Indoor homogeneous and heterogeneous NO_2 chemistry.

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Homogeneous NO_2 chemistry

Gas phase equilibrium of NO_2 with O_3

1. $NO_2 + h\upsilon \rightarrow NO + O, \quad \lambda < 420$ nm
2. $O + O_2 \rightarrow O_3$

$= NO_2 + O_2 \rightarrow NO + O_3$

Indoors:
- little UV- light
- no NO emission

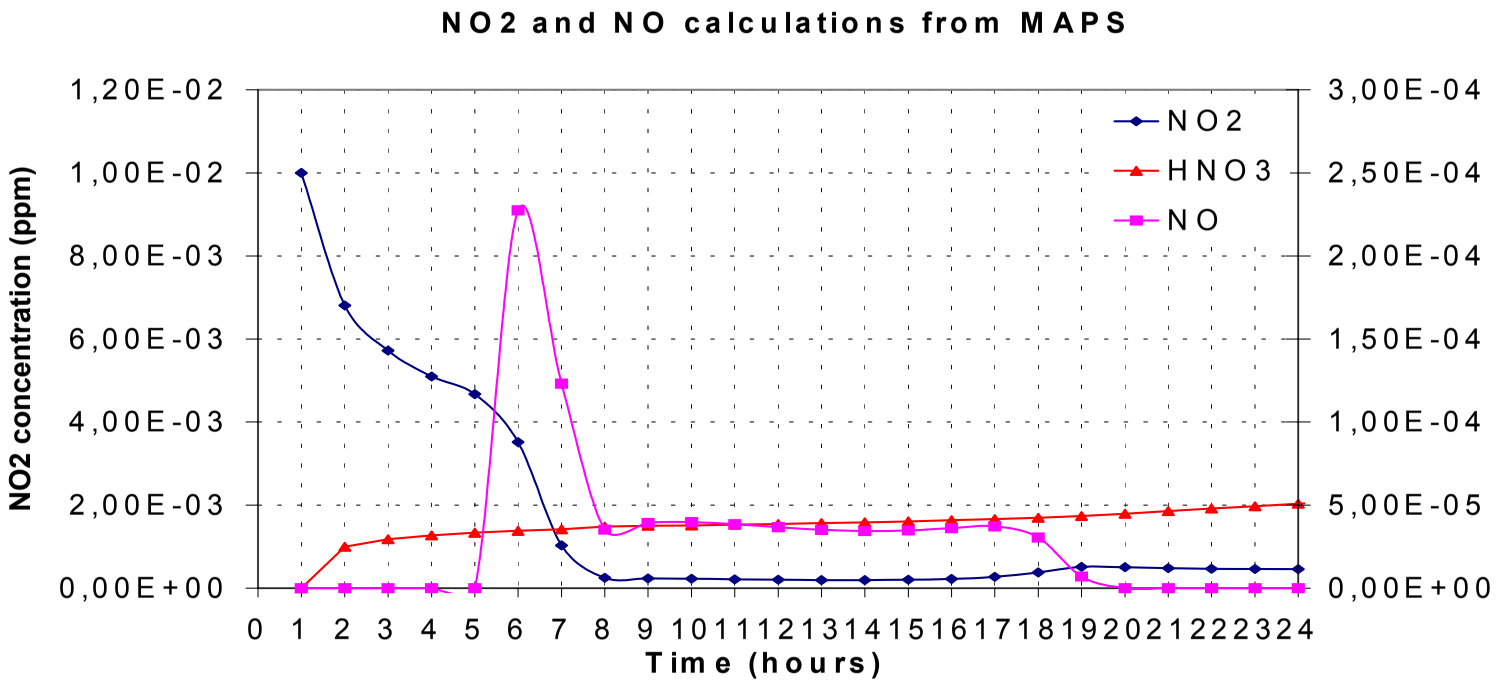
Calculation of indoor NO_2 and O_3 concentrations from the MAPS model.

