Supplementary material

Explicit modelling of SOA formation from α-pinene photooxidation : sensitivity to vapour pressure estimation

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– Figure S1 : Time evolution of α-pinene/O_3/NO_x for the low, intermediate and high-NO_x experiments.

– Figure S2 : The extra OH source issue in the high-NOx experiment.

– Figure S3 : Contribution of the top 10, top 100 and top 1000 organic species to the total simulated SOA mass for the intermediate-NO_x experiment and for the high-NO_x experiment obtained with MY, SIM and NAN.

– Figure S4 : Comparisons of the ranks of the simulated top 100 organic species between the various methods in the intermediate and high-NO_x experiments.

– Table S1 : Top 10 species in simulated SOA with SIM in the intermediate NO_x experiment, with their rank and contribution to the total simulated SOA mass.

– Table S2 : Top 10 species in simulated SOA with SIM in the high NO_x experiment, with their rank and contribution to the total simulated SOA mass.

– References.

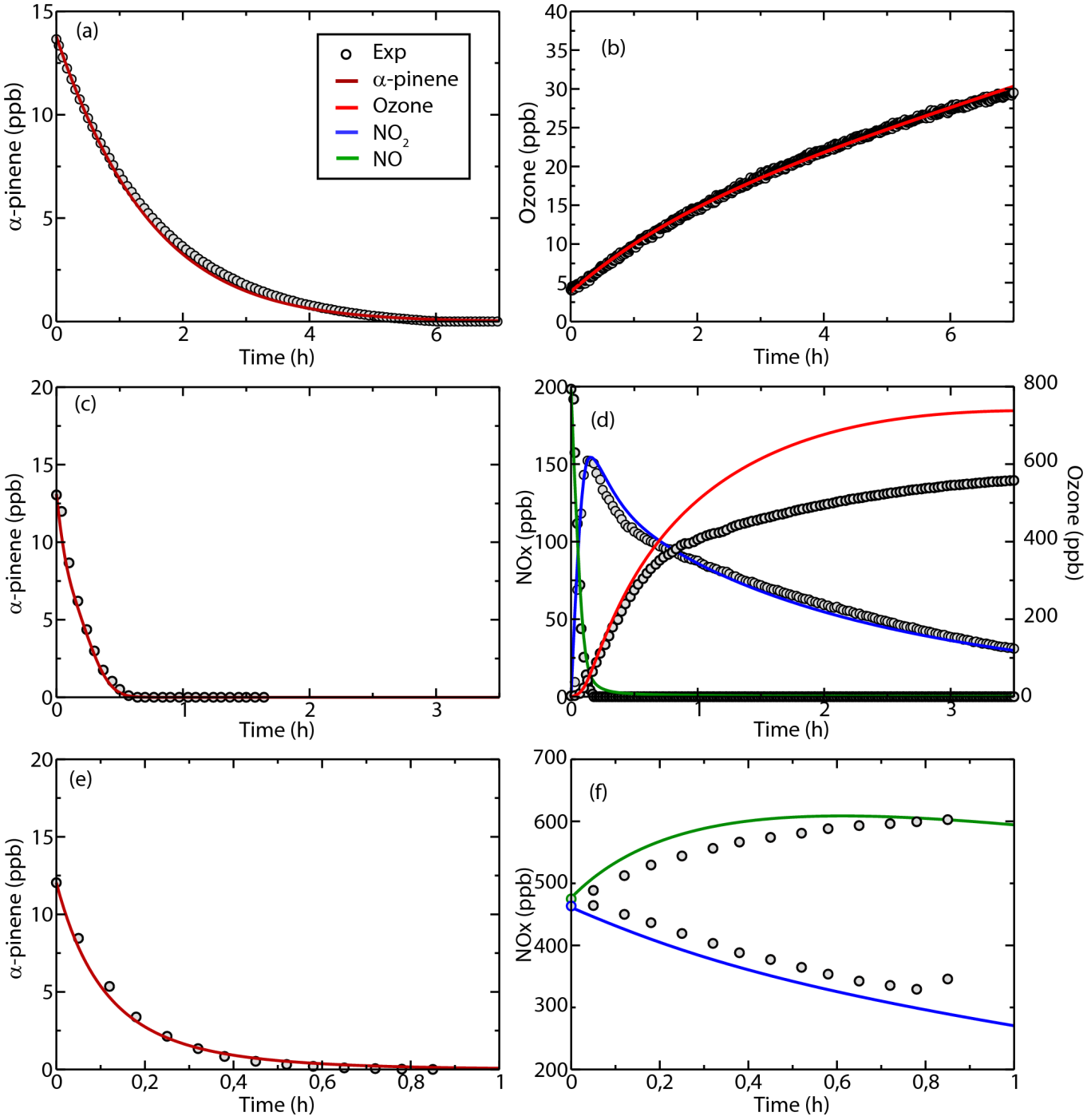


Figure S 1 – Time evolution of α-pinene/O3/NO_x for (a-b) the low-, (c-d) intermediate- and (e-f) high-NO_x experiments. Dots and lines represent measured and modelled compounds respectively. Modelled results are obtained with MY scheme. Similar results are observed with NAN and SIM and are therefore not represented.

