Run BOXMOX experiments online

mechanism: use example:

Click on

new experiment

Edit Experiment settings

Run time (s): 86400

time step (s): 60

You can also download files here,
look at formats, modify them
and/or re-upload new files.

Click “run”

When the run is finished, you can download the .conc, .rates and .jacobian files.

BOXMOX Online Examples

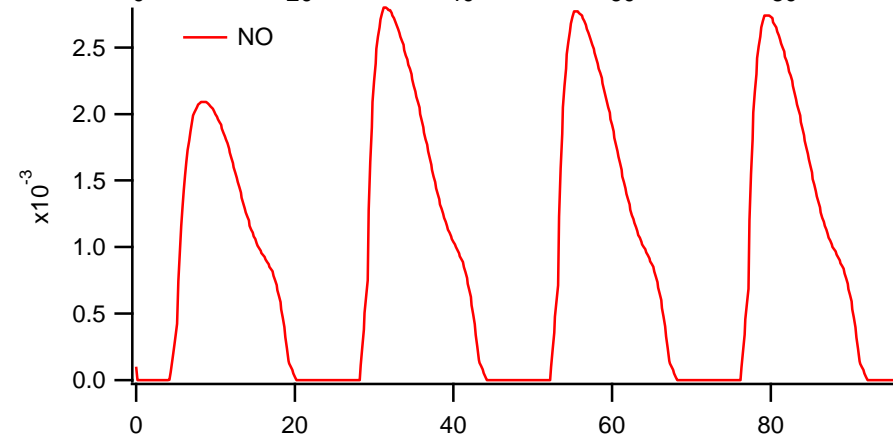
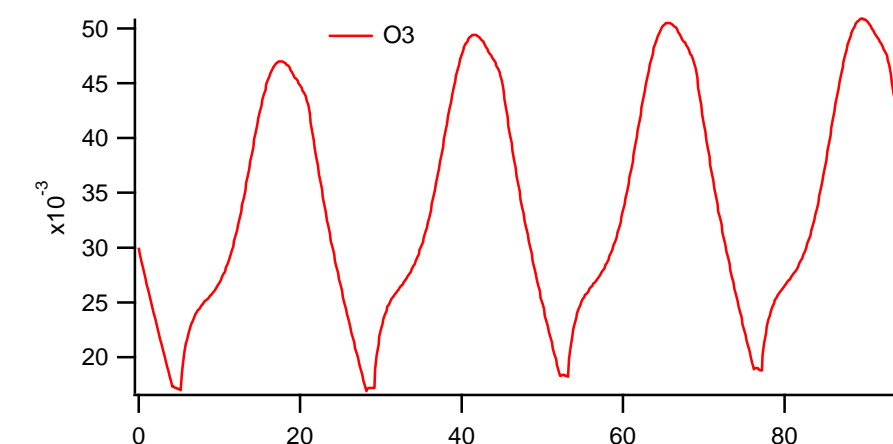
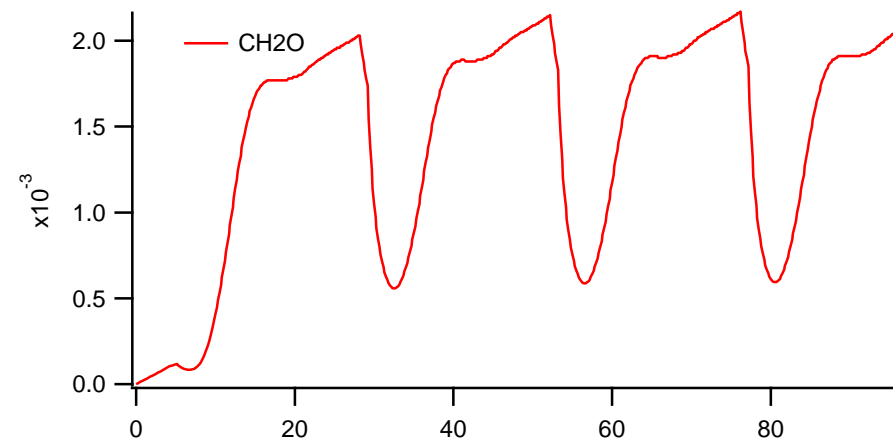
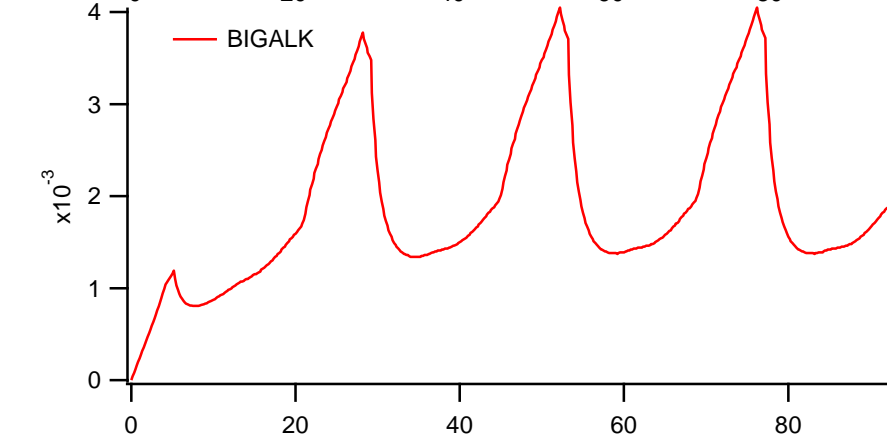
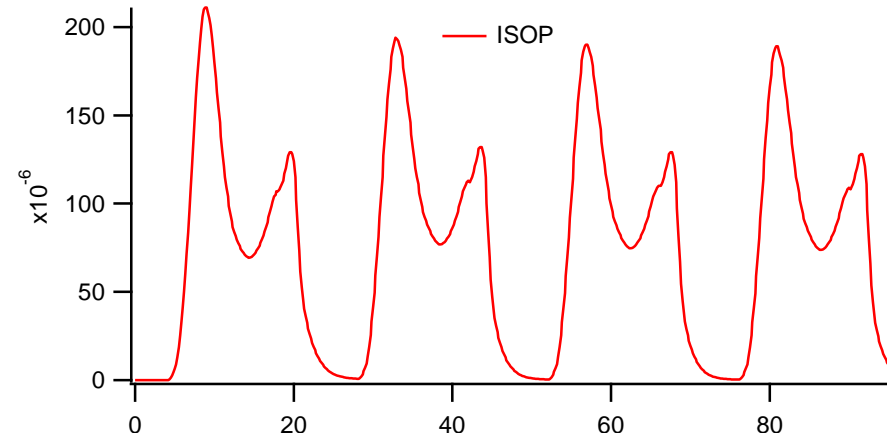
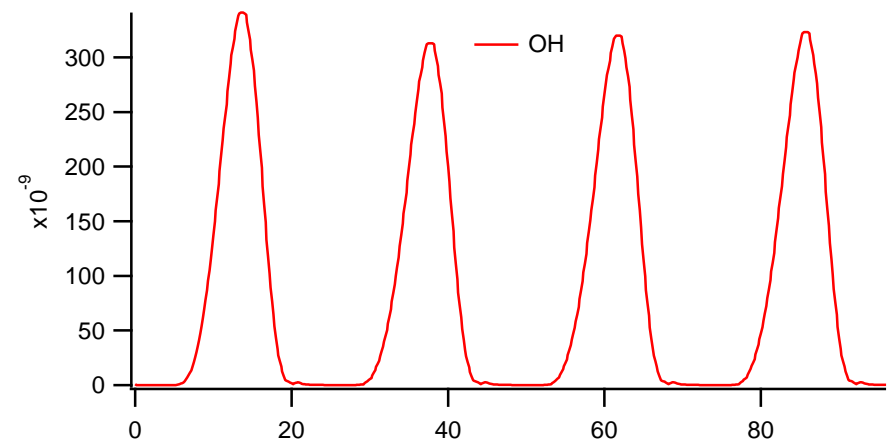
Take a look through the .conc files generated... use EXCEL, IGOR, or whatever program you prefer

Hint – rename the file generated to something unique.

