A new isoprene mechanism MIM2 for atmospheric modelling

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Table 1: MIM2 species. For the lumped species based on isomers in MCM only the condensed formulae are shown. For lumped species representing non-isomeric species the condensed formulae are not shown.

MIM2 name	**Formula**	**Description**	**Transported**
C_5 **Stable species**			
C5H8	CH_2=C(CH_3)CH=CH_2	2-methyl-1,3-butadiene (isoprene)	yes
LISOPACOOH	$C_5H_{10}O_3$ lumped	see Tab. 2	yes
ISOPBOOH	HOCH_2C(CH_3)(OOH)CH=CH_2	β-hydroxyperoxide	yes
ISOPDOOH	CH_2=C(CH_3)CHOOHCH_2OH	β-hydroxyperoxide	yes
ISOPAOH	HOCH_2C(CH_3)=CHCH_2OH	E-2-methyl-2-butene-1,4-diol	yes
ISOPBOH	HOCH_2C(CH_3)OHCH=CH_2	2-methyl-3-butene-1,2-diol	yes
ISOPDOH	CH_2=C(CH_3)CHOHCH_2OH	3-methyl-3-butene-1,2-diol	yes
LISOPACNO3	$C_5H_{10}NO_4$ lumped	see Tab. 2	yes
ISOPBNO3	HOCH_2C(CH_3)ONO_2CH=CH_2	alkyl nitrate	yes
ISOPDNO3	CH_2=C(CH_3)CHONO_2CH_2OH	alkyl nitrate	yes
NISOPOOH	O_2NOCH_2C(CH_3)=CHCH_2OOH	nitro-hydro-peroxide	yes
NC4CHO	O_2NOCH_2C(CH_3)=CHCHO	nitro-aldehyde	yes
LNISOOH	$C_5H_7NO_{6.5}$ lumped	see Tab. 2	yes
LHC4ACCHO	$C_5H_8O_2$ lumped	see Tab. 2	yes
LC578OOH	$C_5H_10O_5$ lumped	see Tab. 2	yes
LHC4ACCO2H	$C_5H_8O_3$ lumped	see Tab. 2	yes
LHC4ACCO3H	$C_5H_8O_4$ lumped	see Tab. 2	yes
LC5PAN1719	$C_5H_7NO_6$ lumped	see Tab. 2	yes
HCOC5	CH_2=C(CH_3)COCH_2OH		yes
C59OOH	HOCH_2C(CH3)(OOH)COCH_2OH		yes
C_5**-peroxy radicals**			
LISOPACO2	$C_5H_9O_3$ lumped	δ-hydroxyperoxy radical see Tab. 2	no
ISOPBO2	HOCH_2CO_2(CH_3)CH=CH2	β-hydroxyperoxy radical	no
ISOPDO2	CH_2=C(CH_3)CO_2CH_2OH	β-hydroxyperoxy radical	no
NISOPO2	O_2NOCH_2C(CH_3)=CHCH_2O_2	nitro-peroxy radical	no
LNISO3	$C_5H_7NO_{6.5}$ lumped	nitro-peroxy radical see Tab. 2	no
LHC4ACCO3	$C_5H_7O_4$ lumped	δ-hydroxyperoxyacyl radical see Tab. 2	no
LC578O2	$C_5H_9O_5$ lumped	see Tab. 2	no
C59O2	$C_5H_9O_5$	alkyl peroxy radicals from the C_5-hydroxy ketone (HCOC5)	no
C_4 **Stable species**			
MACR	CH_2=C(CH_3)CHO	methacrolein	yes
MACROOH	HOCH_2C(CH_3)(OOH)CHO	methacrolein peroxide	yes
MACROH	HOCH_2C(CH_3)(OH)CHO	1,2-dihydroxy-2-methyl-propanaldehyde	yes
MACO2H	CH_2=C(CH_3)CO_2H	methacroleic acid	yes
MACO3H	CH_2=C(CH_3)CO_3H	methacroleic peroxyacid	yes
MPAN	CH_2=C(CH_3)C(O)OONO_2	peroxy methacroleil nitrate	yes

Table 1: MIM2 species (continued)

MIM2 name	Formula	Description	Transported
C_4 **Stable species**			
MVK	CH_2=CHC(O)CH_3	butenone (methyl vinyl ketone)	yes
LHMVKABOOH	$C_4H_8O_4$ lumped	see Tab. 2	yes
MVKOH	CH_2=CHC(O)CH_2OH	β-hydroxy methyl vinyl ketone	yes
LMVKOHABOOH	$C_4H_8O_5$ lumped	see Tab. 2	yes
CO2H3CHO	CH_3COCH_2(OH)CHO		yes
CO2H3CO3H	$CH_3COCH_2(OH)CO_3H$		yes
BIACETOH	CH_3C(O)C(O)CH_2OH		yes
HO12CO3C4	CH_3C(O)CH(OH)CH_2OH		yes
C_4 **Peroxy radicals**			
MACRO2	$HOCH_2C(CH_3)(O_2)$CHO		no
MACO3	$CH_2=C(CH_3)CO_3$		no
LHMVKABO2	$C_4H_7O_4$ lumped	see Tab. 2	no
LMVKOHABO2	$C_4H_7O_5$ lumped	see Tab. 2	no
CO2H3CO3	$CH_3COCH_2(OH)CO_3$		no
C_3 **Stable species**			
C3H6	C_3H_6	propene	yes
HYPROPO2H	CH_3CH(OOH)CH_2OH	β-hydroxyhydroperoxides	yes
PR2O2HNO3	$CH_3CH(OOH)CH_2ONO_2$		yes
ACETOL	CH_3C(O)CH_2OH	hydroxyacetone	yes
MGLYOX	CH_3C(O)CHO	methylglyoxal	yes
NOA	$CH_3C(O)CH_2ONO_2$	α-nitrooxy acetone	yes
HOCH2COCHO	$HOCH_2$C(O)CHO		yes
HOCH2COCO2H	$HOCH_2C(O)CO_2H$		yes
C_3 **Peroxy radicals**			
HYPROPO2	$CH_3CH(O_2)CH_2OH$	β-hydroxy peroxy radical	no
PRONO3BO2	$CH_3CH(O_2)CH_2ONO_2$	nitro peroxy radical from C3H6	no
C_2 **compounds**			
CH3CHO	CH_3CHO	acetaldehyde	yes
CH3CO2H	CH_3CO_2H	acetic acid	yes
CH3CO3H	CH_3CO_3H	peroxy acetic acid	yes
PAN	$CH_3C(O)OONO_2$	peroxy acetyl nitrate	yes
HOCH2CHO	$HOCH_2CHO$	glycolaldehyde	yes
HOCH2CO2H	$HOCH_2CO_2H$	carboxilic acid from HOCH2CHO	yes
HOCH2CO3H	$HOCH_2CO_3H$	peroxy carboxilic acid from HOCH2CHO	yes
PHAN	$HOCH_2C(O)OONO_2$	homologues of PAN for HOCH2CHO	yes
GLYOX	CHOCHO	glyoxal	yes
HCOCO2H	$HCOCO_2H$	carboxilic acid from GLYOX	yes
HCOCO3H	$HCOCO_3H$	peroxy carboxilic acid from GLYOX	yes
C_2 **Peroxy radicals**			
CH3CO3	CH_3CO_3	peroxy acetyl radical	no
HOCH2CO3	$HOCH_2CO_3$	peroxy acyl radical from HOCH2CHO	no
HCOCO3	$HCOCO_3$	peroxy acyl radical from GLYOX	no