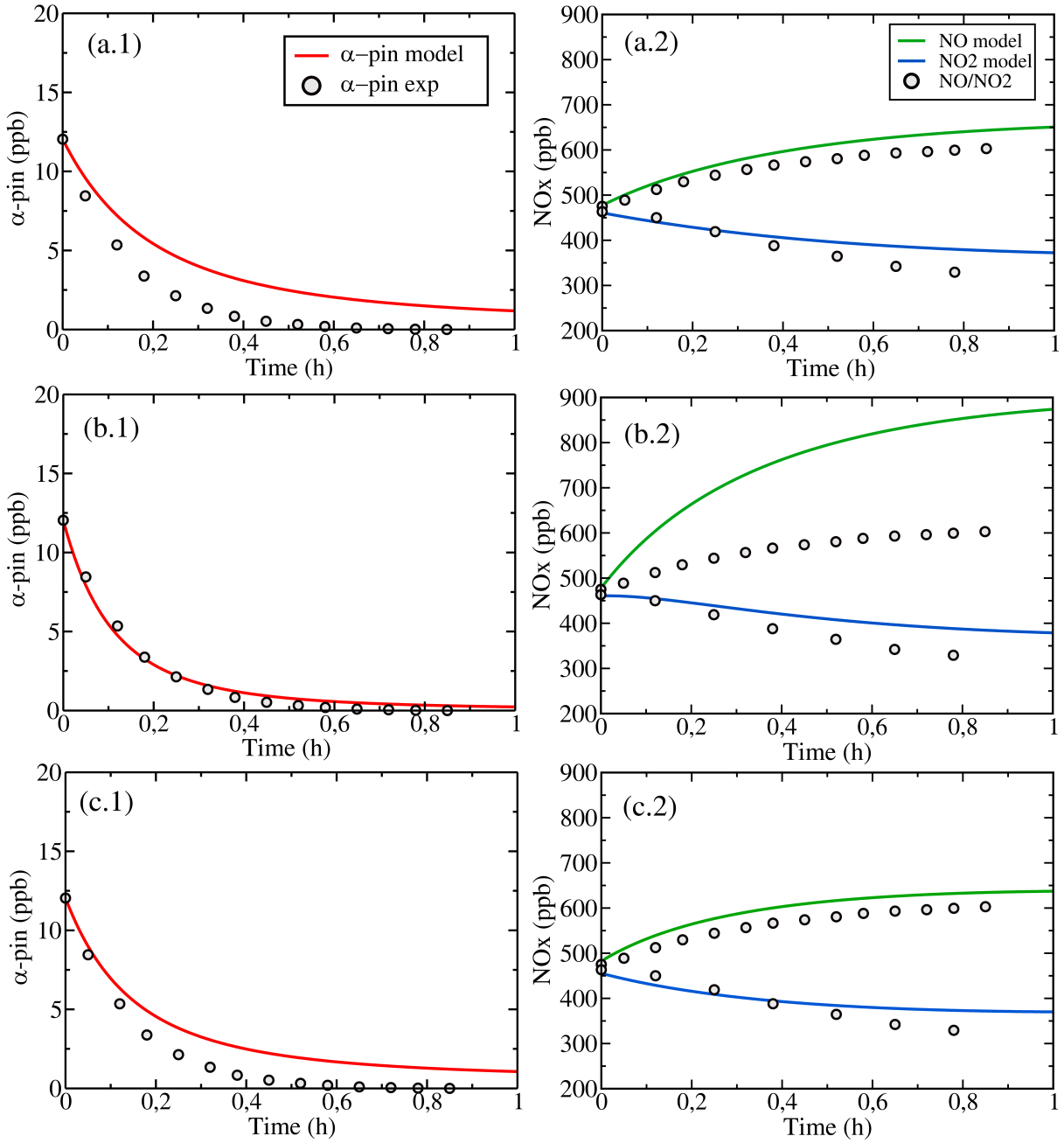


Figure S 2 – Figures show time evolution of α-pinene and NO_x in the high-NO_x experiment. Dots and lines represent measured and modelled compounds respectively. Modelled results are obtained with MY scheme. Figures *a* show results of simulation obtained using 300 ppb of initial HONO concentration. This is the estimated value required to adjust the initial OH concentration retrieved from the initial α-pinene decay. This simulation highlights a missing OH source as seen from the underestimation of the simulated α-pinene decay. Figure *b* show results obtained using an initial concentration of HONO of 800 ppb. This initial HONO concentration leads to a fair representation of the α-pinene decay but overestimates the NOx concentrations. Figure *c* show results obtained using the MCM organic scheme (Saunders et al., 2003) with an initial concentration of HONO of 300 ppb. A similar disagreement is observed in the α-pinene decay. Note that including the typical Teflon wall chamber reactions described by Metzger et al. (2008) does not reconcile the simulated and observed concentration. In the context of this smog chamber experiment, these reactions were found to be negligible. An extra OH source was therefore added for this experiment as described in the text.

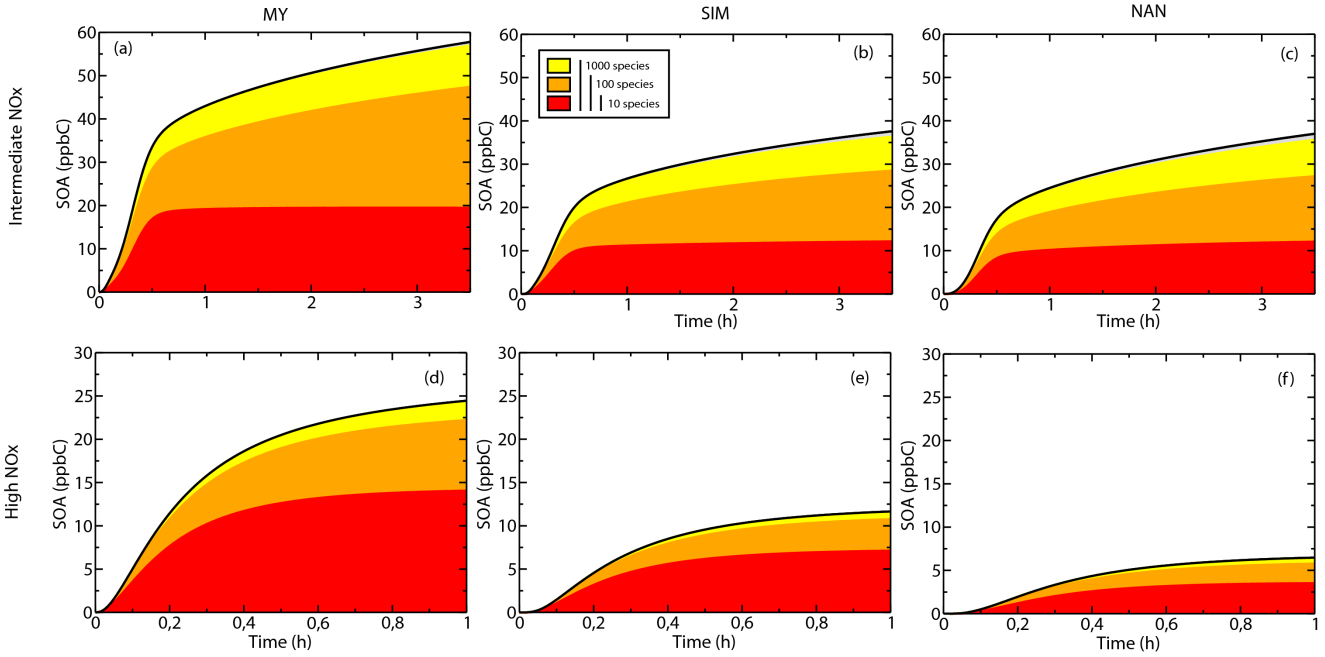


Figure S 3 – Contribution of the top 10 (red), top 100 (red+orange) and top 1000 (red+orange+yellow) organic species to the total simulated SOA mass for the intermediate-NO_x experiment obtained with MY (a), SIM (b) and NAN (c) and for the high-NO_x experiment obtained with MY (d), SIM (e) and NAN (f).

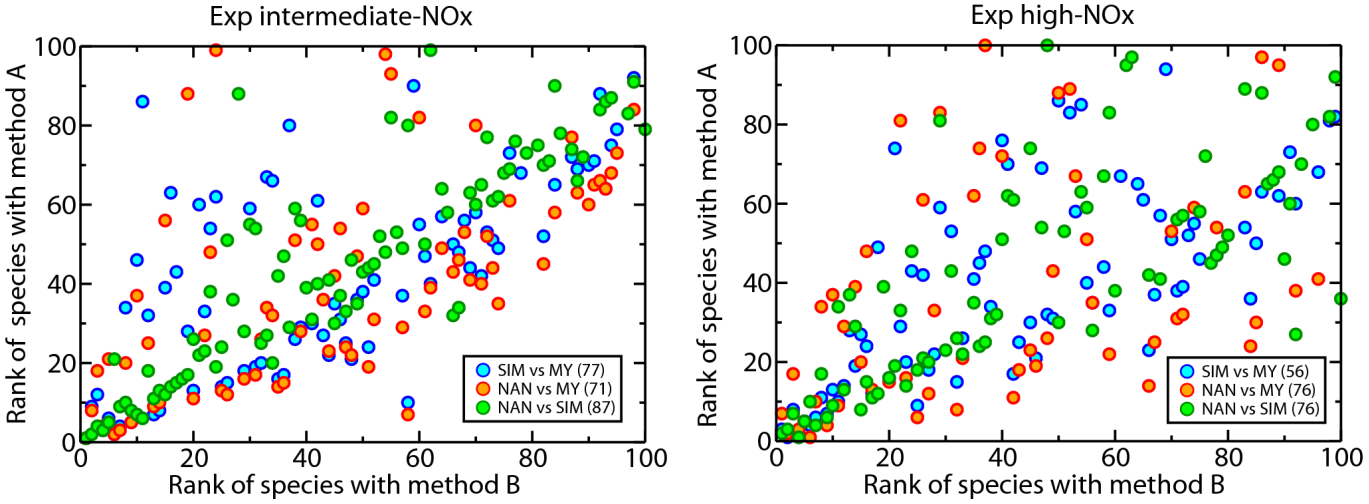
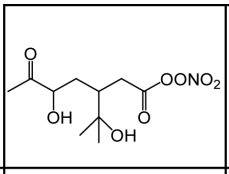
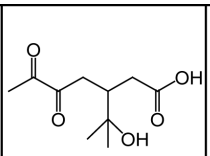
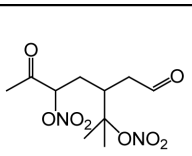
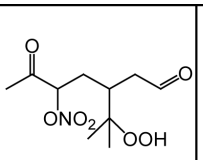
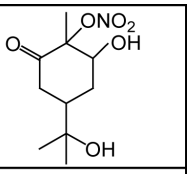


Figure S 4 – Comparisons of the ranks of the simulated top 100 organic species between the various methods in the intermediate and high-NO_x experiments.

Table S1 : Top 10 species in simulated SOA with SIM in the intermediate-NO_x experiment, with their rank and contribution to the total simulated SOA mass.

						
SIM	rank	1	2	3	4	5
	contrib	9%	5%	4%	4%	4%
MY	rank	1	6	4	7	9
	contrib	6%	4%	5%	3%	3%
NAN	rank	1	2	4	3	5
	contrib	8%	6%	3%	5%	3%

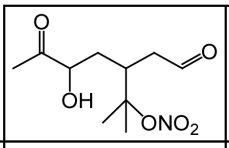
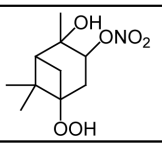
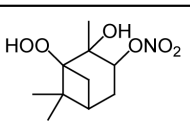
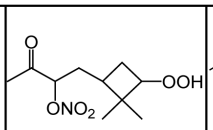
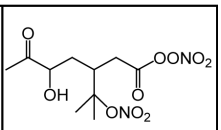
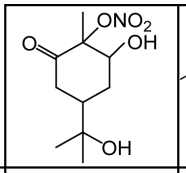
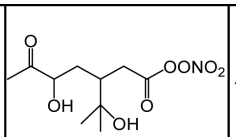
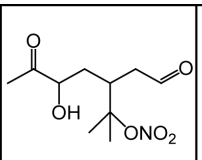
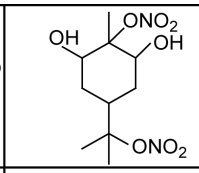
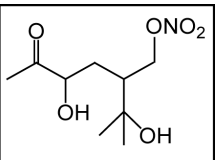
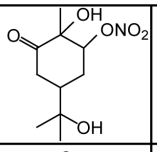
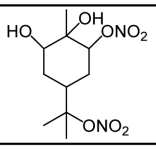
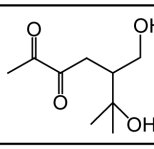
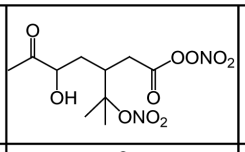
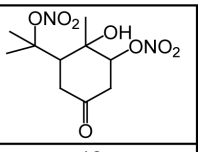
						
SIM	rank	6	7	8	9	10
	contrib	3%	2%	2%	2%	2%
MY	rank	5	13	14	2	58
	contrib	4%	1%	1%	5%	< 1%
NAN	rank	21	9	10	8	7
	contrib	1%	2%	2%	3%	3%

Table S2 : Top 10 species in simulated SOA with SIM in the high-NO_x experiment, with their rank and contribution to the total simulated SOA mass.

						
SIM	rank	1	2	3	4	5
	contrib	15%	13%	10%	7%	5%
MY	rank	2	4	1	6	5
	contrib	10%	9%	16%	4%	4%
NAN	rank	2	3	7	1	5
	contrib	11%	10%	4%	12%	4%

						
SIM	rank	6	7	8	9	10
	contrib	4%	4%	2%	2%	2%
MY	rank	7	9	3	25	11
	contrib	2%	2%	10%	1%	2%
NAN	rank	10	4	17	6	9
	contrib	2%	6%	1%	4%	2%

References

Metzger, A., Dommen, J., Gaeggeler, K., Duplissy, J., Prevot, A. S. H., Kleffmann, J., Elshorbany, Y., Wisthaler, A., and Baltensperger, U.: Evaluation of 1,3,5 trimethylbenzene degradation in the detailed tropospheric chemistry mechanism, MCMv3.1, using environmental chamber data, Atmos. Chem. Phys., 8, 6453-6468, 2008.

Saunders, S. M., Jenkin, M. E., Derwent, R. G., and Pilling, M. J.: Protocol for the development of the Master Chemical Mechanism, MCM v3 (Part A): tropospheric degradation of non-aromatic volatile organic compounds, Atmos. Chem. Phys., 3, 161-180, 2003.