Initial conditions

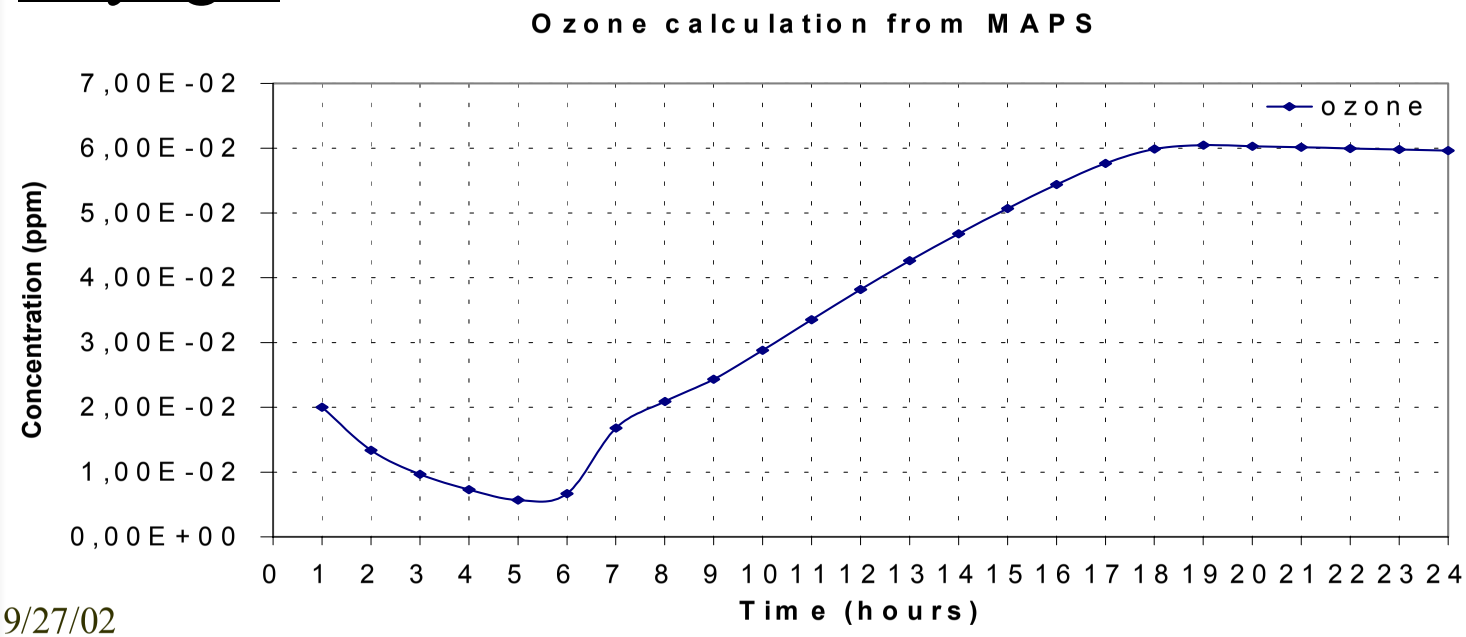
32 chemical species.
No air exchange
No aerosol chemistry.
Deposition velocity, $v_d = 0$.
$O_3(t = 0) = 20$ ppb.
$NO_2(t = 0) = 10$ ppb.

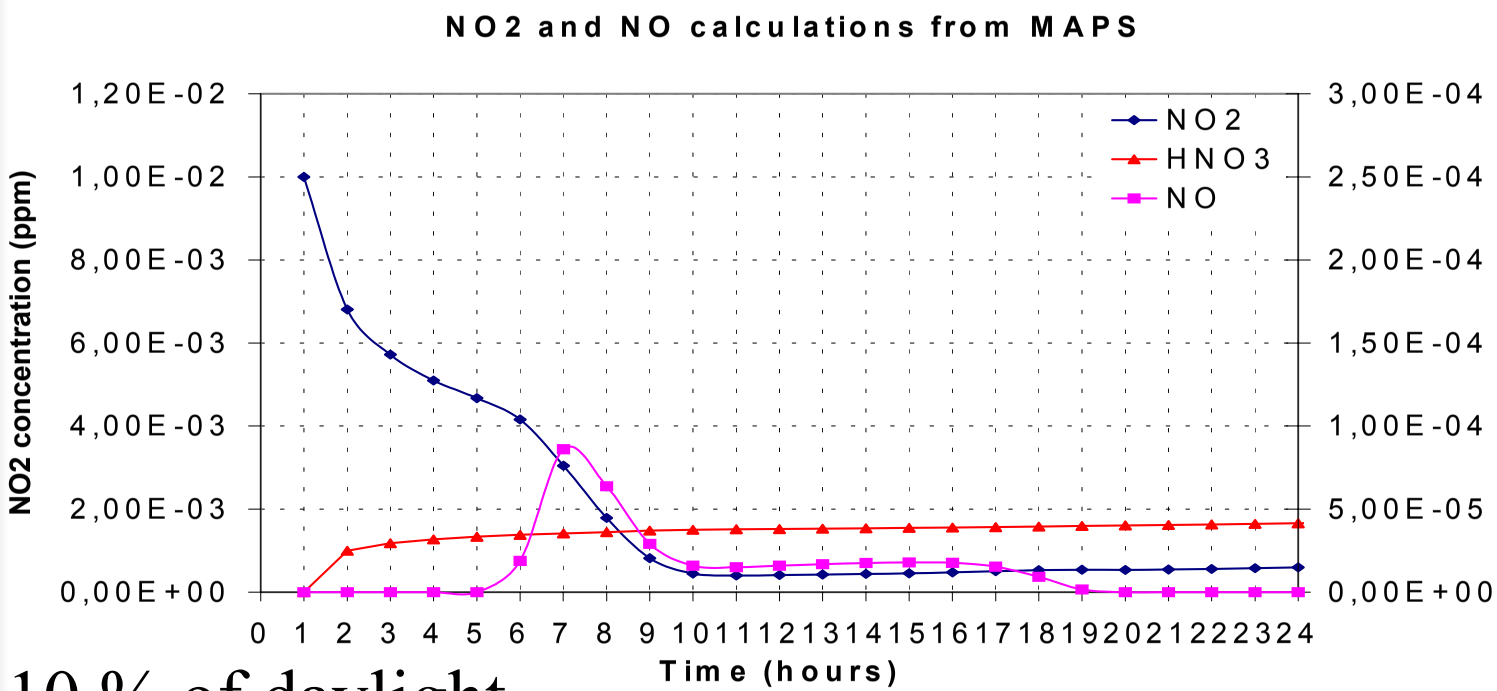
$NO(t = 0) = 0$ ppb
HNO_3 $(t = 0) = 1.0$ ppb
Terpenes = 0.4 ppb
$T = 13^oC$
RH = 68 %