Table 2: Composition of lumped species in MIM2 is given in terms of MCM species.

Lumped species	**Compositions**	Kind
LISOPACO2	0.5 ISOPAO2 + 0.5 ISOPCO2	δ-hydroxyperoxy radical (internal double bond)
LISOPACOOH	0.5 ISOPAOOH + 0.5 ISOPCOOH	δ-hydroxyperoxides (internal double bond)
LISOPACNO3	0.5 ISOPANO3 + 0.5 ISOPCNO3	alky nitrates (internal double bond)
LNISO3	0.5 C510O2 + 0.5 NC4CO3	nitro-peroxy radicals from NC4CHO
LNISOOH	0.5 C510OOH + 0.5 NC4CO3H	nitro-peroxides from LNISO3
LHC4ACCO3	0.5 HC4ACO3 + 0.5 HC4CCO3	acyl peroxy radicals from C_5-hydroxy aldehydes
LHC4ACCHO	0.5 HC4ACHO + 0.5 HC4CCHO	carbonyls (internal double bond)
LHC4ACCO2H	0.5 HC4ACO2H + 0.5 HC4CCO2H	carboxylic acids (internal double bond)
LHC4ACCO3H	0.5 HC4ACO3H + 0.5 HC4CCO3H	percarboxylic acids (internal double bond)
LC5PAN1719	0.5 C5PAN17 + 0.5 C5PAN19	homologues of PAN from LHC4ACCO3
LC578O2	0.5 C57O2 + 0.5 C58O2	peroxy radicals from C_5-hydroxy aldehydes
LC578OOH	0.5 C57OOH + 0.5 C58OOH	hydroperoxides from LC578O2
LHMVKABO2	0.3 HMVKAO2 + 0.7 HMVKBO2	peroxy radicals from MVK
LHMVKABOOH	0.3 HMVKAOOH + 0.7 HMVKBOOH	hydroperoxides from LHMVKABO2
LMVKOHABO2	0.3 MVKOHAO2 + 0.7 MVKOHBO2	peroxy radicals from MVKOH
LMVKOHABOOH	0.3 MVKOHAOOH + 0.7 MVKOHBOOH	hydroperoxides from LMVKOHABO2

Table 3: List of MIM2 reactions. The expressions for the simple MCM rate coefficients (KRO2NO, KRO2HO2, KAPHO2, KAPNO, KRO2NO3, KNO3AL) are shown in Tab. 4. The expressions for the complex MCM rate coefficients (KFPAN, KBPAN and KMT16) are shown in Tab. 5. M is the concentration of air in molec cm^{-3} and T is the temperature in K.

Chemical reaction			**Rate coefficient**
C_5 **compounds**			
C5H8 + OH	→	0.25 LISOPACO2 + 0.491 ISOPBO2 + 0.259 ISOPDO2	2.54E-11× exp(410/T)
C5H8 + O3	→	0.051 CH3O2 + 0.1575 CH3CO3 + 0.054 LHMVK-ABO2 + 0.522 CO + 0.06875 HCOOH + 0.11 H2O2 + 0.32475 MACR + 0.1275 C3H6 + 0.2625 HO2 + 0.255 CO2 + 0.74975 HCHO + 0.04125 MACO2H + 0.27 OH + 0.244 MVK	7.86E-15× exp(-1913/T)
C5H8 + NO3	→	NISOPO2	3.03E-12× exp(-446/T)
LISOPACO2 + HO2	→	LISOPACOOH	0.706×KRO2HO2
LISOPACO2 + NO	→	0.892 LHC4ACCHO + 0.892 HO2 + 0.892 NO2 + 0.108 LISOPACNO3	KRO2NO
LISOPACO2 + NO3	→	LHC4ACCHO + HO2 + NO2	KRO2NO3
LISOPACO2	→	0.9 LHC4ACCHO + 0.8 HO2 + 0.1 ISOPAOH	2.4E-12×RO2
LISOPACOOH + OH	→	LHC4ACCHO + OH	1.07E-10
LISOPACOOH + hν	→	LHC4ACCHO + HO2 + OH	J(41)
ISOPAOH + OH	→	LHC4ACCHO + HO2	9.30E-11
LISOPACNO3 + OH	→	LHC4ACCHO + NO2	8.91E-11
LISOPACNO3 + hν	→	LHC4ACCHO + HO2 + NO2	J(53)
ISOPBO2 + HO2	→	ISOPBOOH	0.706×KRO2HO2
ISOPBO2 + NO	→	0.696 MVK + 0.232 MVKOH + 0.696 HCHO + 0.696 HO2 + 0.232 CH3O2 + 0.928 NO2 + 0.072 ISOPBNO3	KRO2NO
ISOPBO2 + NO3	→	0.75 MVK + 0.25 MVKOH + 0.75 HCHO + 0.75 HO2 + 0.25 CH3O2 + NO2	KRO2NO3
ISOPBO2	→	0.6 MVK + 0.2 MVKOH + 0.6 HCHO + 0.6 HO2 + 0.2 CH3O2 + 0.2 ISOPBOH	8.E-13×RO2
ISOPBOOH + OH	→	ISOPBO2	4.2E-11
ISOPBOOH + hν	→	0.75 MVK + 0.25 MVKOH + 0.75 HCHO + 0.75 HO2 + 0.25 CH3O2 + OH	J(41)
ISOPBOH + OH	→	0.75 MVK + 0.25 MVKOH + 0.75 HCHO + 0.75 HO2 + 0.25 CH3O2	3.85E-11
ISOPBNO3 + OH	→	MVK + HCHO + NO2	3.55E-11
ISOPBNO3 + hν	→	0.75 MVK + 0.25 MVKOH + 0.75 HCHO + 0.75 HO2 + 0.25 CH3O2 + NO2	J(55)
ISOPDO2 + HO2	→	ISOPDOOH	0.706×KRO2HO2
ISOPDO2 + NO	→	0.855 MACR + 0.855 HCHO + 0.855 HO2 + 0.855 NO2 + 0.145 ISOPDNO3	KRO2NO
ISOPDO2 + NO3	→	MACR + HCHO + HO2 + NO2	KRO2NO3
ISOPDO2	→	0.8 MACR + 0.8 HCHO + 0.8 HO2 + 0.1 HCOC5 + 0.1 ISOPDOH	2.9E-12×RO2
ISOPDOOH + OH	→	HCOC5 + OH	1.07E-10
ISOPDOOH + hν	→	MACR + HCHO + HO2 + OH	J(41)
ISOPDOH + OH	→	HCOC5 + HO2	7.38E-11
ISOPDNO3 + OH	→	HCOC5 + NO2	6.1E-11
ISOPDNO3 + hν	→	MACR + HCHO + HO2 + NO2	J(54)