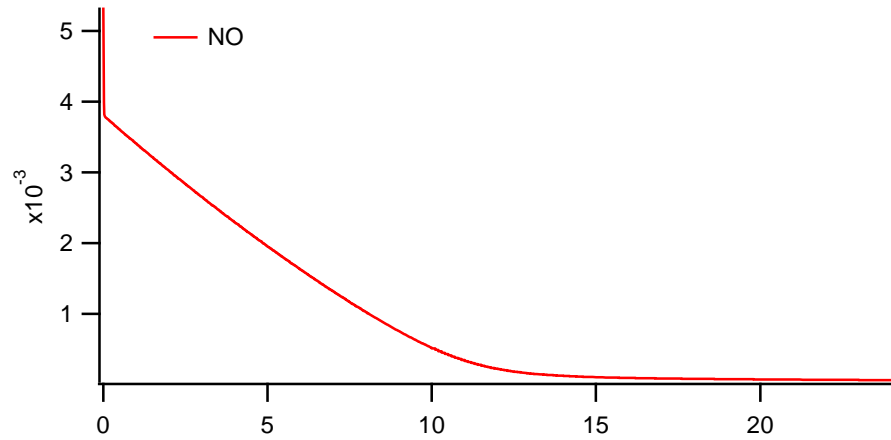
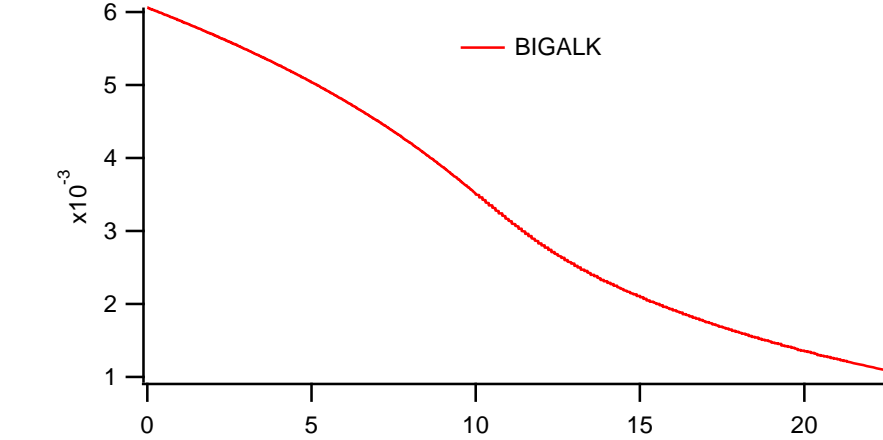
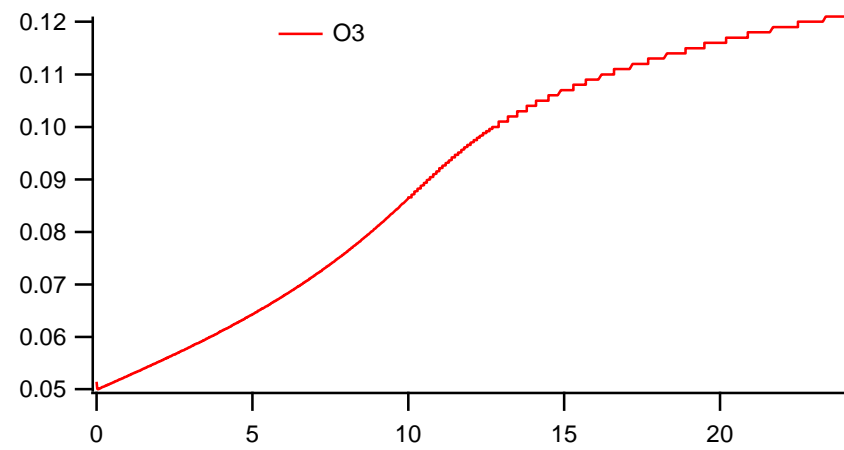
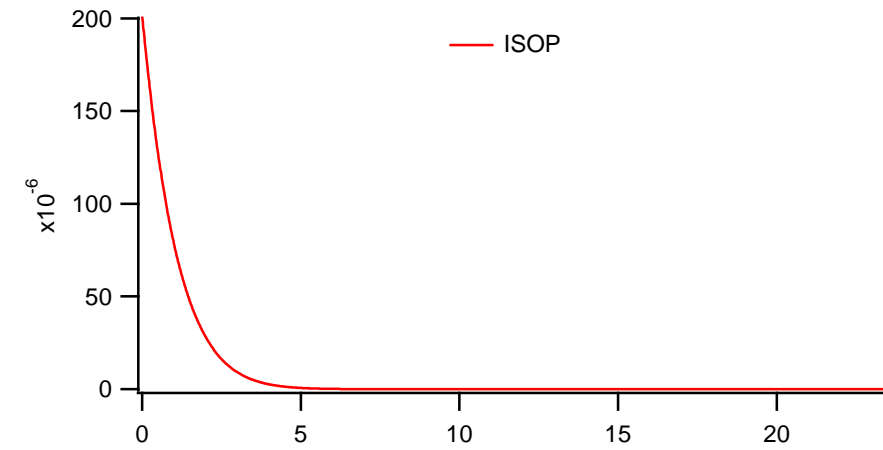