(http://acd.ucar.edu/~^durlak/MAPShome.html)

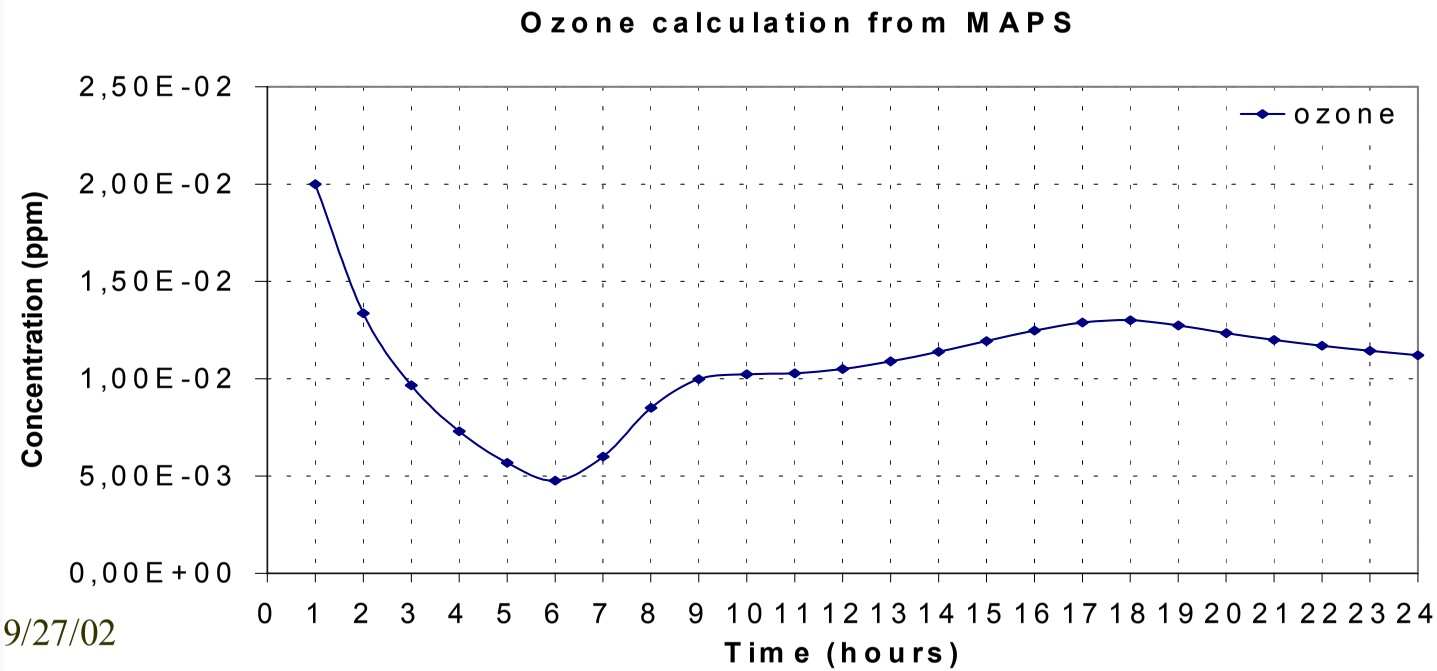

NO2 and NO calculations from MAPS
NO2 concentration (ppm)
NO concentration (ppm)
1,20E-02
1,00E-02
8,00E-03
6,00E-03
4,00E-03
2,00E-03
0,00E+00
3,00E-04
2,50E-04
2,00E-04
1,50E-04
1,00E-04
5,00E-05
0,00E+00
NO2
HNO3
NO
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
Time (hours)