Table 3: MIM2 reactions (continued)

Chemical reaction			**Rate coefficient**
C_5 **compounds**			
NISOPO2	→	0.8 NC4CHO + 0.6 HO2 + 0.2 LISOPACNO3	1.3E-12×RO2
NISOPO2 + NO	→	NC4CHO + HO2 + NO2	KRO2NO
NISOPO2 + NO3	→	NC4CHO + HO2 + NO2	KRO2NO3
NISOPO2 + HO2	→	NISOPOOH	.706×KRO2HO2
NISOPOOH + OH	→	NC4CHO + OH	1.03E-10
NISOPOOH + hν	→	NC4CHO + HO2 + OH	J(41)
NC4CHO + OH	→	LNISO3	4.16E-11
NC4CHO + O3	→	0.445 NO2 + 0.89 CO + 0.075625 H2O2 + 0.034375 HCOCO2H + 0.555 NOA + 0.445 HO2 + 0.520625 GLYOX + 0.89 OH + 0.445 MGLYOX	2.40E-17
NC4CHO + NO3	→	LNISO3 + HNO3	KNO3AL×4.25
NC4CHO + hν	→	NOA + 2 CO + 2 HO2	J(18)
LNISO3 + NO	→	NOA + 0.5 GLYOX + 0.5 CO + HO2 + NO2 + 0.5 CO2	(KAPNO + KRO2NO)/2
LNISO3 + NO3	→	NOA + 0.5 GLYOX + 0.5 CO + HO2 + NO2 + 0.5 CO2	1.3×KRO2NO
LNISO3 + HO2	→	LNISOOH	(0.706×KRO2HO2 + KAPHO2)/2
LNISOOH + OH	→	LNISO3	2.65E-11
LNISOOH + hν	→	NOA + OH + 0.5 GLYOX + 0.5 CO + HO2 + 0.5 CO2	J(41)
LHC4ACCHO + OH	→	0.52 LC578O2 + 0.48 LHC4ACCO3	4.52E-11
LHC4ACCHO + O3	→	0.2225 CH3CO3 + 0.89 CO + 0.0171875 HOCH2CO2H + 0.075625 H2O2 + 0.0171875 HCOCO2H + 0.2775 ACETOL + 0.6675 HO2 + 0.2603125 GLYOX + 0.2225 HCHO + 0.89 OH + 0.2603125 HOCH2CHO + 0.5 MGLYOX	2.40E-17
LHC4ACCHO + NO3	→	LHC4ACCO3 + HNO3	KNO3AL×4.25
LHC4ACCHO + hν	→	0.5 LHC4ACCO3 + 0.25 ACETOL + 0.25 HOCH2CHO + 0.25 CH3CO3 + 0.75 CO + 1.25 HO2	2×J(19)
LC578O2	→	0.5 ACETOL + 0.5 MGLYOX + 0.5 GLYOX + 0.5 HOCH2CHO + HO2	9.20E-14×RO2
LC578O2 + HO2	→	LC578OOH	KRO2HO2×0.706
LC578O2 + NO	→	0.5 ACETOL + 0.5 MGLYOX + 0.5 GLYOX + 0.5 HOCH2CHO + HO2 + NO2	KRO2NO
LC578O2 + NO3	→	0.5 ACETOL + 0.5 MGLYOX + 0.5 GLYOX + 0.5 HOCH2CHO + HO2 + NO2	KRO2NO3
LC578OOH + OH	→	LC578O2	3.16E-11
LC578OOH + hν	→	0.5 ACETOL + 0.5 MGLYOX + 0.5 GLYOX + 0.5 HOCH2CHO + HO2 + OH	J(41)

Table 3: MIM2 reactions (continued)