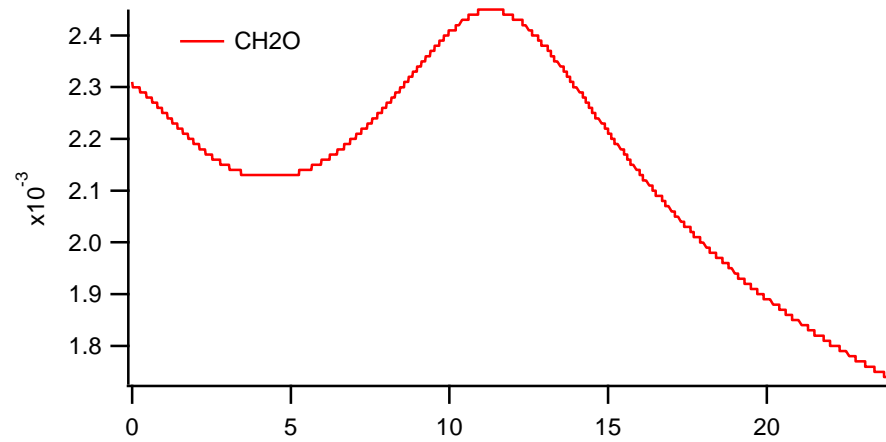
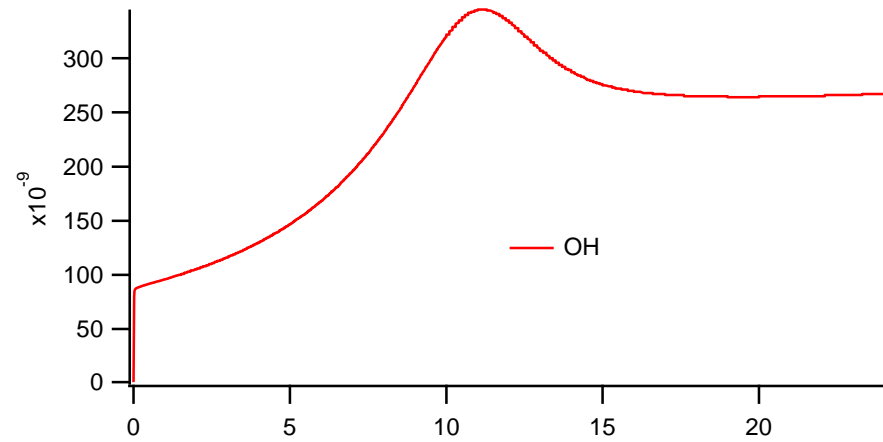
After, try running the other two examples using the default settings:

