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Supplement to Yields of oxidized volatile organic compounds during the OH radical initiated oxidation of isoprene, methyl vinyl ketone, and methacrolein under high–NO_x conditions

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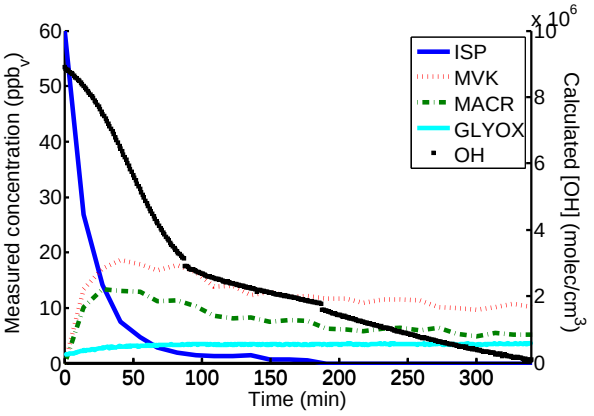

Fig. S1. OH calculated from isoprene, MVK, and MACR from Exp. 7. Note the sudden changes in OH at t=87 and t=187 and as a result of changes OH calculation method (see Sect. 3.2 for details).

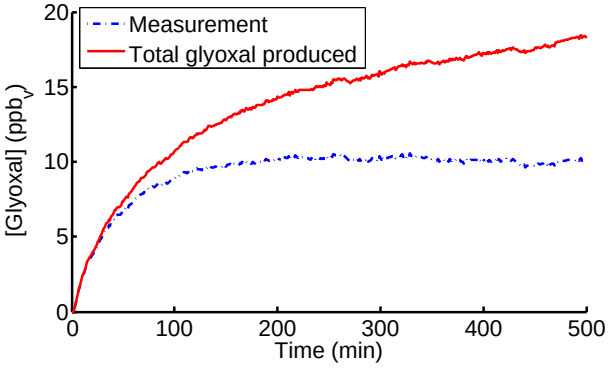

Fig. S2. Total produced glyoxal, corrected for loss to reaction with OH and photolysis from Exp. 3.

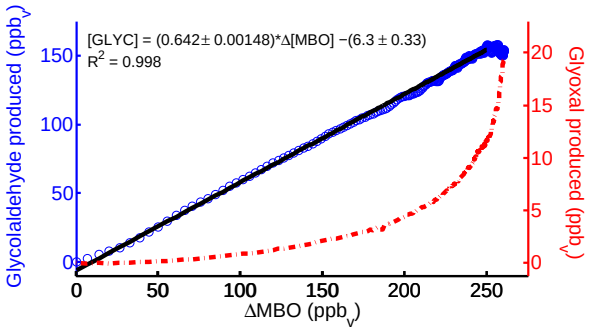

Fig. S3. Glycolaldehyde and glyoxal production as a function of MBO reacted (Exp. C3). Formation of glycolaldehyde, a first generation oxidation product, has a linear relationship with reacted MBO. Glyoxal, a second generation oxidation product, produced primarily via oxidation of glycolaldehyde, has a nonlinear relationship and appears with a lag with respect to reacted MBO. The slope of the line observed for loss-corrected glycolaldehyde production versus reacted-MBO corresponds to the first generation yield.

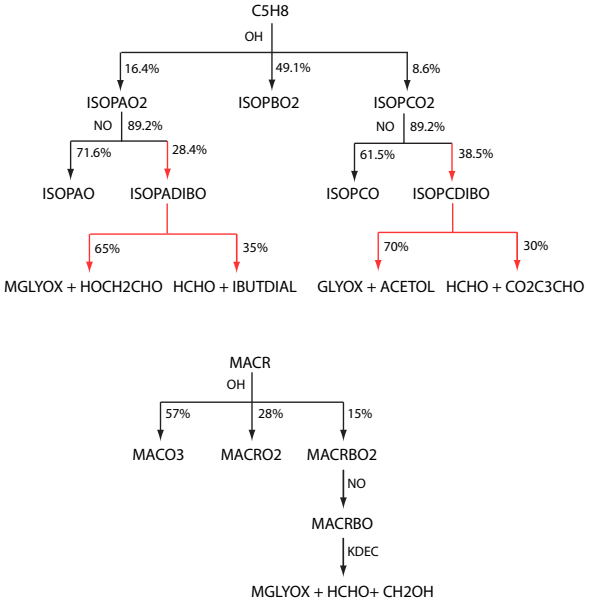

Fig. S4. Details of modifications of the MCM to incorporate first generation production of glyoxal, methylglyoxal, hydroxyacetone and glycolaldehyde and first generation production of methylglyoxal from methacrolein. Pathways highlighted in red are added reactions. Yields of competing pathways were adjusted to assure carbon balance. Isoprene pathways are inferred from Paulot et al. (2009) and MACR pathways from Orlando et al. (1999).

Table S1. MBO experiments, previously published by Chan et al. (2009) and low NO_x isoprene, MVK, and MACR experiments.

Exp. #	Date (mm/dd/yy)	Compound	Initial conc. (ppb)	Initial NO (ppb)	RH (%)	T (K)	Lights	OH source
C3		MBO	288	304	4	295	10%	HONO
C4		MBO	255	422	4	295	10%	HONO
C5		MBO	239	539	66	293	10%	HONO
C6		MBO	299	>2	6	298	50%	H_2O_2
C7		MBO	289	>2	6	298	50%	H_2O_2
S1	10/18/09	Isoprene	22.22	1	10	294	50%	H_2O_2
S2	10/20/09	MVK	25.59	1	10	293	50%	H_2O_2
S3	10/22/09	MACR	40.40	1	10	293	50%	H_2O_2
S4	10/24/09	Blank	None	1	8	294	50%	H_2O_2

Table S2. Assessment of model to measurement agreement for all experiments.

Exp. #	Init cmpd	MBO		C5H8		MVK		MACR		HOCH2CHO		ACETOL		GLYOX		MGLYOX	
		Early	Late	Early	Late	Early	Late	Early	Late	Early	Late	Early	Late	Early	Late	Early	Late
C3	MBO	E	G							E	G			E	E		
C4	MBO	G	G							G	G			G	F		
C6	MBO	E	G							P	P			G	F		
C7	MBO	E	F							P	P			F	G		
S1	Isoprene			E	E	G	G	G	G	P	P	F	F	G	G	ND	ND
S2	MVK					E	E			G	F	F	F	G	G	G	P
S3	MACR							E	E			E	G			G	F
2	Isoprene			E	E	ND	ND	ND	ND	ND	ND	ND	ND	G	G	ND	ND
3	Isoprene			E	E	ND	ND	ND	ND	ND	ND	ND	ND	E	G	ND	ND
4	Isoprene			G	P					F	G	F	F	ND	ND	ND	ND
5	Isoprene			E	E	G	G	G	F	G	G	F	G	G	G	ND	ND
6	Isoprene			G	P	P	G	P	G	F	G	G	G	G	G	ND	ND
7	Isoprene			E	E	G	G	F	F	G	G	F	F	G	G	ND	ND
8	MVK					E	E			G	G	P	P	G	G	G	F
9	MVK					E	F			F	P	P	P	G	G	G	P
10	MACR							E	E			F	G			G	F

E=Excellent

G=Good

F=Fair

P=Poor

ND=No data