Table S1. Detailed information about MCM v 3.3.1 mechanism update.

MCM v3.3.1	MCM v3.3.1g
ethene	
% 9.1D-15*EXP(-2580/TEMP): C2H4 + O3 = HCHO + CH2OOA; % KDEC*0.37: CH2OOA = CH2OO; % KDEC*0.50: CH2OOA = CO; % KDEC*0.13: CH2OOA = HO2 + CO + OH;	6.82D-15*EXP(-2500/TEMP): C2H4 + O3 = HCHO + CH2OOA; % KDEC*0.42: CH2OOA = CH2OO; % KDEC*0.18: CH2OOA = CO; % KDEC*0.17: CH2OOA = HO2 + CO + OH; % KDEC*0.18: CH2OOA = H2; % KDEC*0.05: CH2OOA = HO2 + HO2;
propene	
% 5.5D-15*EXP(-1880/TEMP)*0.5 : O3 + C3H6 = CH2OOB + CH3CHO ; % 5.5D-15*EXP(-1880/TEMP)*0.5 : O3 + C3H6 = CH3CHOOA + HCHO ; % KDEC*0.24 : CH2OOB = CH2OO ; % KDEC*0.40 : CH2OOB = CO ; % KDEC*0.36 : CH2OOB = HO2 + CO + OH ; % KDEC*0.24 : CH3CHOOA = CH3CHOO ; % KDEC*0.36 : CH3CHOOA = CH3O2 + CO + OH ;	% 5.77D-15*EXP(-1880/TEMP)*0.38 : O3 + C3H6 = CH2OOB + CH3CHO ; % 5.77D-15*EXP(-1880/TEMP)*0.62 : O3 + C3H6 = CH3CHOOA + HCHO ; % KDEC*0.53: CH2OOB = CH2OO ; % KDEC*0.13: CH2OOB = CO ; % KDEC*0.17: CH2OOB = HO2 + CO + OH ; % KDEC*0.12: CH2OOB = H2 ; % KDEC*0.05: CH2OOB = HO2 + HO2 ; % KDEC*0.08: CH3CHOOA = CH3OH + CO ; % KDEC*0.13: CH3CHOOA = CH3CHOO; % KDEC*0.48: CH3CHOOA = HCOCH2O2 + OH ; % KDEC*0.16: CH3CHOOA = CH4 ;
but-1-ene	
% 3.55D-15*EXP(-1745/TEMP)*0.5 : BUT1ENE + O3 = C2H5CHOOA + HCHO ; % 3.55D-15*EXP(-1745/TEMP)*0.5 : BUT1ENE + O3 = CH2OOB + C2H5CHO ; % KDEC*0.24 : C2H5CHOOA = C2H5CHOO ; % KDEC*0.36 : C2H5CHOOA = C2H5O2 + CO + OH ;	%3.55D-15*EXP(-1750/TEMP)*0.65 : BUT1ENE + O3 = C2H5CHOOA + HCHO ; %3.55D-15*EXP(-1750/TEMP)*0.35 : BUT1ENE + O3 = CH2OOA + C2H5CHO ; % KDEC*0.13 : C2H5CHOOA = C2H5CHOO ; %KDEC*0.49: C2H5CHOOA = OH + PROPALO2; % KDEC*0.08 : C2H5CHOOA = C2H5OH + CO ; % KDEC*0.15 : C2H5CHOOA = C2H6 ;
cis-but-2-ene	
% 3.22D-15*EXP(-968/TEMP) : CBUT2ENE + O3 = CH3CHO + CH3CHOOB ; % KDEC*0.18 : CH3CHOOB = CH3CHOO ; % KDEC*0.57 : CH3CHOOB = CH3O2 + CO + OH ; % KDEC*0.125 : CH3CHOOB = CH3O2 + HO2 ;	% 3.37D-15*EXP(-970/TEMP) : CBUT2ENE + O3 = CH3CHO + CH3CHOOB ; % KDEC*0.20 : CH3CHOOB = CH3CHOO ; % KDEC*0.33 : CH3CHOOB = HCOCH2O2 + OH ; % KDEC*0.10 : CH3CHOOB = CH3OH + CO ;

% KDEC*0.125 : CH3CHOOB = CH4 ; trans-but-2-ene	% KDEC*0.3 : CH3CHOOB = CH4 ;
% 6.64D-15*EXP(-1059/TEMP) : TBUT2ENE + O3 = CH3CHO + CH3CHOOB ;	%7.0D-15*EXP(-1060/TEMP) : TBUT2ENE + O3 = CH3CHO + CH3CHOOC; % KDEC*0.22 : CH3CHOOC = CH3CHOO ; % KDEC*0.60 : CH3CHOOC = HCOCH2O2 + OH ; % KDEC*0.07 : CH3CHOOC = CH3OH + CO ; % KDEC*0.11 : CH3CHOOC = CH4 ;
2-methylpropene	