- Urban plume
- PBL diurnal

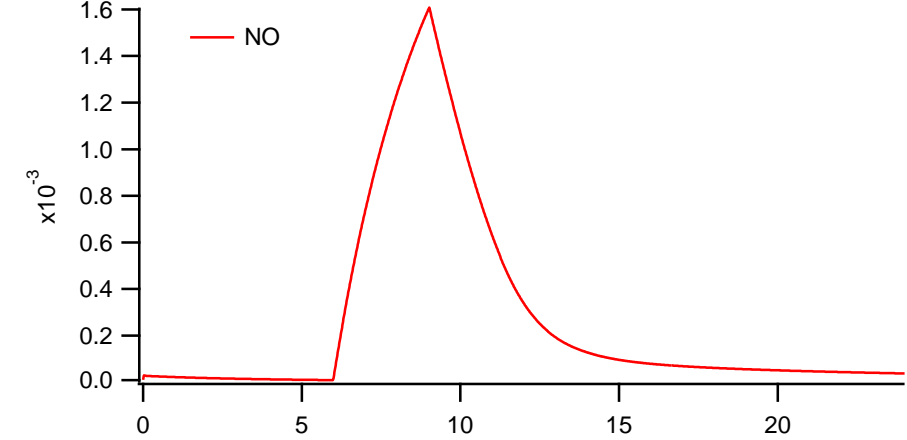
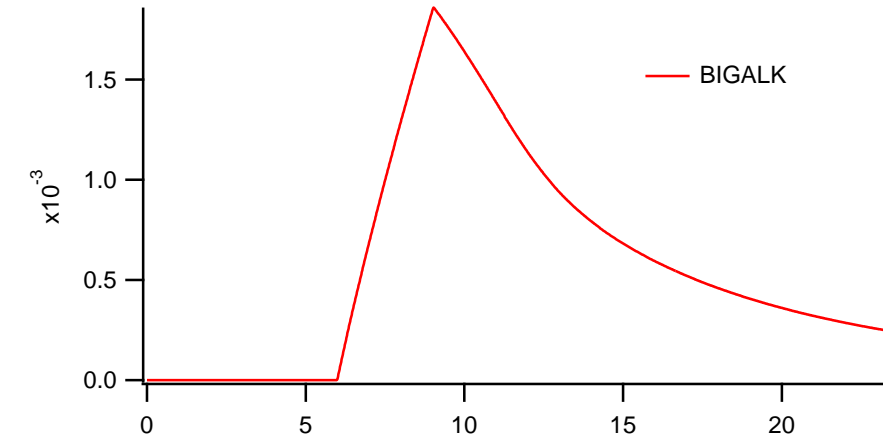
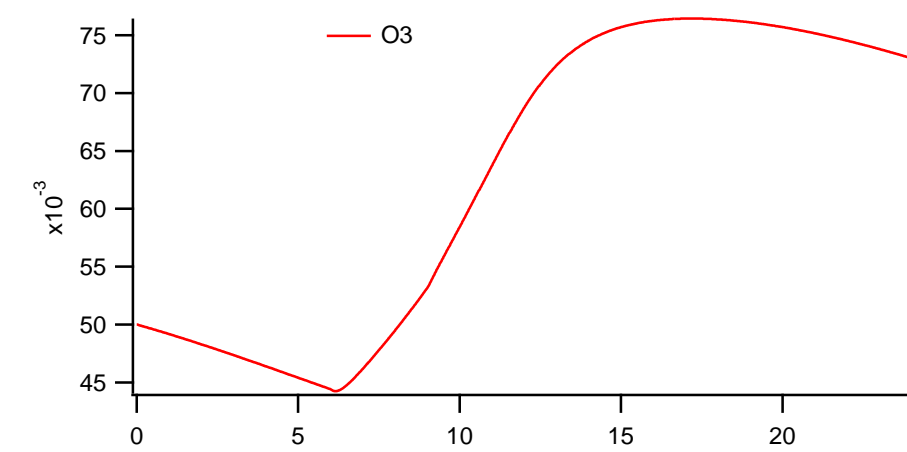
