Supplementary material

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

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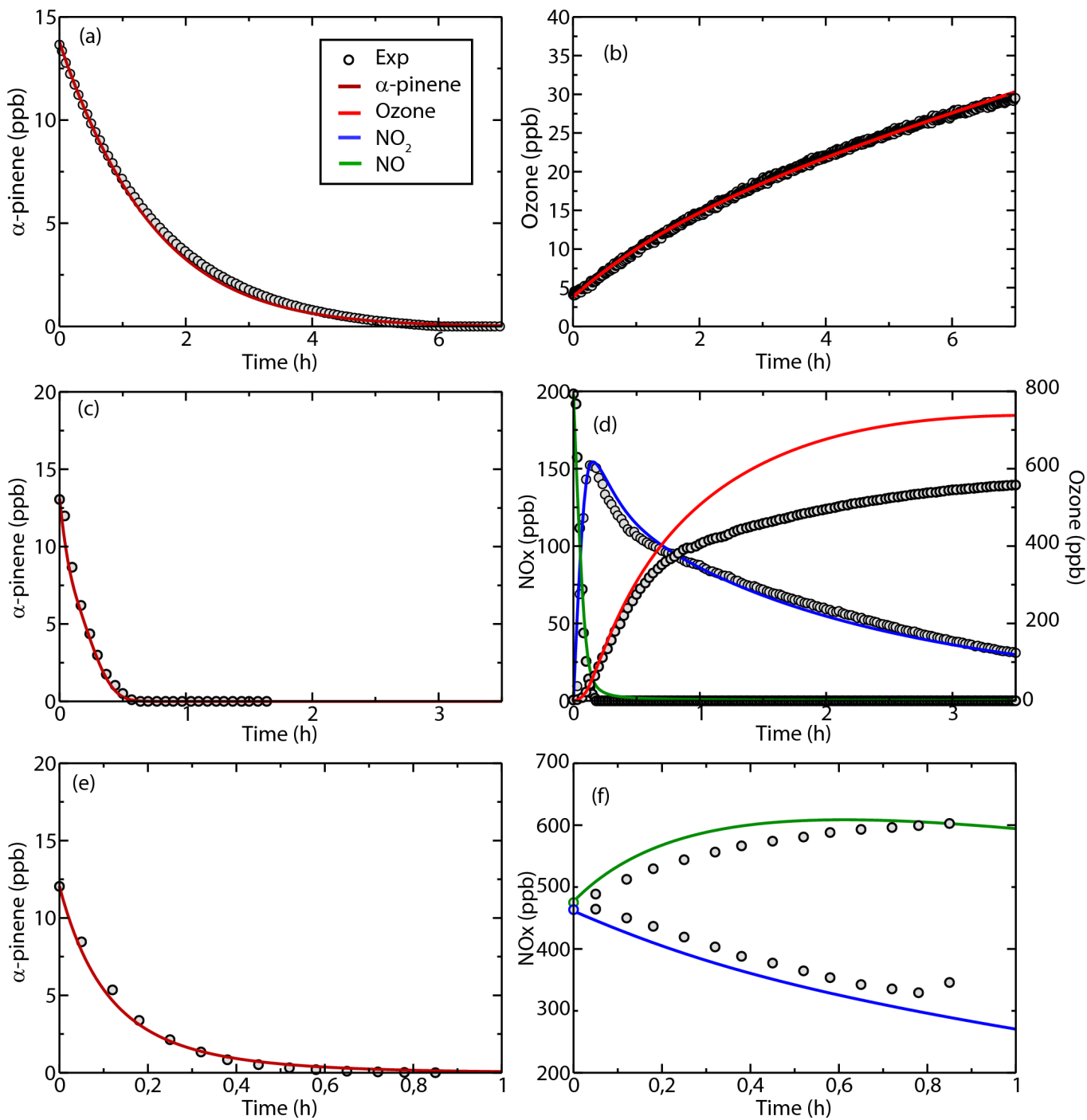
Figure S 1 – Time evolution of α-pinene/O3/NO$_x$ for (a-b) the low-, (c-d) intermediate- and (e-f) high-NO$_x$ experiments. Dots and lines represent measured and modelled compounds respectively. Modelled results are obtained with JR/MY scheme. Similar results are observed with NAN/NAN and SIM and are therefore not represented.