Chemical reaction			**Rate coefficient**
C_5 **compounds**			
LHC4ACCO3	→	0.3 LHC4ACCO2H + 0.35 ACETOL + 0.35 HOCH2CHO + 0.35 CH3CO3 + 0.35 CO + 0.35 HO2 + 0.7 CO2	1.00E-11× RO2
LHC4ACCO3 + HO2	→	0.71 LHC4ACCO3H + 0.29 LHC4ACCO2H + 0.29 O3	KAPHO2
LHC4ACCO3 + NO	→	0.5 ACETOL + 0.5 HOCH2CHO + 0.5 CH3CO3 + 0.5 CO + 0.5 HO2 + NO2 + CO2	KAPNO
LHC4ACCO3 + NO3	→	0.5 ACETOL + 0.5 HOCH2CHO + 0.5 CH3CO3 + 0.5 CO + 0.5 HO2 + NO2 + CO2	1.6×KRO2NO3
LHC4ACCO3 + NO2	→	LC5PAN1719	KFPAN(T,M)
LHC4ACCO2H + OH	→	0.5 ACETOL + 0.5 HOCH2CHO + 0.5 CH3CO3 + 0.5 CO + 0.5 HO2 + CO2	2.52E-11
LHC4ACCO3H + OH	→	LHC4ACCO3	2.88E-11
LHC4ACCO3H + hν	→	0.5 ACETOL + 0.5 HOCH2CHO + 0.5 CH3CO3 + 0.5 CO + 0.5 HO2 + OH + CO2	J(41)
LC5PAN1719	→	LHC4ACCO3 + NO2	KBPAN(T,M)
LC5PAN1719 + OH	→	0.5 MACROH + 0.5 HO12CO3C4 + CO + NO2	2.52E-11
HCOC5 + OH	→	C59O2	3.81E-11
HCOC5 + hν	→	CH3CO3 + HCHO + HOCH2CO3	J(24)
C59O2	→	ACETOL + HOCH2CO3	9.20E-14×RO2
C59O2 + NO	→	ACETOL + HOCH2CO3 + NO2	KRO2NO
C59O2 + NO3	→	ACETOL + HOCH2CO3 + NO2	KRO2NO3
C59O2 + HO2	→	C59OOH	KRO2HO2×0.706
C59OOH + OH	→	C59O2	9.7E-12
C59OOH + hν	→	ACETOL + HOCH2CO3 + OH	J(22)+J(41)
C_4 **compounds**			
MACR + OH	→	0.57 MACO3 + 0.43 MACRO2	1.86E-11× exp(175/T)
MACR + O3	→	0.59 MGLYOX + 0.41 CH3CO3 + 0.03375 HCOOH + 0.55625 HCHO + 0.82 CO + 0.12375 H2O2 + 0.41 HO2 + 0.82 OH	1.36E-15× exp(-2112/T)
MACR + NO3	→	MACO3 + HNO3	KNO3AL×2.0
MACR + hν	→	0.5 MACO3 + 0.5 CH3CO3 + 0.5 HCHO + 0.5 CO + HO2	J(18)+J(19)
MACO3	→	0.7 CH3CO3 + 0.7 HCHO + 0.7 CO2 + 0.3 MACO2H	1.00E-11×RO2
MACO3 + HO2	→	0.71 MACO3H + 0.29 MACO2H + 0.29 O3	KAPHO2
MACO3 + NO	→	CH3CO3 + HCHO + NO2 + CO2	8.70E-12× exp(290/T)
MACO3 + NO3	→	CH3CO3 + HCHO + NO2 + CO2	1.6×KRO2NO3
MACO3 + NO2	→	MPAN	KFPAN(T,M)
MACRO2	→	0.7 ACETOL + 0.7 HCHO + 0.7 HO2 + 0.3 MACROH	9.20E-14×RO2
MACRO2 + NO	→	ACETOL + HCHO + HO2 + NO2	KRO2NO
MACRO2 + NO3	→	ACETOL + HCHO + HO2 + NO2	KRO2NO3
MACRO2 + HO2	→	MACROOH	KRO2HO2×0.625

Table 3: MIM2 reactions (continued)

Chemical reaction			Rate coefficient
C_4 **compounds**			
MACROOH + OH	→	MACRO2	2.82E-11
MACROOH + hν	→	ACETOL + HCHO + HO2 + OH	J(41)
MACROOH + hν	→	ACETOL + CO + HO2 + OH	J(17)
MACROH + OH	→	ACETOL + HCHO + HO2	2.46E-11
MACROH + hν	→	ACETOL + CO + HO2 + HO2	J(17)
MPAN	→	MACO3 + NO2	KBPAN(T,M)
MPAN + OH	→	ACETOL + CO + NO2	3.60E-12
MACO2H + OH	→	CH3CO3 + HCHO + CO2	1.51E-11
MACO3H + OH	→	MACO3	1.87E-11
MACO3H + hν	→	CH3CO3 + HCHO + OH + CO2	J(41)
MVK + OH	→	LHMVKABO2	4.13E-12× exp(452/T)
MVK + O3	→	0.28 CH3CO3 + 0.56 CO + 0.225 LCARBON + 0.075 HCOOH + 0.09 H2O2 + 0.28 HO2 + 0.1 CO2 + 0.1 CH3CHO + 0.645 HCHO + 0.36 OH + 0.545 MGLYOX	7.51E-16× exp(-1521/T)
MVK + hν	→	0.5 C3H6 + 0.5 CH3CO3 + 0.5 HCHO + CO + 0.5 HO2	2×J(23)
LHMVKABO2	→	0.06 CO2H3CHO + 0.18 HO2 + 0.18 HCHO + 0.18 MGLYOX + 0.42 CH3CO3 + 0.42 HOCH2CHO+ 0.2 HO12CO3C4 + 0.14 BIACETOH	(0.3×2.00E-12 + 0.7×8.80E-13)×RO2
LHMVKABO2 + HO2	→	LHMVKABOOH	KRO2HO2×0.625
LHMVKABO2 + NO	→	0.3 MGLYOX + 0.7 HOCH2CHO + 0.7 CH3CO3 + 0.3 HCHO + 0.3 HO2 + NO2	KRO2NO
LHMVKABO2 + NO3	→	0.3 MGLYOX + 0.7 HOCH2CHO + 0.7 CH3CO3 + 0.3 HCHO + 0.3 HO2 + NO2	KRO2NO3
LHMVKABOOH + OH	→	0.3 CO2H3CHO + 0.7 BIACETOH + OH	0.3×5.77E-11 + 0.7×3.95E-11
LHMVKABOOH + hν	→	0.3 MGLYOX + 0.7 CH3CO3 + 0.7 HOCH2CHO + 0.3 HCHO + 0.3 HO2 + OH	J(41)
MVKOH + OH	→	LMVKOHABO2	4.60E-12× exp(452/T)
MVKOH + O3	→	0.56 CO + 0.545 HOCH2COCHO + 0.075 HOCH2COCO2H + 0.075 HCOOH + 0.09 H2O2 + 0.28 HOCH2CO3 + 0.28 HO2 + 0.2 CO2 + 0.545 HCHO + 0.36 OH + 0.1 HOCH2CHO	7.51E-16× exp(-1521/T)
MVKOH + hν	→	0.5 HCHO + 0.5 HO2 + 0.5 HOCH2CO3 + CO + 1.5 LCARBON	2×J(23)
LMVKOHABO2	→	0.7 HOCH2CHO + 0.7 HOCH2CO3 + 0.3 HOCH2COCHO + 0.3 HCHO + 0.3 HO2	(0.3×2.00E-12+.7× 8.80E-13)×RO2
LMVKOHABO2 + NO	→	0.3 HOCH2COCHO + 0.3 HCHO + 0.3 HO2 + 0.7 HOCH2CHO + 0.7 HOCH2CO3 + NO2	KRO2NO
LMVKOHABO2 + NO3	→	0.3 HOCH2COCHO + 0.3 HCHO + 0.3 HO2 + 0.7 HOCH2CHO + 0.7 HOCH2CO3 + NO2	KRO2NO3
LMVKOHABO2 + HO2	→	LMVKOHABOOH	KRO2HO2×0.625
LMVKOHABOOH + OH	→	0.7 HO12CO3C4 + 0.3 CO2H3CHO + OH	5.98E-11
LMVKOHABOOH + hν	→	0.3 HOCH2COCHO + 0.3 HCHO + 0.3 HO2 + 0.7 HOCH2CHO + 0.7 HOCH2CO3 + OH	J(22)+J(41)