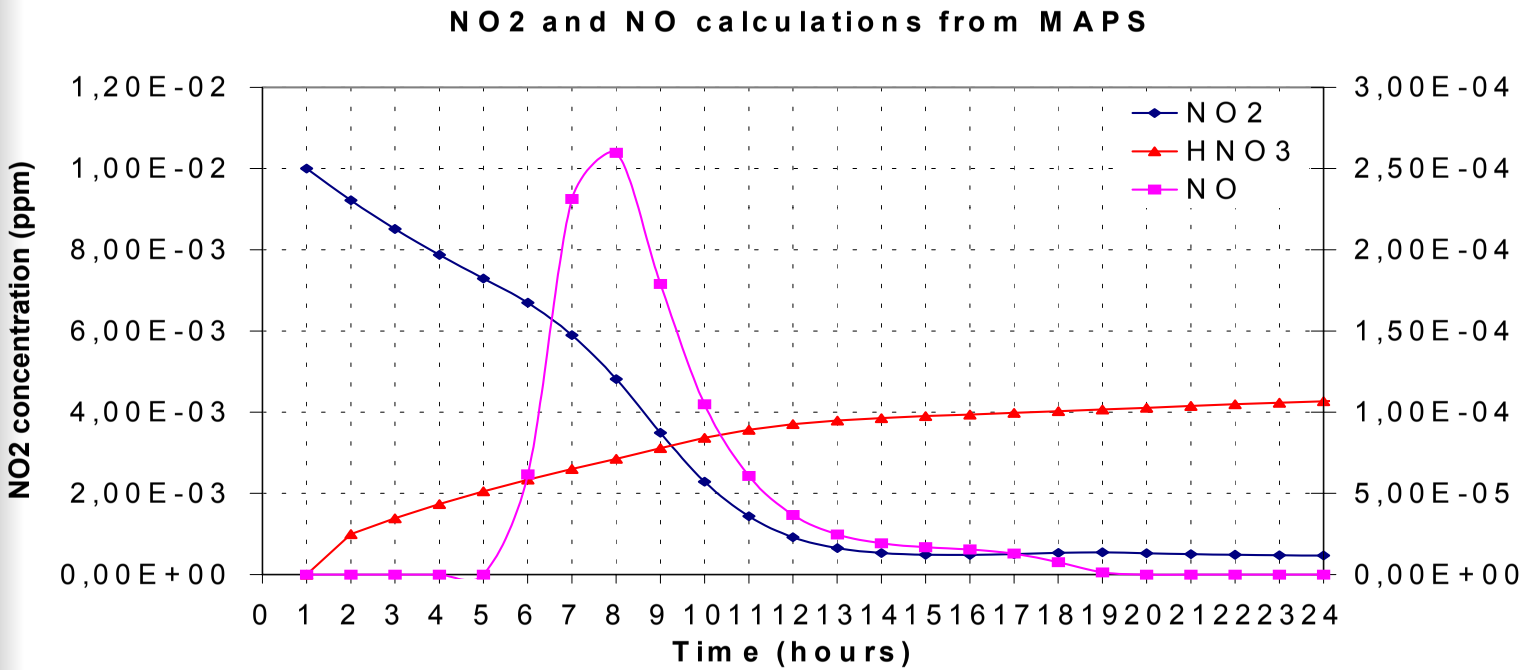
Daylight


Ozone calculation from MAPS
Concentration (ppm)
7,00E-02
6,00E-02
5,00E-02
4,00E-02
3,00E-02
2,00E-02
1,00E-02
0,00E+00
ozone
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
Time (hours)

