Paper title: Chemical Kinetic Mechanism for Pyrolysis of Bio-oil Surrogate

1. APPENDIX

Reference	Number of species and reactions	Validation domain	Mechanism validation	Toluene	Ethanol	Acetic acid
Sivaramakrishnan et al. [1]	87 species 262 reactions	1200-1900 K 27-45 bar	ST	x		
Dagaut et al. [2]	120 species 920 reactions	1000-1375 K 1 bar ϕ = 0.5-1.5	PSR, LFS	x		
Colket and Seery [3]	98 species 529 reactions	1200-1850 K 10.0 bar	ST	x		
Emdee et al. [4]	130 reactions	1100-1190 K 1 bar ϕ = 0.65-1.38	FR	x		
Lindstedt and Maurice [5]	141 species 743 reactions	1515-2100 K 0.3-7.01 bar ϕ = 0.63-1.4	TR	x		
Metcalfe et al. [6]	329 species 1888 reactions	800-1500 K 1-550 bar ϕ = 0.3-5.0	ST, FR JSR, LFS	x		
Huang et al. [7]	120 species 531 reactions	K 0.04-80 bar ϕ = 0.5-1.5	ST, LFS, LPF, HCCI, CFF, EA	x		
Cai and Pitsch [8]	335 species 1610 reactions	300-1250 K 1-40 bar ϕ = 0.5-2.0	ST, LFS, JSR	x	x	
Leplat and Vandooren [9]	43 species 270 reactions	400 K 0.05 bar ϕ = 0.77, 0.9, 1.05	LPF			x
Christensen and Konnov [10]	100 species 1140 reactions	338-358 K 0.05, 1 bar ϕ = 0.7-1.3	LFS, LPF		x	x
Marinov [11]	57 species 387 reactions	1000-1700 K 1-4.5 bar ϕ = 0.5-2.0	ST, JSR FR, CFF		x	
Saxena and Williams [12]	36 species 192 reactions	$\leq$ 1000 K $\leq$ 100 bar ϕ =$\leq$ 3.0	CFF, ST		x	
Cancino et al. [13]	136 species 1349 reactions	650-1220 K 30-50 bar ϕ = 0.3-1.0	ST		x	
Leplat et al. [14]	36 species 252 reactions	890-1250 K 1 bar ϕ = 0.25-2.0	LPF, JSR ST		x	
Present work	180 species 1495 reactions	300-2000 K 1-100 bar ϕ = 0.5-1.5	ST LFS	x	x	x

Table A1: Non-exhaustive list of available chemical schemes for toluene, ethanol and acetic acid. ST: shock tubes, PSR: perfectly stirred reactor, LFS: laminar flame speed, , FR: flow reactors, TR: turbulent reactor, JSR: jet-stirred reactor, LPF: laminar premixed flames, HCCI: homogeneous charge compression ignition, CFF: counterflow flame, EA: engine application.