Table 3: MIM2 reactions (continued)

Chemical reaction			**Rate coefficient**
C_4 **compounds**			
CO2H3CHO + OH	→	CO2H3CO3	2.45E-11
CO2H3CHO + NO3	→	CO2H3CO3 + HNO3	KNO3AL×4.0
CO2H3CHO + hν	→	MGLYOX + CO + HO2 + HO2	J(15)
CO2H3CO3	→	MGLYOX + HO2 + CO2	1.00E-11×RO2
CO2H3CO3 + HO2	→	CO2H3CO3H	KAPHO2
CO2H3CO3 + NO	→	MGLYOX + HO2 + NO2 + CO2	KAPNO
CO2H3CO3 + NO3	→	MGLYOX + HO2 + NO2 + CO2	1.6×KRO2NO3
CO2H3CO3H + OH	→	CO2H3CO3	7.34E-12
CO2H3CO3H + hν	→	MGLYOX + HO2 + OH + CO2	J(41)
CO2H3CO3H + hν	→	CH3CO3 + HO2 + HCOCO3H	J(22)
HO12CO3C4 + OH	→	BIACETOH + HO2	1.88E-11
HO12CO3C4 + hν	→	CH3CO3 + HOCH2CHO + HO2	J(22)
BIACETOH + hν	→	CH3CO3 + HOCH2CO3	J(35)
C_3 **compounds**			
C3H6 + OH	→	HYPROPO2	KMT16(T,M)
C3H6 + O3	→	0.28 CH3O2 + 0.1 CH4 + 0.075 CH3CO2H + 0.56 CO + 0.075 HCOOH + 0.09 H2O2 + 0.28 HO2 + 0.2 CO2 + 0.545 CH3CHO + 0.545 HCHO + 0.36 OH	5.51E-15× exp(-1878/T)
C3H6 + NO3	→	PRONO3BO2	9.4E-15
HYPROPO2 + HO2	→	HYPROPO2H	KRO2HO2×0.520
HYPROPO2 + NO	→	CH3CHO + HCHO + HO2 + NO2	KRO2NO
HYPROPO2 + NO3	→	CH3CHO + HCHO + HO2 + NO2	KRO2NO3
HYPROPO2	→	CH3CHO + HCHO + HO2	8.80E-13×RO2
HYPROPO2H + OH	→	HYPROPO2	1.90E-12× exp(190/T)
HYPROPO2H + OH	→	ACETOL + OH	2.44E-11
HYPROPO2H + hν	→	CH3CHO + HCHO + HO2 + OH	J(41)
PRONO3BO2 + NO	→	NOA + HO2 + NO2	KRO2NO
PRONO3BO2 + NO3	→	NOA + HO2 + NO2	KRO2NO3
PRONO3BO2 + HO2	→	PR2O2HNO3	KRO2HO2×0.520
PR2O2HNO3 + OH	→	PRONO3BO2	1.90E-12× exp(190/T)
PR2O2HNO3 + OH	→	NOA + OH	3.47E-12
PR2O2HNO3 + hν	→	NOA + HO2 + OH	J(41)
ACETOL + OH	→	MGLYOX + HO2	3.00E-12
ACETOL + hν	→	CH3CO3 + HCHO + HO2	J(22)
MGLYOX + OH	→	CH3CO3 + CO	1.72E-11
MGLYOX + NO3	→	CH3CO3 + CO + HNO3	KNO3AL×2.4
MGLYOX + hν	→	CH3CO3 + CO + HO2	J(34)
NOA + OH	→	MGLYOX + NO2	1.30E-13
NOA + hν	→	CH3CO3 + HCHO + NO2	J(56)+J(57)
HOCH2COCHO + OH	→	HOCH2CO3 + CO	1.44E-11
HOCH2COCHO + NO3	→	HOCH2CO3 + CO + HNO3	KNO3AL×2.4
HOCH2COCHO + hν	→	HOCH2CO3 + CO + HO2	J(34)
HOCH2COCO2H + OH	→	HOCH2CO3 + CO2	2.89E-12
HOCH2COCO2H + hν	→	HOCH2CO3 + HO2 + CO2	J(34)

Table 3: MIM2 reactions (continued)