%2.7D-15*EXP(-1630/TEMP)*0.5 : MEPROPENE + O3 = CH2OOC + CH3COCH3 ; %2.7D-15*EXP(-1630/TEMP)*0.5 : MEPROPENE + O3 = CH3CCH3OOA + HCHO ; % KDEC*0.18: CH2OOC = CH2OO ; % KDEC*0.82 : CH2OOC = HO2 + CO + OH ; % KDEC*0.18:CH3CCH3OOA = CH3CCH3OO ; % KDEC*0.82:CH3CCH3OOA = CH3COCH2O2 + OH ;	%2.92D-15*EXP(-1650/TEMP)*0.32 : MEPROPENE + O3 = CH2OOA + CH3COCH3 ; %2.92D-15*EXP(-1650/TEMP)*0.68 : MEPROPENE + O3 = CH3CCH3OOA + HCHO ; %KDEC*0.10: CH3CCH3OOA = CH3CCH3OO ; %KDEC*0.90: CH3CCH3OOA = CH3COCH2O2 + OH ;
isoprene	
% 1.03D-14*EXP(-1995/TEMP)*0.3 : O3 + C5H8 = CH2OOE + MACR ; % 1.03D-14*EXP(-1995/TEMP)*0.2 : O3 + C5H8 = CH2OOE + MVK ; % 1.03D-14*EXP(-1995/TEMP)*0.3 : O3 + C5H8 = HCHO + MACROOA ; % 1.03D-14*EXP(-1995/TEMP)*0.2 : O3 + C5H8 = HCHO + MVKOOA ; % KDEC*0.095 : MACROOA = C3H6 ; % KDEC*0.095 : MACROOA = CH3CO3 + HCHO + HO2 ; % KDEC*0.56 : MACROOA = MACROO ; % KDEC*0.25 : MACROOA = OH + CO + CH3CO3 + HCHO ; % KDEC*0.095 : MVKOOA = C3H6 ; % KDEC*0.095 : MVKOOA = CH3O2 + HCHO + CO + HO2 ; % KDEC*0.56 : MVKOOA = MVKOO ; % KDEC*0.25 : MVKOOA = OH + MVKO2 ; % KDEC*0.56 : CH2OOE = CH2OO ; % KDEC*0.19 : CH2OOE = CO ; % KDEC*0.25 : CH2OOE = HO2 + CO + OH ;	% 1.05D-14*EXP(-2000/TEMP)*0.41 : O3 + C5H8 = CH2OOE + MACR ; % 1.05D-14*EXP(-2000/TEMP)*0.17 : O3 + C5H8 = CH2OOE + MVK ; % 1.05D-14*EXP(-2000/TEMP)*0.19 : O3 + C5H8 = HCHO + MACROOA ; % 1.05D-14*EXP(-2000/TEMP)*0.23 : O3 + C5H8 = HCHO + MVKOOA ; % KDEC*0.10 : MACROOA = C3H6 ; % KDEC*0.11 : MACROOA = CH3CO3 + HCHO + HO2 ; % KDEC*0.16 : MACROOA = MACROO ; % KDEC*0.63 : MACROOA = OH + CO + CH3CO3 + HCHO ; % KDEC*0.08 : MVKOOA = C3H6 ; % KDEC*0.09 : MVKOOA = CH3O2 + HCHO + CO + HO2 ; % KDEC*0.33 : MVKOOA = MVKOO ; % KDEC*0.50 : MVKOOA = OH + MVKO2 ; % KDEC*0.95: CH2OOE = CH2OO ; % KDEC*0.05: CH2OOE = HO2 + CO + OH ;

CH2OO	
% 1.20D-15 : CH2OO + CO = HCHO ;	% 1.20D-15 : CH2OO + CO = HCHO ;
% 1.00D-14 : CH2OO + NO = HCHO + NO2 ;	% 1.00D-14 : CH2OO + NO = HCHO + NO2 ;
% 1.00D-15 : CH2OO + NO2 = HCHO + NO3 ;	% 3.00D-12 : CH2OO + NO2 = HCHO + NO3 ;
% 7.00D-14 : CH2OO + SO2 = HCHO + SO3 ;	% 3.70D-11 : CH2OO + SO2 = HCHO + SO3 ;
% 6.00D-18*H2O : CH2OO = HCHO + H2O2 ;	% 2.80D-16*0.5*H2O : CH2OO = HCHO + H2O2 ;
% 1.00D-17*H2O : CH2OO = HCOOH ;	% 2.80D-16*0.5*H2O : CH2OO = HCOOH ;
	% 6.40D-16*0.5*H2O: CH2OO = HCHO + H2O2 ;
	% 6.40D-16*0.5*H2O : CH2OO = HCOOH ;
CH3CHOO	
% 1.20D-15 : CH3CHOO + CO = CH3CHO ;	% 1.20D-15: CH3CHOO + CO = CH3CHO ;
% 1.00D-14 : CH3CHOO + NO = CH3CHO + NO2 ;	% 1.00D-14: CH3CHOO + NO = CH3CHO + NO2 ;
% 1.00D-15 : CH3CHOO + NO2 = CH3CHO + NO3 ;	% 2.00D-12: CH3CHOO + NO2 = CH3CHO + NO3 ;
% 7.00D-14 : CH3CHOO + SO2 = CH3CHO + SO3 ;	% 1.40D-10: CH3CHOO + SO2 = CH3CHO + SO3 ;
% 6.00D-18*H2O : CH3CHOO = CH3CHO + H2O2 ;	% 1.30D-14*0.5*H2O: CH3CHOO = CH3CHO + H2O2 ;
% 1.00D-17*H2O : CH3CHOO = CH3CO2H ;	% 1.30D-14*0.5*H2O: CH3CHOO = CH3CO2H ;
	% 4.40D-15*0.5*H2O: CH3CHOO = CH3CHO + H2O2 ;
	% 4.40D-15*0.5*H2O: CH3CHOO = CH3CO2H ;
C2H5CHOO	
% 1.20D-15 : C2H5CHOO + CO = C2H5CHO ;	% 1.20D-15 : C2H5CHOO + CO = C2H5CHO ;
% 1.00D-14 : C2H5CHOO + NO = C2H5CHO + NO2 ;	% 1.00D-14 : C2H5CHOO + NO = C2H5CHO + NO2 ;
% 1.00D-15 : C2H5CHOO + NO2 = C2H5CHO + NO3 ;	% 2.00D-12 : C2H5CHOO + NO2 = C2H5CHO + NO3 ;
% 7.00D-14 : C2H5CHOO + SO2 = C2H5CHO + SO3 ;	% 1.40D-10 : C2H5CHOO + SO2 = C2H5CHO + SO3 ;
% 6.00D-18*H2O : C2H5CHOO = C2H5CHO + H2O2 ;	% 1.30D-14*0.5*H2O: C2H5CHOO = C2H5CHO + H2O2 ;
% 1.00D-17*H2O : C2H5CHOO = PROPACID ;	% 1.30D-14*0.5*H2O: C2H5CHOO = PROPACID ;
	% 4.40D-15*0.5*H2O: C2H5CHOO = C2H5CHO + H2O2 ;
	% 4.40D-15*0.5*H2O: C2H5CHOO = PROPACID ;
CH3CCH3OO	
% 1.20D-15: CH3CCH3OO + CO = CH3COCH3 ;	% 1.20D-15: CH3CCH3OO + CO = CH3COCH3 ;

% 1.00D-14 : CH3CCH3OO + NO = CH3COCH3 + NO2 ;	% 1.00D-14 : CH3CCH3OO + NO = CH3COCH3 + NO2 ;
%1.00D-15 : CH3CCH3OO + NO2 = CH3COCH3 + NO3 ;	%2.10D-12 : CH3CCH3OO + NO2 = CH3COCH3 + NO3 ;
% 7.00D-14 : CH3CCH3OO + SO2 = CH3COCH3 + SO3 ;	% 1.55D-10 : CH3CCH3OO + SO2 = CH3COCH3 + SO3 ;
% 6.00D-18*H2O : CH3CCH3OO = CH3COCH3 + H2O2 ;	% 6.00D-17*H2O : CH3CCH3OO = CH3COCH3 + H2O2 ;
	% 6.00D-18*H2O : CH3CCH3OO = CH3COCH3 + H2O2 ;
MACROO	
% 1.2D-15 : MACROO + CO = MACR ;	% 1.2D-15 : MACROO + CO = MACR ;
% 1.0D-14 : MACROO + NO = MACR + NO2 ;	% 1.0D-14 : MACROO + NO = MACR + NO2 ;
% 1.0D-15 : MACROO + NO2 = MACR + NO3 ;	% 1.0D-15 : MACROO + NO2 = MACR + NO3 ;
% 7.0D-14 : MACROO + SO2 = MACR + SO3 ;	% 1.4D-10 : MACROO + SO2 = MACR + SO3 ;
% 1.0D-17*H2O : MACROO = MACO2H ;	% 1.43D-16*0.5*H2O : MACROO = MACO2H ;
% 6.0D-18*H2O : MACROO = MACR + H2O2 ;	% 1.43D-16*0.5*H2O : MACROO = MACR + H2O2 ;
	% 2.79D-17*0.5*H2O : MACROO = MACO2H ;
	% 2.79D-17*0.5*H2O : MACROO = MACR + H2O2 ;
	% 3.02D+01 : MACROO = ;
MVKOO	
% 1.2D-15 : MVKOO + CO = MVK ;	% 1.2D-15 : MVKOO + CO = MVK ;
% 1.0D-14 : MVKOO + NO = MVK + NO2 ;	% 1.0D-14 : MVKOO + NO = MVK + NO2 ;
% 1.0D-15 : MVKOO + NO2 = MVK + NO3 ;	% 1.0D-15 : MVKOO + NO2 = MVK + NO3 ;
% 7.0D-14 : MVKOO + SO2 = MVK + SO3 ;	% 4.2D-11 : MVKOO + SO2 = MVK + SO3 ;
% 6.0D-18*H2O : MVKOO = MVK + H2O2 ;	% 7.89D-20*H2O : MVKOO = MVK + H2O2 ;
	% 3.06D-20*H2O : MVKOO = MVK + H2O2 ;
	% 5.13D+01 : MVKOO = ;