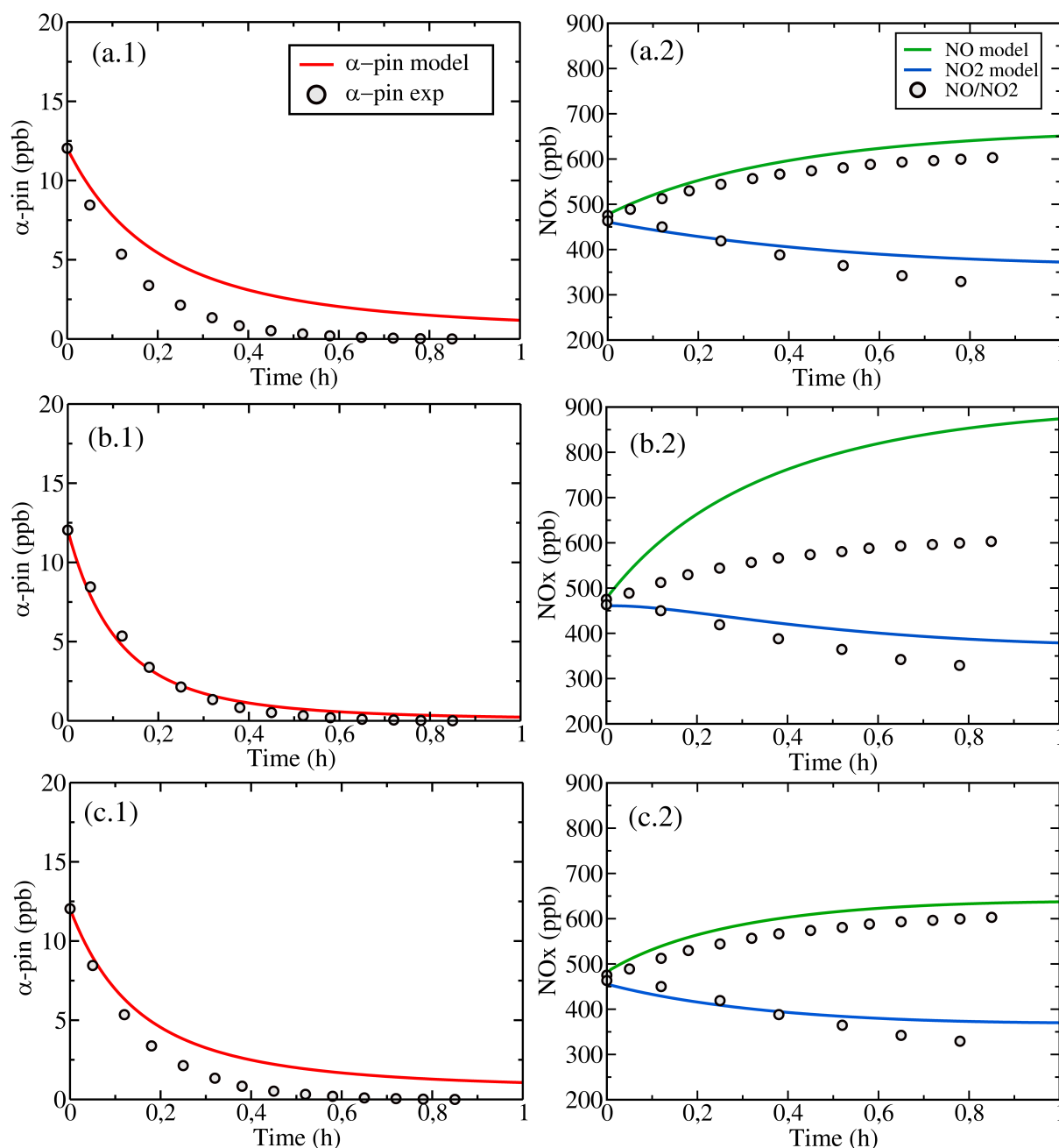
Figure S 2 – Figures show time evolution of α-pinene and NO_x in the high-NO_x experiment. Dots and lines represent measured and modelled compounds respectively. Modelled results are obtained with JR/MY scheme. Figures a show results of simulation obtained using 300 ppb of initial HONO concentration. 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 shows 