Chemical reaction			**Rate coefficient**
C_2 **compounds**			
CH3CO3	→	0.7 CH3O2 + 0.3 CH3CO2H	1.00E-11×RO2
CH3CO3 + HO2	→	0.71 CH3CO3H + 0.29 CH3CO2H + 0.29 O3	KAPHO2
CH3CO3 + NO2	→	PAN	KFPAN(T,M)
CH3CO3 + NO	→	NO2 + CH3O2 + CO2	KAPNO
CH3CO3 + NO3	→	NO2 + CH3O2 + CO2	KRO2NO3×1.60
CH3CO2H + OH	→	CH3O2 + CO2	8.00E-13
CH3CO3H + OH	→	CH3CO3	3.70E-12
CH3CO3H + hν	→	CH3O2 + OH + CO2	J(41)
CH3CHO + OH	→	CH3CO3	5.55E-12× exp(311/T)
CH3CHO + NO3	→	CH3CO3 + HNO3	KNO3AL
CH3CHO + hν	→	CH3O2 + HO2 + CO	J(13)
PAN	→	CH3CO3 + NO2	KBPAN(T,M)
PAN + OH	→	HCHO + CO + NO2	9.50E-13× exp(-650/T)
HOCH2CHO + OH	→	0.8 HOCH2CO3 + 0.2 GLYOX + 0.2 HO2	1.00E-11
HOCH2CHO + NO3	→	HOCH2CO3 + HNO3	KNO3AL
HOCH2CHO + hν	→	HO2 + HCHO + HO2 + CO	J(15)
HOCH2CO3 + NO2	→	PHAN	KFPAN(T,M)
HOCH2CO3 + HO2	→	0.71 HOCH2CO3H + 0.29 HOCH2CO2H + 0.29 O3	KAPHO2
HOCH2CO3	→	0.7 HCHO + 0.7 CO2 + 0.7 HO2 + 0.3 HOCH2CO2H	1.00E-11×RO2
HOCH2CO3 + NO	→	NO2 + HO2 + HCHO + CO2	KAPNO
HOCH2CO3 + NO3	→	NO2 + HO2 + HCHO + CO2	1.6×KRO2NO3
HOCH2CO2H + OH	→	HCHO + HO2 + CO2	2.73E-12
HOCH2CO3H + OH	→	HOCH2CO3	6.19E-12
HOCH2CO3H + hν	→	HCHO + HO2 + OH + CO2	J(41)
PHAN	→	HOCH2CO3 + NO2	KBPAN(T,M)
PHAN + OH	→	HCHO + CO + NO2	1.12E-12
GLYOX + OH	→	1.2 CO + 0.6 HO2 + 0.4 HCOCO3	1.14E-11
GLYOX + NO3	→	1.2 CO + 0.6 HO2 + 0.4 HCOCO3 + HNO3	KNO3AL
GLYOX + hν	→	2 CO + H2	J(31)
GLYOX + hν	→	HCHO + CO	J(32)
GLYOX + hν	→	2 CO + 2 HO2	J(33)
HCOCO3	→	0.7 CO + 0.7 HO2 + 0.7 CO2 + 0.3 HCOCO2H	1.00E-11×RO2
HCOCO3 + HO2	→	0.71 HCOCO3H + 0.29 HCOCO2H + 0.29 O3	KAPHO2
HCOCO3 + NO	→	HO2 + CO + NO2 + CO2	KAPNO
HCOCO3 + NO3	→	HO2 + CO + NO2 + CO2	1.6×KRO2NO3
HCOCO2H + OH	→	CO + HO2 + CO2	1.23E-11
HCOCO2H + hν	→	2 HO2 + CO + CO2	J(34)
HCOCO3H + OH	→	HCOCO3	1.58E-11
HCOCO3H + hν	→	HO2 + CO + OH + CO2	J(41)+J(15)

The total peroxy radicals are defined as: RO2 = LISOPACO2 + ISOPBO2 + ISOPDO2 + NISOPO2 + LHC4ACCO3 + LC578O2 + C59O2 + LNISO3 + LHMVKABO2 + LMVKOHABO2 + MACO3 + MACRO2 + CO2H3CO3 + HYPROPO2 + PRONO3BO2 + CH3CO3 + HOCH2CO3 + HCOCO3 + CH3O2.

Table 4: MCM simple rate constants. T is the temperature in K.

name	expression
KRO2NO	2.54E-12$\times$ exp($360/T$)
KRO2HO2	2.91E-13$\times$ exp($1300/T$)
KAPHO2	4.30E-13$\times$ exp($1040/T$)
KAPNO	8.10E-12$\times$ exp($270/T$)
KRO2NO3	2.50E-12
KNO3AL	1.44E-12$\times$ exp($-1862/T$)

Table 5: Parameters for the MCM complex rate constants used in MIM2. M is the concentration of air in molec cm^{-3} and T is the temperature in K.

rate constant	parameters
KMT16	
K0	$8.00 \times 10^{-27} \times (T/300)^{-3.5} \times M$
KI	3.00×10^{-11}
FC	0.5
KFPAN	
K0	$2.70 \times 10^{-28} \times (T/300)^{-7.1} \times M$
KI	$1.20 \times 10^{-11} \times (T/300)^{-0.9}$
FC	0.3
KBPAN	
K0	$4.90 \times 10^{-03} \times \exp(-12100/T) \times M$
KI	$5.40 \times 10^{+16} \times \exp(-13830/T)$
FC	0.3

The rate constants are then calculated according to the follwing expressions: $k_{comp} = K0 \cdot KI \cdot F/(K0 + KI)$, where $F = 10^{\log FC/(1+(\log krd/nu)^2)}$ and $nu = 0.75 - 1.27 \cdot \log FC$.

Table 6: Photolysis Parameters (l, m and n) from MCM and used in the box model evaluation (Saunders et al., 2003). They J-values (in s^{-1}) are computed with the expression $J = l \times (cos(\theta))^m \times \exp(-n\sec(\theta))$, where θ is the solar zenith angle.

J	l	m	n
$J(1)$	6.073E-05	1.743	0.474
$J(2)$	4.775E-04	0.298	0.080
$J(3)$	1.041E-05	0.723	0.279
$J(4)$	1.165E-02	0.244	0.267
$J(5)$	2.485E-02	0.168	0.108
$J(6)$	1.747E-01	0.155	0.125
$J(7)$	2.644E-03	0.261	0.288
$J(8)$	9.312E-07	1.230	0.307
$J(11)$	4.642E-05	0.762	0.353
$J(12)$	6.853E-05	0.477	0.323
$J(13)$	7.344E-06	1.202	0.417
$J(14)$	2.879E-05	1.067	0.358
$J(15)$	2.792E-05	0.805	0.338
$J(16)$	1.675E-05	0.805	0.338
$J(17)$	7.914E-05	0.764	0.364
$J(18)$	1.140E-05	0.396	0.298
$J(19)$	1.140E-05	0.396	0.298
$J(21)$	7.992E-07	1.578	0.271
$J(22)$	5.804E-06	1.092	0.377
$J(23)$	1.836E-05	0.395	0.296
$J(24)$	1.836E-05	0.395	0.296
$J(31)$	6.845E-05	0.130	0.201
$J(32)$	1.032E-05	0.130	0.201
$J(33)$	3.802E-05	0.644	0.312
$J(34)$	1.537E-04	0.170	0.208
$J(35)$	3.326E-04	0.148	0.215
$J(41)$	7.649E-06	0.682	0.279
$J(51)$	1.588E-06	1.154	0.318
$J(52)$	1.907E-06	1.244	0.335
$J(53)$	2.485E-06	1.196	0.328
$J(54)$	4.095E-06	1.111	0.316
$J(55)$	1.135E-05	0.974	0.309
$J(56)$	7.549E-06	1.015	0.324
$J(57)$	3.363E-06	1.296	0.322
$J(61)$	7.537E-04	0.499	0.266