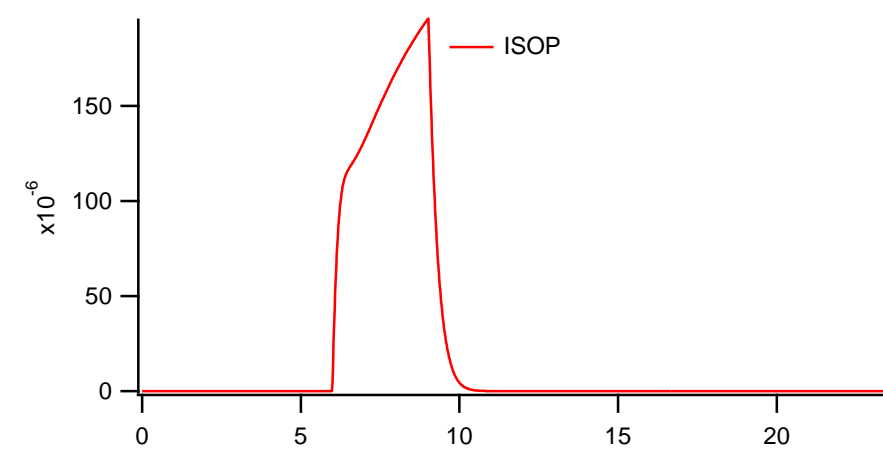
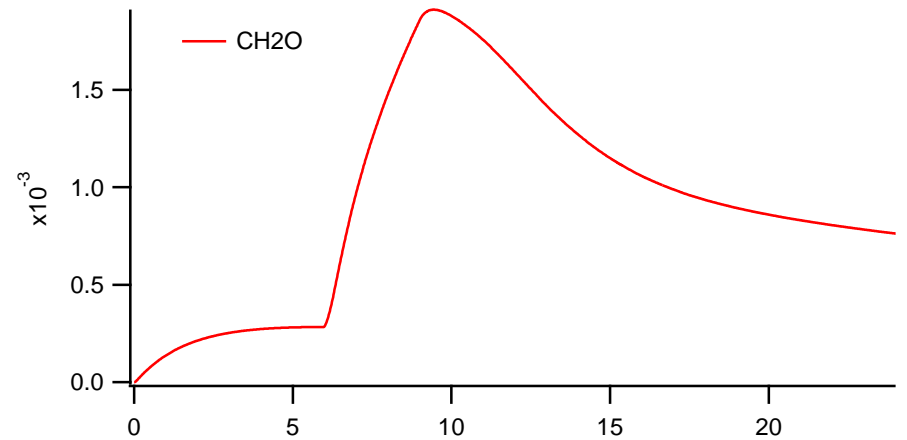
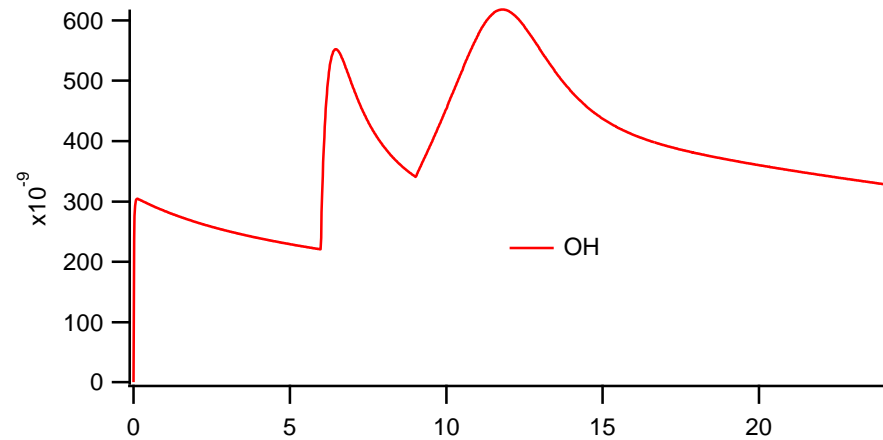
PBL – diurnal results...