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 shows 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.
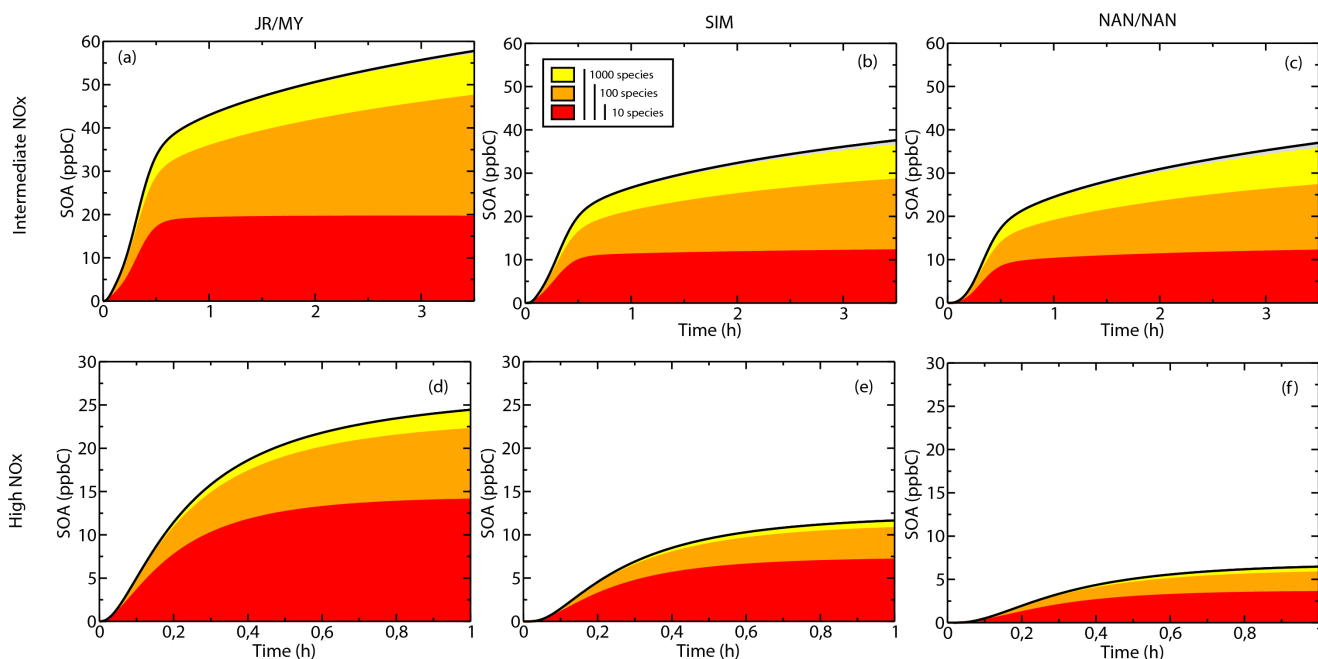
Figure S 3 – Contribution of the top 10 (red), top 100 (red+orange) and top 1000 (red+orange+yellow) organic species to the total simulated SOA mass for the intermediate-NO_x experiment obtained with JR/MY (a), SIM (b) and NAN/NAN (c) and for the high-NO_x experiment obtained with JR/MY (d), SIM (e) and NAN/NAN (f).