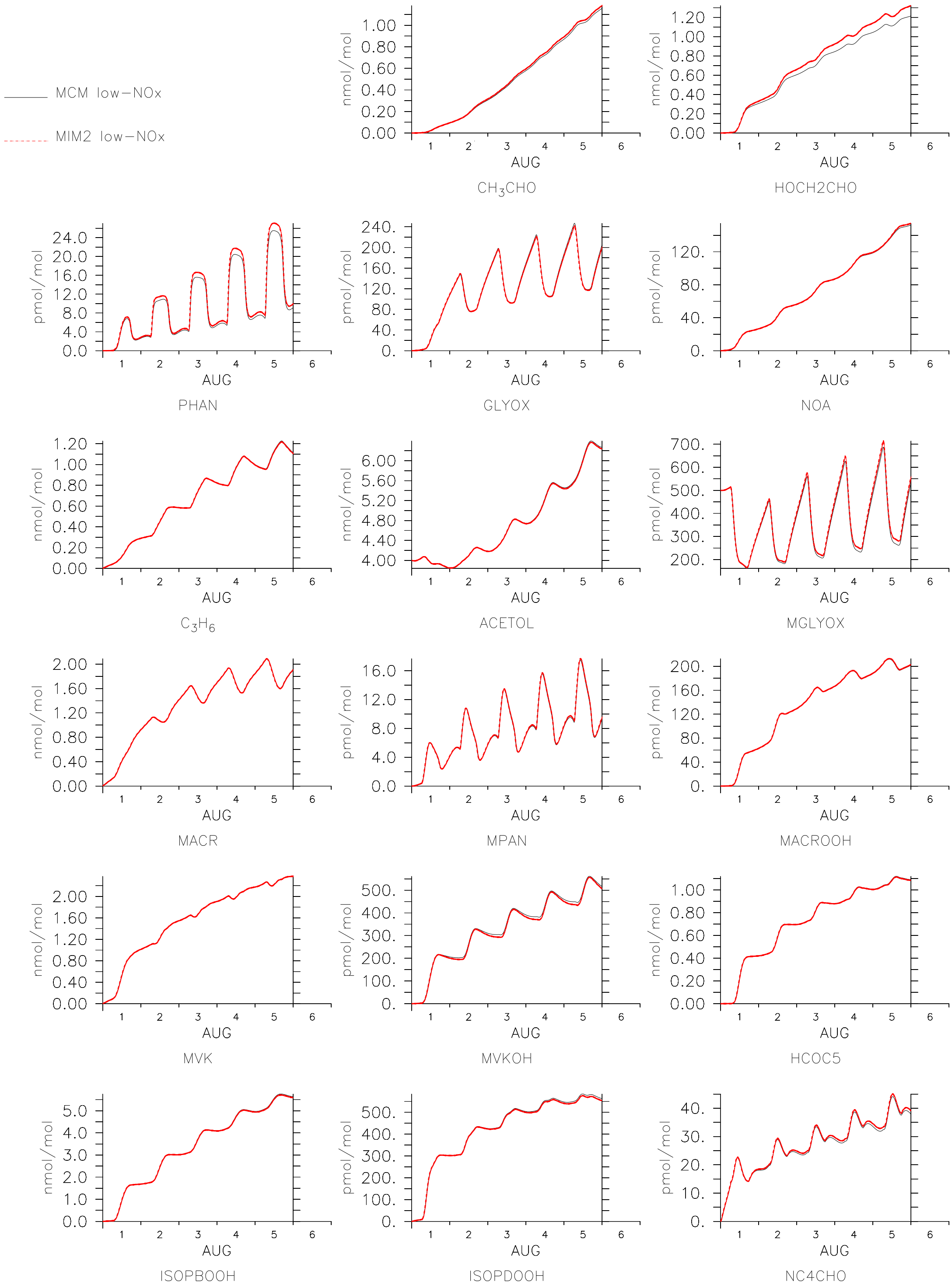

Figure 1: A selection of the most prominent among the news species present now in MIM2. A comparison between MIM2 and MCM in the low-NO_x scenario is shown.

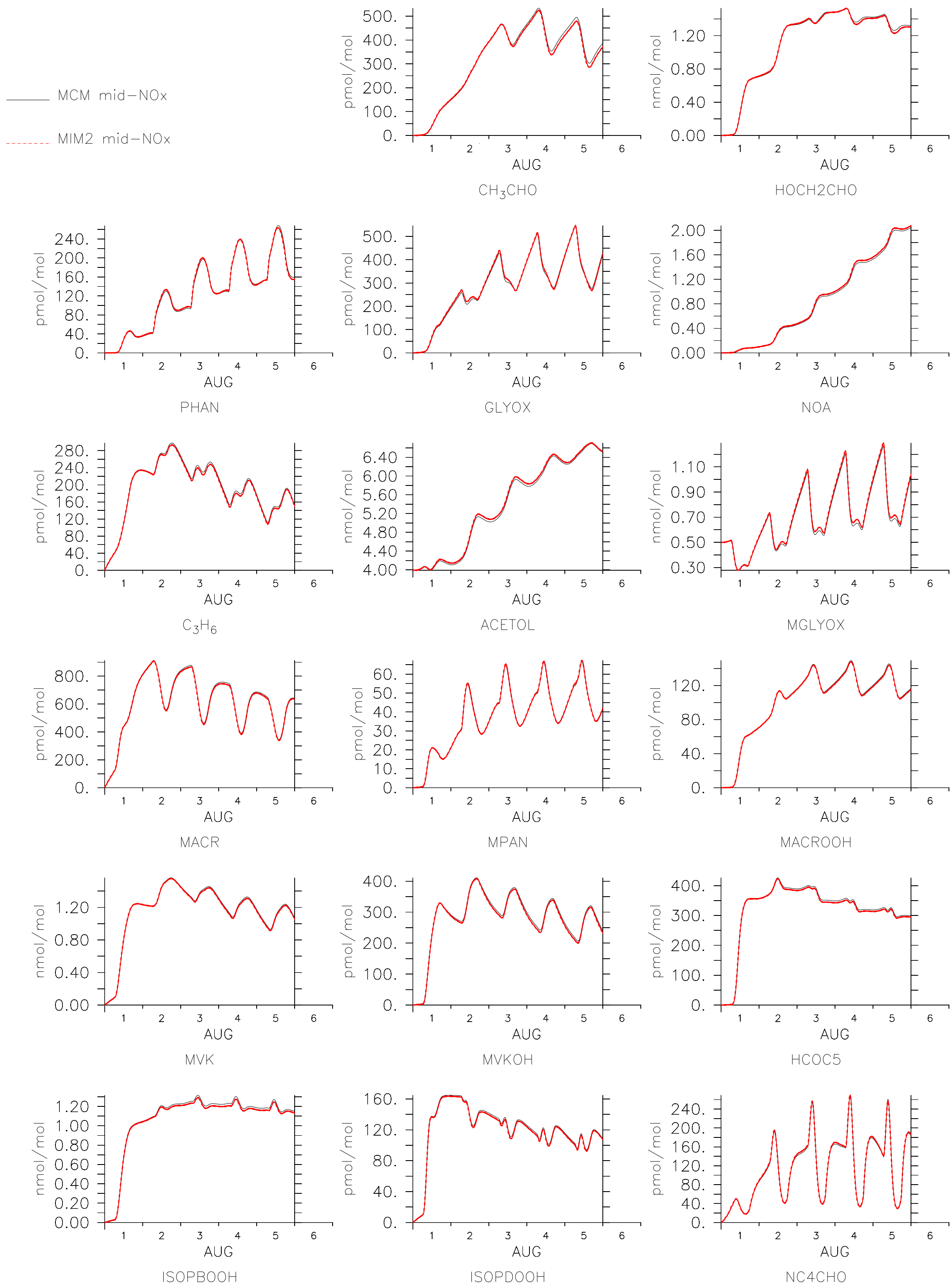

Figure 2: A selection of the most prominent among the news species present now in MIM2. A comparison between MIM2 and MCM in the mid-NO_x scenario is shown.

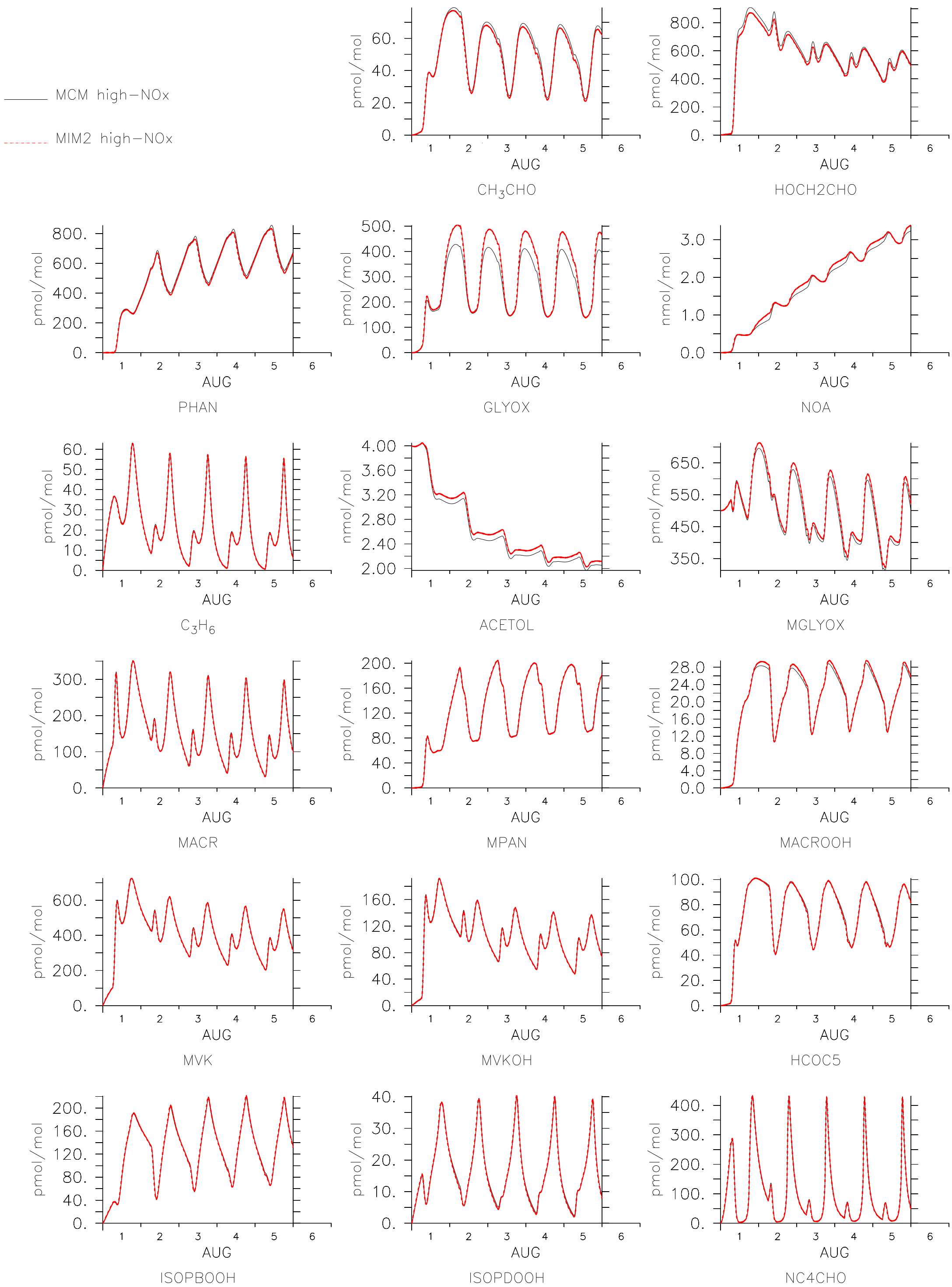

Figure 3: A selection of the most prominent among the news species present now in MIM2. A comparison between MIM2 and MCM in the high-NO_x scenario is shown.

References

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., 34, 161–180, 2003.