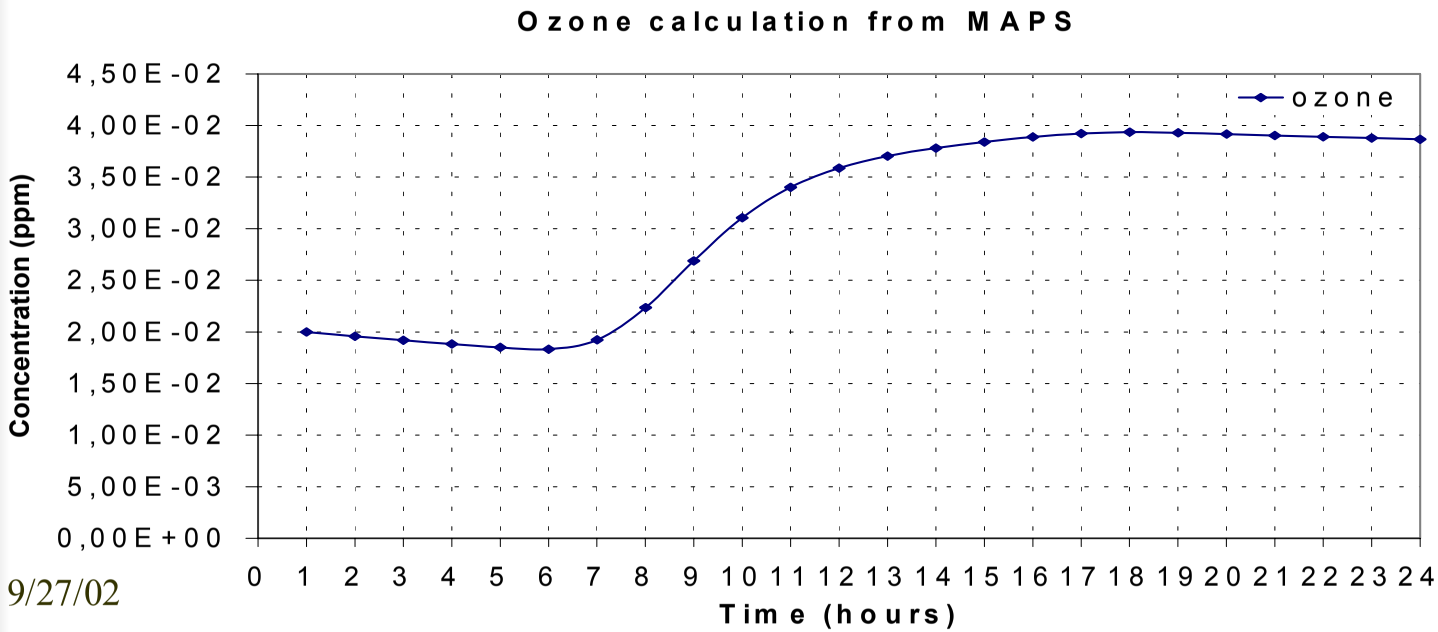


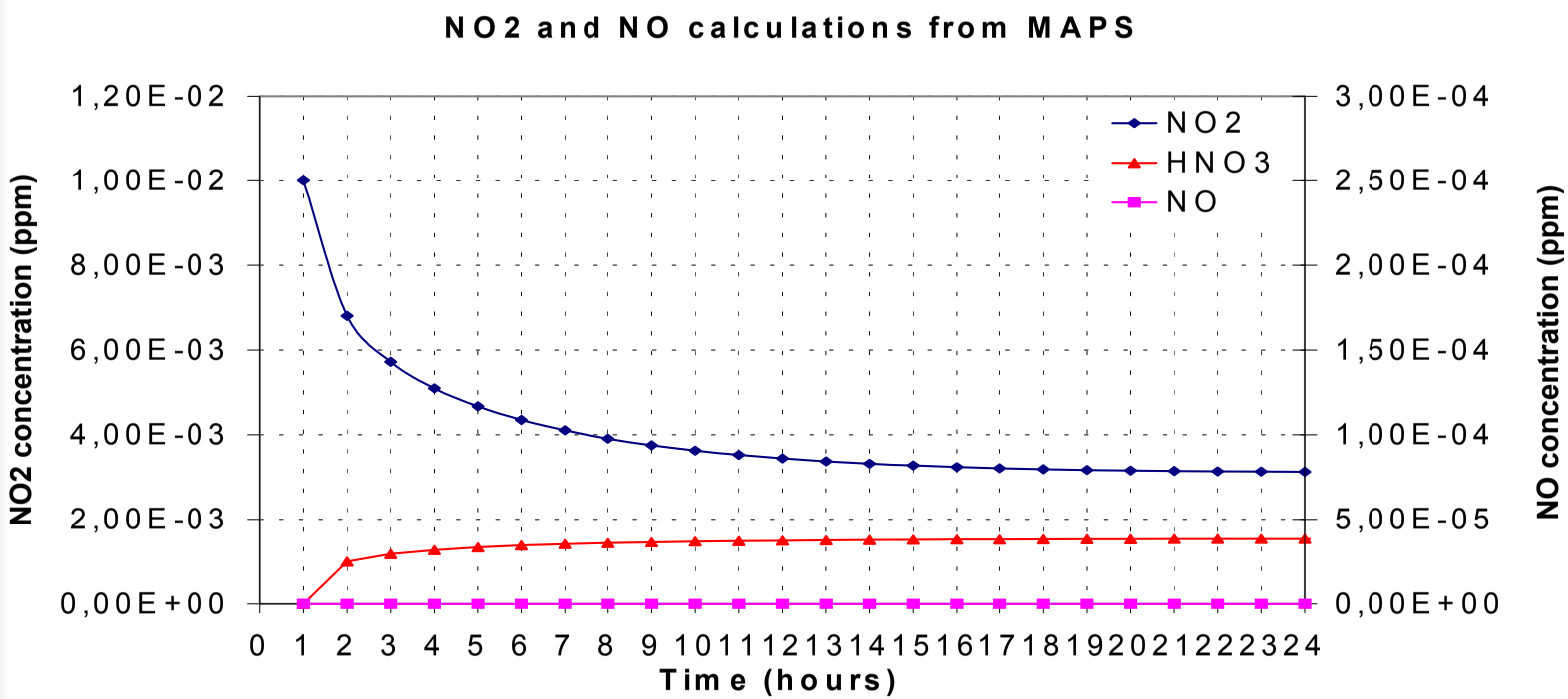
10 % of daylight



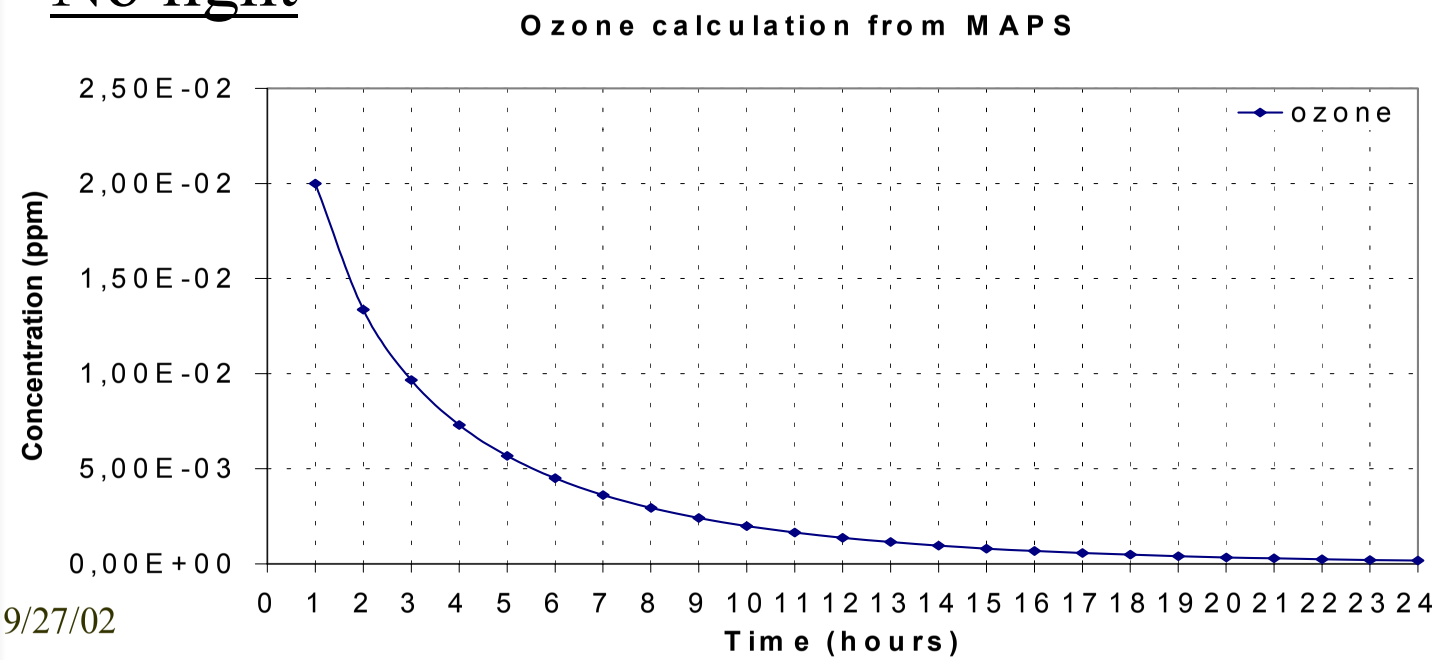


10 % of daylight, no terpenes




NO2 and NO calculations from MAPS
NO2 concentration (ppm)
NO concentration (ppm)
1,20E-02
1,00E-02
8,00E-03
6,00E-03
4,00E-03
2,00E-03
0,00E+00
3,00E-04
2,50E-04
2,00E-04
1,50E-04
1,00E-04
5,00E-05
0,00E+00
NO2
HNO3
NO
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
Time (hours)

No light


Ozone calculation from MAPS
Concentration (ppm)
2,50E-02
2,00E-02
1,50E-02
1,00E-02
5,00E-03
0,00E+00
ozone
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
Time (hours)

Concentrations at noon (ppb)

The effect of light with 40 ppb terpenes:

	1. Daylight	2. 10 % of daylight	3. Indoor scenario	4. No light
O_3	38.2	10.5		1.37
NO_2	0.203	0.41	?	3.44
HNO_3	1.56	1.53		1.49
NO	0.0367	0.016		$9.71 \cdot 10^{-7}$

The effect of terpenes at 10 % daylight:

	1. 0 ppb	2. 40 ppb	3. Indoor scenario	4. 100 ppb
O_3	35.9	10.5		3.0
NO_2	0.92	0.41	?	0.43
HNO_3	3.71	1.53		1.19
NO	0.037	0.016		0.016

Conclusion

Indoor concentrations of:

O_3: Concentration varies strongly with light intensity (+) and terpenes (-).
- Very strong temperature dependence. (NILU-CTM)
- Little humidity dependence. (NILU-CTM)

NO_2: Concentration decreases. It varies with light intensity (-) and with terpenes(-). Products are HNO_3 and organic nitrates that may deposit.