Chamber Experiment



Urban Plume



BOXMOX Uploading input files to run online

Next – let's generate some files to run online:

http://boxmodeling.meteo.physik.uni-muenchen.de/online_tools/inbox.html

FRAPPE

Tags

Tag: RIFLE

Mechanism: MOZART_T1

“constant” (don't check diurnal cycle)

Download:

Environment.csv, InitialConditions.csv, PhotolysisRates.csv


Edit the filenames appropriately so you can find them in the next step.

BOXMOX Uploading input files to run online

Once you have the files,

Go to **Online tools** pulldown menu
Select **Run BOXMOX online**

Mechanism: MOZART_T1

Click on 

One at a time, upload the files you renamed from:

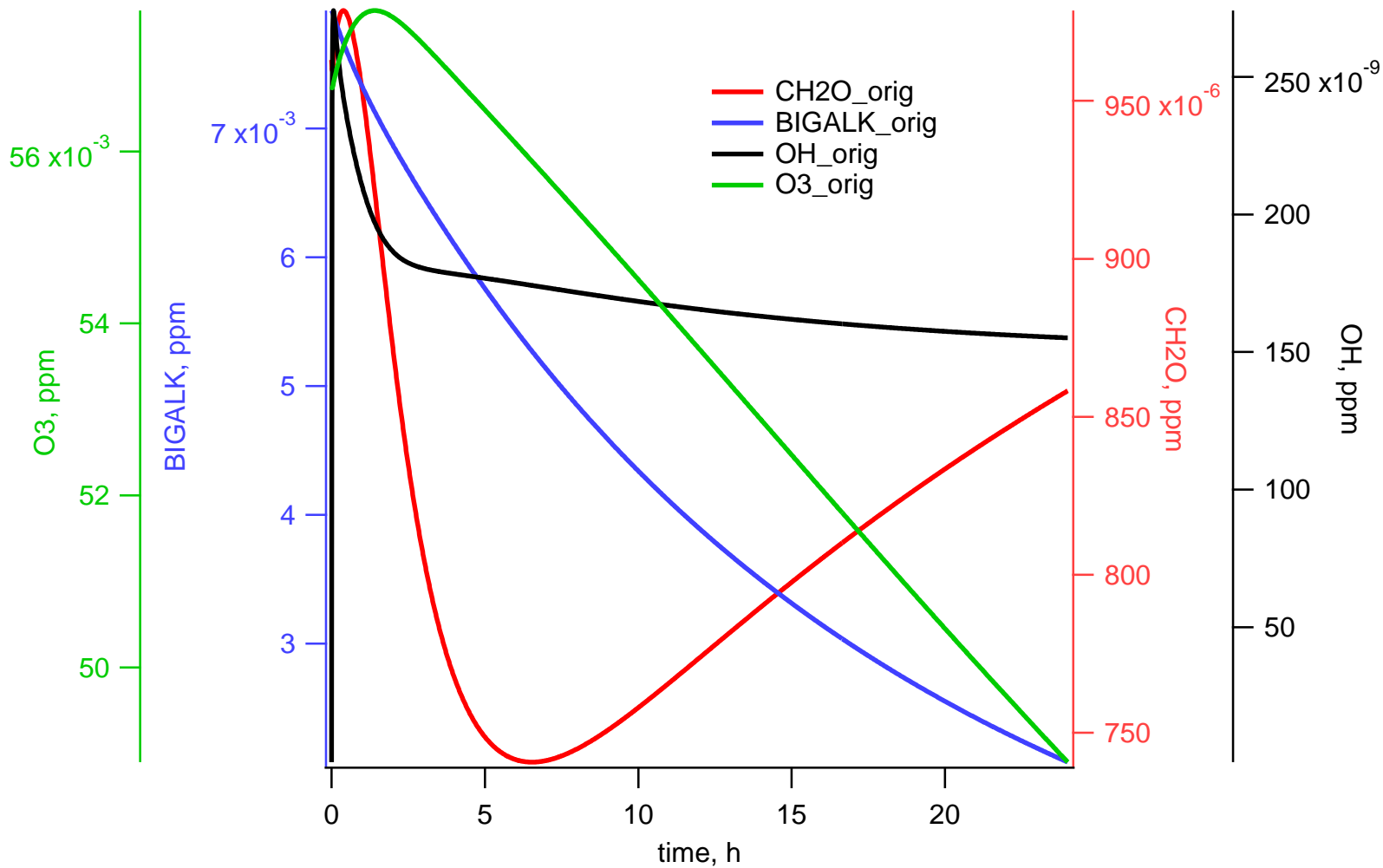
Environment.csv, InitialConditions.csv, PhotolysisRates.csv