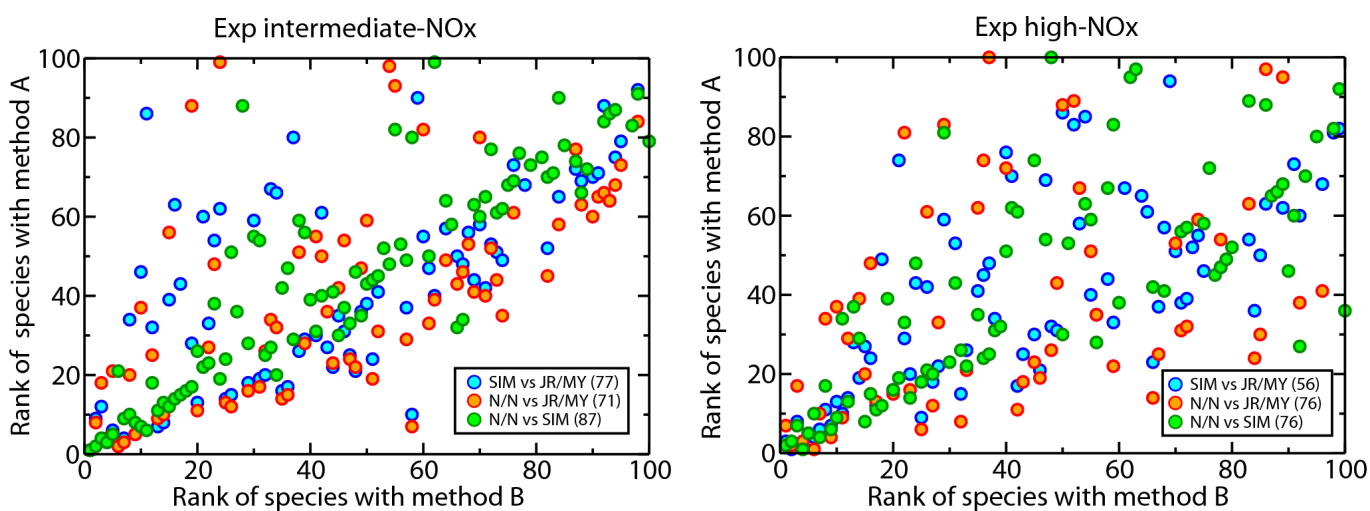

Figure S 4 – Comparisons of the ranks of the simulated top 100 organic species between the various methods in the intermediate and high-NO_x experiments.
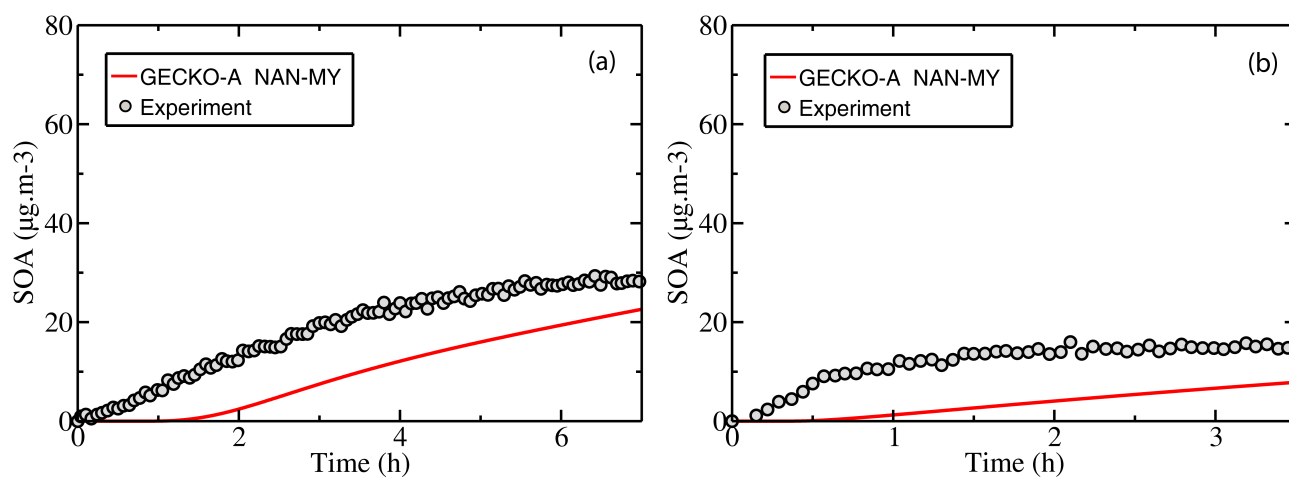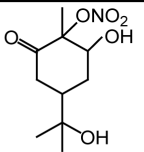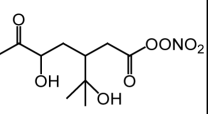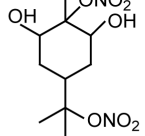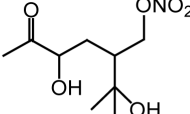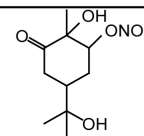
Figure S 5 – Comparisons of observed and simulated SOA in the (a) low- and (b) intermediate-NO$_x$ experiments. Boiling points of organics are estimated with the Nannoolal et al. method (2004) and vapour pressure are estimated with the Myrdal and Yalkowsky method (1997). No SOA is simulated with this method in the high-NO$_x$ experiment.

Table S1 : Top 10 species in simulated SOA with SIM in the intermediate-NO$_x$ experiment, with their rank, contribution to the total simulated SOA mass, vapour pressure and fraction in condensed phase (taken at the end of the experiment).

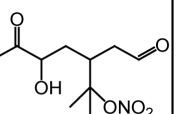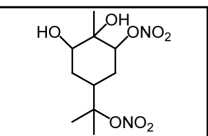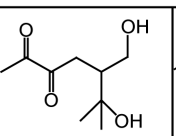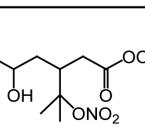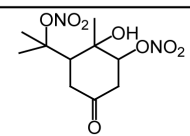|						
SIM	rank	1	2	3	4	5
	contrib	9%	5%	4%	4%	4%
	log(P^{vap})	-9,97	-9,91	-8,98	-9,24	-9,85
	ξ_i^{aer}	0,98	0,98	0,85	0,91	0,97
JR/MY	rank	1	6	4	7	9
	contrib	6%	4%	5%	3%	3%
	log(P^{vap})	-12,16	-11,28	-10,32	-10,79	-11,71
	ξ_i^{aer}	0,99	0,99	0,99	0,99	0,99
NAN/NAN	rank	1	2	4	3	5
	contrib	8%	6%	3%	5%	3%
	log(P^{vap})	-9,32	-9,81	-8,67	-9,45	-9,07
	ξ_i^{aer}	0,93	0,98	0,74	0,96	0,88

SIM	rank	6	7	8	9	10
	contrib	3%	2%	2%	2%	2%
	log(P^{vap})	-8,98	-9,20	-9,20	-7,94	-9,98
	ξ_i^{aer}	0,85	0,90	0,90	0,32	0,98
JR/MY	rank	5	13	14	2	58
	contrib	4%	1%	1%	5%	< 1%
	log(P^{vap})	-10,10	-10,42	-10,42	-9,37	-12,63
	ξ_i^{aer}	0,99	0,99	0,99	0,96	1,00
NAN/NAN	rank	21	9	10	8	7
	contrib	1%	2%	2%	3%	3%
	log(P^{vap})	-8,39	-8,92	-8,92	-7,92	-9,76
	ξ_i^{aer}	0,60	0,87	0,87	0,40	0,97

Table S2 : Top 10 species in simulated SOA with SIM in the high-NO$_x$ experiment, with their rank, contribution to the total simulated SOA mass, vapour pressure and fraction in condensed phase (taken at the end of the experiment).

		(structure 1)	(structure 2)	(structure 3)	(structure 4)	(structure 5)
SIM	rank	1	2	3	4	5
	contrib	15%	13%	10%	7%	5%
	log(P^{vap})	-9,85	-9,97	-8,98	-11,09	-9,41
	ξ_i^{aer}	0,89	0,92	0,54	0,99	0,75
JR/MY	rank	2	4	1	6	5
	contrib	10%	9%	16%	4%	4%
	log(P^{vap})	-11,71	-12,16	-10,10	-12,83	-10,84
	ξ_i^{aer}	0,99	0,99	0,97	0,99	0,99
NAN/NAN	rank	2	3	7	1	5
	contrib	11%	10%	4%	12%	4%
	log(P^{vap})	-9,07	-9,32	-8,39	-10,60	-8,90
	ξ_i^{aer}	0,44	0,59	0,15	0,96	0,36

		(structure 6)	(structure 7)	(structure 8)	(structure 9)	(structure 10)
SIM	rank	6	7	8	9	10
	contrib	4%	4%	2%	2%	2%
	log(P^{vap})	-9,85	-11,09	-8,17	-9,98	-9,86
	ξ_i^{aer}	0,89	0,99	0,15	0,92	0,88
JR/MY	rank	7	9	3	25	11
	contrib	2%	2%	10%	1%	2%
	log(P^{vap})	-11,71	-12,83	-9,26	-12,63	-12,11
	ξ_i^{aer}	0,99	0,99	0,80	0,99	0,99
NAN/NAN	rank	10	4	17	6	9
	contrib	2%	6%	1%	4%	2%
	log(P^{vap})	-8,85	-10,37	-7,80	-9,76	-9,37
	ξ_i^{aer}	0,32	0,94	0,04	0,8	0,61