Air exchange rate is very important

Heterogeneous NO_2 chemistry

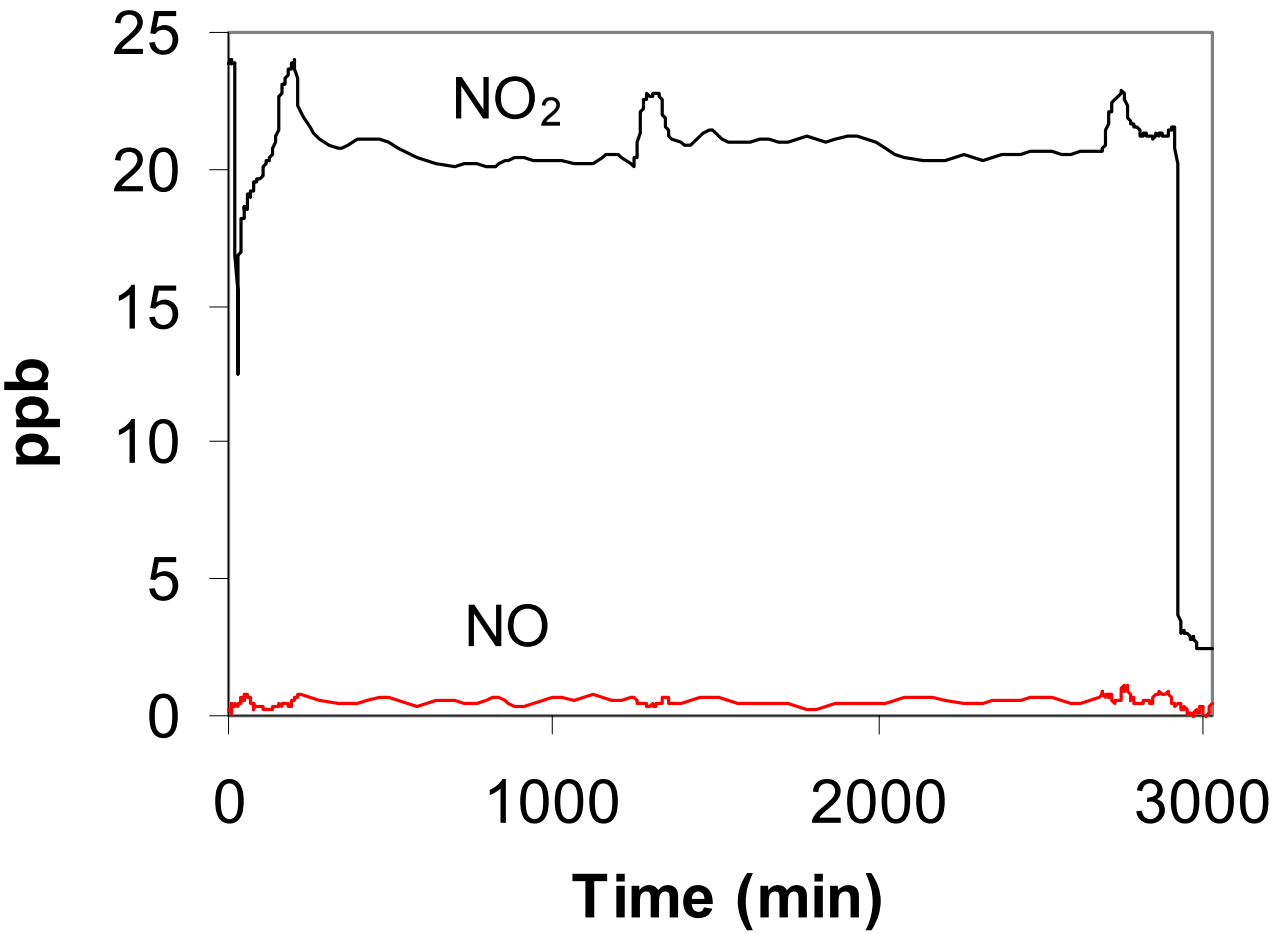
Formation of nitric acid, HNO_3, and deposition on indoor surfaces.

With ozone	hν	VOC
$NO_2 + O_3 \rightarrow NO_3\cdot + O_2$, $\tau_{NO2} \approx 10$ h.		
1. $NO_3\cdot + RH \rightarrow HNO_3 + R\cdot$	–	+
2. $NO_3\cdot + NO_2 \rightarrow N_2O_5$ (highly soluble)	–	
$N_2O_5 + H_2O + M \rightarrow 2HNO_3$ (rapid)		

Without ozone		
3. $NO_2 + OH\cdot \rightarrow HNO_3$, $\tau_{NO2} \approx 1$ day.	+	
$OH\cdot$ formation at $\lambda < 319$ nm		
4. $NO_2 + H_2O \rightarrow HNO_2 + HNO_3$	Of minor importance	
$NO_2 + HNO_2 \rightarrow NO + HNO_3$	(Low solub. of NO_2)	

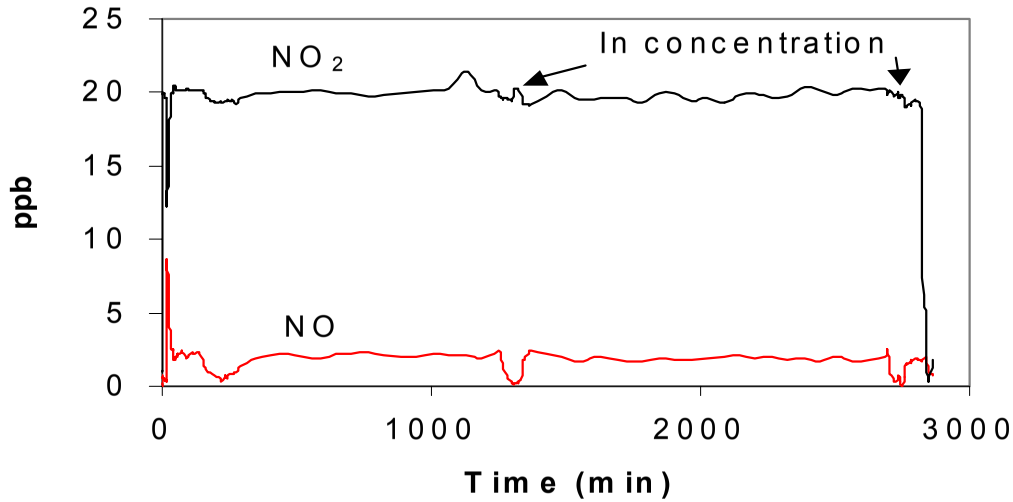
(Seinfeld and Pandis 1998)

Deposition of NO_2 on a rough concrete floor tile. RH = 90 %.