Run time (s): 86400

Time step (s): 60

Click on Run, then download the .conc file when it is done.

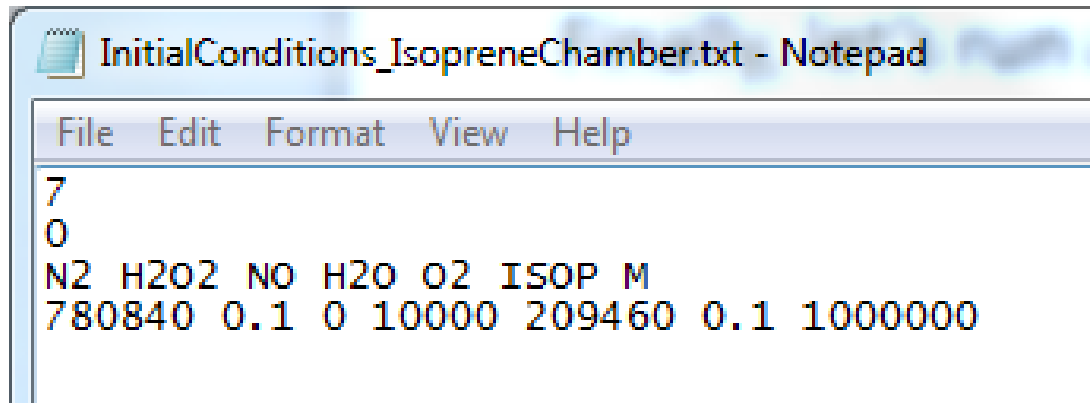
RIFLE, constant photolysis



Simple Isoprene Chamber Experiment

Finally, let's run a simulation using own simple set of initial conditions.

In a text editor, create a file with the following:



```
InitialConditions_IsopreneChamber.txt - Notepad
File Edit Format View Help
7
0
N2 H2O2 NO H2O O2 ISOP M
780840 0.1 0 10000 209460 0.1 1000000
```

** all concentrations are in ppm*

Save this file as a .txt and then rename this file to a .csv in an explorer window.

Using the environment.csv and the PhotolysisRates.csv that you generated for the Rifle Experiment, run for 86400 s with a timestep of 60 s.

Simple Isoprene Chamber Experiment