	Huang et al. [7]			Christensen and Konnov [10]		
Reactions	A	n	E	A	n	E
$H_2 + M = 2H + M$	4.577E19	-1.4	1.044E5	7.000E+17^{rev}	-1.0000^{rev}	0.00^{rev}
$2O + M = O_2 + M$	6.165E15	-0.5	0.0E0	1.000E+17	-1.0000	0.00
$O + H + M = OH + M$	4.714E18	-1.0	0.0E0	6.750E+18	-1.0000	0.00
$H + OH + M = H_2O + M$	3.5E22	-2.0	0.0E0	6.060E+27^{rev}	-3.3120^{rev}	120769.99^{rev}
H + O$_2$(+M) = HO$_2$(+M)	4.65E12	0.44	0.0E0	4.660E+12	0.4400	0.00
H$_2$O$_2$(+M) = 2OH(+M)	2.0E12	0.9	4.875E4	2.000E+12	0.9000	48749.99
O + H$_2$ = H + OH	5.08E4	2.67	6.292E3	5.080E+04	2.6700	6292.00
H + O$_2$ = O + OH	1.04E14	0.0	1.529E4	1.040E+14	0.0000	15286.00
$OH + H_2 = H + H_2O$	4.38E13	0.0	6.99E3	2.140E+08	1.5200	3450.00
$O + H_2O = 2OH$	2.97E6	2.02	1.34E4	3.340E+04^{rev}	2.4200^{rev}	-1930.00^{rev}
$HO_2 + O = OH + O_2$	3.25E13	0.0	0.0E0	2.850E+10	1.0000	-723.90
HO$_2$ + H = 2OH	7.079E13	0.0	2.95E2	7.080E+13	0.0000	300.00
$H_2 + O_2 = H + HO_2$	5.176E5	2.433	5.35E4	7.400E+05	2.4300	53499.99
$HO_2 + OH = H_2O + O_2$	2.456E13	0.0	-4.97E2	7.000E+12	0.0000	-1093.00
$HO_2 + OH = H_2O + O_2$	2.456E13	0.0	-4.97E2	4.500E+14	0.0000	10930.00
$H_2O_2 + H = H_2 + HO_2$	2.15E10	1.0	6.0E3	5.020E+06	2.0700	4300.00
$H_2O_2 + H = H_2O + OH$	2.41E13	0.0	3.97E3	2.030E+07	2.0200	2620.00
H$_2$O$_2$ + O = OH + HO$_2$	9.55E6	2.0	3.97E3	9.550E+06	2.0000	3970.00

Table B1: Package 1 (Species H_2, H_20, HO_2, H_2O_2). Reaction rate coefficients given in the form $k = AT^n exp(-E/RT)$. Units are mol cm cal s. Highlighted reactions correspond to those with similar Arrhenius constants for both models. Superscript ^{rev} in Christensen and Konnov [10] corresponds to the reverse reactions constants, as for these reactions, the reactives in Huang et al. [7] correspond to the products in Christensen and Konnov [10], and vice versa.

	Huang et al. [7]			Christensen and Konnov [10]		
Reactions	A	n	E	A	n	E
$CH + O = CO + H$	5.7E13	0.0	0.0E0	4.000E+13	0.0000	0.00
CH + OH = HCO + H	3.0E13	0.0	0.0E0	3.000E+13	0.0000	0.00
$CH_2 + H = CH + H_2$	1.0E18	-1.56	0.0E0	$1.750E+14^{rev}$	0.0000^{rev}	3320.00^{rev}
$CH + H_2O = H + CH_2O$	1.713E13	0.0	-7.55E2	1.770E+16	-1.2200	24.00
$CH + O_2 = HCO + O$	3.3E13	0.0	0.0E0	4.800E+12	0.0000	0.00
$CH_2 + O => CO + 2H$	5.0E13	0.0	0.0E0	1.000E+14	0.0000	536.00
$CH_2 + OH = CH + H_2O$	1.13E7	2.0	3.0E3	8.630E+05	2.0190	6776.00
$CH_2 + O_2 = HCO + OH$	1.06E13	0.0	1.5E3	1.650E+12	0.0000	1737.00
$CH_2 + O_2 => CO_2 + 2H$	2.64E12	0.0	1.5E3	8.250E+11	0.0000	1737.00
$CH_3 + O = CH_2O + H$	5.54E13	0.05	-1.36E2	4.432E+13	0.0500	-136.00
$CH_3 + O_2 = CH_3O + O$	7.546E12	0.0	2.832E4	2.110E+13	0.0000	32471.00
$CH_3 + O_2 = CH_2O + OH$	2.641E0	3.283	8.105E3	6.390E+11	0.0000	13515.00
$CH_3 + O_2(+M) = CH_3O_2(+M)$	7.812E9	0.9	0.0E0	7.810E+09	0.9000	0.00
$CH_3 + HO_2 = CH_3O + OH$	1.0E12	0.269	-6.875E2	1.000E+12	0.2688	-688.00
$CH_3 + HO_2 = CH_4 + O_2$	1.16E5	2.23	-3.022E3	1.190E+05	2.2280	-3023.00
$2CH_3 = H + C_2H_5$	2.109E5	2.297	1.215E4	5.400E+13	0.0000	16055.00
$2CH_3(+M) = C_2H_6(+M)$	2.277E15	-0.69	1.749E2	3.610E+13	0.0000	0.00
$CH_3 + H(+M) = CH_4(+M)$	1.27E16	-0.63	3.83E2	2.890E+13	0.1930	-10.00
$CH_4 + H = CH_3 + H_2$	6.14E5	2.5	9.587E3	6.140E+05	2.5000	9590.00
$CH_4 + O = CH_3 + OH$	1.02E9	1.5	8.6E3	4.400E+05	2.5000	6577.00
$CH_4 + OH = CH_3 + H_2O$	5.83E4	2.6	2.19E3	1.000E+06	2.1800	2462.00
$CH_4 + HO_2 = CH_3 + H_2O_2$	1.695E1	3.74	2.101E4	1.130E+01	3.7400	21000.00
$CO + O(+M) = CO_2(+M)$	1.362E10	0.0	2.384E3	1.060E+13	-0.3080	6943.00
$CO + OH = CO_2 + H$	7.015E4	2.053	-3.557E2	2.230E+05	1.9000	-1160.00
$CO + O_2 = CO_2 + O$	1.119E12	0.0	4.77E4	5.060E+13	0.0000	63189.99
$CO + HO_2 = CO_2 + OH$	1.57E5	2.18	1.794E4	1.570E+05	2.1800	17940.00
$HCO + M = H + CO + M$	5.7E11	0.66	1.487E4	4.750E+11	0.6600	14870.00
$HCO + H = CO + H_2$	7.34E13	0.0	0.0E0	1.200E+14	0.0000	0.00
HCO + O = CO + OH	3.02E13	0.0	0.0E0	3.000E+13	0.0000	0.00
$HCO + O = CO_2 + H$	3.0E13	0.0	0.0E0	3.000E+13	0.0000	0.00
$HCO + OH = CO + H_2O$	1.02E14	0.0	0.0E0	1.100E+14	0.0000	0.00
$HCO + O_2 = CO + HO_2$	7.58E12	0.0	4.1E2	6.920E+06	1.9000	-1370.00
$HCO + HO_2 => CO_2 + H + OH$	3.0E13	0.0	0.0E0	3.000E+13	0.0000	0.00
$HCO + CH_3 = CH_4 + CO$	2.65E13	0.0	0.0E0	1.849E+20	-2.3000	4781.00
$2HCO = CH_2O + CO$	1.8E13	0.0	0.0E0	1.800E+13	0.0000	0.00
$2HCO => H_2 + 2CO$	3.0E12	0.0	0.0E0	3.000E+12	0.0000	0.00

Table B2: Package 2 (Species CO, CO_2, HCO, CH, CH_2, CH_3, CH_4). Reaction rate coefficients given in the form $k = AT^n exp(-E/RT)$. Units are mol cm cal s. Highlighted reactions correspond to those with similar Arrhenius constants for both models. Superscript ^{rev} in Christensen and Konnov [10] corresponds to the reverse reactions constants, as for these reactions, the reactives in Huang et al. [7] correspond to the products in Christensen and Konnov [10], and vice versa.

	Huang et al. [7]			Christensen and Konnov [10]		
Reactions	A	n	E	A	n	E
$HCO + H(+M) = CH_2O(+M)$	1.09E12	0.48	-2.6E2	1.260E+36^{rev}	-5.5000^{rev}	93993.99^{rev}
$CO + H_2(+M) = CH_2O(+M)$	4.3E7	1.5	7.96E4	4.400E+38^{rev}	-6.1000^{rev}	93993.99^{rev}
$CH_2O + H = HCO + H_2$	5.74E7	1.9	2.74E3	5.860E+03	3.1300	1514.00
$CH_2O + O = HCO + OH$	6.26E9	1.15	2.26E3	4.160E+11	0.5700	2762.00
$CH_2O + OH = HCO + H_2O$	7.82E7	1.63	-1.055E3	2.390E+07	1.8300	-1117.00
$CH_2O + O_2 = HCO + HO_2$	8.07E15	0.0	5.342E4	2.440E+05	2.5000	36465.00
$CH_2O + HO_2 = HCO + H_2O_2$	1.88E4	2.7	1.152E4	4.100E+04	2.5000	10210.00
$CH + CH_2O = H + CH_2CO$	9.46E13	0.0	-5.15E2	1.460E+16	-0.8000	-81.80
$CH_2O + CH_3 = HCO + CH_4$	3.83E1	3.36	4.312E3	3.190E+01	3.3600	4312.00
$CH_3O(+M) = CH_2O + H(+M)$	6.8E13	0.0	2.617E4	1.130E+10	1.2100	24085.00
$CH_3O + H = CH_2O + H_2$	2.0E13	0.0	0.0E0	3.780E+13	0.0000	596.00
$CH_3O + O_2 = CH_2O + HO_2$	4.38E-19	9.5	-5.501E3	2.290E+03	2.4000	413.00
$CH_3O + CH_3 = CH_2O + CH_4$	1.2E13	0.0	0.0E0	2.410E+13	0.0000	0.00
$CH_2O + CH_3O = CH_3OH + HCO$	6.62E11	0.0	2.294E3	6.600E+11	0.0000	2300.00
$2CH_3O = CH_3OH + CH_2O$	6.03E13	0.0	0.0E0	7.800E+12	0.0000	0.00
$CH_2O + H(+M) = CH_2OH(+M)$	5.4E11	0.454	3.6E3	7.370E+10^{rev}	0.8110^{rev}	39585.00^{rev}
$CH_2OH + H = CH_2O + H_2$	6.0E12	0.0	0.0E0	3.000E+13	0.0000	0.00
$O + CH_2OH = OH + CH_2O$	4.2E13	0.0	0.0E0	6.560E+12	0.0000	-693.00
$OH + CH_2OH = H_2O + CH_2O$	2.4E13	0.0	0.0E0	2.400E+13	0.0000	0.00
$CH_2OH + HO_2 = CH_2O + H_2O_2$	1.2E13	0.0	0.0E0	6.300E+11	0.2800	-813.00
$CH_2OH + HO_2 = CH_2O + H_2O_2$	1.2E13	0.0	0.0E0	6.800E+11	0.2100	-454.00
$CH_2OH + HCO = 2CH_2O$	1.8E14	0.0	0.0E0	1.500E+13	0.0000	0.00
$CH_3OH + HCO = CH_2OH + CH_2O$	9.63E3	2.9	1.311E4	5.480E+03^{rev}	2.8100^{rev}	5862.00^{rev}
$CH_2OH + CH_3O = CH_2O + CH_3OH$	2.4E13	0.0	0.0E0	2.400E+13	0.0000	0.00
$2CH_2OH = CH_2O + CH_3OH$	3.0E12	0.0	0.0E0	9.000E+12	0.0000	0.00
$CH_3OH(+M) = CH_3 + OH(+M)$	2.084E18	-0.615	9.254E4	2.080E+18	-0.6148	92549.99
$CH_3OH(+M) = CH_2OH + H(+M)$	7.896E-3	5.038	8.447E4	7.900E-03	5.0380	84475.99
$CH_3OH + H = CH_2OH + H_2$	3.07E5	2.55	5.44E3	3.040E+14	-0.1690	7796.00
$CH_3OH + H = CH_3O + H_2$	1.99E5	2.56	1.03E4	7.470E+14	-0.4010	12774.00
$CH_3OH + O = CH_2OH + OH$	3.88E5	2.5	3.08E3	5.300E+04	2.6100	1870.00
$CH_3OH + OH = CH_2OH + H_2O$	3.08E4	2.65	-8.067E2	5.140E+04	2.6200	-682.00
$CH_3OH + OH = CH_3O + H_2O$	1.5E2	3.03	-7.63E2	5.710E+03	2.6200	-682.00
$CH_3OH + O_2 = CH_2OH + HO_2$	2.05E13	0.0	4.49E4	3.580E+05	2.2700	42764.00
$CH_3OH + HO_2 = CH_2OH + H_2O_2$	1.08E4	2.55	1.053E4	3.500E-04	4.8500	10134.00
$CH_3OH + CH_3 = CH_2OH + CH_4$	3.19E1	3.17	7.172E3	7.100E+00	3.4800	7055.00
$CH_3 + CH_3OH = CH_4 + CH_3O$	1.44E1	3.1	6.935E3	4.290E+02	2.6400	7101.00
$CH_3O + CH_3OH = CH_2OH + CH_3OH$	3.0E11	0.0	4.074E3	3.000E+11	0.0000	4070.00
$CH + CO_2 = HCO + CO$	1.7E12	0.0	6.85E2	6.360E+07	1.5100	-715.00
$CH_3O_2 + H = CH_3O + OH$	9.6E13	0.0	0.0E0	9.600E+13	0.0000	0.00
$CH_3O_2 + O = CH_3O + O_2$	3.6E13	0.0	0.0E0	2.600E+13	0.0000	0.00
$CH_3O_2 + OH = CH_3OH + O_2$	6.0E13	0.0	0.0E0	6.000E+13	0.0000	0.00
$CH_3O_2 + HO_2 = CH_3O_2H + O_2$	2.47E11	0.0	-1.57E3	2.530E+11	0.0000	-1490.00
$CH_3O_2 + CH_3 = 2CH_3O$	5.08E12	0.0	-1.411E3	5.000E+12	0.0000	-1410.00
$CH_4 + CH_3O_2 = CH_3 + CH_3O_2H$	9.6E-1	3.77	1.781E4	1.210E+01	3.7500	21200.00
$CH_3O_2 + CH_2O = CH_3O_2H + HCO$	1.99E12	0.0	1.166E4	2.000E+12	0.0000	11660.00
$CH_3OH + CH_3O_2 = CH_2OH + CH_3O_2H$	1.81E12	0.0	1.371E4	1.810E+11	0.0000	13700.00
$2CH_3O_2 => CH_2O + CH_3OH + O_2$	3.11E14	-1.61	-1.051E3	2.240E+15	-1.8700	-541.00
$2CH_3O_2 => O_2 + 2CH_3O$	1.4E16	-1.61	1.86E3	5.870E+16	-1.8700	1700.00
$H_2 + CH_3O_2 = H + CH_3O_2H$	1.5E14	0.0	2.603E4	8.790E+10^{rev}	0.0000^{rev}	1860.00^{rev}

Table B3: Package 3 (Species CH_2O, CH_3O, CH_2OH, CH_3OH, CH_3O_2, CH_3O_2H). Reaction rate coefficients given in the form $k = AT^n exp(-E/RT)$. Units are mol cm cal s. Highlighted reactions correspond to those with similar Arrhenius constants for both models. Superscript ^{rev} in Christensen and Konnov [10] corresponds to the reverse reactions constants, as for these reactions, the reactives in Huang et al. [7] correspond to the products in Christensen and Konnov [10], and vice versa.

	Huang et al. [7]			Christensen and Konnov [10]		
Reactions	A	n	E	A	n	E
$H_2 + C_2H$ <=> $C_2H_2 + H$	0.1080E+14	0.0000	0.2165E+04	2.100E+06	2.3200	880.00
$C_2H + OH$ <=> $CH_2 + CO$	0.1810E+14	0.0000	0.0000E+00	1.800E+13	0.0000	0.00
$C_2H_2 + O = CH_2 + CO$	7.395E8	1.28	2.472E3	2.350E+08	1.4000	2200.00
$C_2H_2 + O = HCCO + H$	2.958E9	1.28	2.472E3	9.400E+08	1.4000	2200.00
$C_2H_2 + OH = CH_3 + CO$	1.00E7	1.432	4.315E3	1.280E+09	0.7300	2579.00
$C_2H_2 + OH$ <=> $C_2H + H_2O$	0.6000E+14	0.0000	0.1292E+05	2.630E+06	2.1400	17060.00
$C_2H_2 + OH = CH_2CO + H$	1.50E5	2.132	4.048E3	7.530E+06	1.5500	2106.00
$C_2H_2 + CH_2$ <=> $C_3H_3 + H$	0.1200E+14	0.0000	0.6577E+04	1.200E+13	0.0000	6620.00
$C_2H_2 + H(+M) = C_2H_3(+M)$	1.71E10	1.266	2.709E3	3.860E+08^{rev}	1.6200^{rev}	37060.00^{rev}
$C_2H_3 + H(+M) = C_2H_4(+M)$	6.08E12	0.27	2.8E2	6.080E+12	0.2700	280.00
$C_2H_3 + H = C_2H_2 + H_2$	9.0E13	0.0	0.0E0	4.200E+13	0.0000	0.00
$C_2H_3 + OH = C_2H_2 + H_2O$	3.011E13	0.0	0.0E0	3.000E+13	0.0000	0.00
$C_2H_3 + O_2$ <=> $C_2H_2 + HO_2$	0.1120E+15	-0.8330	0.2541E+04	5.190E+15	-1.2600	3310.00
$C_2H_3 + O_2$ <=> $C_2H_2 + HO_2$	0.1120E+15	-0.8330	0.2541E+04	2.120E-06	6.0000	9484.00
$C_2H_3 + O_2 = CH_2O + HCO$	1.7E29	-5.312	6.503E3	4.150E+12	0.0000	-240.00
$CH_3 + C_2H_3 = C_3H_5 + H$	1.5E24	-2.83	1.861855E4	1.500E+24	-2.8300	18618.00
$C_2H_3 + CH_2O$ <=> $C_2H_4 + HCO$	0.5420E+04	2.8100	0.5824E+04	5.420E+03	2.8100	5862.00
$C_2H_4 + CH_3O = C_2H_3 + CH_3OH$	1.2E11	0.0	6.75E3	1.440E+01^{rev}	3.1000^{rev}	6940.00^{rev}
$C_2H + C_2H_3$ <=> $2C_2H_2$	0.1900E+14	0.0000	0.0000E+00	3.000E+13	0.0000	0.00
$2C_2H_3 = C_2H_2 + C_2H_4$	9.6E11	0.0	0.0E0	1.450E+13	0.0000	0.00
$C_2H_4 + H = C_2H_3 + H_2$	5.07E7	1.93	1.295E4	2.340E+02	3.6200	11270.00
$C_2H_4 + O = CH_3 + HCO$	7.453E6	1.88	1.83E2	8.100E+06	1.8800	180.00
$C_2H_4 + OH = CH_2O + CH_3$	5.00E+11	0.0	960.	1.780E+05	1.6800	2061.00
$C_2H_4 + OH = C_2H_3 + H_2O$	2.23E4	2.745	2.216E3	1.310E-01	4.2000	-860.00
$C_2H_4 + O_2 = C_2H_3 + HO_2$	4.22E13	0.0	5.762E4	4.220E+13	0.0000	57629.99
$C_2H_3 + H_2O_2$ <=> $C_2H_4 + HO_2$	0.1210E+11	0.0000	-.5901E+03	4.800E+04^{rev}	2.5000^{rev}	27620.00^{rev}
$C_2H_4 + CH_3 = C_2H_3 + CH_4$	6.62E0	3.7	9.5E3	6.000E+07	1.5600	16630.00
$C_2H_4 + CH_3O_2 = C_2H_3 + CH_3O_2H$	8.59E0	3.754	2.713E4	1.000E+13	0.0000	25000.00
$2C_2H_4 = C_2H_5 + C_2H_3$	4.82E14	0.0	7.153E4	4.820E+14	0.0000	71539.99
$C_2H_4 + H(+M) = C_2H_5(+M)$	9.569E8	1.463	1.355E3	1.110E+10^{rev}	1.0370^{rev}	36767.00^{rev}
$C_2H_5 + H = C_2H_4 + H_2$	2.0E12	0.0	0.0E0	1.700E+12	0.0000	0.00
$C_2H_5 + O_2 = C_2H_4 + HO_2$	7.561E14	-1.01	4.749E3	2.560E+19	-2.7700	1980.00
$CH_3 + C_2H_5 = CH_4 + C_2H_4$	1.18E4	2.45	-2.921E3	9.000E+11	0.0000	0.00
$C_2H_6 + CH_3O = C_2H_5 + CH_3OH$	2.41E11	0.0	7.09E3	1.440E+01^{rev}	3.1000^{rev}	8942.00^{rev}
$C_2H_5 + H(+M) = C_2H_6(+M)$	5.21E17	-0.99	1.58E3	8.850E+20^{rev}	-1.2280^{rev}	102209.99^{rev}
$C_2H_6 + H = C_2H_5 + H_2$	1.15E8	1.9	7.53E3	1.400E+09	1.5000	7400.00
$C_2H_6 + O = C_2H_5 + OH$	3.55E6	2.4	5.83E3	3.550E+06	2.4000	5830.00
$C_2H_6 + OH = C_2H_5 + H_2O$	1.48E7	1.9	9.5E2	7.200E+06	2.0000	870.00
$C_2H_6 + O_2 = C_2H_5 + HO_2$	6.03E13	0.0	5.187E4	7.260E+05	2.5000	49159.99
$C_2H_6 + HO_2 = C_2H_5 + H_2O_2$	3.46E1	3.61	1.692E4	7.080E+04	2.5000	16850.00
$C_2H_6 + CH_3 = C_2H_5 + CH_4$	5.48E-1	4.0	8.28E3	5.600E+10	0.0000	9420.00
$C_2H_6 + CH_3 = C_2H_5 + CH_4$	5.48E-1	4.0	8.28E3	8.400E+14	0.0000	22250.00
$C_2H_6 + CH_3O_2 = C_2H_5 + CH_3O_2H$	1.94E1	3.64	1.71E4	2.950E+11	0.0000	14940.00

Table B4: Package 4 (Species C_2H, C_2H_2, C_2H_3, C_2H_4, C_2H_5, C_2H_6). Reaction rate coefficients given in the form $k = AT^n exp(-E/RT)$. Units are mol cm cal s. Highlighted reactions correspond to those with similar Arrhenius constants for both models. Superscript ^{rev} in Christensen and Konnov [10] corresponds to the reverse reactions constants, as for these reactions, the reactives in Huang et al. [7] correspond to the products in Christensen and Konnov [10], and vice versa.

	Huang et al. [7]			Christensen and Konnov [10]		
Reactions	A	n	E	A	n	E
$HCCO + O => H + 2CO$	8.0E13	0.0	0.0E0	1.000E+14	0.0000	0.00
$HCCO + O_2 => CO_2 + CO + H$	4.78E12	-0.142	1.15E3	4.760E+12	-0.1420	1150.00
$HCCO + O_2 => OH + 2CO$	1.91E11	-0.02	1.02E3	1.900E+11	-0.0200	1023.00
$CH + HCCO = CO + C_2H_2$	5.0E13	0.0	0.0E0	5.000E+13	0.0000	0.00
$CH_2 + CO(+M) = CH_2CO(+M)$	8.1E11	0.0	0.0E0	3.000E+14	0.0000	70999.99
$CH_2CO + H = CH_3 + CO$	7.704E13	-0.171	4.183E3	7.770E+08	1.4500	2780.00
$CH_2CO + H = HCCO + H_2$	1.401E15	-0.171	8.783E3	1.000E+14	0.0000	12300.00
$CH_2CO + O = HCCO + OH$	1.0E13	0.0	8.0E3	1.870E+14	0.0000	16690.00
$CH_2CO + O = CH_2 + CO_2$	1.75E12	0.0	1.35E3	1.080E+12	0.0000	1350.00
$CH_2CO + OH = CH_2OH + CO$	2.0E12	0.0	-1.01E3	2.640E+12	0.0000	-550.00
$CH_2CO + OH = HCCO + H_2O$	1.0E13	0.0	2.0E3	1.780E+13	0.0000	5840.00
$CH_2CO + CH_3 = C_2H_5 + CO$	4.769E4	2.312	9.468E3	2.400E+12	0.0000	8000.00
$CH_3CO + H = CH_2CO + H_2$	2.0E13	0.0	0.0E0	1.150E+13	0.0000	0.00
$CH_3CO + H <=> CH_3 + HCO$	0.2100E+14	0.0000	0.0000E+00	2.150E+13	0.0000	0.00
$CH_3CO + O = CH_2CO + OH$	2.0E13	0.0	0.0E0	5.250E+13	0.0000	0.00
$CH_3CO + OH <=> CH_2CO + H_2O$	0.1200E+14	0.0000	0.0000E+00	2.800E+13	0.0000	0.00
$CH_3CO + CH_3 = CH_2CO + CH_4$	5.0E13	0.0	0.0E0	6.100E+12	0.0000	0.00
$CH_3COCH_3 = CH_3CO + CH_3$	5.113E30	-4.194	8.978E4	4.040E+15	-0.8000	0.00
$C_3H_2 + O <=> C_2H + H + CO$	0.6800E+14	0.0000	0.0000E+00	3.000E+13	0.0000	0.00
$C_3H_3 + O <=> C_2H_2 + CO + H$	0.1390E+15	0.0000	0.0000E+00	7.000E+13	0.0000	0.00
$C_3H_3 + O <=> CH_2O + C_2H$	0.1400E+15	0.0000	0.0000E+00	2.000E+13	0.0000	0.00
$C_3H_3 + OH <=> HCO + C_2H_3$	0.4000E+14	0.0000	0.0000E+00	1.330E+13	0.0000	0.00
$C_3H_3 + O_2 = CH_2CO + HCO$	3.0E10	0.0	2.86807E3	3.010E+10	0.0000	2870.00
$C_3H_3 + HO_2 = OH + CO + C_2H_3$	8.0E11	0.0	0.0E0	8.000E+11	0.0000	0.00
$C_3H_5 + H(+M) = C_3H_6(+M)$	2.0E14	0.0	0.0E0	2.000E+14	0.0000	0.00
$C_3H_6 + H = C_3H_5 + H_2$	1.7E5	2.5	2.49283E3	6.457E+12	0.0000	4445.00
$C_3H_6 + H = C_2H_4 + CH_3$	1.6E22	-2.39	1.118547E4	2.600E+08	1.5000	2000.00
$C_3H_6 + O = C_2H_5 + HCO$	3.5E7	1.65	-9.7275E2	6.833E+06	1.5700	-628.00
$C_3H_6 + OH = C_3H_5 + H_2O$	3.1E6	2.0	-2.9828E2	3.120E+06	2.0000	-300.00
$C_3H_5 + HO_2 = C_3H_6 + O_2$	2.66E12	0.0	0.0E0	1.080E+04	2.5000	35730.00
$NC_3H7 = CH_3 + C_2H_4$	2.284E14	-0.55	2.84E4	1.260E+13	0.0000	30404.00
$NC_3H7 + H = C_2H_5 + CH_3$	3.7E24	-2.92	1.25E4	3.700E+24	-2.9200	12505.00
$NC_3H7 + OH = C_3H_6 + H_2O$	2.4E13	0.0	0.0E0	2.400E+13	0.0000	0.00
$NC_3H7 + O_2 = C_3H_6 + HO_2$	1.71E42	-9.211	1.979E4	1.000E+12	0.0000	5000.00
$C_2H_3CO = C_2H_3 + CO$	1.37E21	-2.179	3.941E4	2.000E+13	0.0000	28700.00

Table B5: Package 5 (Species $HCCO$, CH_2CO, CH_3CO, C_3H_2, C_3H_3, C_3H_5, C_3H_6, NC_3H_7, C_2H_3CO, CH_3COCH_3). Reaction rate coefficients given in the form $k = AT^n exp(-E/RT)$. Units are mol cm cal s. Highlighted reactions correspond to those with similar Arrhenius constants for both models. Superscript ^{rev} in Christensen and Konnov [10] corresponds to the reverse reactions constants, as for these reactions, the reactives in Huang et al. [7] correspond to the products in Christensen and Konnov [10], and vice versa.

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