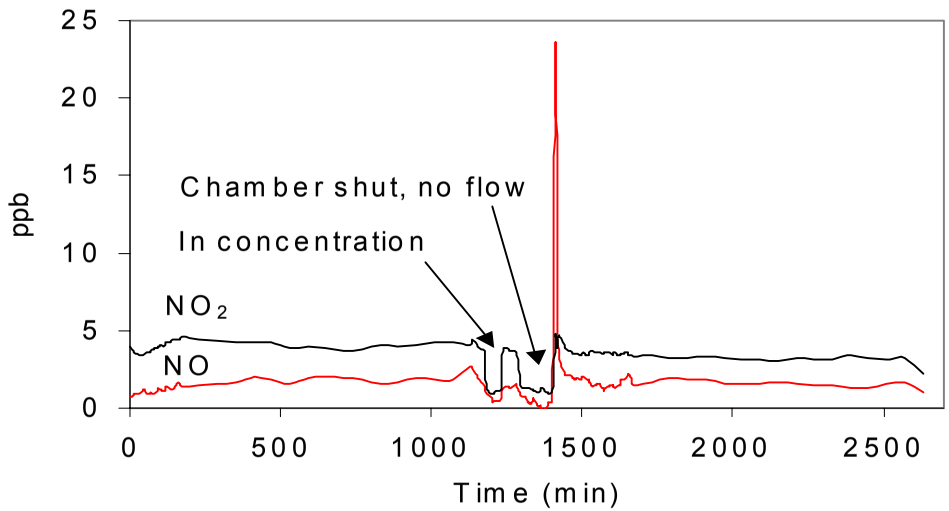


Desorption of NO_2 and NO from wool carpet (Sainsbury center) RH = 90 %

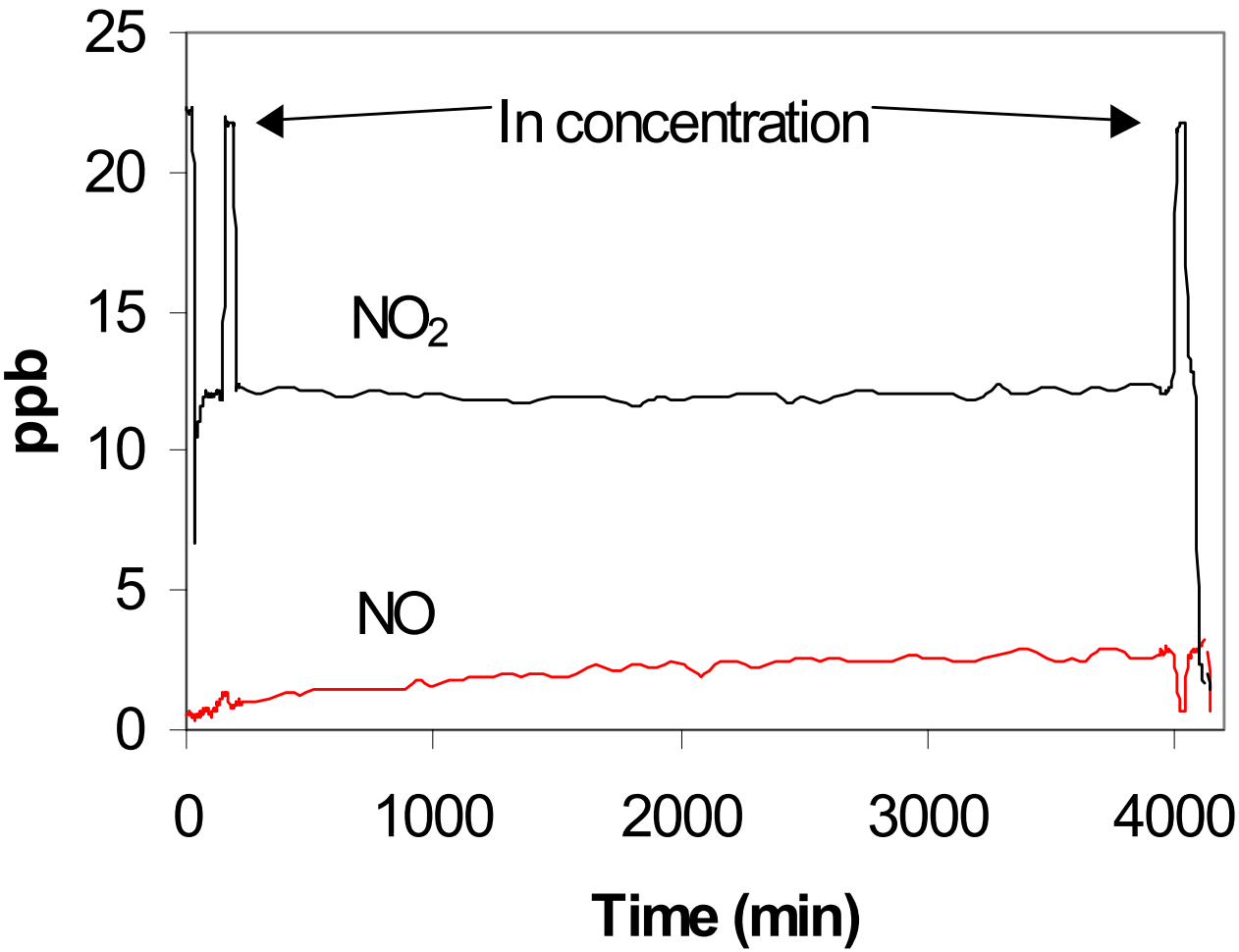
NO_2 flow into the chamber:



No NO_2 flow into the chamber:



Deposition of NO_2 and desorption of NO from an active carbon impregnated cloth. RH = 90 %



Deposition velocities on untreated chipboard: